

6. Process or Product Monitoring and Control

This chapter presents techniques for monitoring and controlling processes and signaling when corrective actions are necessary.

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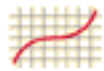
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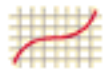
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6.1. Introduction

*Contents of
Section*

This section discusses the basic concepts of statistical process control, quality control and process capability.

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6.1.1. How did Statistical Quality Control Begin?

Historical perspective

Quality Control has been with us for a long time. How long? It is safe to say that when manufacturing began and competition accompanied manufacturing, consumers would compare and choose the most attractive product (barring a monopoly of course). If manufacturer A discovered that manufacturer B's profits soared, the former tried to improve his/her offerings, probably by improving the quality of the output, and/or lowering the price. Improvement of quality did not necessarily stop with the product - but also included the *process* used for making the product.

The process was held in high esteem, as manifested by the medieval guilds of the Middle Ages. These guilds mandated long periods of training for apprentices, and those who were aiming to become master craftsmen had to demonstrate evidence of their ability. Such procedures were, in general, aimed at the maintenance and improvement of the quality of the process.

In modern times we have professional societies, governmental regulatory bodies such as the Food and Drug Administration, factory inspection, etc., aimed at assuring the quality of products sold to consumers. *Quality Control* has thus had a long history.

Science of statistics is fairly recent

On the other hand, *statistical* quality control is comparatively new. The science of statistics itself goes back only two to three centuries. And its greatest developments have taken place during the 20th century. The earlier applications were made in astronomy and physics and in the biological and social sciences. It was not until the 1920s that statistical theory began to be applied effectively to quality control as a result of the development of sampling theory.

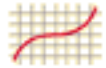
The concept of quality control in manufacturing was first advanced by Walter Shewhart

The first to apply the newly discovered statistical methods to the problem of quality control was Walter A. Shewhart of the Bell Telephone Laboratories. He issued a memorandum on May 16, 1924 that featured a sketch of a modern control chart.

Shewhart kept improving and working on this scheme, and in 1931 he published a book on statistical quality control, "*Economic Control of Quality of Manufactured Product*", published by Van Nostrand in New York. This book set the tone for subsequent applications of statistical methods to process control.

Contributions of Dodge and Romig to sampling inspection

Two other Bell Labs statisticians, H.F. Dodge and H.G. Romig spearheaded efforts in applying statistical theory to sampling inspection. The work of these three pioneers constitutes much of what nowadays comprises the theory of statistical quality and control. There is much more to say about the history of statistical quality control and the interested reader is invited to peruse one or more of the references. A very good summary of the historical background of SQC is found in chapter 1 of "[*Quality Control and Industrial Statistics*](#)", by Acheson J. Duncan. See also [Juran \(1997\)](#).



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6.1.2. What are Process Control Techniques?

Statistical Process Control (SPC)

*Typical
process
control
techniques*

There are many ways to implement process control. Key monitoring and investigating tools include:

- [Histograms](#)
- Check Sheets
- Pareto Charts
- Cause and Effect Diagrams
- Defect Concentration Diagrams
- [Scatter Diagrams](#)
- [Control Charts](#)

All these are described in Montgomery (2000). This chapter will focus ([Section 3](#)) on control chart methods, specifically:

- [Classical Shewhart Control charts,](#)
- [Cumulative Sum \(CUSUM\) charts](#)
- [Exponentially Weighted Moving Average \(EWMA\) charts](#)
- [Multivariate control charts](#)

Underlying concepts

The underlying concept of statistical process control is based on a comparison of what is happening today with what happened previously. We take a snapshot of how the process typically performs or build a model of how we think the process will perform and calculate control limits for the expected measurements of the output of the process. Then we collect data from the process and compare the data to the control limits. The majority of measurements should fall within the control limits. Measurements that fall outside the control limits are examined to see if they belong to the same population as our initial snapshot or model. Stated differently, we use historical data to compute the initial control limits. Then the data are compared against these initial limits. Points that fall outside of the limits are investigated and, perhaps, some will later be discarded. If so, the limits would be recomputed and the process repeated. This is referred to as Phase I. Real-time process monitoring, using the limits from the end of Phase I, is Phase II.

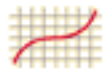
Statistical Quality Control (SQC)*Tools of statistical quality control*

Several techniques can be used to investigate the product for defects or defective pieces after all processing is complete. Typical tools of SQC ([described in section 2](#)) are:

- Lot Acceptance sampling plans
- Skip lot sampling plans
- Military (MIL) Standard sampling plans

Underlying concepts of statistical quality control

The purpose of statistical quality control is to ensure, in a cost efficient manner, that the product shipped to customers meets their specifications. Inspecting every product is costly and inefficient, but the consequences of shipping non conforming product can be significant in terms of customer dissatisfaction. Statistical Quality Control is the process of inspecting enough product from given lots to probabilistically ensure a specified quality level.



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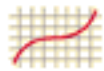
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6.1.3. What is Process Control?

Two types of intervention are possible -- one is based on engineering judgment and the other is automated

Process Control is the active changing of the process based on the results of process monitoring. Once the process monitoring tools have detected an out-of-control situation, the person responsible for the process makes a change to bring the process back into control.

1. *Out-of-control Action Plans (OCAPS)* detail the action to be taken once an out-of-control situation is detected. A specific flowchart, that leads the process engineer through the corrective procedure, may be provided for each unique process.
2. *Advanced Process Control Loops* are automated changes to the process that are programmed to correct for the size of the out-of-control measurement.



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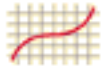
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6.1.4. What to do if the process is "Out of Control"?

Reactions to out-of-control conditions

If the process is out-of-control, the process engineer looks for an assignable cause by following the out-of-control action plan (OCAP) associated with the control chart. Out-of-control refers to rejecting the assumption that the current data are from the same population as the data used to create the initial control chart limits.

For classical Shewhart charts, a set of rules called the Western Electric Rules ([WECO Rules](#)) and a set of [trend rules](#) often are used to determine out-of-control.

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6.1.5. What to do if "In Control" but Unacceptable?

In control means process is predictable

"In Control" only means that the process is predictable in a statistical sense. What do you do if the process is "in control" but the average level is too high or too low or the variability is unacceptable?

Process improvement techniques

Process improvement techniques such as

- [experiments](#)
- [calibration](#)
- re-analysis of historical database

can be initiated to put the process on target or reduce the variability.

Process must be stable

Note that the process must be stable before it can be centered at a target value or its overall variation can be reduced.

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6.1.6. What is Process Capability?

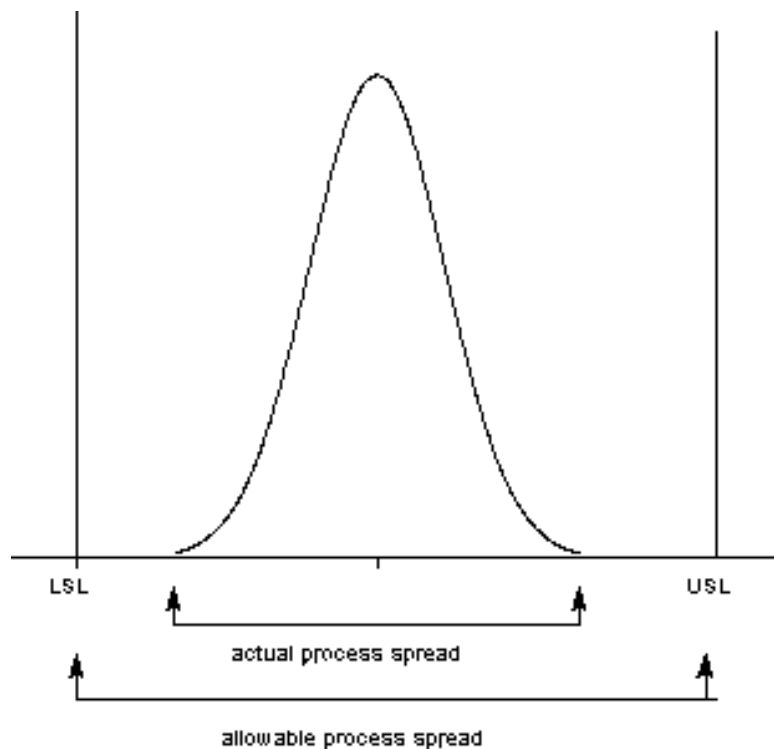
Process capability compares the output of an *in-control* process to the specification limits by using *capability indices*. The comparison is made by forming the ratio of the spread between the process specifications (the specification "width") to the spread of the process values, as measured by 6 process standard deviation units (the process "width").

Process Capability Indices

A process capability index uses both the process variability and the process specifications to determine whether the process is "capable"

We are often required to compare the output of a stable process with the process specifications and make a statement about how well the process meets specification. To do this we compare the natural variability of a stable process with the process specification limits.

A capable process is one where almost all the measurements fall inside the specification limits. This can be represented pictorially by the plot below:



There are several statistics that can be used to measure the capability of a process: C_p , C_{pk} , C_{pm}

Most capability indices estimates are valid only if the sample size used is 'large enough'. Large enough is generally thought to be about 50 independent data values.

The C_p , C_{pk} , and C_{pm} statistics assume that the population of data values is normally distributed. Assuming a two-sided specification, if μ and σ are the mean and standard deviation, respectively, of the normal data and USL, LSL, and T are the upper and lower specification limits and the target value, respectively, then the population capability indices are defined as follows:

Definitions of various process capability indices

$$C_p = \frac{USL - LSL}{6\sigma}$$

$$C_{pk} = \min \left[\frac{USL - \mu}{3\sigma}, \frac{\mu - LSL}{3\sigma} \right]$$

$$C_{pm} = \frac{USL - LSL}{6\sqrt{\sigma^2 + (\mu - T)^2}}$$

Sample estimates of capability indices

Sample estimators for these indices are given below. (Estimators are indicated with a "hat" over them).

$$\hat{C}_p = \frac{USL - LSL}{6s}$$

$$\hat{C}_{pk} = \min \left[\frac{USL - \bar{x}}{3s}, \frac{\bar{x} - LSL}{3s} \right]$$

$$\hat{C}_{pm} = \frac{USL - LSL}{6\sqrt{s^2 + (\bar{x} - T)^2}}$$

The estimator for C_{pk} can also be expressed as $C_{pk} = C_p(1-k)$, where k is a scaled distance between the midpoint of the specification range, m , and the process mean, μ .

Denote the midpoint of the specification range by $m = (USL+LSL)/2$. The distance between the process mean, μ , and the optimum, which is m , is $\mu - m$, where $m \leq \mu \leq LSL$. The scaled distance is

$$k = \frac{|\mu - m|}{(USL - LSL)/2}, \quad 0 \leq k \leq 1$$

(the absolute sign takes care of the case when $LSL \leq \mu \leq m$). To determine the estimated value, \hat{k} , we estimate μ by \bar{x} . Note that $\bar{x} \leq USL$.

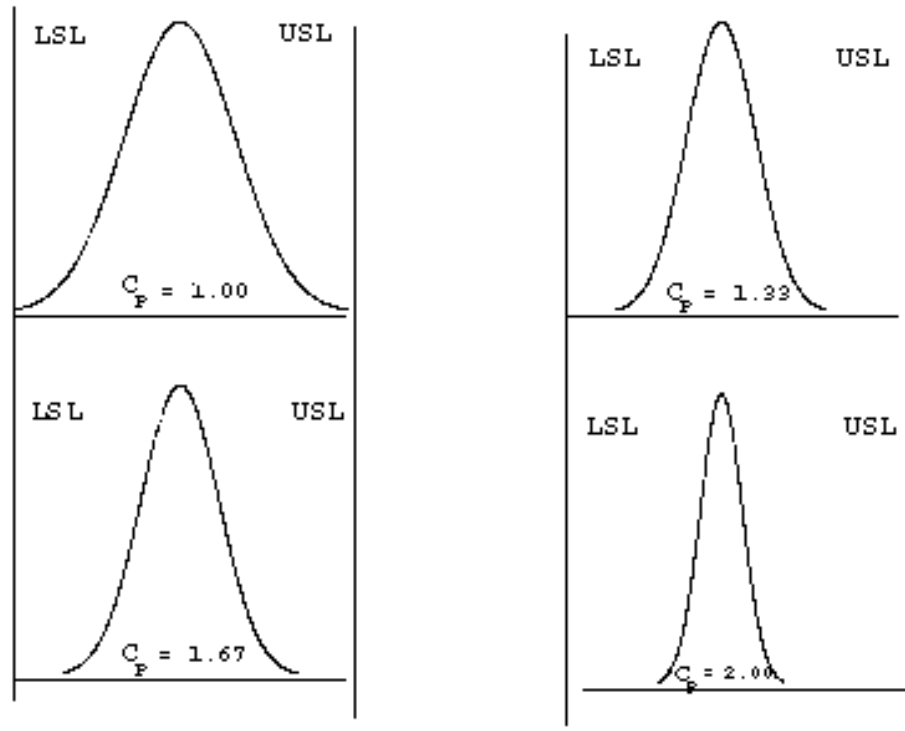
The estimator for the C_p index, adjusted by the k factor, is

$$\hat{C}_{pk} = \hat{C}_p(1 - \hat{k})$$

Since $0 \leq k \leq 1$, it follows that $\hat{C}_{pk} \leq \hat{C}_p$

Plot showing C_p for varying process widths

To get an idea of the value of the C_p statistic for varying process widths, consider the following plot



This can be expressed numerically by the table below:

Translating capability into "rejects"

$USL - LSL$	6σ	8σ	10σ	12σ
C_p	1.00	1.33	1.66	2.00
Rejects	.27%	64 ppm	.6 ppm	2 ppb
% of spec used	100	75	60	50

where ppm = parts per million and ppb = parts per billion. Note that the reject figures are based on the assumption that the distribution is centered at μ .

We have discussed the situation with two spec. limits, the USL and LSL. This is known as the *bilateral* or two-sided case. There are many cases where only the lower or upper specifications are used. Using one spec limit is called *unilateral* or one-sided. The corresponding capability indices are

One-sided specifications and the corresponding capability indices

$$C_{pu} = \frac{\text{allowable upper spread}}{\text{actual upper spread}} = \frac{USL - \mu}{3\sigma}$$

and

$$C_{pl} = \frac{\text{allowable lower spread}}{\text{actual lower spread}} = \frac{\mu - LSL}{3\sigma}$$

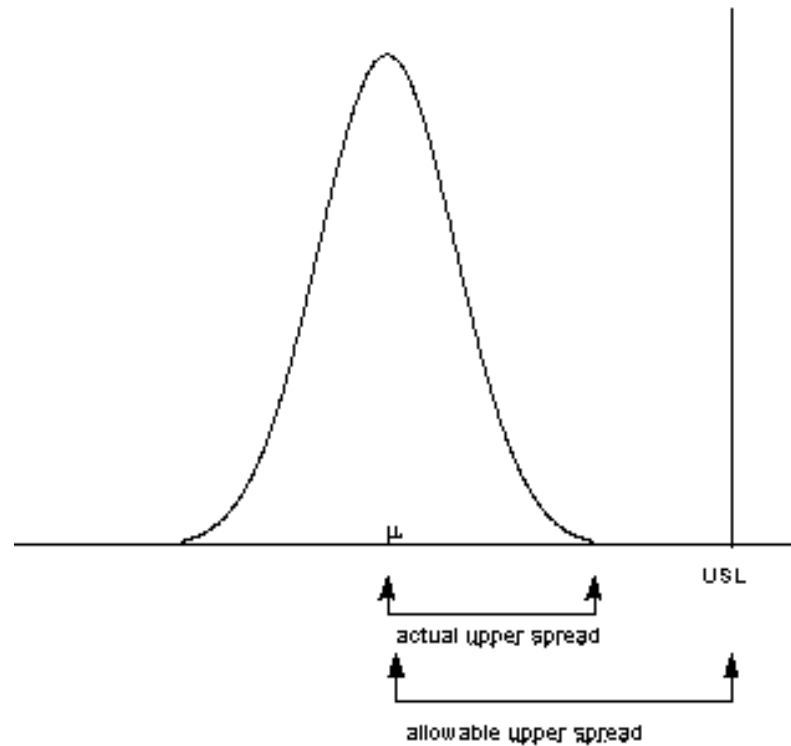
where μ and σ are the process mean and standard deviation, respectively.

Estimators of C_{pu} and C_{pl} are obtained by replacing μ and σ by \bar{x} and s , respectively.

The following relationship holds

$$C_p = (C_{pu} + C_{pl}) / 2.$$

This can be represented pictorially by



Note that we also can write:

$$C_{pk} = \min \{C_{pl}, C_{pu}\}.$$

Confidence Limits For Capability Indices

Confidence intervals for indices

Assuming normally distributed process data, the distribution of the sample \hat{C}_p follows

from a Chi-square distribution and \hat{C}_{pu} and \hat{C}_{pl} have distributions related to the non-central t distribution. Fortunately, approximate confidence limits related to the normal distribution have been derived. Various approximations to the distribution of \hat{C}_{pk} have been proposed, including those given by Bissell (1990), and we will use a normal approximation.

The resulting formulas for confidence limits are given below:

100(1- α)% Confidence Limits for C_p

$$Pr\{\hat{C}_p(L_1) \leq C_p \leq \hat{C}_p(L_2)\} = 1 - \alpha$$

where

$$L_1 = \sqrt{\frac{\chi_{(\nu, \alpha/2)}^2}{\nu}} \quad L_2 = \sqrt{\frac{\chi_{(\nu, 1-\alpha/2)}^2}{\nu}}$$

ν = degrees of freedom

Confidence Intervals for C_{pu} and C_{pl}

Approximate 100(1- α)% confidence limits for C_{pu} with sample size n are:

$$C_{pu}(\text{lower}) = \hat{C}_{pu} - z_{1-\beta} \sqrt{\frac{1}{9n} + \frac{\hat{C}_{pu}^2}{2(n-1)}}$$

$$C_{pu}(\text{upper}) = \hat{C}_{pu} + z_{1-\alpha} \sqrt{\frac{1}{9n} + \frac{\hat{C}_{pu}^2}{2(n-1)}}$$

with z denoting the percent point function of the standard normal distribution. If β is not known, set it to α .

Limits for C_{pl} are obtained by replacing \hat{C}_{pu} by \hat{C}_{pl} .

Confidence
Interval for
 C_{pk}

[Zhang et al. \(1990\)](#) derived the exact variance for the estimator of C_{pk} as well as an approximation for large n . The reference paper is Zhang, Stenback and Wardrop (1990), "Interval Estimation of the process capability index", *Communications in Statistics: Theory and Methods*, 19(21), 4455-4470.

The variance is obtained as follows:

Let

$$c = \sqrt{n}[\mu - (USL + LSL)/2]\sigma$$

$$d = (USL - LSL)/\sigma$$

$$\Phi(-c) = \int_{-\infty}^{-c} \frac{1}{\sqrt{2\pi}} \exp -\frac{1}{2}z^2 dz$$

Then

$$\begin{aligned} &Var(\hat{C}_{pk}) \\ &= (d^2/36)(n-1)(n-3) \\ &\quad - (d/9\sqrt{n})(n-1)(n-3)\{\sqrt{2\pi} \exp(-c^2/2) + c[1 - 2\Phi(-c)]\} \\ &\quad + [(1/9)(n-1)/(n(n-3))](1+c^2) \\ &\quad - [(n-1)/(72n)]\left\{\frac{\Gamma((n-2)/2)}{\Gamma((n-1)/2)}\right\}^2 \\ &\quad * \{d\sqrt{n} - 2\sqrt{2\pi} \exp(-c^2/2) - 2c[1 - 2\Phi(-c)]\}^2 \end{aligned}$$

Their approximation is given by:

$$Var(\hat{C}_{pk}) = \frac{n-1}{n-3} - 0.5\left\{\frac{\Gamma((n-2)/2)}{\Gamma((n-1)/2)}\right\}^2$$

where

$$n \geq 25, 0.75 \leq C_{pk} \leq 4, |c| \leq 100, \text{ and } d \leq 24$$

The following approximation is commonly used in practice

$$C_{pk} = \hat{C}_{pk} \pm z_{1-\alpha/2} \sqrt{\frac{1}{9n} + \frac{\hat{C}_{pk}^2}{2(n-1)}}$$

It is important to note that the sample size should be at least 25 before these approximations are valid. In general, however, we need $n \geq 100$ for capability studies. Another point to observe is that variations are not negligible due to the randomness of capability indices.

Capability Index Example

An example

For a certain process the $USL = 20$ and the $LSL = 8$. The observed process average, $\bar{X} = 16$, and the standard deviation, $s = 2$. From this we obtain

$$\hat{C}_p = \frac{USL - LSL}{6s} = \frac{20 - 8}{6(2)} = 1.0$$

This means that the process is capable as long as it is located at the midpoint, $m = (USL + LSL)/2 = 14$.

But it doesn't, since $\bar{x} = 16$. The \hat{k} factor is found by

$$\hat{k} = \frac{|m - \bar{x}|}{(USL - LSL)/2} = \frac{2}{6} = 0.3333$$

and

$$\hat{C}_{pk} = \hat{C}_p(1 - \hat{k}) = 0.6667$$

We would like to have \hat{C}_{pk} at least 1.0, so this is not a good process. If possible,

reduce the variability or/and center the process. We can compute the \hat{C}_{pu} and \hat{C}_{pl}

$$\hat{C}_{pu} = \frac{USL - \bar{x}}{3s} = \frac{20 - 16}{3(2)} = 0.6667$$

$$\hat{C}_{pl} = \frac{\bar{x} - LSL}{3s} = \frac{16 - 8}{3(2)} = 1.3333$$

From this we see that the \hat{C}_{pu} , which is the smallest of the above indices, is 0.6667.

Note that the formula $\hat{C}_{pk} = \hat{C}_p(1 - \hat{k})$ is the algebraic equivalent of the $\min\{\hat{C}_{pu}, \hat{C}_{pl}\}$ definition.

What happens if the process is not approximately normally distributed?

What you can do with non-normal data

The indices that we considered thus far are based on normality of the process distribution. This poses a problem when the process distribution is not normal. Without going into the specifics, we can list some remedies.

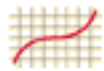
1. Transform the data so that they become approximately normal. A popular transformation is the [Box-Cox transformation](#)
2. Use or develop another set of indices, that apply to nonnormal distributions. One statistic is called C_{npk} (for non-parametric C_{pk}). Its estimator is calculated by

$$\hat{C}_{pk} = \min \left[\frac{USL - median}{p(.995) - median}, \frac{median - LSL}{median - p(.005)} \right]$$

where $p(0.995)$ is the 99.5th percentile of the data and $p(0.005)$ is the 0.5th percentile of the data.

For additional information on nonnormal distributions, see [Johnson and Kotz \(1993\)](#).

There is, of course, much more that can be said about the case of nonnormal data. However, if a Box-Cox transformation can be successfully performed, one is encouraged to use it.



6. [Process or Product Monitoring and Control](#)

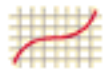
6.2. Test Product for Acceptability: Lot Acceptance Sampling

This section describes how to make decisions on a lot-by-lot basis whether to accept a lot as likely to meet requirements or reject the lot as likely to have too many defective units.

Contents of section 2

This section consists of the following topics.

1. [What is Acceptance Sampling?](#)
2. [What kinds of Lot Acceptance Sampling Plans \(LASPs\) are there?](#)
3. [How do you Choose a Single Sampling Plan?](#)
 1. [Choosing a Sampling Plan: MIL Standard 105D](#)
 2. [Choosing a Sampling Plan with a given OC Curve](#)
4. [What is Double Sampling?](#)
5. [What is Multiple Sampling?](#)
6. [What is a Sequential Sampling Plan?](#)
7. [What is Skip Lot Sampling?](#)

[6. Process or Product Monitoring and Control](#)[6.2. Test Product for Acceptability: Lot Acceptance Sampling](#)

6.2.1. What is Acceptance Sampling?

Contributions of Dodge and Romig to acceptance sampling

Acceptance sampling is an important field of statistical quality control that was popularized by Dodge and Romig and originally applied by the U.S. military to the testing of bullets during World War II. If every bullet was tested in advance, no bullets would be left to ship. If, on the other hand, none were tested, malfunctions might occur in the field of battle, with potentially disastrous results.

Definition of Lot Acceptance Sampling

Dodge reasoned that a sample should be picked at random from the lot, and on the basis of information that was yielded by the sample, a decision should be made regarding the disposition of the lot. In general, the decision is either to accept or reject the lot. This process is called *Lot Acceptance Sampling* or just *Acceptance Sampling*.

"Attributes" (i.e., defect counting) will be assumed

Acceptance sampling is "the middle of the road" approach between no inspection and 100% inspection. There are two major classifications of acceptance plans: by *attributes* ("go, no-go") and by *variables*. The attribute case is the most common for acceptance sampling, and will be assumed for the rest of this section.

Important point

A point to remember is that the main purpose of acceptance sampling is to decide whether or not the lot is likely to be acceptable, not to estimate the quality of the lot.

Scenarios leading to acceptance sampling

Acceptance sampling is employed when one or several of the following hold:

- Testing is destructive
- The cost of 100% inspection is very high
- 100% inspection takes too long

*Acceptance
Quality
Control and
Acceptance
Sampling*

It was pointed out by Harold Dodge in 1969 that Acceptance Quality Control is not the same as Acceptance Sampling. The latter depends on specific sampling plans, which when implemented indicate the conditions for acceptance or rejection of the immediate lot that is being inspected. The former may be implemented in the form of an Acceptance Control Chart. The control limits for the Acceptance Control Chart are computed using the specification limits and the standard deviation of what is being monitored (see [Ryan, 2000](#) for details).

*An
observation
by Harold
Dodge*

In 1942, Dodge stated:

"...basically the "acceptance quality control" system that was developed encompasses the concept of protecting the consumer from getting unacceptable defective product, and encouraging the producer in the use of process quality control by: varying the quantity and severity of acceptance inspections in direct relation to the importance of the characteristics inspected, and in the inverse relation to the goodness of the quality level as indication by those inspections."

To reiterate the difference in these two approaches: acceptance sampling plans are one-shot deals, which essentially test short-run effects. Quality control is of the long-run variety, and is part of a well-designed system for lot acceptance.

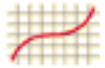
*An
observation
by Ed
Schilling*

Schilling (1989) said:

"An individual sampling plan has much the effect of a lone sniper, while the sampling plan scheme can provide a fusillade in the battle for quality improvement."

*Control of
product
quality using
acceptance
control charts*

According to the ISO standard on acceptance control charts ([ISO 7966, 1993](#)), an acceptance control chart combines consideration of control implications with elements of acceptance sampling. It is an appropriate tool for helping to make decisions with respect to process acceptance. The difference between acceptance sampling approaches and acceptance control charts is the emphasis on process acceptability rather than on product disposition decisions.



6. [Process or Product Monitoring and Control](#)

6.2. [Test Product for Acceptability: Lot Acceptance Sampling](#)

6.2.2. What kinds of Lot Acceptance Sampling Plans (LASPs) are there?

LASP is a sampling scheme and a set of rules

A lot acceptance sampling plan (LASP) is a sampling scheme and a set of rules for making decisions. The decision, based on counting the number of defectives in a sample, can be to accept the lot, reject the lot, or even, for multiple or sequential sampling schemes, to take another sample and then repeat the decision process.

Types of acceptance plans to choose from

LASPs fall into the following categories:

- **Single sampling plans:** One sample of items is selected at random from a lot and the disposition of the lot is determined from the resulting information. These plans are usually denoted as (n,c) plans for a sample size n , where the lot is rejected if there are more than c defectives. *These are the most common (and easiest) plans to use although not the most efficient in terms of average number of samples needed.*
- **Double sampling plans:** After the first sample is tested, there are three possibilities:
 1. Accept the lot
 2. Reject the lot
 3. No decision

If the outcome is (3), and a second sample is taken, the procedure is to combine the results of both samples and make a final decision based on that information.
- **Multiple sampling plans:** This is an extension of the double sampling plans where more than two samples are needed to reach a conclusion. The advantage of multiple sampling is smaller sample sizes.
- **Sequential sampling plans:** . This is the ultimate extension of multiple sampling where items are selected from a lot one at a time and after inspection of each item a decision is made to accept or reject the lot or select another unit.
- **Skip lot sampling plans:** . Skip lot sampling means that only a

fraction of the submitted lots are inspected.

*Definitions
of basic
Acceptance
Sampling
terms*

Deriving a plan, within one of the categories listed above, is discussed in the pages that follow. All derivations depend on the properties you want the plan to have. These are described using the following terms:

- **Acceptable Quality Level (AQL):** The AQL is a percent defective that is the base line requirement for the quality of the producer's product. The producer would like to design a sampling plan such that there is a *high probability of accepting* a lot that has a defect level less than or equal to the AQL.
- **Lot Tolerance Percent Defective (LTPD):** The LTPD is a designated high defect level that would be unacceptable to the consumer. The consumer would like the sampling plan to have a *low probability of accepting* a lot with a defect level as high as the LTPD.
- **Type I Error (Producer's Risk):** This is the probability, for a given (n,c) sampling plan, of rejecting a lot that has a defect level equal to the AQL. The producer suffers when this occurs, because a lot with acceptable quality was rejected. The symbol α is commonly used for the Type I error and typical values for α range from 0.2 to 0.01.
- **Type II Error (Consumer's Risk):** This is the probability, for a given (n,c) sampling plan, of accepting a lot with a defect level equal to the LTPD. The consumer suffers when this occurs, because a lot with unacceptable quality was accepted. The symbol β is commonly used for the Type II error and typical values range from 0.2 to 0.01.
- **Operating Characteristic (OC) Curve:** This curve plots the probability of accepting the lot (Y-axis) versus the lot fraction or percent defectives (X-axis). *The OC curve is the primary tool for displaying and investigating the properties of a LASP.*
- **Average Outgoing Quality (AOQ):** A common procedure, when sampling and testing is non-destructive, is to 100% inspect rejected lots and replace all defectives with good units. In this case, all rejected lots are made perfect and the only defects left are those in lots that were accepted. AOQ's refer to the long term defect level for this combined LASP and 100% inspection of rejected lots process. If all lots come in with a defect level of exactly p , and the OC curve for the chosen (n,c) LASP indicates a probability p_a of accepting such a lot, over the long run the AOQ can easily be shown to be:

$$AOQ = \frac{p_a P(N - n)}{N}$$

where N is the lot size.

- **Average Outgoing Quality Level (AOQL):** A plot of the AOQ (Y-axis) versus the incoming lot p (X-axis) will start at 0 for $p = 0$, and return to 0 for $p = 1$ (where every lot is 100% inspected and rectified). In between, it will rise to a maximum. This maximum, which is the worst possible long term AOQ , is called the $AOQL$.
- **Average Total Inspection (ATI):** When rejected lots are 100% inspected, it is easy to calculate the ATI if lots come consistently with a defect level of p . For a LASP (n, c) with a probability p_a of accepting a lot with defect level p , we have

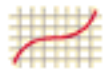
$$ATI = n + (1 - p_a)(N - n)$$

where N is the lot size.

- **Average Sample Number (ASN):** For a single sampling LASP (n, c) we know each and every lot has a sample of size n taken and inspected or tested. For double, multiple and sequential LASP's, the amount of sampling varies depending on the the number of defects observed. For any given double, multiple or sequential plan, a long term ASN can be calculated assuming all lots come in with a defect level of p . A plot of the ASN , versus the incoming defect level p , describes the sampling efficiency of a given LASP scheme.

The final choice is a tradeoff decision

Making a final choice between single or multiple sampling plans that have acceptable properties is a matter of deciding whether the average sampling savings gained by the various multiple sampling plans justifies the additional complexity of these plans and the uncertainty of not knowing how much sampling and inspection will be done on a day-by-day basis.



6. [Process or Product Monitoring and Control](#)

6.2. [Test Product for Acceptability: Lot Acceptance Sampling](#)

6.2.3. How do you Choose a Single Sampling Plan?

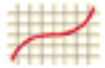
Two methods for choosing a single sample acceptance plan

A single sampling plan, as [previously defined](#), is specified by the pair of numbers (n, c) . The sample size is n , and the lot is rejected if there are more than c defectives in the sample; otherwise the lot is accepted.

There are two widely used ways of picking (n, c) :

1. Use tables (such as [MIL STD 105D](#)) that focus on either the [AQL](#) or the [LTPD](#) desired.
2. [Specify 2 desired points](#) on the [OC curve](#) and solve for the (n, c) that uniquely determines an OC curve going through these points.

The next two pages describe these methods in detail.



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- 6.2. [Test Product for Acceptability: Lot Acceptance Sampling](#)
- 6.2.3. [How do you Choose a Single Sampling Plan?](#)

6.2.3.1. Choosing a Sampling Plan: MIL Standard 105D

The AQL or Acceptable Quality Level is the baseline requirement

Sampling plans are typically set up with reference to an acceptable quality level, or [AQL](#). The *AQL* is the base line requirement for the quality of the producer's product. The producer would like to design a sampling plan such that the [OC curve](#) yields a high probability of acceptance at the *AQL*. On the other side of the OC curve, the consumer wishes to be protected from accepting poor quality from the producer. So the consumer establishes a criterion, the *lot tolerance percent defective* or [LTPD](#). Here the idea is to only accept poor quality product with a very low probability. Mil. Std. plans have been used for over 50 years to achieve these goals.

The U.S. Department of Defense Military Standard 105E

Military Standard 105E sampling plan

Standard military sampling procedures for inspection by attributes were developed during World War II. Army Ordnance tables and procedures were generated in the early 1940's and these grew into the Army Service Forces tables. At the end of the war, the Navy also worked on a set of tables. In the meanwhile, the Statistical Research Group at Columbia University performed research and outputted many outstanding results on attribute sampling plans.

These three streams combined in 1950 into a standard called Mil. Std. 105A. It has since been modified from time to time and issued as 105B, 195C and 105D. Mil. Std. 105D was issued by the U.S. government in 1963. It was adopted in 1971 by the American National Standards Institute as ANSI Standard Z1.4 and in 1974 it was adopted (with minor changes) by the International Organization for Standardization as ISO Std. 2859. The latest revision is Mil. Std 105E and was issued in 1989.

These three similar standards are continuously being updated and revised, but the basic tables remain the same. Thus the discussion that follows of the germane aspects of Mil. Std. 105E also applies to the

other two standards.

Description of Mil. Std. 105D

Military Standard 105D sampling plan

This document is essentially a set of individual plans, organized in a system of sampling schemes. A sampling scheme consists of a combination of a normal sampling plan, a tightened sampling plan, and a reduced sampling plan plus rules for switching from one to the other.

AQL is foundation of standard

The foundation of the Standard is the acceptable quality level or *AQL*. In the following scenario, a certain military agency, called the Consumer from here on, wants to purchase a particular product from a supplier, called the Producer from here on.

In applying the Mil. Std. 105D it is expected that there is perfect agreement between Producer and Consumer regarding what the *AQL* is for a given product characteristic. It is understood by both parties that the Producer will be submitting for inspection a number of lots whose quality level is typically as good as specified by the Consumer. Continued quality is assured by the acceptance or rejection of lots following a particular sampling plan and also by providing for a shift to another, tighter sampling plan, when there is evidence that the Producer's product does not meet the agreed-upon *AQL*.

Standard offers 3 types of sampling plans

Mil. Std. 105E offers three types of sampling plans: single, double and multiple plans. The choice is, in general, up to the inspectors.

Because of the three possible selections, the standard does not give a sample size, but rather a sample code letter. This, together with the decision of the type of plan yields the specific sampling plan to be used.

Inspection level

In addition to an initial decision on an *AQL* it is also necessary to decide on an "inspection level". This determines the relationship between the lot size and the sample size. The standard offers three general and four special levels.

Steps in the standard

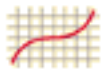
The steps in the use of the standard can be summarized as follows:

1. Decide on the *AQL*.
2. Decide on the inspection level.
3. Determine the lot size.
4. Enter the table to find sample size code letter.
5. Decide on type of sampling to be used.
6. Enter proper table to find the plan to be used.
7. Begin with normal inspection, follow the switching rules and the rule for stopping the inspection (if needed).

Additional information

There is much more that can be said about Mil. Std. 105E, (and 105D). The interested reader is referred to references such as ([Montgomery \(2000\)](#), [Schilling](#), tables 11-2 to 11-17, and [Duncan](#), pages 214 - 248).

There is also (currently) a [web site](#) developed by Galit Shmueli that will develop sampling plans interactively with the user, according to Military Standard 105E (ANSI/ASQC Z1.4, ISO 2859) Tables.



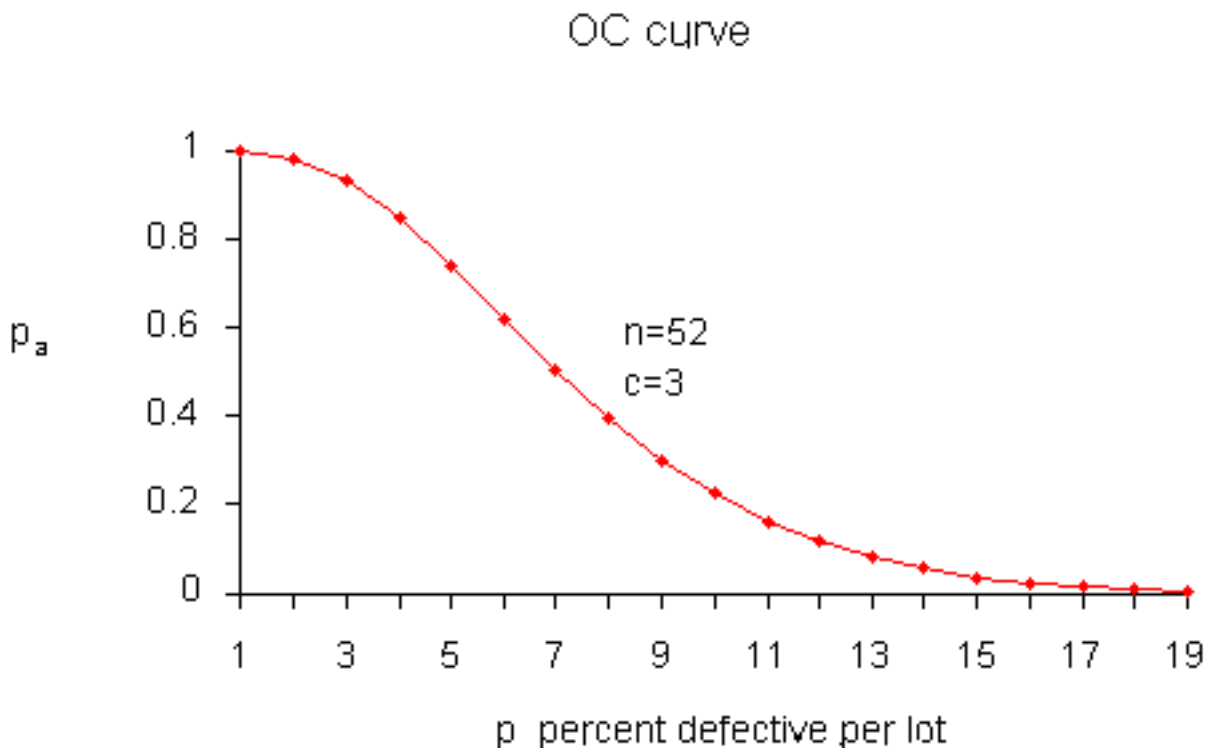
6. [Process or Product Monitoring and Control](#)

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6.2.3. [How do you Choose a Single Sampling Plan?](#)

6.2.3.2. Choosing a Sampling Plan with a given OC Curve

Sample OC curve We start by looking at a typical [OC curve](#). The OC curve for a (52,3) sampling plan is shown below.



Number of defectives is approximately binomial

It is instructive to show how the points on this curve are obtained, once we have a sampling plan (n,c) - later we will demonstrate how a sampling plan (n,c) is obtained.

We assume that the lot size N is very large, as compared to the sample size n , so that removing the sample doesn't significantly change the remainder of the lot, no matter how many defects are in the sample. Then the distribution of the number of defectives, d , in a random sample of n items is approximately binomial with parameters n and p , where p is the fraction of defectives per lot.

The probability of observing exactly d defectives is given by

The binomial distribution

$$P(d) = f(d) = \frac{n!}{d!(n-d)!} p^d (1-p)^{n-d}$$

The probability of acceptance is the probability that d , the number of defectives, is less than or equal to c , the accept number. This means that

$$P_a = P\{d \leq c\} = \sum_{d=0}^c \frac{n!}{d!(n-d)!} p^d (1-p)^{n-d}$$

Sample table for P_a , P_d using the binomial distribution

Using this formula with $n = 52$ and $c=3$ and $p = .01, .02, \dots, .12$ we find

P_a	P_d
.998	.01
.980	.02
.930	.03
.845	.04
.739	.05
.620	.06
.502	.07
.394	.08
.300	.09
.223	.10
.162	.11
.115	.12

Solving for (n,c)

Equations for calculating a sampling plan with a given OC curve

In order to design a sampling plan with a specified OC curve one needs two designated points. Let us design a sampling plan such that the probability of acceptance is $1-\alpha$ for lots with fraction defective p_1 and the probability of acceptance is β for lots with fraction defective p_2 . Typical choices for these points are: p_1 is the [AQL](#), p_2 is the [LTPD](#) and α , β are the [Producer's Risk \(Type I error\)](#) and [Consumer's Risk \(Type II error\)](#), respectively.

If we are willing to assume that binomial sampling is valid, then the sample size n , and the acceptance number c are the solution to

$$1 - \alpha = \sum_{d=0}^c \frac{n!}{d!(n-d)!} p_1^d (1-p_1)^{n-d}$$

$$\beta = \sum_{d=0}^c \frac{n!}{d!(n-d)!} p_2^d (1-p_2)^{n-d}$$

These two simultaneous equations are nonlinear so there is no simple, direct solution. There are however a number of iterative techniques available that give approximate solutions so that composition of a computer program poses few problems.

Average Outgoing Quality (AOQ)

Calculating AOQ's

We can also calculate the [AOQ](#) for a (n,c) sampling plan, provided rejected lots are 100% inspected and defectives are replaced with good parts.

Assume all lots come in with exactly a p_0 proportion of defectives.

After screening a rejected lot, the final fraction defectives will be zero for that lot. However, accepted lots have fraction defective p_0 .

Therefore, the outgoing lots from the inspection stations are a mixture of lots with fractions defective p_0 and 0. Assuming the lot size is N , we have.

$$AOQ = \frac{p_a P(N-n)}{N}$$

For example, let $N = 10000$, $n = 52$, $c = 3$, and p , the quality of incoming lots, = 0.03. Now at $p = 0.03$, we glean from the OC curve table that $p_a = 0.930$ and

$$AOQ = (.930)(.03)(10000-52) / 10000 = 0.02775.$$

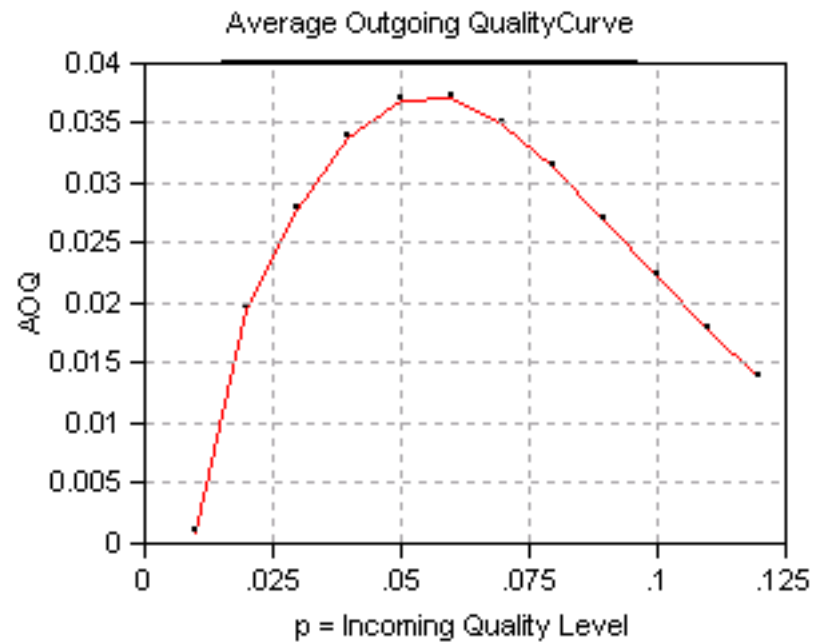
*Sample table
of AOQ
versus p*

Setting $p = .01, .02, \dots, .12$, we can generate the following table

AOQ	p
.0010	.01
.0196	.02
.0278	.03
.0338	.04
.0369	.05
.0372	.06
.0351	.07
.0315	.08
.0270	.09
.0223	.10
.0178	.11
.0138	.12

*Sample plot
of AOQ
versus p*

A plot of the AOQ versus p is given below.



*Interpretation
of AOQ plot*

From examining this curve we observe that when the incoming quality is very good (very small fraction of defectives coming in), then the outgoing quality is also very good (very small fraction of defectives going out). When the incoming lot quality is very bad, most of the lots are rejected and then inspected. The "duds" are eliminated or replaced by good ones, so that the quality of the outgoing lots, the *AOQ*, becomes very good. In between these extremes, the *AOQ* rises, reaches a maximum, and then drops.

The maximum ordinate on the *AOQ* curve represents the worst possible quality that results from the rectifying inspection program. It is called the **average outgoing quality limit**, ([*AOQL*](#)).

From the table we see that the $AOQL = 0.0372$ at $p = .06$ for the above example.

One final remark: if $N \gg n$, then the $AOQ \sim p_a p$.

The Average Total Inspection (ATI)

*Calculating
the Average
Total
Inspection*

What is the total amount of inspection when rejected lots are screened?

If all lots contain zero defectives, no lot will be rejected.

If all items are defective, all lots will be inspected, and the amount to be inspected is N .

Finally, if the lot quality is $0 < p < 1$, the average amount of inspection per lot will vary between the sample size n , and the lot size N .

Let the quality of the lot be p and the probability of lot acceptance be p_a , then the *ATI* per lot is

$$ATI = n + (1 - p_a)(N - n)$$

For example, let $N = 10000$, $n = 52$, $c = 3$, and $p = .03$. We know from the OC table that $p_a = 0.930$. Then $ATI = 52 + (1 - 0.930)(10000 - 52) = 753$. (Note that while 0.930 was rounded to three decimal places, 753 was obtained using more decimal places.)

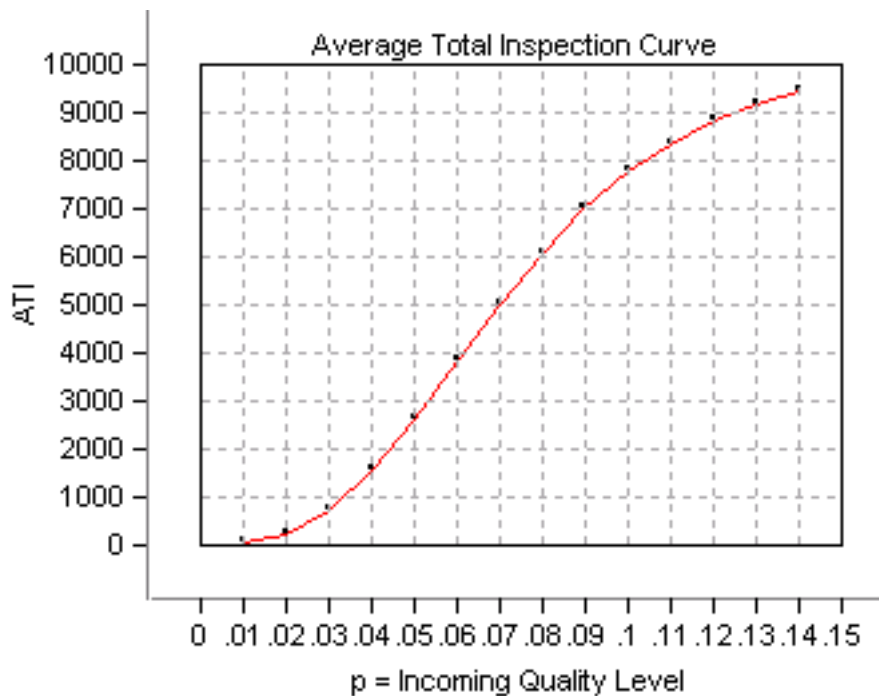
Sample table
of ATI versus
 p

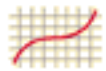
Setting $p = .01, .02, \dots, .14$ generates the following table

ATI	P
70	.01
253	.02
753	.03
1584	.04
2655	.05
3836	.06
5007	.07
6083	.08
7012	.09
7779	.10
8388	.11
8854	.12
9201	.13
9453	.14

Plot of ATI
versus p

A plot of ATI versus p , the Incoming Lot Quality (ILQ) is given below.





6. [Process or Product Monitoring and Control](#)

6.2. [Test Product for Acceptability: Lot Acceptance Sampling](#)

6.2.4. What is Double Sampling?

Double Sampling Plans

How double sampling plans work

Double and multiple sampling plans were invented to give a questionable lot another chance. For example, if in double sampling the results of the first sample are not conclusive with regard to accepting or rejecting, a second sample is taken. Application of double sampling requires that a first sample of size n_1 is taken at random from the (large) lot. The number of defectives is then counted and compared to the first sample's acceptance number a_1 and rejection number r_1 . Denote the number of defectives in sample 1 by d_1 and in sample 2 by d_2 , then:

If $d_1 \leq a_1$, the lot is accepted.

If $d_1 \geq r_1$, the lot is rejected.

If $a_1 < d_1 < r_1$, a second sample is taken.

If a second sample of size n_2 is taken, the number of defectives, d_2 , is counted. The total number of defectives is $D_2 = d_1 + d_2$. Now this is compared to the acceptance number a_2 and the rejection number r_2 of sample 2. In double sampling, $r_2 = a_2 + 1$ to ensure a decision on the sample.

If $D_2 \leq a_2$, the lot is accepted.

If $D_2 \geq r_2$, the lot is rejected.

Design of a Double Sampling Plan

Design of a double sampling plan

The parameters required to construct the OC curve are similar to the single sample case. The two points of interest are $(p_1, 1-\alpha)$ and (p_2, β) , where p_1 is the lot fraction defective for plan 1 and p_2 is the lot fraction defective for plan 2. As far as the respective sample sizes are concerned, the second sample size must be equal to, or an even multiple of, the first sample size.

There exist a variety of tables that assist the user in constructing double and multiple sampling plans. The index to these tables is the p_2/p_1 ratio, where $p_2 > p_1$. One set of tables, taken from the [Army Chemical Corps Engineering Agency](#) for $\alpha = .05$ and $\beta = .10$, is given below:

Tables for $n_1 = n_2$

$R = p_2/p_1$	accept numbers		approximation of pn_1	values for
	c_1	c_2	$P = .95$	$P = .10$
11.90	0	1	0.21	2.50
7.54	1	2	0.52	3.92
6.79	0	2	0.43	2.96
5.39	1	3	0.76	4.11
4.65	2	4	1.16	5.39
4.25	1	4	1.04	4.42
3.88	2	5	1.43	5.55
3.63	3	6	1.87	6.78
3.38	2	6	1.72	5.82
3.21	3	7	2.15	6.91
3.09	4	8	2.62	8.10
2.85	4	9	2.90	8.26
2.60	5	11	3.68	9.56
2.44	5	12	4.00	9.77
2.32	5	13	4.35	10.08
2.22	5	14	4.70	10.45
2.12	5	16	5.39	11.41

Tables for $n_2 = 2n_1$

$R = p_2/p_1$	accept numbers		approximation of pn_1	values for
	c_1	c_2	$P = .95$	$P = .10$
14.50	0	1	0.16	2.32
8.07	0	2	0.30	2.42
6.48	1	3	0.60	3.89

5.39	0	3	0.49	2.64
5.09	0	4	0.77	3.92
4.31	1	4	0.68	2.93
4.19	0	5	0.96	4.02
3.60	1	6	1.16	4.17
3.26	1	8	1.68	5.47
2.96	2	10	2.27	6.72
2.77	3	11	2.46	6.82
2.62	4	13	3.07	8.05
2.46	4	14	3.29	8.11
2.21	3	15	3.41	7.55
1.97	4	20	4.75	9.35
1.74	6	30	7.45	12.96

Example

*Example of
a double
sampling
plan*

We wish to construct a double sampling plan according to

$$p_1 = 0.01 \quad \alpha = 0.05 \quad p_2 = 0.05 \quad \beta = 0.10 \quad \text{and } n_1 = n_2$$

The plans in the corresponding table are indexed on the ratio

$$R = p_2/p_1 = 5$$

We find the row whose R is closet to 5. This is the 5th row ($R = 4.65$). This gives $c_1 = 2$ and $c_2 = 4$. The value of n_1 is determined from either of the two columns labeled pn_1 .

The left holds α constant at 0.05 ($P = 0.95 = 1 - \alpha$) and the right holds β constant at 0.10. ($P = 0.10$). Then holding α constant we find $pn_1 = 1.16$ so $n_1 = 1.16/p_1 = 116$. And, holding β constant we find $pn_1 = 5.39$, so $n_1 = 5.39/p_2 = 108$. Thus the desired sampling plan is

$$n_1 = 108 \quad c_1 = 2 \quad n_2 = 108 \quad c_2 = 4$$

If we opt for $n_2 = 2n_1$, and follow the same procedure using the appropriate table, the plan is:

$$n_1 = 77 \quad c_1 = 1 \quad n_2 = 154 \quad c_2 = 4$$

The first plan needs less samples if the number of defectives in sample 1 is greater than 2, while the second plan needs less samples if the number of defectives in sample 1 is less than 2.

ASN Curve for a Double Sampling Plan

*Construction
of the ASN
curve*

Since when using a double sampling plan the sample size depends on whether or not a second sample is required, an important consideration for this kind of sampling is the Average Sample Number (*ASN*) curve. This curve plots the *ASN* versus p' , the true fraction defective in an incoming lot.

We will illustrate how to calculate the *ASN* curve with an example. Consider a double-sampling plan $n_1 = 50$, $c_1 = 2$, $n_2 = 100$, $c_2 = 6$, where n_1 is the sample size for plan 1, with accept number c_1 , and n_2 , c_2 , are the sample size and accept number, respectively, for plan 2.

Let $p' = .06$. Then the probability of acceptance on the first sample, which is the chance of getting two or less defectives, is .416 (using binomial tables). The probability of rejection on the second sample, which is the chance of getting more than six defectives, is $(1 - .971) = .029$. The probability of making a decision on the first sample is .445, equal to the sum of .416 and .029. With complete inspection of the second sample, the *average* size sample is equal to the size of the first sample times the probability that there will be only one sample plus the size of the combined samples times the probability that a second sample will be necessary. For the sampling plan under consideration, the *ASN* with complete inspection of the second sample for a p' of .06 is

$$50(.445) + 150(.555) = 106$$

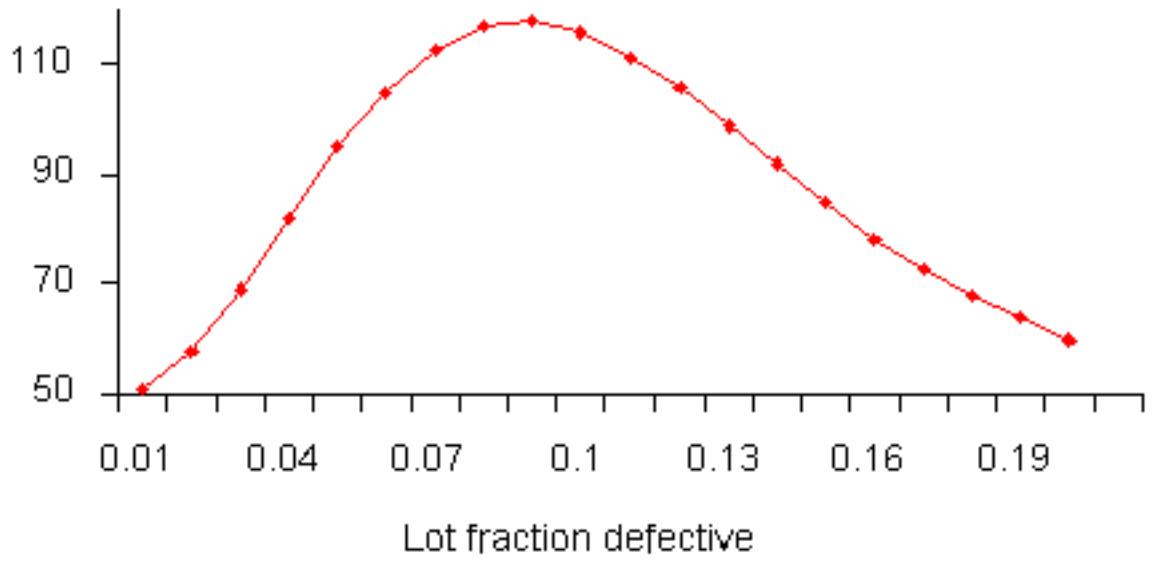
The general formula for an average sample number curve of a double-sampling plan with complete inspection of the second sample is

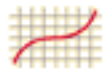
$$ASN = n_1 P_1 + (n_1 + n_2)(1 - P_1) = n_1 + n_2(1 - P_1)$$

where P_1 is the probability of a decision on the first sample. The graph below shows a plot of the *ASN* versus p' .

*The ASN
curve for a
double
sampling
plan*

Average Sample Number





6. [Process or Product Monitoring and Control](#)

6.2. [Test Product for Acceptability: Lot Acceptance Sampling](#)

6.2.5. What is Multiple Sampling?

Multiple Sampling is an extension of the double sampling concept

Multiple sampling is an extension of double sampling. It involves inspection of 1 to k successive samples as required to reach an ultimate decision.

Mil-Std 105D suggests $k = 7$ is a good number. Multiple sampling plans are usually presented in tabular form:

Procedure for multiple sampling

The procedure commences with taking a random sample of size n_1 from a large lot of size N and counting the number of defectives, d_1 .

if $d_1 \leq a_1$ the lot is accepted.

if $d_1 \geq r_1$ the lot is rejected.

if $a_1 < d_1 < r_1$, another sample is taken.

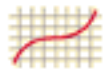
If subsequent samples are required, the first sample procedure is repeated sample by sample. For each sample, the total number of defectives found at any stage, say stage i , is

$$D_i = \sum_{j=1}^i d_j$$

This is compared with the acceptance number a_i and the rejection number r_i for that stage until a decision is made. Sometimes acceptance is not allowed at the early stages of multiple sampling; however, rejection can occur at any stage.

Efficiency measured by the ASN

Efficiency for a multiple sampling scheme is measured by the *average sample number (ASN)* required for a given [Type I](#) and [Type II](#) set of errors. The number of samples needed when following a multiple sampling scheme may vary from trial to trial, and the *ASN* represents the average of what might happen over many trials with a fixed incoming defect level.

6. [Process or Product Monitoring and Control](#)6.2. [Test Product for Acceptability: Lot Acceptance Sampling](#)

6.2.6. What is a Sequential Sampling Plan?

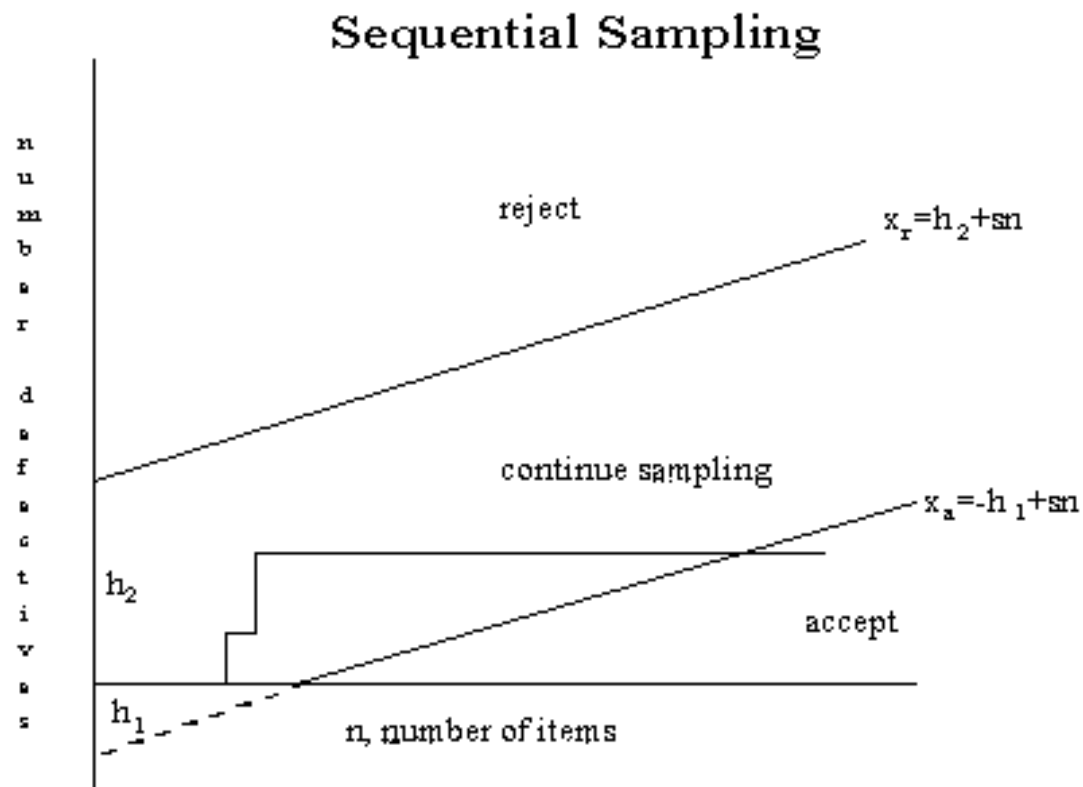
Sequential Sampling

Sequential sampling is different from single, double or multiple sampling. Here one takes a sequence of samples from a lot. How many total samples looked at is a function of the results of the sampling process.

Item-by-item and group sequential sampling

The sequence can be one sample at a time, and then the sampling process is usually called *item-by-item* sequential sampling. One can also select sample sizes greater than one, in which case the process is referred to as *group* sequential sampling. Item-by-item is more popular so we concentrate on it. The operation of such a plan is illustrated below:

Diagram of item-by-item sampling



Description of sequential sampling graph

The cumulative observed number of defectives is plotted on the graph. For each point, the x-axis is the total number of items thus far selected, and the y-axis is the total number of observed defectives. If the plotted point falls within the parallel lines the process continues by drawing another sample. As soon as a point falls on or above the upper line, the lot is rejected. And when a point falls on or below the lower line, the lot is accepted. The process can theoretically last until the lot is 100% inspected. However, as a rule of thumb, sequential-sampling plans are truncated after the number inspected reaches three times the number that would have been inspected using a corresponding single sampling plan.

Equations for the limit lines

The equations for the two limit lines are functions of the parameters p_1 , α , p_2 , and β .

$$\begin{aligned}x_a &= -h_1 + sn \quad (\text{acceptance line}) \\x_r &= h_2 + sn \quad (\text{rejection line})\end{aligned}$$

where

$$h_1 = (\log \frac{1 - \alpha}{\beta}) / k$$

$$h_2 = (\log \frac{1 - \beta}{\alpha}) / k$$

$$k = \log \frac{p_2(1 - p_1)}{p_1(1 - p_2)}$$

$$s = (\log [\frac{1 - p_1}{1 - p_2}]) / k$$

Instead of using the graph to determine the fate of the lot, one can resort to generating tables (with the help of a computer program).

Example of a sequential sampling plan

As an example, let $p_1 = .01$, $p_2 = .10$, $\alpha = .05$, $\beta = .10$. The resulting equations are

$$\begin{aligned}x_a &= -0.939 + 0.04n \\x_r &= 1.205 + 0.04n\end{aligned}$$

Both acceptance numbers and rejection numbers must be integers. The acceptance number is the next integer less than or equal to x_a and the rejection number is the next integer greater than or equal to x_r . Thus for $n = 1$, the acceptance number = -1, which is impossible, and the rejection number = 2, which is also impossible. For $n = 24$, the acceptance number is 0 and the rejection number = 3.

The results for $n = 1, 2, 3 \dots 26$ are tabulated below.

	n	n	n	n	n	n
	inspect	accept	reject	inspect	accept	reject
1	x	x	14	x	2	
2	x	2	15	x	2	
3	x	2	16	x	3	
4	x	2	17	x	3	
5	x	2	18	x	3	
6	x	2	19	x	3	
7	x	2	20	x	3	
8	x	2	21	x	3	
9	x	2	22	x	3	
10	x	2	23	x	3	
11	x	2	24	0	3	
12	x	2	25	0	3	
13	x	2	26	0	3	

So, for $n = 24$ the acceptance number is 0 and the rejection number is 3. The "x" means that acceptance or rejection is not possible.

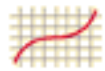
Other sequential plans are given below.

n	n	n
inspect	accept	reject
49	1	3
58	1	4
74	2	4
83	2	5
100	3	5
109	3	6

The corresponding single sampling plan is (52,2) and double sampling plan is (21,0), (21,1).

Efficiency measured by ASN

Efficiency for a sequential sampling scheme is measured by the *average sample number (ASN)* required for a given [Type I](#) and [Type II](#) set of errors. The number of samples needed when following a sequential sampling scheme may vary from trial to trial, and the ASN represents the average of what might happen over many trials with a fixed incoming defect level. Good software for designing sequential sampling schemes will calculate the ASN curve as a function of the incoming defect level.



6. [Process or Product Monitoring and Control](#)

6.2. [Test Product for Acceptability: Lot Acceptance Sampling](#)

6.2.7. What is Skip Lot Sampling?

Skip Lot Sampling

Skip Lot sampling means that only a fraction of the submitted lots are inspected. This mode of sampling is of the cost-saving variety in terms of time and effort. However skip-lot sampling should only be used when it has been demonstrated that the quality of the submitted product is very good.

Implementation of skip-lot sampling plan

A skip-lot sampling plan is implemented as follows:

1. [Design a single sampling plan](#) by specifying the alpha and beta risks and the consumer/producer's risks. This plan is called "the reference sampling plan".
2. Start with normal lot-by-lot inspection, using the reference plan.
3. When a pre-specified number, i , of consecutive lots are accepted, switch to inspecting only a fraction f of the lots. The selection of the members of that fraction is done at random.
4. When a lot is rejected return to normal inspection.

The f and i parameters

The parameters f and i are essential to calculating the probability of acceptance for a skip-lot sampling plan. In this scheme, i , called the *clearance number*, is a positive integer and the sampling fraction f is such that $0 < f < 1$. Hence, when $f = 1$ there is no longer skip-lot sampling. The calculation of the acceptance probability for the skip-lot sampling plan is performed via the following formula

$$P_a(f, i) = \frac{fP + (1-f)P^i}{f + (1-f)P^i}$$

where P is the probability of accepting a lot with a given proportion of incoming defectives p , from the [OC curve](#) of the single sampling plan.

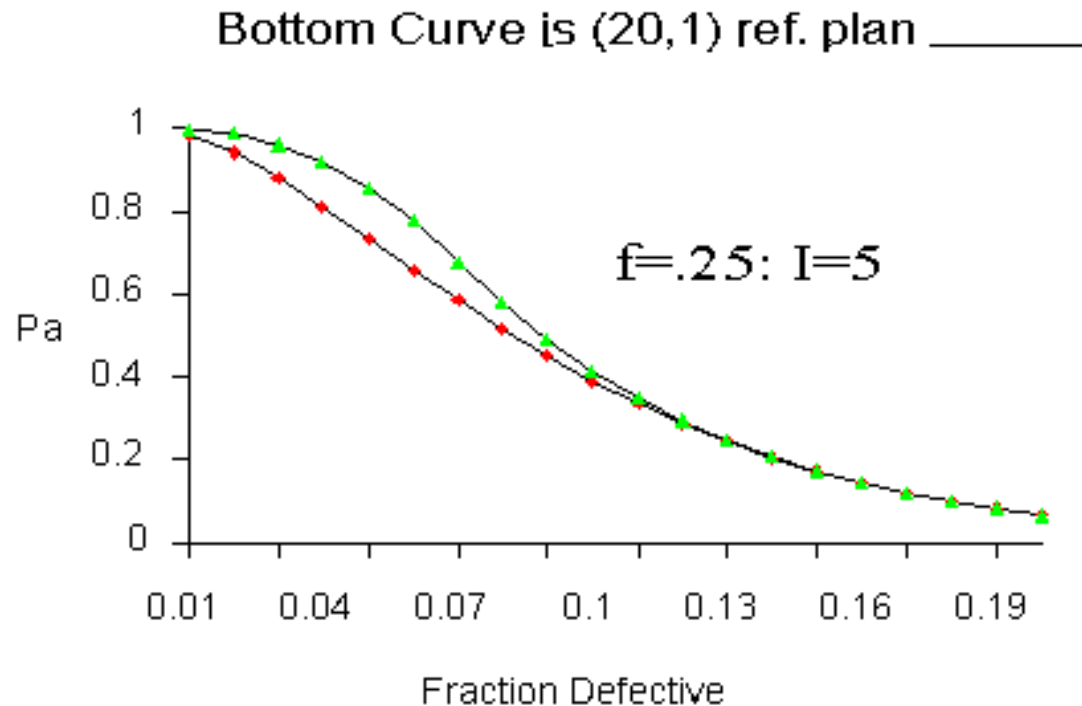
The following relationships hold:

for a given i , the smaller is f , the greater is P_a

for a given f , the smaller is i , the greater is P_a

*Illustration of
a skip lot
sampling plan*

An illustration of a skip-lot sampling plan is given below.



*ASN of skip-lot
sampling plan*

An important property of skip-lot sampling plans is the average sample number ([ASN](#)). The ASN of a skip-lot sampling plan is

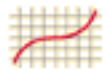
$$ASN_{skip-lot} = (F)(ASN_{reference})$$

where F is defined by

$$F = \frac{f}{(1-f)P^i + f}$$

Therefore, since $0 < F < 1$, it follows that the ASN of skip-lot sampling is smaller than the ASN of the reference sampling plan.

In summary, skip-lot sampling is preferred when the quality of the submitted lots is excellent and the supplier can demonstrate a proven track record.



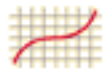
6. [Process or Product Monitoring and Control](#)

6.3. Univariate and Multivariate Control Charts

Contents of section 3

Control charts in this section are classified and described according to three general types: variables, attributes and multivariate.

1. [What are Control Charts?](#)
2. [What are Variables Control Charts?](#)
 1. [Shewhart X bar and R and S Control Charts](#)
 2. [Individuals Control Charts](#)
 3. [Cusum Control Charts](#)
 1. [Cusum Average Run Length](#)
 4. [EWMA Control Charts](#)
3. [What are Attributes Control Charts?](#)
 1. [Counts Control Charts](#)
 2. [Proportions Control Charts](#)
4. [What are Multivariate Control Charts?](#)
 1. [Hotelling Control Charts](#)
 2. [Principal Components Control Charts](#)
 3. [Multivariate EWMA Charts](#)



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.1. What are Control Charts?

Comparison of univariate and multivariate control data

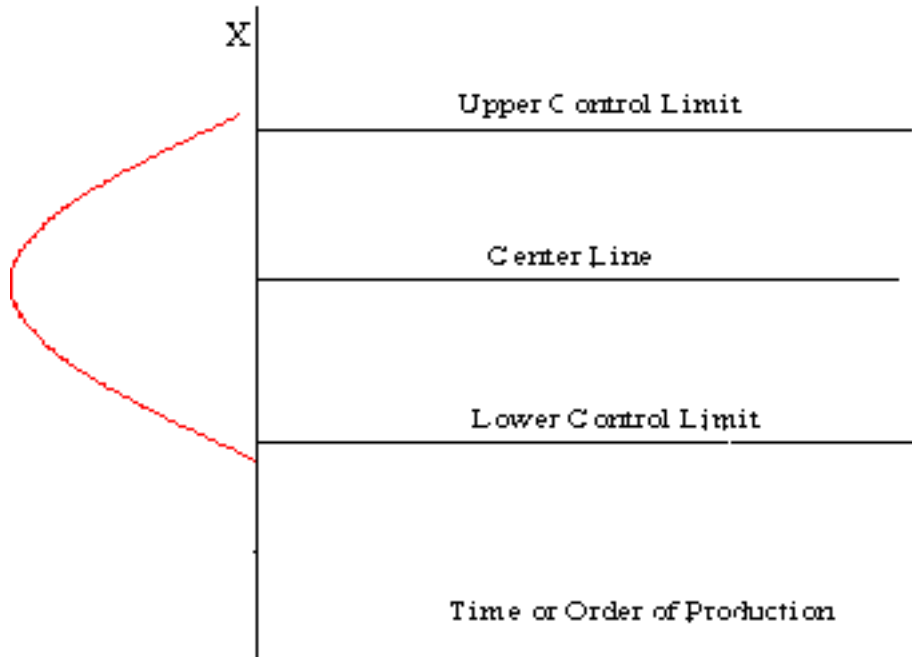
Control charts are used to routinely monitor quality. Depending on the number of process characteristics to be monitored, there are two basic types of control charts. The first, referred to as a univariate control chart, is a graphical display (chart) of one quality characteristic. The second, referred to as a multivariate control chart, is a graphical display of a statistic that summarizes or represents more than one quality characteristic.

Characteristics of control charts

If a single quality characteristic has been measured or computed from a sample, the control chart shows the value of the quality characteristic versus the sample number or versus time. In general, the chart contains a center line that represents the mean value for the in-control process. Two other horizontal lines, called the upper control limit (UCL) and the lower control limit (LCL), are also shown on the chart. These control limits are chosen so that almost all of the data points will fall within these limits as long as the process remains in-control. The figure below illustrates this.

Chart demonstrating basis of control chart

Theoretical Basis for a Control Chart



Why control charts "work"

The control limits as pictured in the graph might be .001 *probability* limits. If so, and if chance causes alone were present, the probability of a point falling above the upper limit would be one out of a thousand, and similarly, a point falling below the lower limit would be one out of a thousand. We would be searching for an assignable cause if a point would fall outside these limits. Where we put these limits will determine the risk of undertaking such a search when in reality there is no assignable cause for variation.

Since two out of a thousand is a very small risk, the 0.001 limits may be said to give practical assurances that, if a point falls outside these limits, the variation was caused by an assignable cause. It must be noted that two out of one thousand is a purely arbitrary number. There is no reason why it could have been set to one out of a hundred or even larger. The decision would depend on the amount of risk the management of the quality control program is willing to take. In general (in the world of quality control) it is customary to use limits that approximate the 0.002 standard.

Letting X denote the value of a process characteristic, if the system of chance causes generates a variation in X that follows the normal distribution, the 0.001 probability limits will be very close to the 3σ limits. From normal tables we glean that the 3σ in one direction is 0.00135, or in both directions 0.0027. For normal distributions, therefore, the 3σ limits are the practical equivalent of 0.001 probability limits.

*Plus or minus
"3 sigma"
limits are
typical*

In the U.S., whether X is normally distributed or not, it is an acceptable practice to base the control limits upon a multiple of the standard deviation. Usually this multiple is 3 and thus the limits are called 3-sigma limits. This term is used whether the standard deviation is the universe or population parameter, or some estimate thereof, or simply a "standard value" for control chart purposes. It should be inferred from the context what standard deviation is involved. (Note that in the U.K., statisticians generally prefer to adhere to probability limits.)

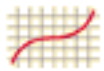
If the underlying distribution is skewed, say in the positive direction, the 3-sigma limit will fall short of the upper 0.001 limit, while the lower 3-sigma limit will fall below the 0.001 limit. This situation means that the risk of looking for assignable causes of positive variation when none exists will be greater than one out of a thousand. But the risk of searching for an assignable cause of negative variation, when none exists, will be reduced. The net result, however, will be an increase in the risk of a chance variation beyond the control limits. How much this risk will be increased will depend on the degree of skewness.

If variation in quality follows a Poisson distribution, for example, for which $np = .8$, the risk of exceeding the upper limit by chance would be raised by the use of 3-sigma limits from 0.001 to 0.009 and the lower limit reduces from 0.001 to 0. For a Poisson distribution the mean and variance both equal np . Hence the upper 3-sigma limit is $0.8 + 3 \text{ sqrt}(.8) = 3.48$ and the lower limit = 0 (here *sqrt* denotes "square root"). For $np = .8$ the probability of getting more than 3 successes = 0.009.

*Strategies for
dealing with
out-of-control
findings*

If a data point falls outside the control limits, we assume that the process is probably out of control and that an investigation is warranted to find and eliminate the cause or causes.

Does this mean that when all points fall within the limits, the process is in control? Not necessarily. If the plot looks non-random, that is, if the points exhibit some form of systematic behavior, there is still something wrong. For example, if the first 25 of 30 points fall above the center line and the last 5 fall below the center line, we would wish to know why this is so. Statistical methods to detect sequences or nonrandom patterns can be applied to the interpretation of control charts. To be sure, "in control" implies that all points are between the control limits and they form a random pattern.



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.2. What are Variables Control Charts?

During the 1920's, Dr. Walter A. Shewhart proposed a general model for control charts as follows:

*Shewhart
Control
Charts for
variables*

Let w be a sample statistic that measures some continuously varying quality characteristic of interest (e.g., thickness), and suppose that the mean of w is μ_w , with a standard deviation of σ_w . Then the center line, the UCL and the LCL are

$$\text{UCL} = \mu_w + k\sigma_w$$

$$\text{Center Line} = \mu_w$$

$$\text{LCL} = \mu_w - k\sigma_w$$

where k is the distance of the control limits from the center line, expressed in terms of standard deviation units. When k is set to 3, we speak of 3-sigma control charts.

Historically, $k = 3$ has become an accepted standard in industry.

The centerline is the process mean, which in general is unknown. We replace it with a *target* or the average of all the data. The quantity that we plot is the sample average, \bar{X} . The chart is called the \bar{X} chart.

We also have to deal with the fact that σ is, in general, unknown. Here we replace σ_w with a given standard value, or we estimate it by a function of the *average standard deviation*. This is obtained by averaging the individual standard deviations that we calculated from each of m preliminary (or present) samples, each of size n . This function will be discussed shortly.

It is equally important to examine the standard deviations in ascertaining whether the process is in control. There is, unfortunately, a slight problem involved when we work with the usual estimator of σ . The following discussion will illustrate this.

*Sample
Variance*

If σ^2 is the unknown variance of a probability distribution, then an unbiased estimator of σ^2 is the sample variance

$$s^2 = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n-1}$$

However, s , the sample standard deviation is *not* an unbiased estimator of σ . If the underlying distribution is normal, then s actually estimates $c_4\sigma$, where c_4 is a constant that depends on the sample size n . This constant is tabulated in most text books on statistical quality control and may be calculated using

C₄ factor

$$c_4 = \sqrt{\frac{2}{n-1}} \frac{\left(\frac{n}{2}-1\right)!}{\left(\frac{n-1}{2}-1\right)!}$$

To compute this we need a *non-integer factorial*, which is defined for $n/2$ as follows:

*Fractional
Factorials*

$$\left(\frac{n}{2}\right)! = \left(\frac{n}{2}\right)\left(\frac{n}{2}-1\right)\left(\frac{n}{2}-2\right)\cdots\left(\frac{1}{2}\right)\sqrt{\pi}$$

For example, let $n = 3.5 = 7/2$. Then

$$\left(\frac{7}{2}\right)! = (3.5)! = (3.5)(2.5)(1.5)(.5)(1.77246) = 11.632$$

With this definition the reader should have no problem verifying that the c_4 factor for $n = 10$ is .9727.

Mean and standard deviation of the estimators

So the mean or expected value of the sample standard deviation is $c_4 \sigma$.

The standard deviation of the sample standard deviation is

$$\sigma_s = \sigma \sqrt{1 - c_4^2}$$

What are the differences between control limits and specification limits ?

Control limits vs. specifications

Control Limits are used to determine if the process is in a state of statistical control (i.e., is producing consistent output).

Specification Limits are used to determine if the product will function in the intended fashion.

How many data points are needed to set up a control chart?

How many samples are needed?

Shewhart gave the following rule of thumb:

"It has also been observed that a person would seldom if ever be justified in concluding that a state of statistical control of a given repetitive operation or production process has been reached until he had obtained, under presumably the same essential conditions, a sequence of not less than twenty five samples of size four that are in control."

It is important to note that control chart properties, such as false alarm probabilities, are generally given under the assumption that the parameters, such as μ and σ , are known. When the control limits are not computed from a large amount of data, the actual properties might be quite different from what is assumed (see, e.g., [Quesenberry, 1993](#)).

When do we recalculate control limits?

When do we recalculate control limits?

Since a control chart "compares" the current performance of the process characteristic to the past performance of this characteristic, changing the control limits frequently would negate any usefulness.

So, only change your control limits if you have a valid, compelling reason for doing so. Some examples of reasons:

- When you have at least 30 more data points to add to the chart and there have been no known changes to the process
 - you get a better estimate of the variability
- If a major process change occurs and affects the way your process runs.
- If a known, preventable act changes the way the tool or process would behave (power goes out, consumable is corrupted or bad quality, etc.)

What are the WECO rules for signaling "Out of Control"?

General rules for detecting out of control or non-random situations

WECO stands for Western Electric Company Rules

Any Point Above +3 Sigma		+3 σ LIMIT
2 Out of the Last 3 Points Above +2 Sigma		+2 σ LIMIT
4 Out of the Last 5 Points Above +1 Sigma		+1 σ LIMIT
8 Consecutive Points on This Side of Control Line		+1 σ LIMIT
CENTER LINE		
8 Consecutive Points on This Side of Control Line		-1 σ LIMIT
4 Out of the Last 5 Points Below - 1 Sigma		-2 σ LIMIT
2 Out of the Last 3 Points Below -2 Sigma		-3 σ LIMIT
Any Point Below -3 Sigma		

Trend Rules: 6 in a row trending up or down. 14 in a row alternating up and down

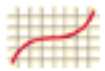
*WECO rules
based on
probabilities*

The WECO rules are based on probability. We know that, for a normal distribution, the probability of encountering a point outside $\pm 3\sigma$ is 0.3%. This is a rare event. Therefore, if we observe a point outside the control limits, we conclude the process has shifted and is unstable. Similarly, we can identify other events that are equally rare and use them as flags for instability. The probability of observing two points out of three in a row between 2σ and 3σ and the probability of observing four points out of five in a row between 1σ and 2σ are also about 0.3%.

*WECO rules
increase
false alarms*

Note: While the WECO rules increase a Shewhart chart's sensitivity to trends or drifts in the mean, there is a severe downside to adding the WECO rules to an ordinary Shewhart control chart that the user should understand. When following the standard Shewhart "out of control" rule (i.e., signal if and only if you see a point beyond the plus or minus 3 sigma control limits) you will have "false alarms" every 371 points on the average (see the description of [Average Run Length or ARL](#) on the next page). Adding the WECO rules increases the frequency of false alarms to about once in every 91.75 points, on the average (see [Champ and Woodall, 1987](#)). The user has to decide whether this price is worth paying (some users add the WECO rules, but take them "less seriously" in terms of the effort put into troubleshooting activities when out of control signals occur).

With this background, the next page will describe how to construct Shewhart variables control charts.



- 6. [Process or Product Monitoring and Control](#)
- 6.3. [Univariate and Multivariate Control Charts](#)
- 6.3.2. [What are Variables Control Charts?](#)

6.3.2.1. Shewhart X-bar and R and S Control Charts

\bar{X} and S Charts

\bar{X} and S Shewhart Control Charts

We begin with \bar{X} and s charts. We should use the s chart first to determine if the distribution for the process characteristic is stable.

Let us consider the case where we have to estimate σ by analyzing past data. Suppose we have m preliminary samples at our disposition, each of size n , and let s_i be the standard deviation of the i th sample. Then the average of the m standard deviations is

$$\bar{s} = \frac{1}{m} \sum_{i=1}^m s_i$$

Control Limits for \bar{X} and S Charts

We make use of the factor c_4 described on the [previous page](#).

The statistic \bar{s}/c_4 is an unbiased estimator of σ . Therefore, the parameters of the S chart would be

$$UCL = \bar{s} + 3 \frac{\bar{s}}{c_4} \sqrt{1 - c_4^2}$$

$$\text{Center Line} = \bar{s}$$

$$LCL = \bar{s} - 3 \frac{\bar{s}}{c_4} \sqrt{1 - c_4^2}$$

Similarly, the parameters of the \bar{X} chart would be

$$UCL = \bar{\bar{x}} + 3 \frac{\bar{s}}{c_4 \sqrt{n}}$$

$$\text{Center Line} = \bar{\bar{x}}$$

$$LCL = \bar{\bar{x}} - 3 \frac{\bar{s}}{c_4 \sqrt{n}}$$

$\bar{\bar{x}}$, the "grand" mean is the average of all the observations.

It is often convenient to plot the \bar{X} and s charts on one page.

\bar{X} and R Control Charts

\bar{X} and R control charts

If the sample size is relatively small (say equal to or less than 10), we can use the range instead of the standard deviation of a sample to construct control charts on \bar{X} and *the range*, R . The range of a sample is simply the difference between the largest and smallest observation.

There is a statistical relationship (Patnaik, 1946) between the mean range for data from a normal distribution and σ , the standard deviation of that distribution. This relationship depends only on the sample size, n . The mean of R is $d_2 \sigma$, where the value of d_2 is also a function of n . An estimator of σ is therefore R/d_2 .

Armed with this background we can now develop the \bar{X} and R control chart.

Let R_1, R_2, \dots, R_k , be the range of k samples. The average range is

$$\bar{R} = \frac{R_1 + R_2 + \dots + R_k}{k}$$

Then an estimate of σ can be computed as

$$\hat{\sigma} = \frac{\bar{R}}{d_2}$$

\bar{X} control charts

So, if we use $\bar{\bar{x}}$ (or a given target) as an estimator of μ and \bar{R}/d_2 as an estimator of σ , then the parameters of the \bar{X} chart are

$$UCL = \bar{\bar{x}} + \frac{3}{d_2\sqrt{n}}\bar{R}$$

$$\text{Center Line} = \bar{\bar{x}}$$

$$LCL = \bar{\bar{x}} - \frac{3}{d_2\sqrt{n}}\bar{R}$$

The simplest way to describe the limits is to define the factor $A_2 = 3/(d_2\sqrt{n})$ and the construction of the \bar{X} becomes

$$UCL = \bar{\bar{x}} + A_2\bar{R}$$

$$\text{Center Line} = \bar{\bar{x}}$$

$$LCL = \bar{\bar{x}} - A_2\bar{R}$$

The factor A_2 depends only on n , and is [tabled below](#).

The R chart **R control charts**

This chart controls the process variability since the sample range is related to the process standard deviation. *The center line of the R chart is the average range.*

To compute the control limits we need an estimate of the true, but unknown standard deviation $W = R/\sigma$. This can be found from the distribution of $W = R/\sigma$ (assuming that the items that we measure follow a normal distribution). The standard deviation of W is d_3 , and is a known function of the sample size, n . It is tabulated in many textbooks on statistical quality control.

Therefore since $R = W\sigma$, the standard deviation of R is $\sigma_R = d_3\sigma$. But since the true σ is unknown, we may estimate σ_R by

$$\hat{\sigma}_R = d_3\frac{\bar{R}}{d_2}$$

As a result, the parameters of the R chart with the customary 3-sigma control limits are

$$UCL = \bar{R} + 3\sigma_{\bar{R}} = \bar{R} + 3d_3 \frac{\bar{R}}{d_2}$$

$$\text{Center Line} = \bar{R}$$

$$LCL = \bar{R} - 3\sigma_{\bar{R}} = \bar{R} - 3d_3 \frac{\bar{R}}{d_2}$$

As was the case with the control chart parameters for the subgroup averages, defining another set of factors will ease the computations, namely:

$D_3 = 1 - 3 d_3 / d_2$ and $D_4 = 1 + 3 d_3 / d_2$. These yield

$$UCL = \bar{R}D_4$$

$$\text{Center Line} = \bar{R}$$

$$LCL = \bar{R}D_3$$

The factors D_3 and D_4 depend only on n , and are tabled below.

Factors for Calculating Limits for \bar{X} and R Charts

n	A₂	D₃	D₄
2	1.880	0	3.267
3	1.023	0	2.575
4	0.729	0	2.282
5	0.577	0	2.115
6	0.483	0	2.004
7	0.419	0.076	1.924
8	0.373	0.136	1.864
9	0.337	0.184	1.816
10	0.308	0.223	1.777

In general, the range approach is quite satisfactory for sample sizes up to around 10. For larger sample sizes, using subgroup standard deviations is preferable. For small sample sizes, the relative efficiency of using the range approach as opposed to using standard deviations is shown in the following table.

*Efficiency of
R versus S*

n	Relative Efficiency
2	1.000
3	0.992
4	0.975
5	0.955
6	0.930
10	0.850

A typical sample size is 4 or 5, so not much is lost by using the range for such sample sizes.

Time To Detection or Average Run Length (ARL)

*Waiting time
to signal
"out of
control"*

Two important questions when dealing with control charts are:

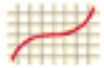
1. How often will there be false alarms where we look for an assignable cause but nothing has changed?
2. How quickly will we detect certain kinds of systematic changes, such as mean shifts?

The ARL tells us, for a given situation, how long on the average we will plot successive control charts points before we detect a point beyond the control limits.

For an \bar{X} chart, with no change in the process, we wait on the average $1/p$ points before a false alarm takes place, with p denoting the probability of an observation plotting outside the control limits. For a normal distribution, $p = .0027$ and the ARL is approximately 371.

A [table](#) comparing Shewhart \bar{X} chart ARL's to Cumulative Sum (CUSUM) ARL's for various mean shifts is given later in this section.

There is also (currently) a [web site](#) developed by Galit Shmueli that will do ARL calculations interactively with the user, for Shewhart charts with or without additional ([Western Electric](#)) rules added.



- 6. [Process or Product Monitoring and Control](#)
- 6.3. [Univariate and Multivariate Control Charts](#)
- 6.3.2. [What are Variables Control Charts?](#)

6.3.2.2. Individuals Control Charts

Samples are Individual Measurements

Moving range used to derive upper and lower limits

Control charts for individual measurements, e.g., the sample size = 1, use the *moving range* of two successive observations to measure the process variability.

The moving range is defined as

$$MR_i = |x_i - x_{i-1}|$$

which is the absolute value of the first difference (e.g., the difference between two consecutive data points) of the data. Analogous to the Shewhart control chart, one can plot both the data (which are the individuals) and the moving range.

Individuals control limits for an observation

For the control chart for individual measurements, the lines plotted are:

$$UCL = \bar{x} + 3 \frac{\overline{MR}}{1.128}$$

$$\text{Center Line} = \bar{x}$$

$$LCL = \bar{x} - 3 \frac{\overline{MR}}{1.128}$$

where \bar{x} is the average of all the individuals and \overline{MR} is the average of all the moving ranges of two observations. Keep in mind that either or both averages may be replaced by a standard or target, if available. (Note that 1.128 is the value of d_2 for $n = 2$).

Example of moving range

The following example illustrates the control chart for individual observations. A new process was studied in order to monitor flow rate. The first 10 batches resulted in

Batch Number	Flowrate x	Moving Range MR
1	49.6	
2	47.6	2.0
3	49.9	2.3
4	51.3	14
5	47.8	3.5
6	51.2	3.4
7	52.6	1.4
8	52.4	0.2
9	53.6	1.2
10	52.1	1.5
	$\bar{X} = 50.81$	$\overline{MR} = 1.8778$

Limits for the moving range chart

This yields the parameters below.

$$UCL = \bar{x} + 3 \frac{\overline{MR}}{1.128} = 50.81 + 3 \frac{1.8778}{1.128} = 55.8041$$

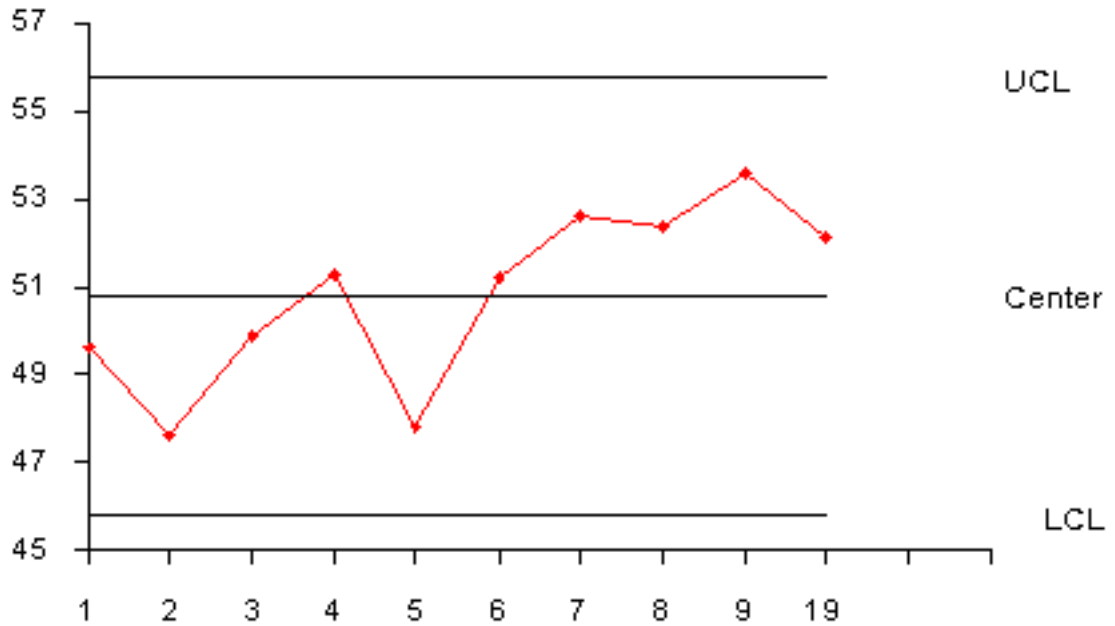
$$\text{Center Line} = \bar{x} = 50.81$$

$$LCL = \bar{x} - 3 \frac{\overline{MR}}{1.128} = 50.81 - 3 \frac{1.8778}{1.128} = 45.8159$$

Example of individuals chart

The control chart is given below

Control Chart for Individuals



The process is in control, since none of the plotted points fall outside either the *UCL* or *LCL*.

*Alternative
for
constructing
individuals
control
chart*

Note: Another way to construct the individuals chart is by using the standard deviation. Then we can obtain the chart from

$$\bar{x} \pm 3s/c_4$$

It is preferable to have the limits computed this way for the start of Phase 2.



6. [Process or Product Monitoring and Control](#)
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6.3.2.3. Cusum Control Charts

CUSUM is an efficient alternative to Shewhart procedures

CUSUM charts, while not as intuitive and simple to operate as Shewhart charts, have been shown to be more efficient in detecting small shifts in the mean of a process. In particular, analyzing [ARL's for CUSUM control charts](#) shows that they are better than Shewhart control charts when it is desired to detect shifts in the mean that are 2 sigma or less.

CUSUM works as follows: Let us collect k samples, each of size n , and compute the mean of each sample. Then the cumulative sum (CUSUM) control chart is formed by plotting one of the following quantities:

Definition of cumulative sum

$$S_m = \sum_{i=1}^m (\bar{x}_i - \hat{\mu}_0) \quad \text{OR} \quad S'_m = \frac{1}{\sigma_{\bar{x}}} \sum_{i=1}^m (\bar{x}_i - \hat{\mu}_0)$$

against the sample number m , where $\hat{\mu}_0$ is the estimate of the in-control mean and $\sigma_{\bar{x}}$ is the known (or estimated) standard deviation of the sample means. The choice of which of these two quantities is plotted is usually determined by the statistical software package. In

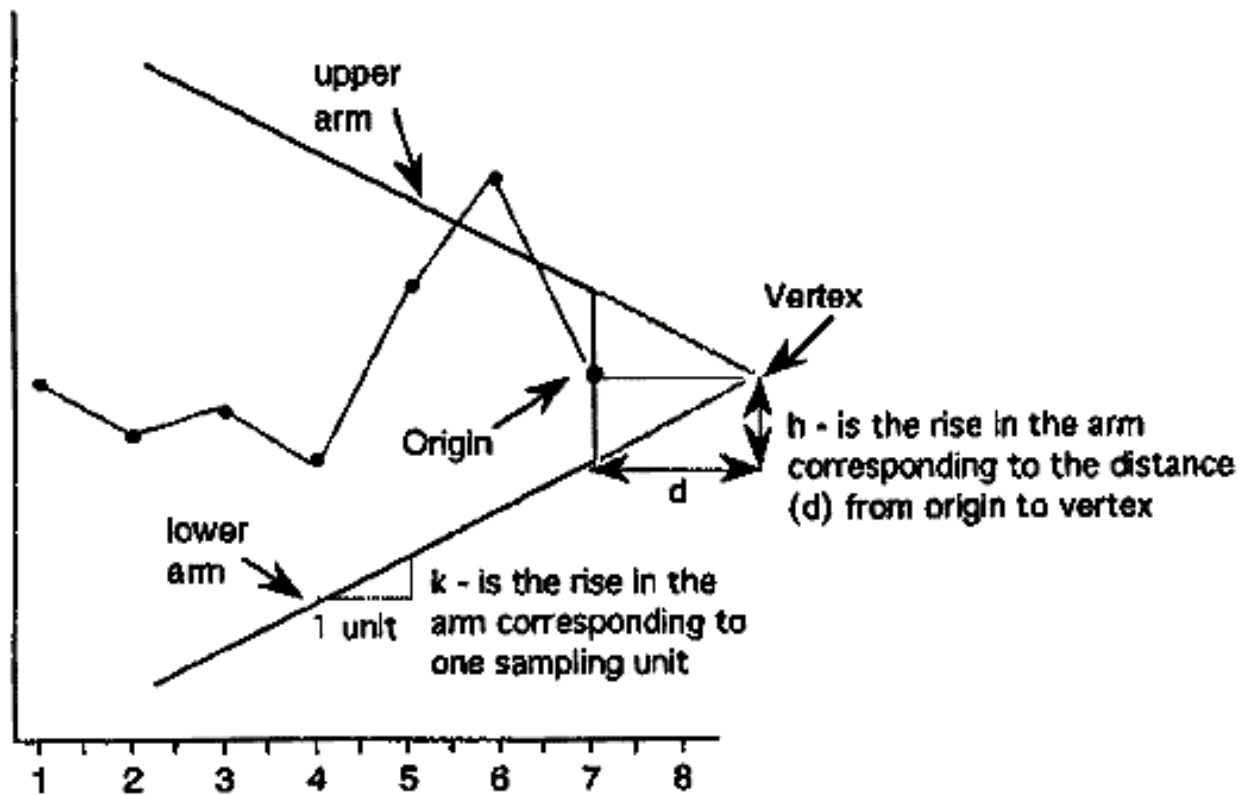
either case, as long as the process remains in control centered at $\hat{\mu}_0$, the cusum plot will show variation in a random pattern centered about zero. If the process mean shifts upward, the charted cusum points will eventually drift upwards, and vice versa if the process mean decreases.

V-Mask used to determine if process is out of control

A visual procedure proposed by Barnard in 1959, known as *the V-Mask*, is sometimes used to determine whether a process is out of control. More often, the tabular form of the V-Mask is preferred. The tabular form is illustrated later in this section.

A V-Mask is an overlay shape in the form of a V on its side that is superimposed on the graph of the cumulative sums. The origin point of the V-Mask (see diagram below) is placed on top of the latest cumulative sum point and past points are examined to see if any fall above or below the sides of the V. As long as all the previous points lie between the sides of the V, the process is in control. Otherwise (even if one point lies outside) the process is suspected of being out of control.

Sample V-Mask demonstrating an out of control process



Interpretation of the V-Mask on the plot

In the diagram above, the V-Mask shows an out of control situation because of the point that lies above the upper arm. By sliding the V-Mask backwards so that the origin point covers other cumulative sum data points, we can determine the first point that signaled an out-of-control situation. This is useful for diagnosing what might have caused the process to go out of control.

From the diagram it is clear that the behavior of the V-Mask is determined by the distance k (which is the slope of the lower arm) and the rise distance h . These are the *design parameters* of the V-Mask. Note that we could also specify d and the vertex angle (or, as is more common in the literature, $\theta = 1/2$ the vertex angle) as the design parameters, and we would end up with the same V-Mask.

In practice, designing and manually constructing a V-Mask is a complicated procedure. A cusum spreadsheet style procedure shown below is more practical, unless you have statistical software that automates the V-Mask methodology. Before describing the spreadsheet approach, we will look briefly at an example of a software V-Mask.

JMP example of V-Mask

An example will be used to illustrate how to construct and apply a V-Mask procedure using JMP. The 20 data points

324.925, 324.675, 324.725, 324.350, 325.350, 325.225, 324.125, 324.525, 325.225, 324.600, 324.625, 325.150, 328.325, 327.250, 327.825, 328.500, 326.675, 327.775, 326.875, 328.350

are each the average of samples of size 4 taken from a process that has an estimated mean of 325. Based on process data, the process standard deviation is 1.27 and therefore the sample means used in the cusum procedure have a standard deviation of $1.27/4^{1/2} = 0.635$.

After inputting the 20 sample means and selecting "control charts" from the pull down "Graph" menu, JMP displays a "Control Charts" screen and a "CUSUM Charts" screen. Since each sample mean is a separate "data point", we choose a constant sample size of 1. We also choose the option for a two sided Cusum plot shown in terms of the original data.

JMP allows us a choice of either designing via the method using h and k or using an α and β design approach. For the latter approach we must specify

- α , the probability of a false alarm, i.e., concluding that a shift in the process has occurred, while in fact it did not
- β , the the probability of not detecting that a shift in the process mean has, in fact, occurred
- δ (delta), the amount of shift in the process mean that we wish to detect, expressed as a multiple of the standard deviation of the data points (which are the sample means).

Note: Technically, alpha and beta are calculated in terms of one sequential trial where we monitor S_m until we have either an out-of-control signal or S_m returns to the starting point (and the monitoring begins, in effect, all over again).

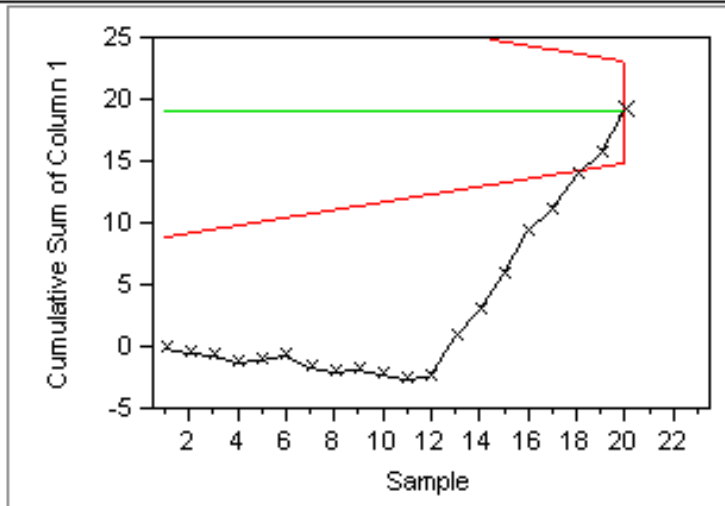
JMP menus for inputting options to the cusum procedure

In our example we choose an α of 0.0027 (equivalent to the plus or minus 3 sigma criteria used in a standard Shewhart chart), and a β of 0.01. Finally, we decide we want to quickly detect a shift as large as 1 sigma, which sets delta = 1. The screen below shows all the inputs.

Column 1	Control Charts		Action
324.925	Select Columns	Cast Columns into Roles	OK
324.675	<input checked="" type="checkbox"/> Column 1	Process: Column 1	Cancel
324.725	Chart Type	Sample Label: optional	Remove
324.35	CUSUM	By: optional	Recall
325.35	<input checked="" type="checkbox"/> Two sided	Sample Size	Help
325.225	<input checked="" type="checkbox"/> Data Units	<input type="radio"/> Sample Grouped by Sample Label	Get Limits
324.125	Parameters	<input checked="" type="radio"/> Sample Size Constant	<input type="checkbox"/> Capability
324.525	<input type="radio"/> K Sigma Beta	1	
325.225	<input checked="" type="radio"/> Alpha 0.01	Specify Stats Delete Stats	
324.6	<input type="radio"/> H		
324.625	0.0027		
325.15	Known Statistics for CUSUM Chart		
328.325	Column 1		
327.25	Target 325		
327.825	Delta 1		
328.5	Shift .		
326.675	Sigma 0.635		
327.775	Head Start .		
326.875			
328.35			

*JMP output
from
CUSUM
procedure*

When we click on chart we see the V-Mask placed over the last data point. The mask clearly indicates an out of control situation.

Control Chart**CUSUM of Column 1****Parameters**

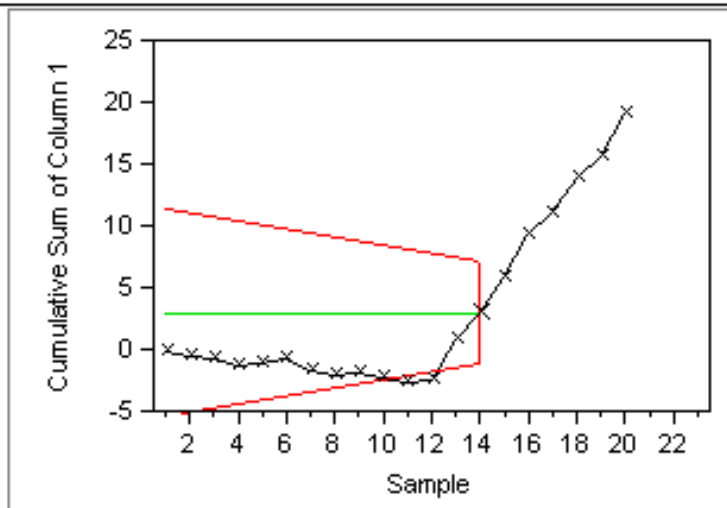
Target	325.0000
Delta	1.0000
Shift	0.6350
Sigma	0.6350
Head Start	0.0000

ARL

ARL (Delta)	6.82922
ARL (0)	63.26935

We next "grab" the V-Mask and move it back to the first point that indicated the process was out of control. This is point number 14, as shown below.

*JMP
CUSUM
chart after
moving
V-Mask to
first out of
control
point*

CUSUM of Column 1

Rule of thumb for choosing h and k

Note: A general rule of thumb ([Montgomery](#)) if one chooses to design with the h and k approach, instead of the alpha and beta method illustrated above, is to choose k to be half the delta shift (.5 in our example) and h to be around 4 or 5.

For more information on cusum chart design, see [Woodall and Adams \(1993\)](#).

Tabular or Spreadsheet Form of the V-Mask

A spreadsheet approach to cusum monitoring

Most users of cusum procedures prefer tabular charts over the V-Mask. The V-Mask is actually a carry-over of the pre-computer era. The tabular method can be quickly implemented by standard spreadsheet software.

To generate the tabular form we use the h and k parameters expressed in the original data units. It is also possible to use sigma units.

The following quantities are calculated:

$$S_{hi}(i) = \max(0, S_{hi}(i-1) + x_i - \hat{\mu}_0 - k)$$

$$S_{lo}(i) = \max(0, S_{lo}(i-1) + \hat{\mu}_0 - k - x_i)$$

where $S_{hi}(0)$ and $S_{lo}(0)$ are 0. When either $S_{hi}(i)$ or $S_{lo}(i)$ exceeds h , the process is out of control.

Example of spreadsheet calculations

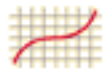
We will construct a cusum tabular chart for the example described above. For this example, the JMP parameter table gave $h = 4.1959$ and $k = .3175$. Using these design values, the tabular form of the example is

	$\hat{\mu}_0$	h	k				
	325	4.1959	0.3175				
			Increase in mean		Decrease in mean		
Group	x	$x-325$	$x-325-k$	S_{hi}	$325-k-x$	S_{lo}	Cusum
1	324.93	-0.07	-0.39	0.00	-0.24	0.00	-0.007
2	324.68	-0.32	-0.64	0.00	0.01	0.01	-0.40
3	324.73	-0.27	-0.59	0.00	-0.04	0.00	-0.67
4	324.35	-0.65	-0.97	0.00	0.33	0.33	-1.32
5	325.35	0.35	0.03	0.03	-0.67	0.00	-0.97
6	325.23	0.23	-0.09	0.00	-0.54	0.00	-0.75
7	324.13	-0.88	-1.19	0.00	0.56	0.56	-1.62
8	324.53	-0.48	-0.79	0.00	0.16	0.72	-2.10
9	325.23	0.23	-0.09	0.00	0.54	0.17	-1.87
10	324.60	-0.40	-0.72	0.00	0.08	0.25	-2.27
11	324.63	-0.38	-0.69	0.00	0.06	0.31	-2.65
12	325.15	0.15	-0.17	0.00	0.47	0.00	-2.50
13	328.33	3.32	3.01	3.01	-3.64	0.00	0.83
14	327.25	2.25	1.93	4.94*	-0.57	0.00	3.08

6.3.2.3. Cusum Control Charts

15	327.83	2.82	2.51	7.45*	-3.14	0.00	5.90
16	328.50	3.50	3.18	10.63*	-3.82	0.00	9.40
17	326.68	1.68	1.36	11.99*	-1.99	0.00	11.08
18	327.78	2.77	2.46	14.44*	-3.09	0.00	13.85
19	326.88	1.88	1.56	16.00*	-2.19	0.00	15.73
20	328.35	3.35	3.03	19.04*	-3.67	0.00	19.08

* = out of control signal



- 6. [Process or Product Monitoring and Control](#)
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- 6.3.2. [What are Variables Control Charts?](#)
- 6.3.2.3. [Cusum Control Charts](#)

6.3.2.3.1. Cusum Average Run Length

The Average Run Length of Cumulative Sum Control Charts

The ARL of CUSUM

The operation of obtaining samples to use with a cumulative sum (CUSUM) control chart consists of taking samples of size n and plotting the cumulative sums

$$S_r = \sum_{i=1}^r (\bar{x}_i - k) \quad \text{or} \quad S_r = \sum_{i=1}^r (\bar{x}_i - \bar{x}) / \sigma_{\bar{x}} \quad (\text{standardized})$$

versus the sample number r , where \bar{x}_i is the sample mean and k is a reference value.

In practice, k might be set equal to $(\hat{\mu}_0 + \mu_1)/2$, where $\hat{\mu}_0$ is the estimated in-control mean, which is sometimes known as the *acceptable quality level*, and μ_1 is referred to as the *rejectable quality level*.

If the distance between a plotted point and the lowest previous point is equal to or greater than h , one concludes that the process mean has shifted (increased).

h is decision limit

Hence, h is referred to as the *decision limit*. Thus the sample size n , reference value k , and decision limit h are the parameters required for operating a one-sided CUSUM chart. If one has to control both positive and negative deviations, as is usually the case, two one-sided charts are used, with respective values k_1, k_2 , ($k_1 > k_2$) and respective decision limits h and $-h$.

*Standardizing
shift in mean
and decision
limit*

The shift in the mean can be expressed as $\mu - k$. If we are dealing with normally distributed measurements, we can standardize this shift by

$$k_s = \frac{(\mu - k)}{\sigma / \sqrt{n}} \text{ or } (\mu - k) \sqrt{n} / \sigma$$

Similarly, the decision limit can be standardized by

$$h_s = \frac{h}{\sigma / \sqrt{n}} = h \sqrt{n} / \sigma$$

*Determination
of the ARL,
given h and k*

The average run length (ARL) at a given quality level is the average number of samples (subgroups) taken before an action signal is given. The standardized parameters k_s and h_s together with the sample size n are usually selected to yield approximate ARL's L_0 and L_1 at acceptable and rejectable quality levels μ_0 and μ_1 respectively. We would like to see a high ARL, L_0 , when the process is on target, (i.e. in control), and a low ARL, L_1 , when the process mean shifts to an unsatisfactory level.

In order to determine the parameters of a CUSUM chart, the acceptable and rejectable quality levels along with the desired respective ARL 's are usually specified. The design parameters can then be obtained by a number of ways. Unfortunately, the calculations of the ARL for CUSUM charts are quite involved.

There are several nomographs available from different sources that can be utilized to find the ARL's when the standardized h and k are given. Some of the nomographs solve the unpleasant integral equations that form the basis of the exact solutions, using an approximation of Systems of Linear Algebraic Equations (SLAE). This Handbook used a computer program that furnished the required ARL's given the standardized h and k . An example is given below:

Example of finding ARL's given the standardized h and k

mean shift ($k = .5$)	$h\sqrt{n}/\sigma$		Shewart
	4	5	\bar{X}
0	336	930	371.00
.25	74.2	140	281.14
.5	26.6	30.0	155.22
.75	13.3	17.0	81.22
1.00	8.38	10.4	44.0
1.50	4.75	5.75	14.97
2.00	3.34	4.01	6.30
2.50	2.62	3.11	3.24
3.00	2.19	2.57	2.00
4.00	1.71	2.01	1.19

Using the table

If $k = .5$, then the shift of the mean (in multiples of the standard deviation of the mean) is obtained by adding .5 to the first column. For example to detect a mean shift of 1 sigma at $h = 4$, the ARL = 8.38. (at first column entry of .5).

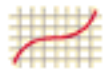
The last column of the table contains the ARL's for a Shewhart control chart at selected mean shifts. The ARL for Shewhart = $1/p$, where p is the probability for a point to fall outside established control limits. Thus, for 3-sigma control limits and assuming normality, the probability to exceed the upper control limit = .00135 and to fall below the lower control limit is also .00135 and their sum = .0027. (These numbers come from standard normal distribution tables or computer programs, setting $z = 3$). Then the ARL = $1/.0027 = 370.37$. This says that when a process is in control one expects an out-of-control signal (false alarm) each 371 runs.

ARL if a 1 sigma shift has occurred

When the means shifts up by 1 sigma, then the distance between the upper control limit and the shifted mean is 2 sigma (instead of 3 σ). Entering normal distribution tables with $z = 2$ yields a probability of $p = .02275$ to exceed this value. The distance between the shifted mean and the lower limit is now 4 sigma and the probability of $\bar{X} < -4$ is only .000032 and can be ignored. The ARL is $1 / .02275 = 43.96$.

Shewhart is better for detecting large shifts, CUSUM is faster for small shifts

The conclusion can be drawn that the Shewhart chart is superior for detecting large shifts and the CUSUM scheme is faster for small shifts. The break-even point is a function of h , as the table shows.



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.2. [What are Variables Control Charts?](#)

6.3.2.4. EWMA Control Charts

EWMA statistic

The Exponentially Weighted Moving Average (EWMA) is a statistic for monitoring the process that averages the data in a way that gives less and less weight to data as they are further removed in time.

Comparison of Shewhart control chart and EWMA control chart techniques

For the [Shewhart chart control](#) technique, the decision regarding the state of control of the process at any time, t , depends solely on the most recent measurement from the process and, of course, the degree of 'trueness' of the estimates of the control limits from historical data. For the EWMA control technique, the decision depends on the EWMA statistic, which is an exponentially weighted average of all prior data, including the most recent measurement.

By the choice of weighting factor, λ , the EWMA control procedure can be made sensitive to a small or gradual drift in the process, whereas the Shewhart control procedure can only react when the last data point is outside a control limit.

Definition of EWMA

The statistic that is calculated is:

$$EWMA_t = \lambda Y_t + (1 - \lambda) EWMA_{t-1} \quad \text{for } t = 1, 2, \dots, n.$$

where

- $EWMA_0$ is the mean of historical data (target)
- Y_t is the observation at time t
- n is the number of observations to be monitored including $EWMA_0$
- $0 < \lambda \leq 1$ is a constant that determines the depth of memory of the EWMA.

The equation is due to Roberts (1959).

Choice of weighting factor

The parameter λ determines the rate at which 'older' data enter into the calculation of the EWMA statistic. A value of $\lambda = 1$ implies that only the most recent measurement influences the EWMA (degrades to Shewhart chart). Thus, a large value of $\lambda = 1$ gives more weight to recent data and less weight to older data; a small value of λ gives more weight to older data. The value of λ is usually set between 0.2 and 0.3 ([Hunter](#)) although this choice is somewhat arbitrary. [Lucas and Saccucci \(1990\)](#) give tables that help the user select λ .

Variance of EWMA statistic

The estimated variance of the EWMA statistic is approximately

$$s_{\text{ewma}}^2 = (\lambda / (2 - \lambda)) s^2$$

when t is not small, where s is the standard deviation calculated from the historical data.

Definition of control limits for EWMA

The center line for the control chart is the target value or EWMA_0 . The control limits are:

$$\text{UCL} = \text{EWMA}_0 + k s_{\text{ewma}}$$

$$\text{LCL} = \text{EWMA}_0 - k s_{\text{ewma}}$$

where the factor k is either set equal 3 or chosen using the [Lucas and Saccucci \(1990\)](#) tables. The data are assumed to be independent and these tables also assume a normal population.

As with all control procedures, the EWMA procedure depends on a database of measurements that are truly representative of the process. Once the mean value and standard deviation have been calculated from this database, the process can enter the monitoring stage, provided the process was in control when the data were collected. If not, then the usual Phase 1 work would have to be completed first.

Example of calculation of parameters for an EWMA control chart

To illustrate the construction of an EWMA control chart, consider a process with the following parameters calculated from historical data:

$$\text{EWMA}_0 = 50$$

$$s = 2.0539$$

with λ chosen to be 0.3 so that $\lambda / (2 - \lambda) = .3 / 1.7 = 0.1765$ and the square root = 0.4201. The control limits are given by

$$\text{UCL} = 50 + 3 (0.4201)(2.0539) = 52.5884$$

$$\text{LCL} = 50 - 3 (0.4201) (2.0539) = 47.4115$$

Sample data Consider the following data consisting of 20 points where 1 - 10 are on the top row from left to right and 11-20 are on the bottom row from left to right:

```

52.0 47.0 53.0 49.3 50.1 47.0
51.0 50.1 51.2 50.5 49.6 47.6
49.9 51.3 47.8 51.2 52.6 52.4
53.6 52.1

```

EWMA statistics for sample data These data represent control measurements from the process which is to be monitored using the EWMA control chart technique. The corresponding EWMA statistics that are computed from this data set are:

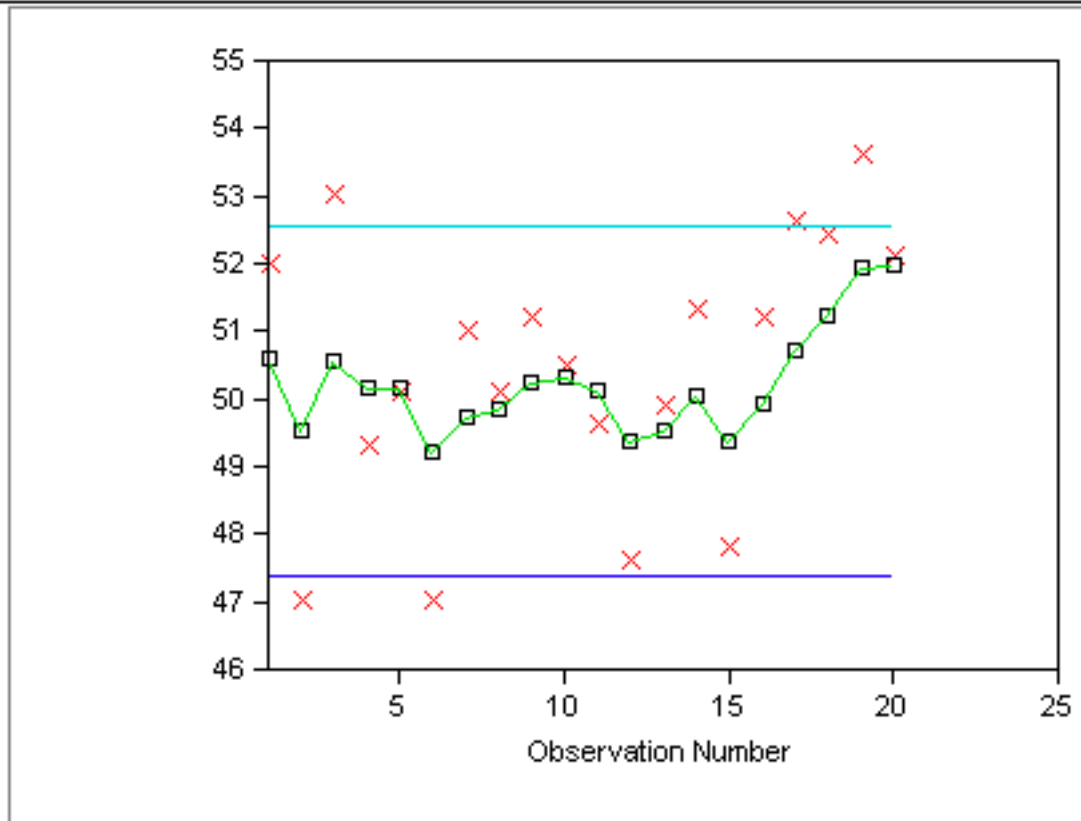
```

50.00 50.60 49.52 50.56 50.18
50.16 49.12 49.75 49.85 50.26
50.33 50.11 49.36 49.52 50.05
49.34 49.92 50.73 51.23 51.94

```

Sample EWMA plot The control chart is given below.

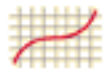
EWMA PLOT



Y x Data ■ EWMA Values
— Lower EWMA Limit — **Upper EWMA Limit**

*Interpretation
of EWMA
control chart*

The red dots are the raw data; the jagged line is the EWMA statistic over time. The chart tells us that the process is in control because all $EWMA_t$ lie between the control limits. However, there seems to be a trend upwards for the last 5 periods.



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.3. What are Attributes Control Charts?

Attributes data arise when classifying or counting observations

The Shewhart control chart plots quality characteristics that can be measured and expressed numerically. We measure weight, height, position, thickness, etc. If we cannot represent a particular quality characteristic numerically, or if it is impractical to do so, we then often resort to using a quality characteristic to sort or classify an item that is inspected into one of two "buckets".

An example of a common quality characteristic classification would be designating units as "conforming units" or "nonconforming units". Another quality characteristic criteria would be sorting units into "non defective" and "defective" categories. Quality characteristics of that type are called *attributes*.

Note that there is a difference between "nonconforming to an engineering specification" and "defective" -- a nonconforming unit may function just fine and be, in fact, not defective at all, while a part can be "in spec" and not function as desired (i.e., be defective).

Examples of quality characteristics that are attributes are the number of failures in a production run, the proportion of malfunctioning wafers in a lot, the number of people eating in the cafeteria on a given day, etc.

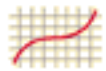
Types of attribute control charts

Control charts dealing with the number of *defects* or *nonconformities* are called [c charts \(for count\)](#).

Control charts dealing with the *proportion* or *fraction* of defective product are called [p charts \(for proportion\)](#).

There is another chart which handles *defects per unit*, called the *u* chart (for unit). This applies when we wish to work with the average number of nonconformities per unit of product.

For additional references, see [Woodall \(1997\)](#) which reviews papers showing examples of attribute control charting, including examples from semiconductor manufacturing such as those examining the spatial dependence of defects.



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.3. [What are Attributes Control Charts?](#)

6.3.3.1. Counts Control Charts

Defective items vs individual defects

The literature differentiates between *defect* and *defective*, which is the same as differentiating between *nonconformity* and *nonconforming units*. This may sound like splitting hairs, but in the interest of clarity let's try to unravel this man-made mystery.

Consider a wafer with a number of chips on it. The wafer is referred to as an "item of a product". The chip may be referred to as "a specific point". There exist certain specifications for the wafers. When a particular wafer (e.g., the item of the product) does not meet at least one of the specifications, it is classified as a nonconforming item. Furthermore, each chip, (e.g., the specific point) at which a specification is not met becomes a defect or nonconformity.

So, a nonconforming or defective item contains at least one defect or nonconformity. It should be pointed out that a wafer can contain several defects but still be classified as conforming. For example, the defects may be located at noncritical positions on the wafer. If, on the other hand, the number of the so-called "unimportant" defects becomes alarmingly large, an investigation of the production of these wafers is warranted.

Control charts involving counts can be either for the *total number* of nonconformities (defects) for the sample of inspected units, or for the *average number* of defects per inspection unit.

Poisson approximation for numbers or counts of defects

Let us consider an assembled product such as a microcomputer. The opportunity for the occurrence of any given defect may be quite large. However, the probability of occurrence of a defect in any one arbitrarily chosen spot is likely to be very small. In such a case, the incidence of defects might be modeled by a [Poisson distribution](#). Actually, the Poisson distribution is an approximation of the [binomial distribution](#) and applies well in this capacity according to the following rule of thumb:

The sample size n should be equal to or larger than 20 and the probability of a single success, p , should be smaller than or equal to .05. If $n \geq 100$, the approximation is excellent if np is also ≤ 10 .

Illustrate Poisson approximation to binomial

To illustrate the use of the Poisson distribution as an approximation of a binomial distribution, consider the following comparison: Let p , the probability of a single success in $n = 200$ trials, be .025.

Find the probability of exactly 3 successes. If we assume that p remains constant then the solution follows the binomial distribution rules, that is:

$$p(x) = \binom{n}{x} p^x (1-p)^{n-x} = \binom{200}{3} .025^3 .975^{197} = 0.1399995$$

By the Poisson approximation we have

$$c = (200)(.025)$$

and

$$p(x) = \frac{e^{-c} c^x}{x!} = \frac{e^{-5} 5^3}{3!} = 0.1403739$$

The inspection unit

Before the control chart parameters are defined there is one more definition: *the inspection unit*. We shall count the number of defects that occur in a so-called inspection unit. More often than not, an inspection unit is a single unit or item of product; for example, a wafer. However, sometimes the inspection unit could consist of five wafers, or ten wafers and so on. The size of the inspection units may depend on the recording facility, measuring equipment, operators, etc.

Suppose that defects occur in a given inspection unit according to the Poisson distribution, with parameter c (often denoted by np or the Greek letter λ). In other words

Control charts for counts, using the Poisson distribution

$$p(x) = \frac{e^{-c}c^x}{x!}$$

where x is the number of defects and $c > 0$ is the parameter of the Poisson distribution. It is known that both the mean and the variance of this distribution are equal to c . Then the k -sigma control chart is

$$UCL = c + k\sqrt{c}$$

$$CenterLine = c$$

$$LCL = c - k\sqrt{c}$$

If the LCL comes out negative, then there is no lower control limit. This control scheme assumes that a standard value for c is available. If this is not the case then c may be estimated as the average of the number of defects in a preliminary sample of inspection units, call it \bar{c} . Usually k is set to 3 by many practitioners.

Control chart example using counts

An example may help to illustrate the construction of control limits for counts data. We are inspecting 25 successive wafers, each containing 100 chips. Here the wafer is the inspection unit. The observed number of defects are

Wafer Number	Number of Defects	Wafer Number	Number of Defects
1	16	14	16
2	14	15	15
3	28	16	13
4	16	17	14
5	12	18	16
6	20	19	11
7	10	20	20

8	12	21	11
9	10	22	19
10	17	23	16
11	19	24	31
12	17	25	13
13	14		

From this table we have

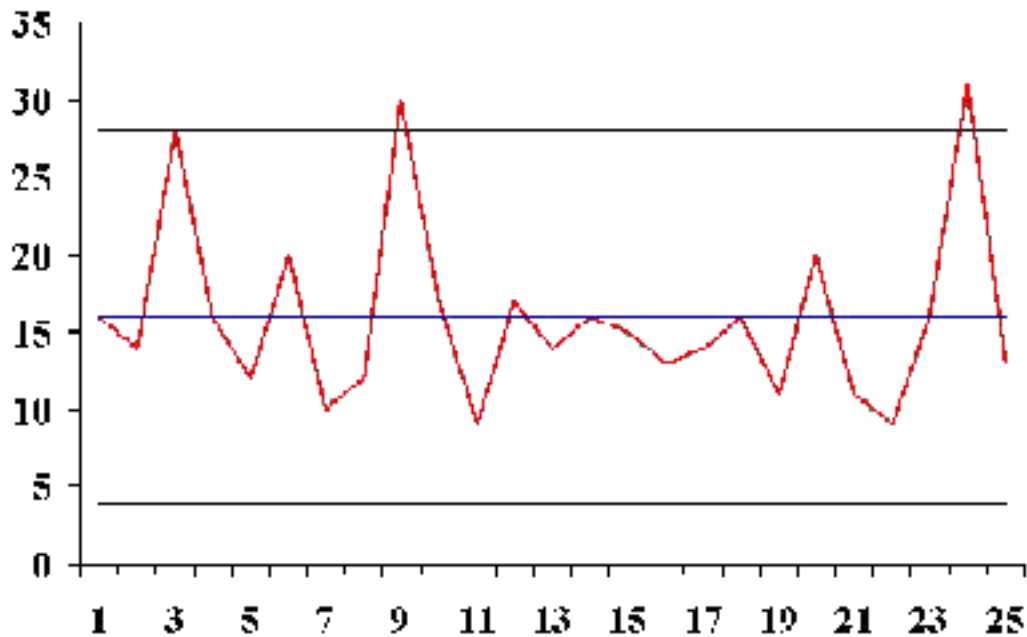
$$\bar{c} = \frac{\text{total number of defects}}{\text{total number of samples}} = \frac{400}{25} = 16$$

$$UCL = \bar{c} + 3\sqrt{\bar{c}} = 16 + 2\sqrt{16} = 28$$

$$LCL = \bar{c} - 3\sqrt{\bar{c}}$$

*Sample
counts
control
chart*

Control Chart for Counts



Transforming Poisson Data

Normal approximation to Poisson is adequate when the mean of the Poisson is at least 5

We have seen that the 3-sigma limits for a c chart, where c represents the number of nonconformities, are given by

$$\bar{c} \pm 3\sqrt{\bar{c}}$$

where it is assumed that the normal approximation to the Poisson distribution holds, hence the symmetry of the control limits. It is shown in the literature that the normal approximation to the Poisson is adequate when the mean of the Poisson is at least 5. When applied to the c chart this implies that the mean of the defects should be at least 5. This requirement will often be met in practice, but still, when the mean is smaller than 9 (solving the above equation) there will be no lower control limit.

Let the mean be 10. Then the lower control limit = 0.513. However, $P(c = 0) = .000045$, using the Poisson formula. This is only 1/30 of the assumed area of .00135. So one has to raise the lower limit so as to get as close as possible to .00135. From Poisson tables or computer software we find that $P(1) = .0005$ and $P(2) = .0027$, so the lower limit should actually be 2 or 3.

Transforming count data into approximately normal data

To avoid this type of problem, we may resort to a transformation that makes the transformed data match the normal distribution better. One such transformation described by Ryan (2000) is

$$Y = 2\sqrt{c}$$

which is, for a large sample, approximately normally distributed with mean = $2\sqrt{\lambda}$ and variance = 1, where λ is the mean of the Poisson distribution.

Similar transformations have been proposed by Anscombe (1948) and Freeman and Tukey (1950). When applied to a c chart these are

$$y_1 = 2\sqrt{c + 3/8} \quad \text{and} \quad y_2 = \sqrt{c} + \sqrt{c + 1}$$

The respective control limits are

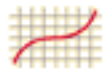
$$\bar{y} \pm 3, \quad \bar{y}_1 \pm 3, \quad \text{and} \quad \bar{y}_2 \pm 3$$

While using transformations may result in meaningful control limits, one has to bear in mind that the user is now working with data on a different scale than the original measurements. There is another way to remedy the problem of symmetric limits applied to non symmetric cases, and that is to use *probability* limits. These can be obtained from tables given by Molina (1973). This allows the user to work with data

on the original scale, but they require special tables to obtain the limits. Of course, software might be used instead.

Warning for highly skewed distributions

Note: In general, it is not a good idea to use 3-sigma limits for distributions that are highly skewed (see [Ryan and Schwertman \(1997\)](#) for more about the possibly extreme consequences of doing this).



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.3. [What are Attributes Control Charts?](#)

6.3.3.2. Proportions Control Charts

p is the fraction defective in a lot or population

The proportion or fraction nonconforming (defective) in a population is defined as the ratio of the number of nonconforming items in the population to the total number of items in that population. The item under consideration may have one or more quality characteristics that are inspected simultaneously. If at least one of the characteristics does not conform to standard, the item is classified as nonconforming.

The fraction or proportion can be expressed as a decimal, or, when multiplied by 100, as a percent. The underlying statistical principles for a control chart for proportion nonconforming are based on the binomial distribution.

Let us suppose that the production process operates in a stable manner, such that the probability that a given unit will not conform to specifications is p . Furthermore, we assume that successive units produced are independent. Under these conditions, each unit that is produced is a realization of a Bernoulli random variable with parameter p . If a random sample of n units of product is selected and if D is the number of units that are nonconforming, the D follows a [binomial distribution](#) with parameters n and p

The binomial distribution model for number of defectives in a sample

$$p\{D = x\} = \binom{n}{x} p^x (1-p)^{n-x} \quad x = 0, 1, \dots, n$$

The mean of D is np and the variance is $np(1-p)$. The *sample* proportion nonconforming is the ratio of the number of nonconforming units in the sample, D , to the sample size n ,

$$\hat{p} = \frac{D}{n}$$

The mean and variance of this estimator are

$$\mu = p$$

and

$$\sigma_{\hat{p}}^2 = \frac{p(1-p)}{n}$$

This background is sufficient to develop the control chart for proportion or fraction nonconforming. The chart is called the p -chart.

*p control
charts for
lot
proportion
defective*

If the true fraction conforming p is known (or a standard value is given), then the center line and control limits of the fraction nonconforming control chart is

$$UCL = p + 3\sqrt{\frac{p(1-p)}{n}}$$

$$\text{Center Line} = p$$

$$LCL = p - 3\sqrt{\frac{p(1-p)}{n}}$$

When the process fraction (proportion) p is not known, it must be estimated from the available data. This is accomplished by selecting m preliminary samples, each of size n . If there are D_i defectives in sample i , the fraction nonconforming in sample i is

$$\hat{p}_i = \frac{D_i}{n} \quad i = 1, 2, \dots, m$$

and the average of these individual sample fractions is

$$\bar{p} = \frac{\sum_{i=1}^m D_i}{mn} = \frac{\sum_{i=1}^m \hat{p}_i}{m}$$

The \bar{p} is used instead of p in the control chart setup.

*Example of
a p-chart*

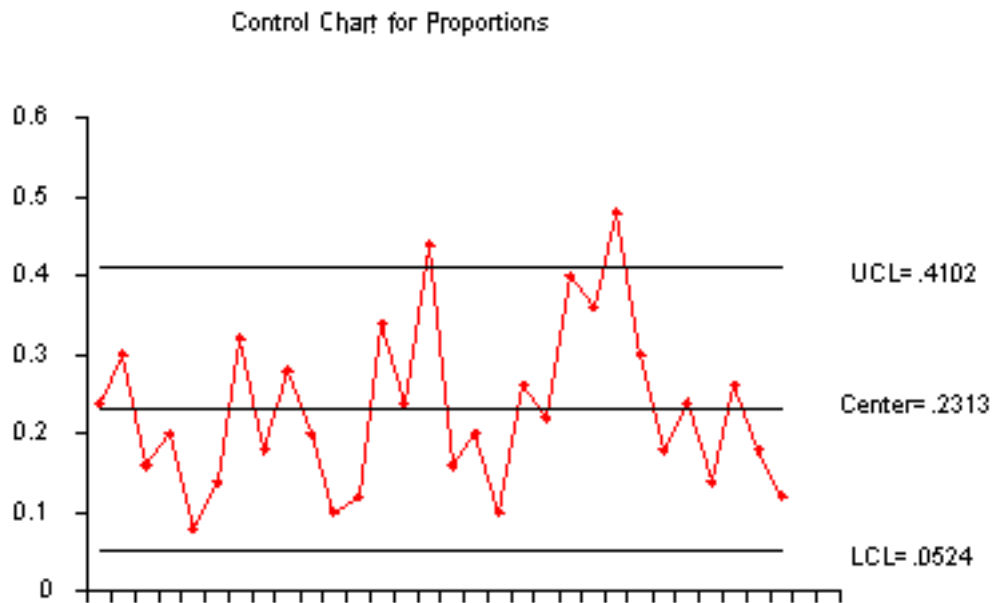
A numerical example will now be given to illustrate the above mentioned principles. The location of chips on a wafer is measured on 30 wafers.

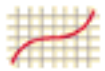
On each wafer 50 chips are measured and a defective is defined whenever a misregistration, in terms of horizontal and/or vertical distances from the center, is recorded. The results are

Sample Number	Fraction Defectives	Sample Number	Fraction Defectives	Sample Number	Fraction Defectives
1	.24	11	.10	21	.40
2	.30	12	.12	22	.36
3	.16	13	.34	23	.48
4	.20	14	.24	24	.30
5	.08	15	.44	25	.18
6	.14	16	.16	26	.24
7	.32	17	.20	27	.14
8	.18	18	.10	28	.26
9	.28	19	.26	29	.18
10	.20	20	.22	30	.12

*Sample
proportions
control
chart*

The corresponding control chart is given below:





6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.4. What are Multivariate Control Charts?

Multivariate control charts and Hotelling's T^2 statistic

It is a fact of life that most data are naturally multivariate. Hotelling in 1947 introduced a statistic which uniquely lends itself to plotting multivariate observations. This statistic, appropriately named Hotelling's T^2 , is a scalar that combines information from the dispersion and mean of several variables. Due to the fact that computations are laborious and fairly complex and require some knowledge of matrix algebra, acceptance of multivariate control charts by industry was slow and hesitant.

Multivariate control charts now more accessible

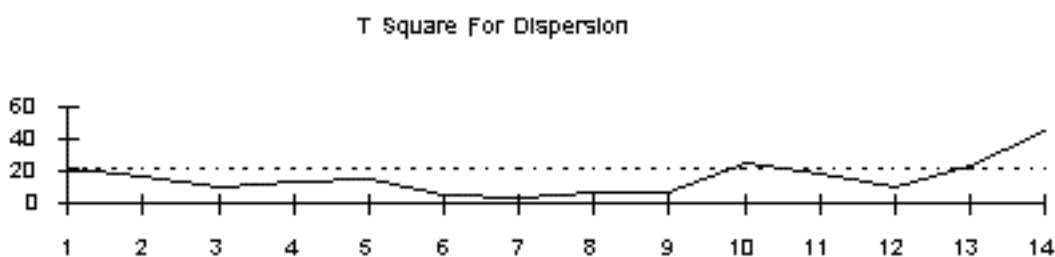
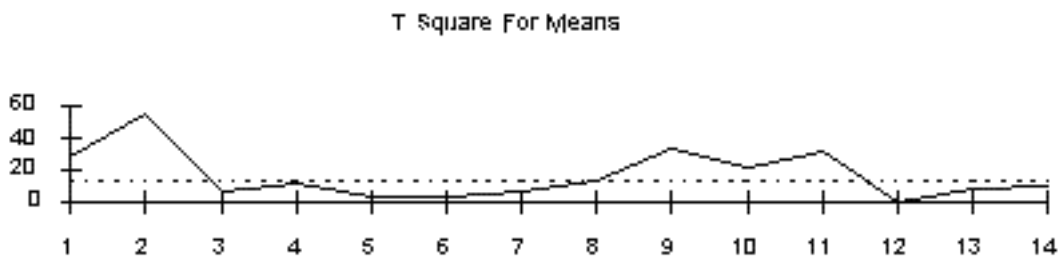
Nowadays, modern computers in general and the PC in particular have made complex calculations accessible and during the last decade, multivariate control charts were given more attention. In fact, the multivariate charts which display the Hotelling T^2 statistic became so popular that they sometimes are called Shewhart charts as well (e.g., Crosier, 1988), although Shewhart had nothing to do with them.

Hotelling charts for both means and dispersion

As in the univariate case, when data are grouped, the T^2 chart can be paired with a chart that displays a measure of variability within the subgroups for all the analyzed characteristics. The combined T^2 and T_d^2 (dispersion) charts are thus a multivariate counterpart of the univariate \bar{X} and S (or \bar{X} and R) charts.

*Hotelling
mean and
dispersion
control
charts*

An example of a Hotelling T^2 and T^2_d pair of charts is given below:

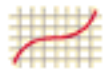


*Interpretation
of sample
Hotelling
control
charts*

Each chart represents 14 consecutive measurements on the means of four variables. The T^2 chart for means indicates an out-of-control state for groups 1,2 and 9-11. The T^2_d chart for dispersions indicate that groups 10, 13 and 14 are also out of control. The interpretation is that the multivariate system is suspect. To find an assignable cause, one has to resort to the individual univariate control charts or some other univariate procedure that should accompany this multivariate chart.

*Additional
discussion*

For more details and examples see the [next page](#) and also Tutorials, section 5, [subsections 4.3](#), 4.3.1 and 4.3.2. An introduction to [Elements of multivariate analysis](#) is also given in the Tutorials.



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.4. [What are Multivariate Control Charts?](#)

6.3.4.1. Hotelling Control Charts

Definition of Hotelling's T^2 "distance" statistic

The Hotelling T^2 distance is a measure that accounts for the covariance structure of a multivariate normal distribution. It was proposed by Harold Hotelling in 1947 and is called Hotelling T^2 . It may be thought of as the multivariate counterpart of the Student's- t statistic.

The T^2 distance is a constant multiplied by a quadratic form. This quadratic form is obtained by multiplying the following three quantities:

1. The vector of deviations between the observations and the mean \mathbf{m} , which is expressed by $(\mathbf{X}-\mathbf{m})'$,
2. The inverse of the covariance matrix, \mathbf{S}^{-1} ,
3. The vector of deviations, $(\mathbf{X}-\mathbf{m})$.

It should be mentioned that for independent variables, the covariance matrix is a diagonal matrix and T^2 becomes proportional to the sum of squared standardized variables.

In general, the higher the T^2 value, the more distant is the observation from the mean. The formula for computing the T^2 is:

$$T^2 = c(\mathbf{X} - \mathbf{m}')\mathbf{S}^{-1}(\mathbf{X} - \mathbf{m})$$

The constant c is the sample size from which the covariance matrix was estimated.

T^2 readily graphable

The T^2 distances lend themselves readily to graphical displays and as a result the T^2 -chart is the most popular among the multivariate control charts.

Estimation of the Mean and Covariance Matrix

*Mean and
Covariance
matrices*

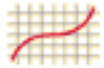
Let $\mathbf{X}_1, \dots, \mathbf{X}_n$ be n p -dimensional vectors of observations that are sampled independently from $N_p(\mathbf{m}, \Sigma)$ with $p < n-1$, with Σ the covariance matrix of \mathbf{X} . The observed mean vector $\bar{\mathbf{X}}$ and the sample dispersion matrix

$$\mathbf{S} = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{X}_i - \bar{\mathbf{X}})(\mathbf{X}_i - \bar{\mathbf{X}})'$$

are the unbiased estimators of \mathbf{m} and Σ , respectively.

*Additional
discussion*

See Tutorials (section 5), [subsections 4.3, 4.3.1](#) and [4.3.2](#) for more details and examples. An introduction to [Elements of multivariate analysis](#) is also given in the Tutorials.



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.4. [What are Multivariate Control Charts?](#)

6.3.4.2. Principal Components Control Charts

Problems with T^2 charts

Although the T^2 chart is the most popular, easiest to use and interpret method for handling multivariate process data, and is beginning to be widely accepted by quality engineers and operators, it is not a panacea. First, unlike the univariate case, the scale of the values displayed on the chart is not related to the scales of any of the monitored variables. Secondly, when the T^2 statistic exceeds the upper control limit (UCL), the user does not know which particular variable(s) caused the out-of-control signal.

Run univariate charts along with the multivariate ones

With respect to scaling, we strongly advise to run individual univariate charts in tandem with the multivariate chart. This will also help in honing in on the culprit(s) that might have caused the signal. However, individual univariate charts cannot explain situations that are a result of some problems in the covariance or correlation between the variables. This is why a dispersion chart must also be used.

Another way to monitor multivariate data: Principal Components control charts

Another way to analyze the data is to use *principal components*. For each multivariate measurement (or observation), the principal components are linear combinations of the standardized p variables (to standardize subtract their respective targets and divide by their standard deviations). The principal components have two important advantages:

1. the new variables are uncorrelated (or almost)
2. very often, a few (sometimes 1 or 2) principal components may capture most of the variability in the data so that we do not have to use all of the p principal components for control.

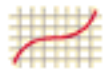
Eigenvalues

Unfortunately, there is one big disadvantage: The identity of the original variables is lost! However, in some cases the specific linear combinations corresponding to the principal components with the largest [eigenvalues](#) may yield meaningful measurement units. What is being used in control charts are the *principal factors*.

A principal factor is the principal component divided by the square root of its eigenvalue.

Additional discussion

More [details and examples](#) are given in the Tutorials (section 5).



6. [Process or Product Monitoring and Control](#)

6.3. [Univariate and Multivariate Control Charts](#)

6.3.4. [What are Multivariate Control Charts?](#)

6.3.4.3. Multivariate EWMA Charts

Multivariate EWMA Control Chart

*Univariate
EWMA model*

The model for a univariate EWMA chart is given by:

$$Z_i = \lambda X_i + (1 - \lambda)Z_{i-1} \quad i = 1, 2, \dots, n$$

where Z_i is the i th EWMA, X_i is the the i th observation, Z_0 is the average from the historical data, and $0 < \lambda \leq 1$.

*Multivariate
EWMA model*

In the multivariate case, one can extend this formula to

$$Z_i = \Lambda X_i + (1 - \Lambda)Z_{i-1}$$

where Z_i is the i th EWMA vector, X_i is the the i th observation vector $i = 1, 2, \dots, n$, Z_0 is the vector of variable values from the historical data, Λ is the $\text{diag}(\lambda_1, \lambda_2, \dots, \lambda_p)$ which is a diagonal matrix with $\lambda_1, \lambda_2, \dots, \lambda_p$ on the main diagonal, and p is the number of variables; that is the number of elements in each vector.

*Illustration of
multivariate
EWMA*

The following illustration may clarify this. There are p variables and each variable contains n observations. The input data matrix looks like:

$$\begin{array}{cccc} X_{11} & X_{12} & \cdots & X_{1p} \\ X_{21} & X_{22} & \cdots & X_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ X_{n1} & X_{n2} & \cdots & X_{np} \end{array}$$

The quantity to be plotted on the control chart is

$$\mathbf{T}_i^2 = \mathbf{Z}_i' \Sigma_z^{-1} \mathbf{Z}_i$$

Simplification It has been shown ([Lowry et al., 1992](#)) that the (k,l) th element of the covariance matrix of the i th EWMA, Σ_{z_i} , is

$$\Sigma_{z_i}(k, l) = \lambda_k \lambda_l \frac{[1 - (1 - \lambda_k)^i (1 - \lambda_l)^i]}{[\lambda_k + \lambda_l - \lambda_k \lambda_l]} \sigma_{k,l}$$

where $\sigma_{k,l}$ is the (k,l) th element of Σ , the covariance matrix of the X's.

If $\lambda_1 = \lambda_2 = \dots = \lambda_p = \lambda$, then the above expression simplifies to

$$\Sigma_{z_i}(k, l) = \frac{\lambda}{2 - \lambda} [1 - (1 - \lambda)^{2i}] \Sigma$$

where Σ is the covariance matrix of the input data.

Further simplification There is a further simplification. When i becomes large, the covariance matrix may be expressed as:

$$\Sigma_{z_i} = \frac{\lambda}{2 - \lambda} \Sigma$$

The question is "What is large?". When we examine the formula with the $2i$ in it, we observe that when $2i$ becomes sufficiently large such that $(1 - \lambda)^{2i}$ becomes almost zero, then we can use the simplified formula.

Table for
selected
values of λ
and i

The following table gives the values of $(1-\lambda)^{2i}$ for selected values of λ and i .

	$2i$									
$1 - \lambda$	4	6	8	10	12	20	30	40	50	
.9	.656	.531	.430	.349	.282	.122	.042	.015	.005	
.8	.410	.262	.168	.107	.069	.012	.001	.000	.000	
.7	.240	.118	.058	.028	.014	.001	.000	.000	.000	
.6	.130	.047	.017	.006	.002	.000	.000	.000	.000	
.5	.063	.016	.004	.001	.000	.000	.000	.000	.000	
.4	.026	.004	.001	.000	.000	.000	.000	.000	.000	
.3	.008	.001	.000	.000	.000	.000	.000	.000	.000	
.2	.002	.000	.000	.000	.000	.000	.000	.000	.000	
.1	.000	.000	.000	.000	.000	.000	.000	.000	.000	

Simplified
formula not
required

It should be pointed out that a well-meaning computer program does not have to adhere to the simplified formula, and potential inaccuracies for low values for λ and i can thus be avoided.

MEWMA
computer
output
for the
Lowry
data

Here is an example of the application of an MEWMA control chart. To facilitate comparison with existing literature, we used data from Lowry et al. The data were simulated from a bivariate normal distribution with unit variances and a correlation coefficient of 0.5. The value for $\lambda = .10$ and the values for T_i^2 were obtained by the equation given above. The covariance of the MEWMA vectors was obtained by using the non-simplified equation. That means that for each MEWMA control statistic, the computer computed a covariance matrix, where $i = 1, 2, \dots, 10$. The results of the computer routine are:

```
*****
*           Multi-Variate EWMA Control Chart           *
*****
```

DATA SERIES		MEWMA Vector		MEWMA
1	2	1	2	STATISTIC
-1.190	0.590	-0.119	0.059	2.1886
0.120	0.900	-0.095	0.143	2.0697
-1.690	0.400	-0.255	0.169	4.8365
0.300	0.460	-0.199	0.198	3.4158
0.890	-0.750	-0.090	0.103	0.7089
0.820	0.980	0.001	0.191	0.9268

-0.300	2.280	-0.029	0.400	4.0018
0.630	1.750	0.037	0.535	6.1657
1.560	1.580	0.189	0.639	7.8554
1.460	3.050	0.316	0.880	14.4158

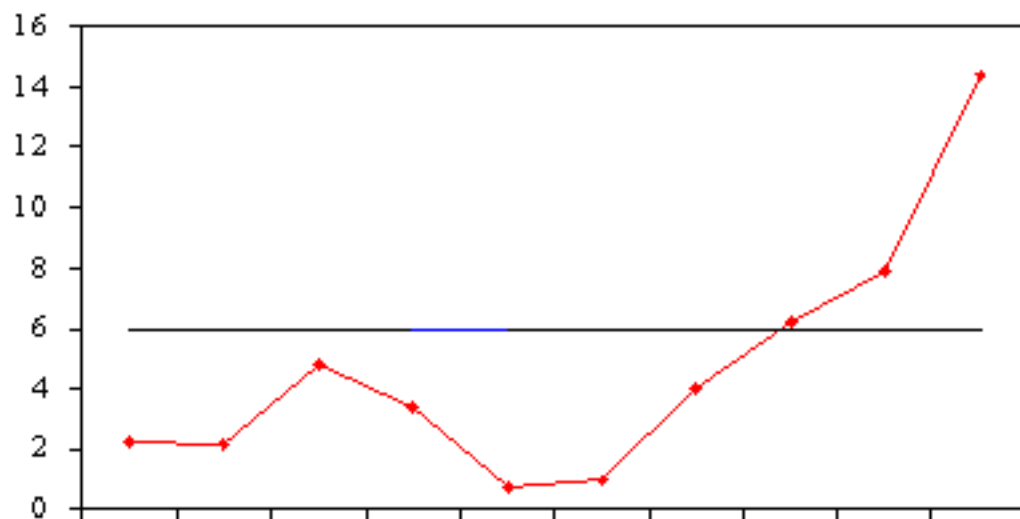
VEC	XBAR	MSE	Lamda
1	.260	1.200	0.100
2	1.124	1.774	0.100

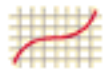
The UCL = 5.938 for $\alpha = .05$. Smaller choices of α are also used.

*Sample
MEWMA
plot*

The following is the plot of the above MEWMA.

Plot of MEWMA's





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6.4. Introduction to Time Series Analysis

Time series methods take into account possible internal structure in the data

Time series data often arise when monitoring industrial processes or tracking corporate business metrics. The essential difference between modeling data via time series methods or using the process monitoring methods discussed earlier in this chapter is the following:

Time series analysis accounts for the fact that data points taken over time may have an internal structure (such as autocorrelation, trend or seasonal variation) that should be accounted for.

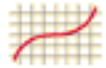
This section will give a brief overview of some of the more widely used techniques in the rich and rapidly growing field of time series modeling and analysis.

Contents for this section

Areas covered are:

1. [Definitions, Applications and Techniques](#)
2. [What are Moving Average or Smoothing Techniques?](#)
 1. [Single Moving Average](#)
 2. [Centered Moving Average](#)
3. [What is Exponential Smoothing?](#)
 1. [Single Exponential Smoothing](#)
 2. [Forecasting with Single Exponential Smoothing](#)
 3. [Double Exponential Smoothing](#)
 4. [Forecasting with Double Exponential Smoothing](#)
 5. [Triple Exponential Smoothing](#)
 6. [Example of Triple Exponential Smoothing](#)
 7. [Exponential Smoothing Summary](#)
4. [Univariate Time Series Models](#)

1. [Sample Data Sets](#)
 2. [Stationarity](#)
 3. [Seasonality](#)
 4. [Common Approaches](#)
 5. [Box-Jenkins Approach](#)
 6. [Box-Jenkins Model Identification](#)
 7. [Box-Jenkins Model Estimation](#)
 8. [Box-Jenkins Model Validation](#)
 9. [SEMPLOT Sample Output for a Box-Jenkins Model Analysis](#)
 10. [SEMPLOT Sample Output for a Box-Jenkins Model Analysis with Seasonality](#)
5. [Multivariate Time Series Models](#)
 1. [Example of Multivariate Time Series Analysis](#)



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6.4. [Introduction to Time Series Analysis](#)

6.4.1. Definitions, Applications and Techniques

Definition

Definition of Time Series: *An ordered sequence of values of a variable at equally spaced time intervals.*

Time series occur frequently when looking at industrial data

Applications: The usage of time series models is twofold:

- Obtain an understanding of the underlying forces and structure that produced the observed data
- Fit a model and proceed to forecasting, monitoring or even feedback and feedforward control.

Time Series Analysis is used for many applications such as:

- Economic Forecasting
- Sales Forecasting
- Budgetary Analysis
- Stock Market Analysis
- Yield Projections
- Process and Quality Control
- Inventory Studies
- Workload Projections
- Utility Studies
- Census Analysis

and many, many more...

There are many methods used to model and forecast time series

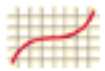
Techniques: The fitting of time series models can be an ambitious undertaking. There are many methods of model fitting including the following:

- [Box-Jenkins ARIMA models](#)
- [Box-Jenkins Multivariate Models](#)
- [Holt-Winters Exponential Smoothing \(single, double, triple\)](#)

The user's application and preference will decide the selection of the appropriate technique. It is beyond the realm and intention of the authors of this handbook to cover all these methods. The overview presented here will start by looking at some basic smoothing techniques:

- Averaging Methods
- Exponential Smoothing Techniques.

Later in this section we will discuss the Box-Jenkins modeling methods and Multivariate Time Series.



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6.4. [Introduction to Time Series Analysis](#)

6.4.2. What are Moving Average or Smoothing Techniques?

Smoothing data removes random variation and shows trends and cyclic components

Inherent in the collection of data taken over time is some form of random variation. There exist methods for reducing or canceling the effect due to random variation. An often-used technique in industry is "smoothing". This technique, when properly applied, reveals more clearly the underlying trend, seasonal and cyclic components.

There are two distinct groups of smoothing methods

- Averaging Methods
- Exponential Smoothing Methods

Taking averages is the simplest way to smooth data

We will first investigate some averaging methods, such as the "simple" average of all past data.

A manager of a warehouse wants to know how much a typical supplier delivers in 1000 dollar units. He/she takes a sample of 12 suppliers, at random, obtaining the following results:

Supplier	Amount	Supplier	Amount
1	9	7	11
2	8	8	7
3	9	9	13
4	12	10	9
5	9	11	11
6	12	12	10

The computed mean or average of the data = 10. The manager decides to use this as the estimate for *expenditure of a typical supplier*.

Is this a good or bad estimate?

Mean squared error is a way to judge how good a model is

We shall compute the "mean squared error":

- The "error" = true amount spent minus the estimated amount.
- The "error squared" is the error above, squared.
- The "SSE" is the sum of the squared errors.
- The "MSE" is the mean of the squared errors.

MSE results for example

The results are:

Error and Squared Errors

The estimate = 10

Supplier	\$	Error	Error Squared
1	9	-1	1
2	8	-2	4
3	9	-1	1
4	12	2	4
5	9	-1	1
6	12	2	4
7	11	1	1
8	7	-3	9
9	13	3	9
10	9	-1	1
11	11	1	1
12	10	0	0

The SSE = 36 and the MSE = $36/12 = 3$.

Table of MSE results for example using different estimates

So how good was the estimator for the amount spent for each supplier? Let us compare the estimate (10) with the following estimates: 7, 9, and 12. That is, we estimate that each supplier will spend \$7, or \$9 or \$12.

Performing the same calculations we arrive at:

Estimator	7	9	10	12
SSE	144	48	36	84
MSE	12	4	3	7

The estimator with the smallest MSE is the best. It can be shown mathematically that the estimator that minimizes the MSE for a set of random data is the mean.

Table showing squared error for the mean for sample data

Next we will examine the mean to see how well it predicts net income over time.

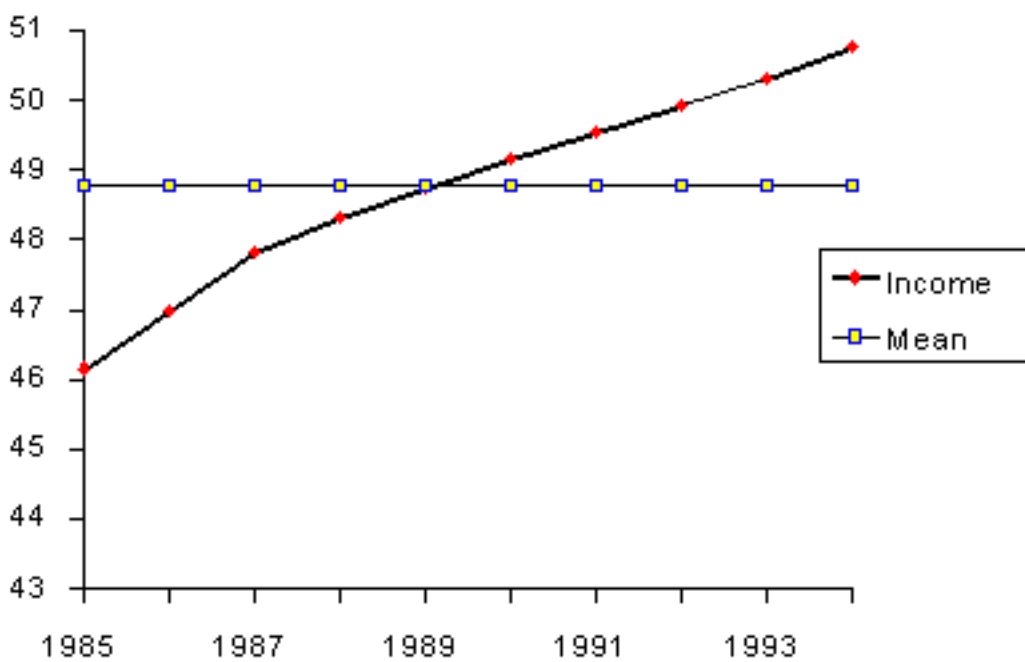
The next table gives the income before taxes of a PC manufacturer between 1985 and 1994.

Year	\$ (millions)	Mean	Error	Squared Error
1985	46.163	48.776	-2.613	6.828
1986	46.998	48.776	-1.778	3.161
1987	47.816	48.776	-0.960	0.922
1988	48.311	48.776	-0.465	0.216
1989	48.758	48.776	-0.018	0.000
1990	49.164	48.776	0.388	0.151
1991	49.548	48.776	0.772	0.596
1992	48.915	48.776	1.139	1.297
1993	50.315	48.776	1.539	2.369
1994	50.768	48.776	1.992	3.968

The MSE = 1.9508.

The mean is not a good estimator when there are trends

The question arises: *can we use the mean to forecast income if we suspect a trend?* A look at the graph below shows clearly that we should not do this.



*Average
weighs all
past
observations
equally*

In summary, we state that

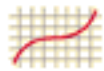
1. The "simple" average or mean of all past observations is only a useful estimate for forecasting when there are no trends. If there are trends, use different estimates that take the trend into account.
2. The average "weighs" all past observations equally. For example, the average of the values 3, 4, 5 is 4. We know, of course, that an average is computed by adding all the values and dividing the sum by the number of values. Another way of computing the average is by adding each value divided by the number of values, or

$$3/3 + 4/3 + 5/3 = 1 + 1.3333 + 1.6667 = 4.$$

The multiplier $1/3$ is called the *weight*. In general:

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i = \left(\frac{1}{n}\right) x_1 + \left(\frac{1}{n}\right) x_2 + \dots + \left(\frac{1}{n}\right) x_n$$

The $\left(\frac{1}{n}\right)$ are the weights and of course they sum to 1.



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6.4.2. [What are Moving Average or Smoothing Techniques?](#)

6.4.2.1. Single Moving Average

Taking a moving average is a smoothing process

An alternative way to summarize the past data is to compute the mean of successive smaller sets of numbers of past data as follows:

Recall the set of numbers 9, 8, 9, 12, 9, 12, 11, 7, 13, 9, 11, 10 which were the dollar amount of [12 suppliers](#) selected at random. Let us set M , the size of the "smaller set" equal to 3. Then the average of the first 3 numbers is: $(9 + 8 + 9) / 3 = 8.667$.

This is called "smoothing" (i.e., some form of averaging). This smoothing process is continued by advancing one period and calculating the next average of three numbers, dropping the first number.

Moving average example

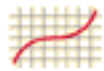
The next table summarizes the process, which is referred to as *Moving Averaging*. The general expression for the moving average is

$$M_t = [X_t + X_{t-1} + \dots + X_{t-N+1}] / N$$

Results of Moving Average

Supplier	\$	MA	Error	Error squared
1	9			
2	8			
3	9	8.667	0.333	0.111
4	12	9.667	2.333	5.444
5	9	10.000	-1.000	1.000
6	12	11.000	1.000	1.000
7	11	10.667	0.333	0.111
8	7	10.000	-3.000	9.000
9	13	10.333	2.667	7.111
10	9	9.667	-0.667	0.444
11	11	11.000	0	0
12	10	10.000	0	0

The MSE = 2.018 as compared to 3 in the previous case.



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6.4.2. [What are Moving Average or Smoothing Techniques?](#)

6.4.2.2. Centered Moving Average

When computing a running moving average, placing the average in the middle time period makes sense

In the [previous example](#) we computed the average of the first 3 time periods and placed it next to period 3. We could have placed the average in the middle of the time interval of three periods, that is, next to period 2. This works well with odd time periods, but not so good for even time periods. So where would we place the first moving average when $M = 4$?

Technically, the Moving Average would fall at $t = 2.5, 3.5, \dots$

To avoid this problem we smooth the MA's using $M = 2$. **Thus we smooth the smoothed values!**

If we average an even number of terms, we need to smooth the smoothed values

The following table shows the results using $M = 4$.

		Interim Steps	
Period	Value	MA	Centered
1	9		
1.5			
2	8		
2.5		9.5	
3	9		9.5
3.5		9.5	
4	12		10.0
4.5		10.5	
5	9		10.750
5.5		11.0	
6	12		
6.5			
7	9		

Final table This is the final table:

Period Value Centered MA

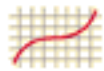
1	9	
2	8	
3	9	9.5
4	12	10.0
5	9	10.75
6	12	
7	11	

Double Moving Averages for a Linear Trend Process

Moving averages are still not able to handle significant trends when forecasting

Unfortunately, neither the mean of all data nor the moving average of the most recent M values, when used as forecasts for the next period, are able to cope with a significant trend.

There exists a variation on the MA procedure that often does a better job of handling trend. It is called *Double Moving Averages for a Linear Trend Process*. It calculates a second moving average from the original moving average, using the same value for M . As soon as both single and double moving averages are available, a computer routine uses these averages to compute a slope and intercept, and then forecasts one or more periods ahead.



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6.4.3. What is Exponential Smoothing?

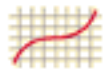
Exponential smoothing schemes weight past observations using exponentially decreasing weights

This is a very popular scheme to produce a smoothed Time Series. Whereas in Single Moving Averages the past observations are weighted equally, Exponential Smoothing assigns *exponentially decreasing weights* as the observation get older.

In other words, *recent observations are given relatively more weight in forecasting than the older observations.*

In the case of moving averages, the weights assigned to the observations are the same and are equal to $1/N$. In exponential smoothing, however, there are one or more *smoothing parameters* to be determined (or estimated) and these choices determine the weights assigned to the observations.

[Single](#), [double](#) and [triple](#) Exponential Smoothing will be described in this section.



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6.4.3. [What is Exponential Smoothing?](#)

6.4.3.1. Single Exponential Smoothing

Exponential smoothing weights past observations with exponentially decreasing weights to forecast future values

This smoothing scheme begins by setting S_2 to y_1 , where S_i stands for smoothed observation or EWMA, and y stands for the original observation. The subscripts refer to the time periods, 1, 2, ..., n . For the third period, $S_3 = \alpha y_2 + (1-\alpha) S_2$; and so on. There is no S_1 ; the smoothed series starts with the smoothed version of the second observation.

For any time period t , the smoothed value S_t is found by computing

$$S_t = \alpha y_{t-1} + (1-\alpha) S_{t-1} \quad 0 < \alpha \leq 1 \quad t \geq 3$$

This is the *basic equation of exponential smoothing* and the constant or parameter α is called the *smoothing constant*.

Note: There is an alternative approach to exponential smoothing that replaces y_{t-1} in the basic equation with y_t , the current observation. That formulation, due to Roberts (1959), is described in the section on [EWMA control charts](#). The formulation here follows Hunter (1986).

Setting the first EWMA

The first forecast is very important

The initial EWMA plays an important role in computing all the subsequent EWMA's. Setting S_2 to y_1 is one method of initialization. Another way is to set it to the target of the process.

Still another possibility would be to average the first four or five observations.

It can also be shown that the smaller the value of α , the more important is the selection of the initial EWMA. The user would be wise to try a few methods, (assuming that the software has them available) before finalizing the settings.

Why is it called "Exponential"?

Expand basic equation

Let us expand the basic equation by first substituting for S_{t-1} in the basic equation to obtain

$$\begin{aligned} S_t &= \alpha y_{t-1} + (1-\alpha) [\alpha y_{t-2} + (1-\alpha) S_{t-2}] \\ &= \alpha y_{t-1} + \alpha (1-\alpha) y_{t-2} + (1-\alpha)^2 S_{t-2} \end{aligned}$$

Summation formula for basic equation

By substituting for S_{t-2} , then for S_{t-3} , and so forth, until we reach S_2 (which is just y_1), it can be shown that the expanding equation can be written as:

$$S_t = \alpha \sum_{i=1}^{t-1} (1-\alpha)^{i-1} y_{t-i} + (1-\alpha)^{t-2} S_2, t \geq 2$$

Expanded equation for S_5

For example, the expanded equation for the smoothed value S_5 is:

$$S_5 = \alpha \left[(1-\alpha)^0 y_{5-1} + (1-\alpha)^1 y_{5-2} + (1-\alpha)^2 y_{5-3} \right] + (1-\alpha)^3 S_2$$

Illustrates exponential behavior

This illustrates the exponential behavior. The weights, $\alpha (1-\alpha)^t$ decrease geometrically, and their sum is unity as shown below, using a property of geometric series:

$$\alpha \sum_{i=0}^{t-1} (1-\alpha)^i = \alpha \left[\frac{1-(1-\alpha)^t}{1-(1-\alpha)} \right] = 1-(1-\alpha)^t$$

From the last formula we can see that the summation term shows that the contribution to the smoothed value S_t becomes less at each consecutive time period.

Example for $\alpha = .3$

Let $\alpha = .3$. Observe that the weights $\alpha (1-\alpha)^t$ decrease exponentially (geometrically) with time.

Value weight		
last	y_1	.2100
	y_2	.1470
	y_3	.1029
	y_4	.0720

What is the "best" value for α ?

How do you choose the weight parameter?

The speed at which the older responses are dampened (smoothed) is a function of the value of α . When α is close to 1, dampening is quick and when α is close to 0, dampening is slow. This is illustrated in the table below:

-----> towards past observations				
α	$(1-\alpha)$	$(1-\alpha)^2$	$(1-\alpha)^3$	$(1-\alpha)^4$
.9	.1	.01	.001	.0001
.5	.5	.25	.125	.0625
.1	.9	.81	.729	.6561

We choose the best value for α so the value which results in the smallest MSE.

Example

Let us illustrate this principle with an example. Consider the following data set consisting of 12 observations taken over time:

Time	y_t	$S (\alpha=.1)$	Error	Error squared
1	71			
2	70	71	-1.00	1.00
3	69	70.9	-1.90	3.61
4	68	70.71	-2.71	7.34
5	64	70.44	-6.44	41.47
6	65	69.80	-4.80	23.04
7	72	69.32	2.68	7.18
8	78	69.58	8.42	70.90
9	75	70.43	4.57	20.88
10	75	70.88	4.12	16.97
11	75	71.29	3.71	13.76
12	70	71.67	-1.67	2.79

The sum of the squared errors (SSE) = 208.94. The mean of the squared errors (MSE) is the SSE /11 = 19.0.

Calculate for different values of α

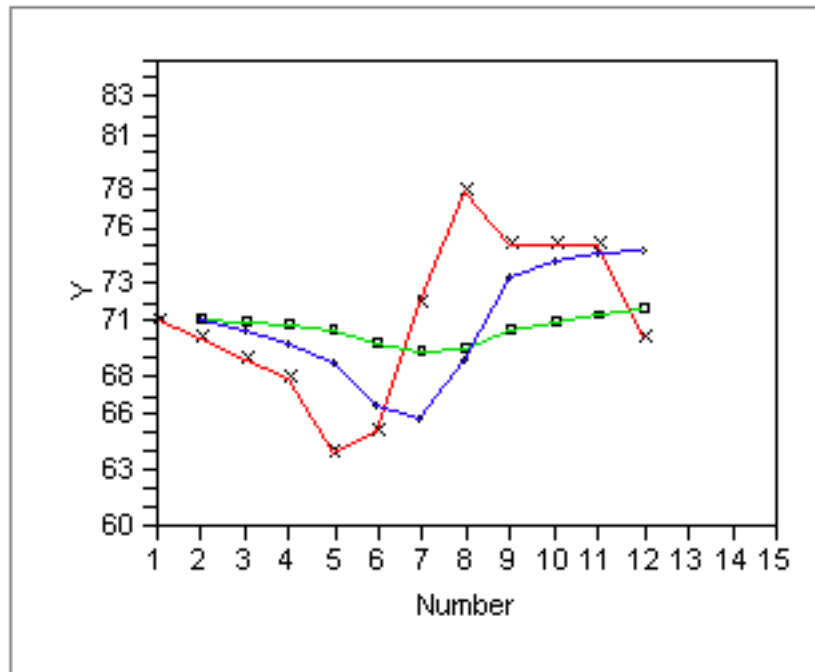
The MSE was again calculated for $\alpha = .5$ and turned out to be 16.29, so in this case we would prefer an α of .5. Can we do better? We could apply the proven trial-and-error method. This is an iterative procedure beginning with a range of α between .1 and .9. We determine the best initial choice for α and then search between $\alpha - \Delta$ and $\alpha + \Delta$. We could repeat this perhaps one more time to find the best α to 3 decimal places.

Nonlinear optimizers can be used

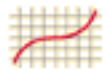
But there are better search methods, such as the Marquardt procedure. This is a nonlinear optimizer that minimizes the sum of squares of residuals. In general, most well designed statistical software programs should be able to find the value of α that minimizes the MSE.

Sample plot showing smoothed data for 2 values of α

Exponential Smoothing: Original and Smoothed Values



Y x- Original Y ■ alpha = .1 ♦ alpha = .5



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6.4.3. [What is Exponential Smoothing?](#)

6.4.3.2. Forecasting with Single Exponential Smoothing

Forecasting Formula

*Forecasting
the next point*

The forecasting formula is the basic equation

$$S_{t+1} = \alpha y_t + (1 - \alpha) S_t \quad 0 < \alpha \leq 1 \quad t > 0$$

*New forecast
is previous
forecast plus
an error
adjustment*

This can be written as:

$$S_{t+1} = S_t + \alpha(\epsilon_t)$$

where ϵ_t is the forecast error (actual - forecast) for period t .

In other words, the new forecast is the old one plus an adjustment for the error that occurred in the last forecast.

Bootstrapping of Forecasts

*Bootstrapping
forecasts*

What happens if you wish to forecast from some origin, usually the last data point, and no actual observations are available? In this situation we have to modify the formula to become:

$$S_{t+1} = \alpha y_{origin} + (1 - \alpha) S_t$$

where y_{origin} remains constant. This technique is known as *bootstrapping*.

Example of Bootstrapping

Example

The last data point in the previous example was 70 and its forecast (smoothed value S) was 71.7. Since we do have the data point **and** the forecast available, we can calculate the next forecast using the regular formula

$$S_{t+1} = \alpha y_{t+1} + (1 - \alpha) S_t$$

$$= .1(70) + .9(71.7) = 71.5 \quad (\alpha = .1)$$

But for the next forecast we have no data point (observation). So now we compute:

$$S_{t+2} = .1(70) + .9(71.5) = 71.35$$

Comparison between bootstrap and regular forecasting

Table comparing two methods

The following table displays the comparison between the two methods:

Period	Bootstrap forecast	Data	Single Smoothing Forecast
13	71.50	75	71.5
14	71.35	75	71.9
15	71.21	74	72.2
16	71.09	78	72.4
17	70.98	86	73.0

Single Exponential Smoothing with Trend

Single Smoothing (short for single exponential smoothing) is not very good when there is a trend. The single coefficient α is not enough.

Sample data set with trend

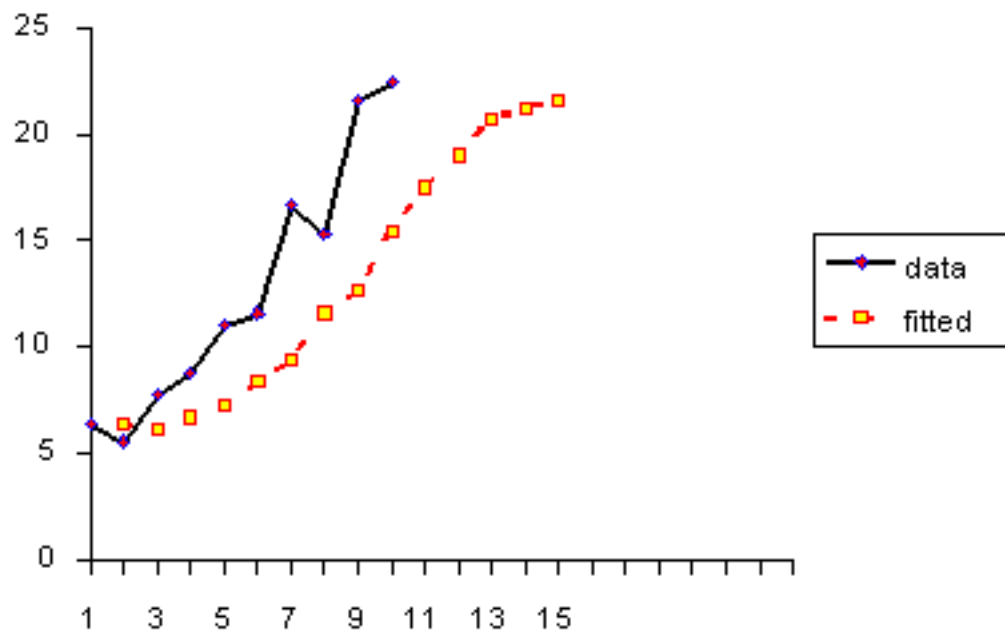
Let us demonstrate this with the following data set smoothed with an α of 0.3:

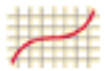
Data Fit

6.4	
5.6	6.4
7.8	6.2
8.8	6.7
11.0	7.3
11.6	8.4
16.7	9.4
15.3	11.6
21.6	12.7
22.4	15.4

Plot demonstrating inadequacy of single exponential smoothing when there is trend

The resulting graph looks like:





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6.4.3. [What is Exponential Smoothing?](#)

6.4.3.3. Double Exponential Smoothing

Double exponential smoothing uses two constants and is better at handling trends

As was [previously observed](#), Single Smoothing does not excel in following the data when there is a trend. This situation can be improved by the introduction of a second equation with a second constant, γ , which must be chosen in conjunction with α .

Here are the two equations associated with Double Exponential Smoothing:

$$S_t = \alpha y_t + (1 - \alpha) (S_{t-1} + b_{t-1}) \quad 0 \leq \alpha \leq 1$$

$$b_t = \gamma (S_t - S_{t-1}) + (1 - \gamma) b_{t-1} \quad 0 \leq \gamma \leq 1$$

Note that the current value of the series is used to calculate its smoothed value replacement in double exponential smoothing.

Initial Values

Several methods to choose the initial values

As in the case for single smoothing, there are a variety of schemes to set initial values for S_t and b_t in double smoothing.

S_1 is in general set to y_1 . Here are three suggestions for b_1 :

$$b_1 = y_2 - y_1$$

$$b_1 = [(y_2 - y_1) + (y_3 - y_2) + (y_4 - y_3)]/3$$

$$b_1 = (y_n - y_1)/(n - 1)$$

Comments

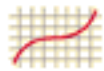
*Meaning of
the
smoothing
equations*

The first smoothing equation adjusts S_t directly for the trend of the previous period, b_{t-1} , by adding it to the last smoothed value, S_{t-1} . This helps to eliminate the lag and brings S_t to the appropriate base of the current value.

The second smoothing equation then updates the trend, which is expressed as the difference between the last two values. The equation is similar to the basic form of single smoothing, but here applied to the updating of the trend.

*Non-linear
optimization
techniques
can be used*

The values for α and γ can be obtained via non-linear optimization techniques, such as the Marquardt Algorithm.



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6.4.3. [What is Exponential Smoothing?](#)

6.4.3.4. Forecasting with Double Exponential Smoothing(LASP)

Forecasting formula

The one-period-ahead forecast is given by:

$$F_{t+1} = S_t + b_t$$

The m-periods-ahead forecast is given by:

$$F_{t+m} = S_t + mb_t$$

Example

Example

Consider once more the data set:

6.4, 5.6, 7.8, 8.8, 11, 11.6, 16.7, 15.3, 21.6, 22.4.

Now we will fit a double smoothing model with $\alpha = .3623$ and $\gamma = 1.0$. These are the estimates that result in the lowest possible MSE when comparing the original series to one step ahead at a time forecasts (since this version of double exponential smoothing uses the current series value to calculate a smoothed value, the smoothed series cannot be used to determine an α with minimum MSE). The chosen starting values are $S_1 = y_1 = 6.4$ and $b_1 = ((y_2 - y_1) + (y_3 - y_2) + (y_4 - y_3))/3 = 0.8$.

For comparison's sake we also fit a single smoothing model with $\alpha = 0.977$ (this results in the lowest MSE for single exponential smoothing).

The MSE for double smoothing is 3.7024.

The MSE for single smoothing is 8.8867.

Forecasting results for the example

The smoothed results for the example are:

Data	Double	Single
6.4	6.4	
5.6	6.6 (Forecast = 7.2)	6.4
7.8	7.2 (Forecast = 6.8)	5.6
8.8	8.1 (Forecast = 7.8)	7.8
11.0	9.8 (Forecast = 9.1)	8.8
11.6	11.5 (Forecast = 11.4)	10.9
16.7	14.5 (Forecast = 13.2)	11.6
15.3	16.7 (Forecast = 17.4)	16.6
21.6	19.9 (Forecast = 18.9)	15.3
22.4	22.8 (Forecast = 23.1)	21.5

Comparison of Forecasts

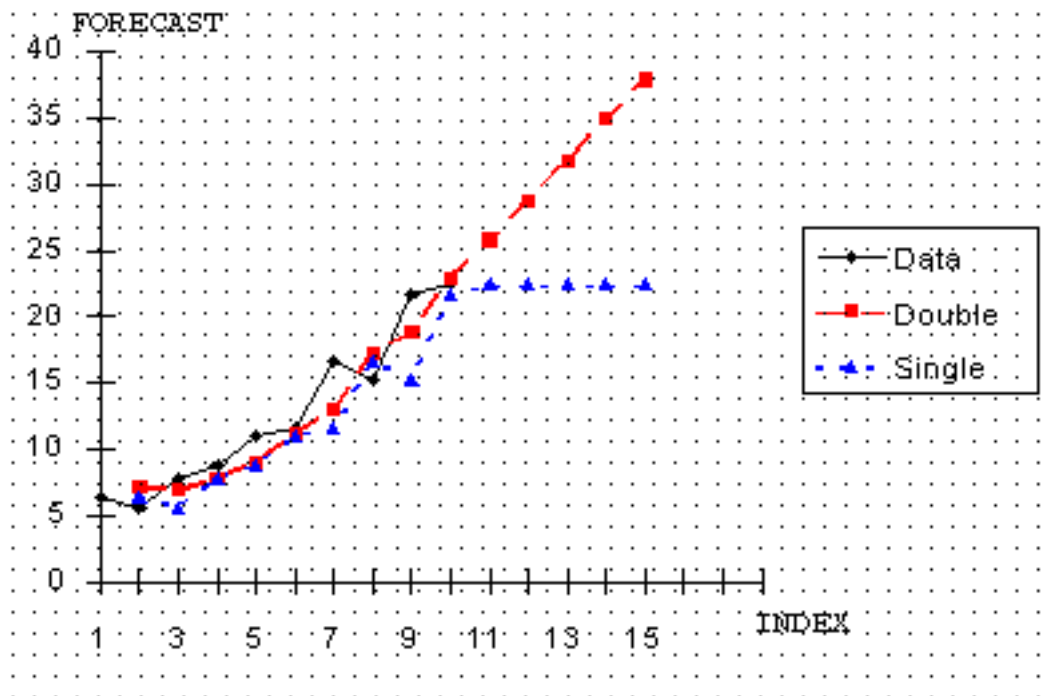
Table showing single and double exponential smoothing forecasts

To see how each method predicts the future, we computed the first five forecasts from the last observation as follows:

Period	Single	Double
11	22.4	25.8
12	22.4	28.7
13	22.4	31.7
14	22.4	34.6
15	22.4	37.6

Plot comparing single and double exponential smoothing forecasts

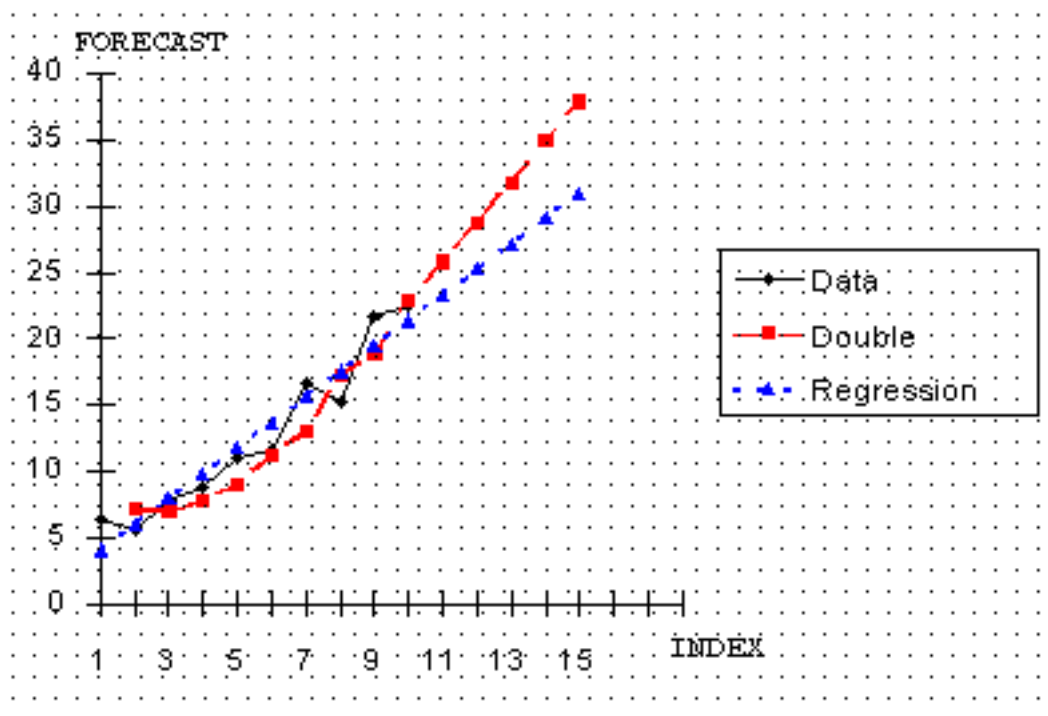
A plot of these results (using the forecasted double smoothing values) is very enlightening.



This graph indicates that double smoothing follows the data much closer than single smoothing. Furthermore, for forecasting single smoothing cannot do better than projecting a straight horizontal line, which is not very likely to occur in reality. So in this case double smoothing is preferred.

Plot comparing double exponential smoothing and regression forecasts

Finally, let us compare double smoothing with linear regression:



This is an interesting picture. Both techniques follow the data in similar fashion, but the regression line is more conservative. That is, there is a slower increase with the regression line than with double smoothing.

Selection of technique depends on the forecaster

The selection of the technique depends on the forecaster. If it is desired to portray the growth process in a more aggressive manner, then one selects double smoothing. Otherwise, regression may be preferable. It should be noted that in linear regression "time" functions as the independent variable. [Chapter 4](#) discusses the [basics](#) of linear regression, and the details of regression [estimation](#).

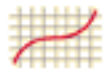
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6.4.3.5. Triple Exponential Smoothing

What happens if the data show trend **and** seasonality?

To handle seasonality, we have to add a third parameter

In this case double smoothing will not work. We now introduce a third equation to take care of seasonality (sometimes called periodicity). The resulting set of equations is called the "Holt-Winters" (HW) method after the names of the inventors.

The basic equations for their method are given by:

$$S_t = \alpha \frac{y_t}{I_{t-L}} + (1 - \alpha)(S_{t-1} + b_{t-1}) \quad \text{OVERALL SMOOTHING}$$

$$b_t = \gamma(S_t - S_{t-1}) + (1 - \gamma)b_{t-1} \quad \text{TREND SMOOTHING}$$

$$I_t = \beta \frac{y_t}{S_t} + (1 - \beta)I_{t-L} \quad \text{SEASONAL SMOOTHING}$$

$$F_{t+m} = (S_t + mb_t) I_{t-L+m} \quad \text{FORECAST}$$

where

- y is the observation
- S is the smoothed observation
- b is the trend factor
- I is the seasonal index
- F is the forecast at m periods ahead
- t is an index denoting a time period

and α , β , and γ are constants that must be estimated in such a way that the MSE of the error is minimized. This is best left to a good software package.

Complete season needed

To initialize the HW method we need at least one complete season's data to determine initial estimates of the seasonal indices I_{t-L} .

L periods in a season

A complete season's data consists of L periods. And we need to estimate the trend factor from one period to the next. To accomplish this, it is advisable to use two complete seasons; that is, $2L$ periods.

Initial values for the trend factor

How to get initial estimates for trend and seasonality parameters

The general formula to estimate the initial trend is given by

$$b = \frac{1}{L} \left(\frac{y_{L+1} - y_1}{L} + \frac{y_{L+2} - y_2}{L} + \dots + \frac{y_{L+L} - y_L}{L} \right)$$

Initial values for the Seasonal Indices

As we will see in the example, we work with data that consist of 6 years with 4 periods (that is, 4 quarters) per year. Then

Step 1: compute yearly averages

Step 1: Compute the averages of each of the 6 years

$$A_p = \sum_{i=1}^4 y_i \quad p = 1, 2, \dots, 6$$

Step 2: divide by yearly averages

Step 2: Divide the observations by the appropriate yearly mean

	1	2	3	4	5	6
	y_1/A_1	y_5/A_2	y_9/A_3	y_{13}/A_4	y_{17}/A_5	y_{21}/A_6
	y_2/A_1	y_6/A_2	y_{10}/A_3	y_{14}/A_4	y_{18}/A_5	y_{22}/A_6
	y_3/A_1	y_7/A_2	y_{11}/A_3	y_{15}/A_4	y_{19}/A_5	y_{23}/A_6
	y_4/A_1	y_8/A_2	y_{12}/A_3	y_{16}/A_4	y_{20}/A_5	y_{24}/A_6

*Step 3:
form
seasonal
indices*

Step 3: Now the seasonal indices are formed by computing the average of each row. Thus the initial seasonal indices (symbolically) are:

$$I_1 = (y_1/A_1 + y_5/A_2 + y_9/A_3 + y_{13}/A_4 + y_{17}/A_5 + y_{21}/A_6)/6$$

$$I_2 = (y_2/A_1 + y_6/A_2 + y_{10}/A_3 + y_{14}/A_4 + y_{18}/A_5 + y_{22}/A_6)/6$$

$$I_3 = (y_3/A_1 + y_7/A_2 + y_{11}/A_3 + y_{15}/A_4 + y_{19}/A_5 + y_{22}/A_6)/6$$

$$I_4 = (y_4/A_1 + y_8/A_2 + y_{12}/A_3 + y_{16}/A_4 + y_{20}/A_5 + y_{24}/A_6)/6$$

We now know the algebra behind the computation of the initial estimates.

The next page contains an [example](#) of triple exponential smoothing.

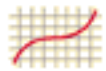
The case of the Zero Coefficients

*Zero
coefficients
for trend
and
seasonality
parameters*

Sometimes it happens that a computer program for triple exponential smoothing outputs a final coefficient for trend (α) or for seasonality (β) of zero. Or worse, both are outputted as zero!

Does this indicate that there is no trend and/or no seasonality?

Of course not! It only means that the initial values for trend and/or seasonality were right on the money. No updating was necessary in order to arrive at the lowest possible MSE. We should inspect the updating formulas to verify this.



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6.4.3.6. Example of Triple Exponential Smoothing

Example comparing single, double, triple exponential smoothing

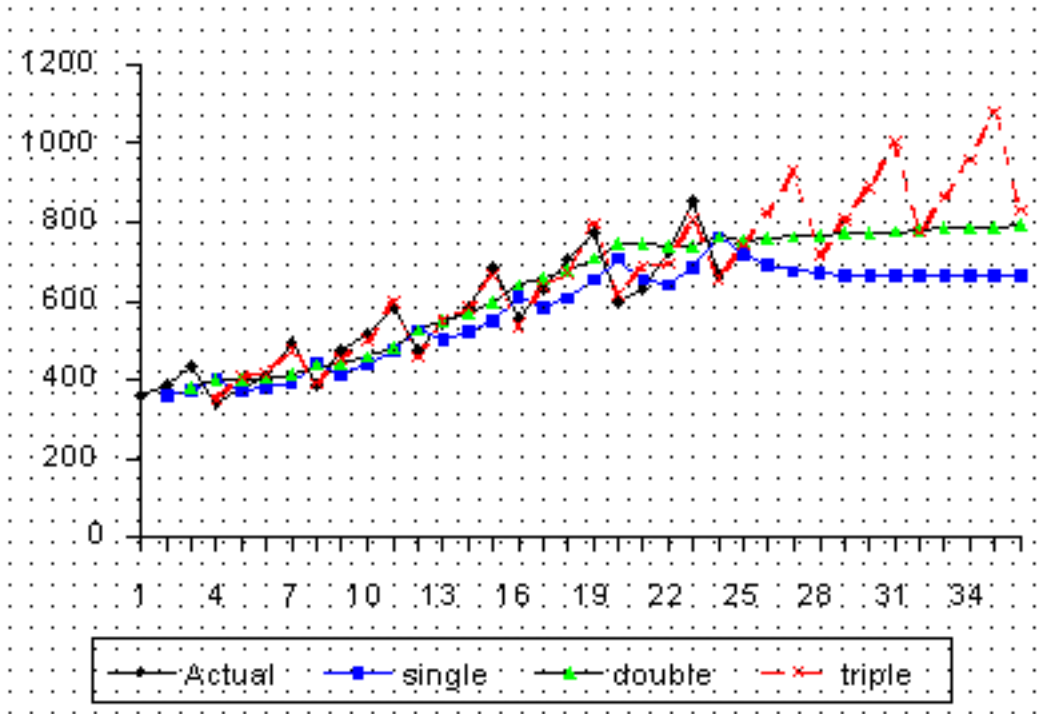
This example shows comparison of single, double and triple exponential smoothing for a data set.

The following data set represents 24 observations. These are six years of quarterly data (each year = 4 quarters).

Table showing the data for the example

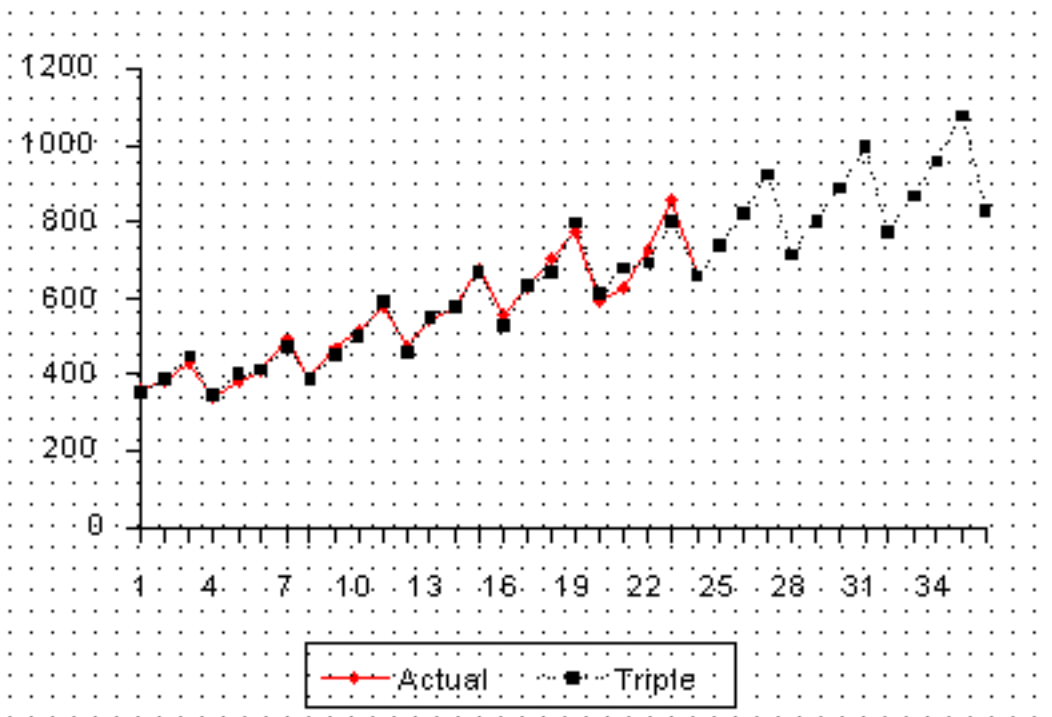
	Quarter	Period	Sales	Quarter	Period	Sales
90	1	1	362	93	1	544
	2	2	385		2	582
	3	3	432		3	681
	4	4	341		4	557
91	1	5	382	94	1	628
	2	6	409		2	707
	3	7	498		3	773
	4	8	387		4	592
92	1	9	473	95	1	627
	2	10	513		2	725
	3	11	582		3	854
	4	12	474		4	661

Plot of raw data with single, double, and triple exponential forecasts



Plot of raw data with triple exponential forecasts

Actual Time Series with forecasts



*Comparison
of MSE's*

	α	γ	β
MSE demand trend seasonality			
6906	.4694		
5054	.1086	1.000	
936	1.000		1.000
520	.7556	0.000	.9837

The updating coefficients were chosen by a computer program such that the MSE for each of the methods was minimized.

Example of the computation of the Initial Trend

*Computation
of initial
trend*

The data set consists of quarterly sales data. The season is 1 year and since there are 4 quarters per year, $L = 4$. Using the formula we obtain:

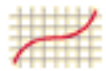
$$\begin{aligned}
 b_1 &= \frac{1}{4} \left[\frac{215-211}{4} \right] + \left[\frac{216-212}{4} \right] + \left[\frac{217-213}{4} \right] + \left[\frac{218-214}{4} \right] \\
 &= \frac{1}{4} \left[\frac{382-362}{4} \right] + \left[\frac{409-385}{4} \right] + \left[\frac{498-432}{4} \right] + \left[\frac{387-341}{4} \right] \\
 &= \frac{5+6+16.5+11.5}{4} = 9.75
 \end{aligned}$$

Example of the computation of the Initial Seasonal Indices

*Table of
initial
seasonal
indices*

	1	2	3	4	5	6
1	362	382	473	544	628	627
2	385	409	513	582	707	725
3	432	498	582	681	773	854
4	341	387	474	557	592	661
\bar{X}	380	419	510.5	591	675	716.75

In this example we used the full 6 years of data. Other schemes may use only 3, or some other number of years. There are also a number of ways to compute initial estimates.

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6.4.3.7. Exponential Smoothing Summary

Summary

Exponential smoothing has proven to be a useful technique

Exponential smoothing has proven through the years to be very useful in many forecasting situations. It was first suggested by C.C. Holt in 1957 and was meant to be used for non-seasonal time series showing no trend. He later offered a procedure (1958) that does handle trends. Winters(1965) generalized the method to include seasonality, hence the name "Holt-Winters Method".

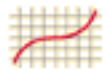
Holt-Winters has 3 updating equations

The Holt-Winters Method has 3 updating equations, each with a constant that ranges from 0 to 1. The equations are intended to give more weight to recent observations and less weights to observations further in the past.

These weights are geometrically decreasing by a constant ratio.

The HW procedure can be made fully automatic by user-friendly software.

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6.4.4. Univariate Time Series Models

Univariate Time Series

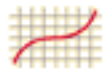
The term "univariate time series" refers to a time series that consists of single (scalar) observations recorded sequentially over equal time increments. Some examples are [monthly CO₂ concentrations](#) and [southern oscillations to predict el nino effects](#).

Although a univariate time series data set is usually given as a single column of numbers, time is in fact an implicit variable in the time series. If the data are equi-spaced, the time variable, or index, does not need to be explicitly given. The time variable may sometimes be explicitly used for plotting the series. However, it is not used in the time series model itself.

The analysis of time series where the data are not collected in equal time increments is beyond the scope of this handbook.

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2. [Stationarity](#)
3. [Seasonality](#)
4. [Common Approaches](#)
5. [Box-Jenkins Approach](#)
6. [Box-Jenkins Model Identification](#)
7. [Box-Jenkins Model Estimation](#)
8. [Box-Jenkins Model Validation](#)
9. [SEMPLOT Sample Output for a Box-Jenkins Analysis](#)
10. [SEMPLOT Sample Output for a Box-Jenkins Analysis with Seasonality](#)

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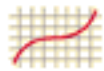
6.4.4.1. Sample Data Sets

*Sample
Data Sets*

The following two data sets are used as examples in the text for this section.

1. [Monthly mean CO₂ concentrations.](#)
2. [Southern oscillations.](#)

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6.4.4. [Univariate Time Series Models](#)

6.4.4.1. [Sample Data Sets](#)

6.4.4.1.1. Data Set of Monthly CO2 Concentrations

Source and Background

This data set contains selected monthly mean CO₂ concentrations at the Mauna Loa Observatory from 1974 to 1987. The CO₂ concentrations were measured by the continuous infrared analyser of the Geophysical Monitoring for Climatic Change division of NOAA's Air Resources Laboratory. The selection has been for an approximation of 'background conditions'. See Thoning et al., "Atmospheric Carbon Dioxide at Mauna Loa Observatory: II Analysis of the NOAA/GMCC Data 1974-1985", *Journal of Geophysical Research* (submitted) for details.

This dataset was received from Jim Elkins of NOAA in 1988.

Data

Each line contains the CO₂ concentration (mixing ratio in dry air, expressed in the WMO X85 mole fraction scale, maintained by the Scripps Institution of Oceanography). In addition, it contains the year, month, and a numeric value for the combined month and year. This combined date is useful for plotting purposes.

CO ₂	Year&Month	Year	Month
333.13	1974.38	1974	5
332.09	1974.46	1974	6
331.10	1974.54	1974	7
329.14	1974.63	1974	8
327.36	1974.71	1974	9
327.29	1974.79	1974	10
328.23	1974.88	1974	11
329.55	1974.96	1974	12
330.62	1975.04	1975	1
331.40	1975.13	1975	2
331.87	1975.21	1975	3

6.4.4.1.1. Data Set of Monthly CO2 Concentrations

333.18	1975.29	1975	4
333.92	1975.38	1975	5
333.43	1975.46	1975	6
331.85	1975.54	1975	7
330.01	1975.63	1975	8
328.51	1975.71	1975	9
328.41	1975.79	1975	10
329.25	1975.88	1975	11
330.97	1975.96	1975	12
331.60	1976.04	1976	1
332.60	1976.13	1976	2
333.57	1976.21	1976	3
334.72	1976.29	1976	4
334.68	1976.38	1976	5
334.17	1976.46	1976	6
332.96	1976.54	1976	7
330.80	1976.63	1976	8
328.98	1976.71	1976	9
328.57	1976.79	1976	10
330.20	1976.88	1976	11
331.58	1976.96	1976	12
332.67	1977.04	1977	1
333.17	1977.13	1977	2
334.86	1977.21	1977	3
336.07	1977.29	1977	4
336.82	1977.38	1977	5
336.12	1977.46	1977	6
334.81	1977.54	1977	7
332.56	1977.63	1977	8
331.30	1977.71	1977	9
331.22	1977.79	1977	10
332.37	1977.88	1977	11
333.49	1977.96	1977	12
334.71	1978.04	1978	1
335.23	1978.13	1978	2
336.54	1978.21	1978	3
337.79	1978.29	1978	4
337.95	1978.38	1978	5
338.00	1978.46	1978	6
336.37	1978.54	1978	7
334.47	1978.63	1978	8
332.46	1978.71	1978	9
332.29	1978.79	1978	10

6.4.4.1.1. Data Set of Monthly CO2 Concentrations

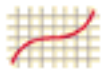
333.76	1978.88	1978	11
334.80	1978.96	1978	12
336.00	1979.04	1979	1
336.63	1979.13	1979	2
337.93	1979.21	1979	3
338.95	1979.29	1979	4
339.05	1979.38	1979	5
339.27	1979.46	1979	6
337.64	1979.54	1979	7
335.68	1979.63	1979	8
333.77	1979.71	1979	9
334.09	1979.79	1979	10
335.29	1979.88	1979	11
336.76	1979.96	1979	12
337.77	1980.04	1980	1
338.26	1980.13	1980	2
340.10	1980.21	1980	3
340.88	1980.29	1980	4
341.47	1980.38	1980	5
341.31	1980.46	1980	6
339.41	1980.54	1980	7
337.74	1980.63	1980	8
336.07	1980.71	1980	9
336.07	1980.79	1980	10
337.22	1980.88	1980	11
338.38	1980.96	1980	12
339.32	1981.04	1981	1
340.41	1981.13	1981	2
341.69	1981.21	1981	3
342.51	1981.29	1981	4
343.02	1981.38	1981	5
342.54	1981.46	1981	6
340.88	1981.54	1981	7
338.75	1981.63	1981	8
337.05	1981.71	1981	9
337.13	1981.79	1981	10
338.45	1981.88	1981	11
339.85	1981.96	1981	12
340.90	1982.04	1982	1
341.70	1982.13	1982	2
342.70	1982.21	1982	3
343.65	1982.29	1982	4

6.4.4.1.1. Data Set of Monthly CO2 Concentrations

344.28	1982.38	1982	5
343.42	1982.46	1982	6
342.02	1982.54	1982	7
339.97	1982.63	1982	8
337.84	1982.71	1982	9
338.00	1982.79	1982	10
339.20	1982.88	1982	11
340.63	1982.96	1982	12
341.41	1983.04	1983	1
342.68	1983.13	1983	2
343.04	1983.21	1983	3
345.27	1983.29	1983	4
345.92	1983.38	1983	5
345.40	1983.46	1983	6
344.16	1983.54	1983	7
342.11	1983.63	1983	8
340.11	1983.71	1983	9
340.15	1983.79	1983	10
341.38	1983.88	1983	11
343.02	1983.96	1983	12
343.87	1984.04	1984	1
344.59	1984.13	1984	2
345.11	1984.21	1984	3
347.07	1984.29	1984	4
347.38	1984.38	1984	5
346.78	1984.46	1984	6
344.96	1984.54	1984	7
342.71	1984.63	1984	8
340.86	1984.71	1984	9
341.13	1984.79	1984	10
342.84	1984.88	1984	11
344.32	1984.96	1984	12
344.88	1985.04	1985	1
345.62	1985.13	1985	2
347.23	1985.21	1985	3
347.62	1985.29	1985	4
348.53	1985.38	1985	5
347.87	1985.46	1985	6
346.00	1985.54	1985	7
343.86	1985.63	1985	8
342.55	1985.71	1985	9
342.57	1985.79	1985	10
344.11	1985.88	1985	11

6.4.4.1.1. Data Set of Monthly CO2 Concentrations

345.49	1985.96	1985	12
346.04	1986.04	1986	1
346.70	1986.13	1986	2
347.38	1986.21	1986	3
349.38	1986.29	1986	4
349.93	1986.38	1986	5
349.26	1986.46	1986	6
347.44	1986.54	1986	7
345.55	1986.63	1986	8
344.21	1986.71	1986	9
343.67	1986.79	1986	10
345.09	1986.88	1986	11
346.27	1986.96	1986	12
347.33	1987.04	1987	1
347.82	1987.13	1987	2
349.29	1987.21	1987	3
350.91	1987.29	1987	4
351.71	1987.38	1987	5
350.94	1987.46	1987	6
349.10	1987.54	1987	7
346.77	1987.63	1987	8
345.73	1987.71	1987	9



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6.4.4.1. [Sample Data Sets](#)

6.4.4.1.2. Data Set of Southern Oscillations

Source and Background

The southern oscillation is defined as the barometric pressure difference between Tahiti and the Darwin Islands at sea level. The southern oscillation is a predictor of el nino which in turn is thought to be a driver of world-wide weather. Specifically, repeated southern oscillation values less than -1 typically defines an el nino. Note: the decimal values in the second column of the data given below are obtained as (month number - 0.5)/12.

Data

Southern

Oscillation	Year + fraction	Year	Month

-0.7	1955.04	1955	1
1.3	1955.13	1955	2
0.1	1955.21	1955	3
-0.9	1955.29	1955	4
0.8	1955.38	1955	5
1.6	1955.46	1955	6
1.7	1955.54	1955	7
1.4	1955.63	1955	8
1.4	1955.71	1955	9
1.5	1955.79	1955	10
1.4	1955.88	1955	11
0.9	1955.96	1955	12
1.2	1956.04	1956	1
1.1	1956.13	1956	2
0.9	1956.21	1956	3
1.1	1956.29	1956	4
1.4	1956.38	1956	5
1.2	1956.46	1956	6

6.4.4.1.2. Data Set of Southern Oscillations

1.1	1956.54	1956	7
1.0	1956.63	1956	8
0.0	1956.71	1956	9
1.9	1956.79	1956	10
0.1	1956.88	1956	11
0.9	1956.96	1956	12
0.4	1957.04	1957	1
-0.4	1957.13	1957	2
-0.4	1957.21	1957	3
0.0	1957.29	1957	4
-1.1	1957.38	1957	5
-0.4	1957.46	1957	6
0.1	1957.54	1957	7
-1.1	1957.63	1957	8
-1.0	1957.71	1957	9
-0.1	1957.79	1957	10
-1.2	1957.88	1957	11
-0.5	1957.96	1957	12
-1.9	1958.04	1958	1
-0.7	1958.13	1958	2
-0.3	1958.21	1958	3
0.1	1958.29	1958	4
-1.3	1958.38	1958	5
-0.3	1958.46	1958	6
0.3	1958.54	1958	7
0.7	1958.63	1958	8
-0.4	1958.71	1958	9
-0.4	1958.79	1958	10
-0.6	1958.88	1958	11
-0.8	1958.96	1958	12
-0.9	1959.04	1959	1
-1.5	1959.13	1959	2
0.8	1959.21	1959	3
0.2	1959.29	1959	4
0.2	1959.38	1959	5
-0.9	1959.46	1959	6
-0.5	1959.54	1959	7
-0.6	1959.63	1959	8
0.0	1959.71	1959	9
0.3	1959.79	1959	10
0.9	1959.88	1959	11
0.8	1959.96	1959	12

6.4.4.1.2. Data Set of Southern Oscillations

0.0	1960.04	1960	1
-0.2	1960.13	1960	2
0.5	1960.21	1960	3
0.9	1960.29	1960	4
0.2	1960.38	1960	5
-0.5	1960.46	1960	6
0.4	1960.54	1960	7
0.5	1960.63	1960	8
0.7	1960.71	1960	9
-0.1	1960.79	1960	10
0.6	1960.88	1960	11
0.7	1960.96	1960	12
-0.4	1961.04	1961	1
0.5	1961.13	1961	2
-2.6	1961.21	1961	3
1.1	1961.29	1961	4
0.2	1961.38	1961	5
-0.4	1961.46	1961	6
0.1	1961.54	1961	7
-0.3	1961.63	1961	8
0.0	1961.71	1961	9
-0.8	1961.79	1961	10
0.7	1961.88	1961	11
1.4	1961.96	1961	12
1.7	1962.04	1962	1
-0.5	1962.13	1962	2
-0.4	1962.21	1962	3
0.0	1962.29	1962	4
1.2	1962.38	1962	5
0.5	1962.46	1962	6
-0.1	1962.54	1962	7
0.3	1962.63	1962	8
0.5	1962.71	1962	9
0.9	1962.79	1962	10
0.2	1962.88	1962	11
0.0	1962.96	1962	12
0.8	1963.04	1963	1
0.3	1963.13	1963	2
0.6	1963.21	1963	3
0.9	1963.29	1963	4
0.0	1963.38	1963	5
-1.5	1963.46	1963	6
-0.3	1963.54	1963	7

6.4.4.1.2. Data Set of Southern Oscillations

-0.4	1963.63	1963	8
-0.7	1963.71	1963	9
-1.6	1963.79	1963	10
-1.0	1963.88	1963	11
-1.4	1963.96	1963	12
-0.5	1964.04	1964	1
-0.2	1964.13	1964	2
0.6	1964.21	1964	3
1.7	1964.29	1964	4
-0.2	1964.38	1964	5
0.7	1964.46	1964	6
0.5	1964.54	1964	7
1.4	1964.63	1964	8
1.3	1964.71	1964	9
1.3	1964.79	1964	10
0.0	1964.88	1964	11
-0.5	1964.96	1964	12
-0.5	1965.04	1965	1
0.0	1965.13	1965	2
0.2	1965.21	1965	3
-1.1	1965.29	1965	4
0.0	1965.38	1965	5
-1.5	1965.46	1965	6
-2.3	1965.54	1965	7
-1.3	1965.63	1965	8
-1.4	1965.71	1965	9
-1.2	1965.79	1965	10
-1.8	1965.88	1965	11
0.0	1965.96	1965	12
-1.4	1966.04	1966	1
-0.5	1966.13	1966	2
-1.6	1966.21	1966	3
-0.7	1966.29	1966	4
-0.6	1966.38	1966	5
0.0	1966.46	1966	6
-0.1	1966.54	1966	7
0.3	1966.63	1966	8
-0.3	1966.71	1966	9
-0.3	1966.79	1966	10
-0.1	1966.88	1966	11
-0.5	1966.96	1966	12
1.5	1967.04	1967	1

6.4.4.1.2. Data Set of Southern Oscillations

1.2	1967.13	1967	2
0.8	1967.21	1967	3
-0.2	1967.29	1967	4
-0.4	1967.38	1967	5
0.6	1967.46	1967	6
0.0	1967.54	1967	7
0.4	1967.63	1967	8
0.5	1967.71	1967	9
-0.2	1967.79	1967	10
-0.7	1967.88	1967	11
-0.7	1967.96	1967	12
0.5	1968.04	1968	1
0.8	1968.13	1968	2
-0.5	1968.21	1968	3
-0.3	1968.29	1968	4
1.2	1968.38	1968	5
1.4	1968.46	1968	6
0.6	1968.54	1968	7
-0.1	1968.63	1968	8
-0.3	1968.71	1968	9
-0.3	1968.79	1968	10
-0.4	1968.88	1968	11
0.0	1968.96	1968	12
-1.4	1969.04	1969	1
0.8	1969.13	1969	2
-0.1	1969.21	1969	3
-0.8	1969.29	1969	4
-0.8	1969.38	1969	5
-0.2	1969.46	1969	6
-0.7	1969.54	1969	7
-0.6	1969.63	1969	8
-1.0	1969.71	1969	9
-1.4	1969.79	1969	10
-0.1	1969.88	1969	11
0.3	1969.96	1969	12
-1.2	1970.04	1970	1
-1.2	1970.13	1970	2
0.0	1970.21	1970	3
-0.5	1970.29	1970	4
0.1	1970.38	1970	5
1.1	1970.46	1970	6
-0.6	1970.54	1970	7
0.3	1970.63	1970	8

6.4.4.1.2. Data Set of Southern Oscillations

1.2	1970.71	1970	9
0.8	1970.79	1970	10
1.8	1970.88	1970	11
1.8	1970.96	1970	12
0.2	1971.04	1971	1
1.4	1971.13	1971	2
2.0	1971.21	1971	3
2.6	1971.29	1971	4
0.9	1971.38	1971	5
0.2	1971.46	1971	6
0.1	1971.54	1971	7
1.4	1971.63	1971	8
1.5	1971.71	1971	9
1.8	1971.79	1971	10
0.5	1971.88	1971	11
0.1	1971.96	1971	12
0.3	1972.04	1972	1
0.6	1972.13	1972	2
0.1	1972.21	1972	3
-0.5	1972.29	1972	4
-2.1	1972.38	1972	5
-1.7	1972.46	1972	6
-1.9	1972.54	1972	7
-1.1	1972.63	1972	8
-1.5	1972.71	1972	9
-1.1	1972.79	1972	10
-0.4	1972.88	1972	11
-1.5	1972.96	1972	12
-0.4	1973.04	1973	1
-1.5	1973.13	1973	2
0.2	1973.21	1973	3
-0.4	1973.29	1973	4
0.3	1973.38	1973	5
1.2	1973.46	1973	6
0.5	1973.54	1973	7
1.2	1973.63	1973	8
1.3	1973.71	1973	9
0.6	1973.79	1973	10
2.9	1973.88	1973	11
1.7	1973.96	1973	12
2.2	1974.04	1974	1
1.5	1974.13	1974	2

6.4.4.1.2. Data Set of Southern Oscillations

2.1	1974.21	1974	3
1.3	1974.29	1974	4
1.3	1974.38	1974	5
0.1	1974.46	1974	6
1.2	1974.54	1974	7
0.5	1974.63	1974	8
1.1	1974.71	1974	9
0.8	1974.79	1974	10
-0.4	1974.88	1974	11
0.0	1974.96	1974	12
-0.6	1975.04	1975	1
0.4	1975.13	1975	2
1.1	1975.21	1975	3
1.5	1975.29	1975	4
0.5	1975.38	1975	5
1.7	1975.46	1975	6
2.1	1975.54	1975	7
2.0	1975.63	1975	8
2.2	1975.71	1975	9
1.7	1975.79	1975	10
1.3	1975.88	1975	11
2.0	1975.96	1975	12
1.2	1976.04	1976	1
1.2	1976.13	1976	2
1.3	1976.21	1976	3
0.2	1976.29	1976	4
0.6	1976.38	1976	5
-0.1	1976.46	1976	6
-1.2	1976.54	1976	7
-1.5	1976.63	1976	8
-1.2	1976.71	1976	9
0.2	1976.79	1976	10
0.7	1976.88	1976	11
-0.5	1976.96	1976	12
-0.5	1977.04	1977	1
0.8	1977.13	1977	2
-1.2	1977.21	1977	3
-1.3	1977.29	1977	4
-1.1	1977.38	1977	5
-2.3	1977.46	1977	6
-1.5	1977.54	1977	7
-1.4	1977.63	1977	8
-0.9	1977.71	1977	9

6.4.4.1.2. Data Set of Southern Oscillations

-1.4	1977.79	1977	10
-1.6	1977.88	1977	11
-1.3	1977.96	1977	12
-0.5	1978.04	1978	1
-2.6	1978.13	1978	2
-0.8	1978.21	1978	3
-0.9	1978.29	1978	4
1.3	1978.38	1978	5
0.4	1978.46	1978	6
0.4	1978.54	1978	7
0.1	1978.63	1978	8
0.0	1978.71	1978	9
-0.8	1978.79	1978	10
-0.1	1978.88	1978	11
-0.2	1978.96	1978	12
-0.5	1979.04	1979	1
0.6	1979.13	1979	2
-0.5	1979.21	1979	3
-0.7	1979.29	1979	4
0.5	1979.38	1979	5
0.6	1979.46	1979	6
1.3	1979.54	1979	7
-0.7	1979.63	1979	8
0.1	1979.71	1979	9
-0.4	1979.79	1979	10
-0.6	1979.88	1979	11
-0.9	1979.96	1979	12
0.3	1980.04	1980	1
0.0	1980.13	1980	2
-1.1	1980.21	1980	3
-1.7	1980.29	1980	4
-0.3	1980.38	1980	5
-0.7	1980.46	1980	6
-0.2	1980.54	1980	7
-0.1	1980.63	1980	8
-0.5	1980.71	1980	9
-0.3	1980.79	1980	10
-0.5	1980.88	1980	11
-0.2	1980.96	1980	12
0.3	1981.04	1981	1
-0.5	1981.13	1981	2
-2.0	1981.21	1981	3

6.4.4.1.2. Data Set of Southern Oscillations

-0.6	1981.29	1981	4
0.8	1981.38	1981	5
1.6	1981.46	1981	6
0.8	1981.54	1981	7
0.4	1981.63	1981	8
0.3	1981.71	1981	9
-0.7	1981.79	1981	10
0.1	1981.88	1981	11
0.4	1981.96	1981	12
1.0	1982.04	1982	1
0.0	1982.13	1982	2
0.0	1982.21	1982	3
-0.1	1982.29	1982	4
-0.6	1982.38	1982	5
-2.5	1982.46	1982	6
-2.0	1982.54	1982	7
-2.7	1982.63	1982	8
-1.9	1982.71	1982	9
-2.2	1982.79	1982	10
-3.2	1982.88	1982	11
-2.5	1982.96	1982	12
-3.4	1983.04	1983	1
-3.5	1983.13	1983	2
-3.2	1983.21	1983	3
-2.1	1983.29	1983	4
0.9	1983.38	1983	5
-0.5	1983.46	1983	6
-0.9	1983.54	1983	7
-0.4	1983.63	1983	8
0.9	1983.71	1983	9
0.3	1983.79	1983	10
-0.1	1983.88	1983	11
-0.1	1983.96	1983	12
0.0	1984.04	1984	1
0.4	1984.13	1984	2
-0.8	1984.21	1984	3
0.4	1984.29	1984	4
0.0	1984.38	1984	5
-1.2	1984.46	1984	6
0.0	1984.54	1984	7
0.1	1984.63	1984	8
0.1	1984.71	1984	9
-0.6	1984.79	1984	10

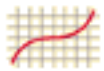
6.4.4.1.2. Data Set of Southern Oscillations

0.3	1984.88	1984	11
-0.3	1984.96	1984	12
-0.5	1985.04	1985	1
0.8	1985.13	1985	2
0.2	1985.21	1985	3
1.4	1985.29	1985	4
-0.2	1985.38	1985	5
-1.4	1985.46	1985	6
-0.3	1985.54	1985	7
0.7	1985.63	1985	8
0.0	1985.71	1985	9
-0.8	1985.79	1985	10
-0.4	1985.88	1985	11
0.1	1985.96	1985	12
0.8	1986.04	1986	1
-1.2	1986.13	1986	2
-0.1	1986.21	1986	3
0.1	1986.29	1986	4
-0.6	1986.38	1986	5
1.0	1986.46	1986	6
0.1	1986.54	1986	7
-0.9	1986.63	1986	8
-0.5	1986.71	1986	9
0.6	1986.79	1986	10
-1.6	1986.88	1986	11
-1.6	1986.96	1986	12
-0.7	1987.04	1987	1
-1.4	1987.13	1987	2
-2.0	1987.21	1987	3
-2.7	1987.29	1987	4
-2.0	1987.38	1987	5
-2.7	1987.46	1987	6
-1.8	1987.54	1987	7
-1.7	1987.63	1987	8
-1.1	1987.71	1987	9
-0.7	1987.79	1987	10
-0.1	1987.88	1987	11
-0.6	1987.96	1987	12
-0.3	1988.04	1988	1
-0.6	1988.13	1988	2
0.1	1988.21	1988	3
0.0	1988.29	1988	4

6.4.4.1.2. Data Set of Southern Oscillations

1.1	1988.38	1988	5
-0.3	1988.46	1988	6
1.1	1988.54	1988	7
1.4	1988.63	1988	8
1.9	1988.71	1988	9
1.5	1988.79	1988	10
1.9	1988.88	1988	11
1.1	1988.96	1988	12
1.5	1989.04	1989	1
1.1	1989.13	1989	2
0.6	1989.21	1989	3
1.6	1989.29	1989	4
1.2	1989.38	1989	5
0.5	1989.46	1989	6
0.8	1989.54	1989	7
-0.8	1989.63	1989	8
0.6	1989.71	1989	9
0.6	1989.79	1989	10
-0.4	1989.88	1989	11
-0.7	1989.96	1989	12
-0.2	1990.04	1990	1
-2.4	1990.13	1990	2
-1.2	1990.21	1990	3
0.0	1990.29	1990	4
1.1	1990.38	1990	5
0.0	1990.46	1990	6
0.5	1990.54	1990	7
-0.5	1990.63	1990	8
-0.8	1990.71	1990	9
0.1	1990.79	1990	10
-0.7	1990.88	1990	11
-0.4	1990.96	1990	12
0.6	1991.04	1991	1
-0.1	1991.13	1991	2
-1.4	1991.21	1991	3
-1.0	1991.29	1991	4
-1.5	1991.38	1991	5
-0.5	1991.46	1991	6
-0.2	1991.54	1991	7
-0.9	1991.63	1991	8
-1.8	1991.71	1991	9
-1.5	1991.79	1991	10
-0.8	1991.88	1991	11

-2.3	1991.96	1991	12
-3.4	1992.04	1992	1
-1.4	1992.13	1992	2
-3.0	1992.21	1992	3
-1.4	1992.29	1992	4
0.0	1992.38	1992	5
-1.2	1992.46	1992	6
-0.8	1992.54	1992	7
0.0	1992.63	1992	8
0.0	1992.71	1992	9
-1.9	1992.79	1992	10
-0.9	1992.88	1992	11
-1.1	1992.96	1992	12



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6.4.4.2. Stationarity

Stationarity

A common assumption in many time series techniques is that the data are stationary.

A stationary process has the property that the mean, variance and autocorrelation structure do not change over time. Stationarity can be defined in precise mathematical terms, but for our purpose we mean a flat looking series, without trend, constant variance over time, a constant autocorrelation structure over time and no periodic fluctuations ([seasonality](#)).

For practical purposes, stationarity can usually be determined from a [run sequence plot](#).

Transformations to Achieve Stationarity

If the time series is not stationary, we can often transform it to stationarity with one of the following techniques.

1. We can difference the data. That is, given the series Z_t , we create the new series

$$Y_i = Z_i - Z_{i-1}$$

The differenced data will contain one less point than the original data. Although you can difference the data more than once, one difference is usually sufficient.

2. If the data contain a trend, we can fit some type of curve to the data and then model the residuals from that fit. Since the purpose of the fit is to simply remove long term trend, a simple fit, such as a straight line, is typically used.
3. For non-constant variance, taking the logarithm or square root of the series may stabilize the variance. For negative data, you can add a suitable constant to make all the data positive before applying the transformation. This constant can then be subtracted from the model to obtain predicted (i.e., the fitted) values and forecasts for future points.

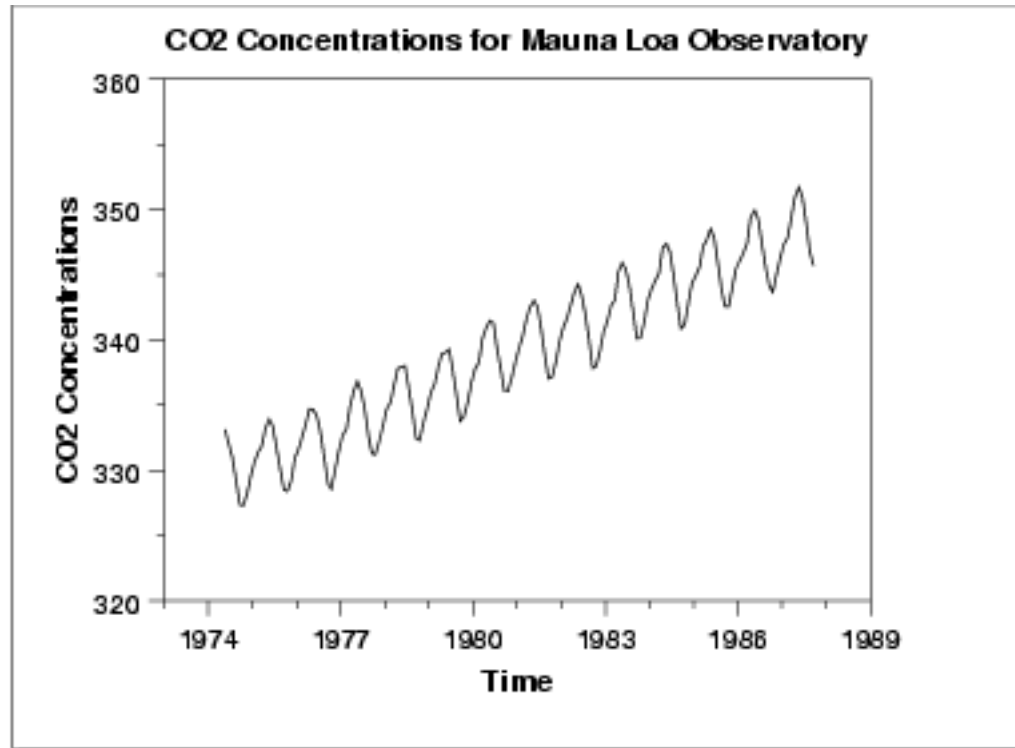
The above techniques are intended to generate series with constant

location and scale. Although seasonality also violates stationarity, this is usually explicitly incorporated into the time series model.

Example

The following plots are from a [data set of monthly CO2 concentrations](#).

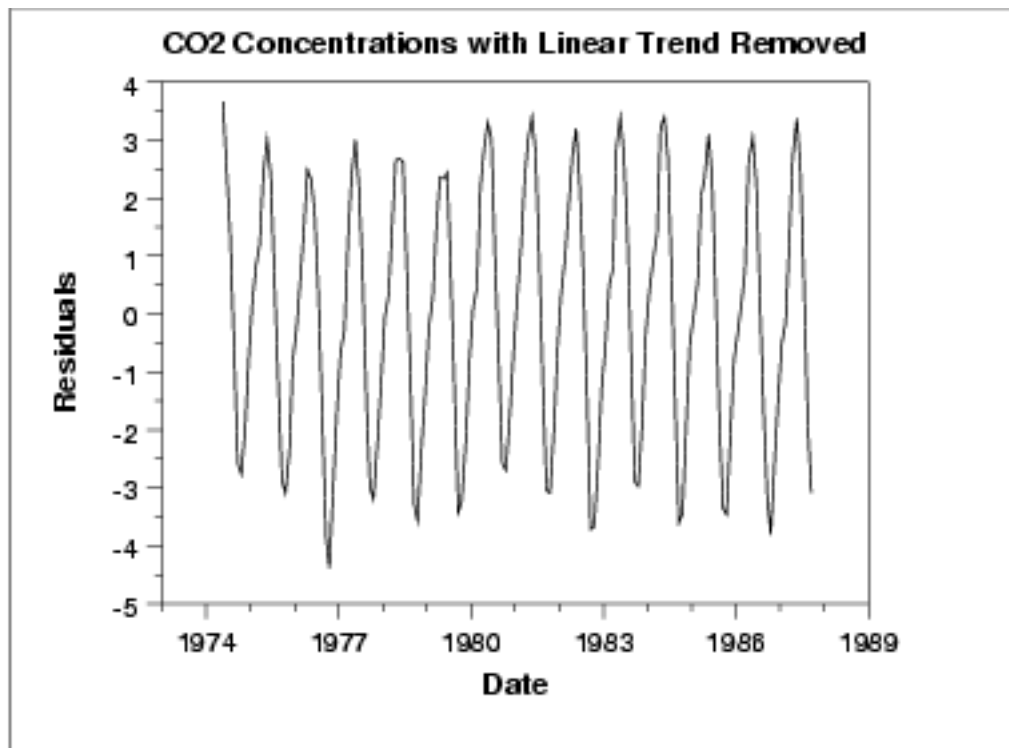
Run Sequence Plot



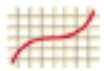
The initial run sequence plot of the data indicates a rising trend. A visual inspection of this plot indicates that a simple linear fit should be sufficient to remove this upward trend.

This plot also shows periodical behavior. This is discussed in the next section.

Linear Trend Removed



This plot contains the residuals from a linear fit to the original data. After removing the linear trend, the run sequence plot indicates that the data have a constant location and variance, although the pattern of the residuals shows that the data depart from the model in a systematic way.



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6.4.4.3. Seasonality

Seasonality

Many time series display seasonality. By seasonality, we mean periodic fluctuations. For example, retail sales tend to peak for the Christmas season and then decline after the holidays. So time series of retail sales will typically show increasing sales from September through December and declining sales in January and February.

Seasonality is quite common in economic time series. It is less common in engineering and scientific data.

If seasonality is present, it must be incorporated into the time series model. In this section, we discuss techniques for detecting seasonality. We defer modeling of seasonality until later sections.

Detecting Seasonality

The following graphical techniques can be used to detect seasonality.

1. A [run sequence plot](#) will often show seasonality.
2. A [seasonal subseries plot](#) is a specialized technique for showing seasonality.
3. Multiple [box plots](#) can be used as an alternative to the seasonal subseries plot to detect seasonality.
4. The [autocorrelation plot](#) can help identify seasonality.

Examples of each of these plots will be shown below.

The run sequence plot is a recommended first step for analyzing any time series. Although seasonality can sometimes be indicated with this plot, seasonality is shown more clearly by the seasonal subseries plot or the box plot. The seasonal subseries plot does an excellent job of showing both the seasonal differences (between group patterns) and also the within-group patterns. The box plot shows the seasonal difference (between group patterns) quite well, but it does not show within group patterns. However, for large data sets, the box plot is usually easier to read than the seasonal subseries plot.

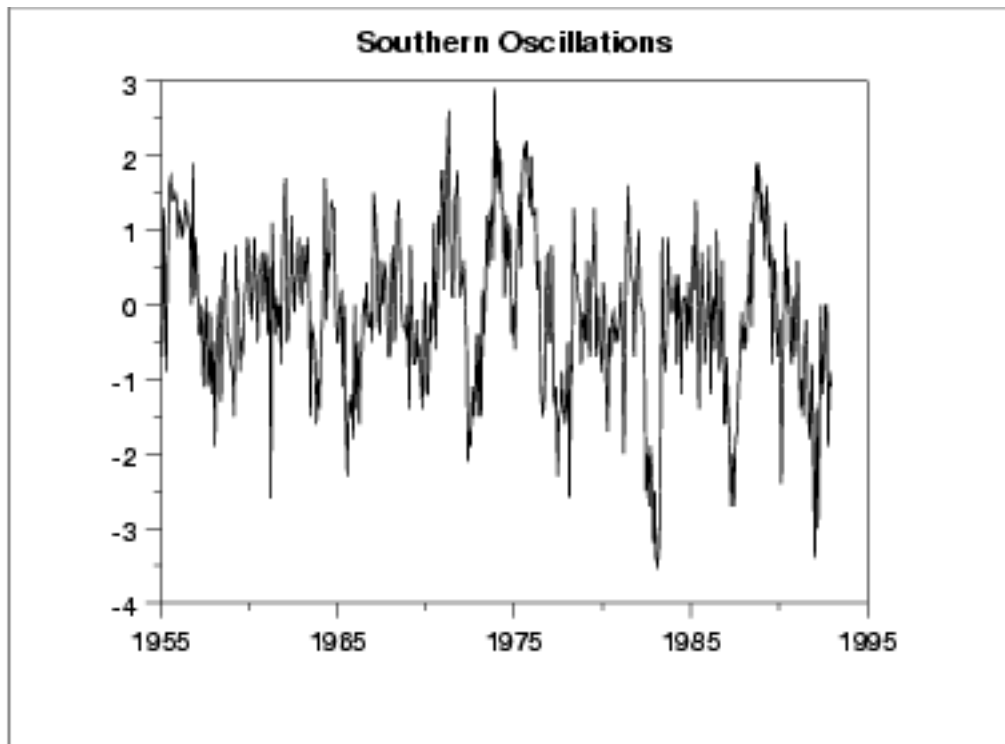
Both the seasonal subseries plot and the box plot assume that the

seasonal periods are known. In most cases, the analyst will in fact know this. For example, for monthly data, the period is 12 since there are 12 months in a year. However, if the period is not known, the autocorrelation plot can help. If there is significant seasonality, the autocorrelation plot should show spikes at lags equal to the period. For example, for monthly data, if there is a seasonality effect, we would expect to see significant peaks at lag 12, 24, 36, and so on (although the intensity may decrease the further out we go).

*Example
without
Seasonality*

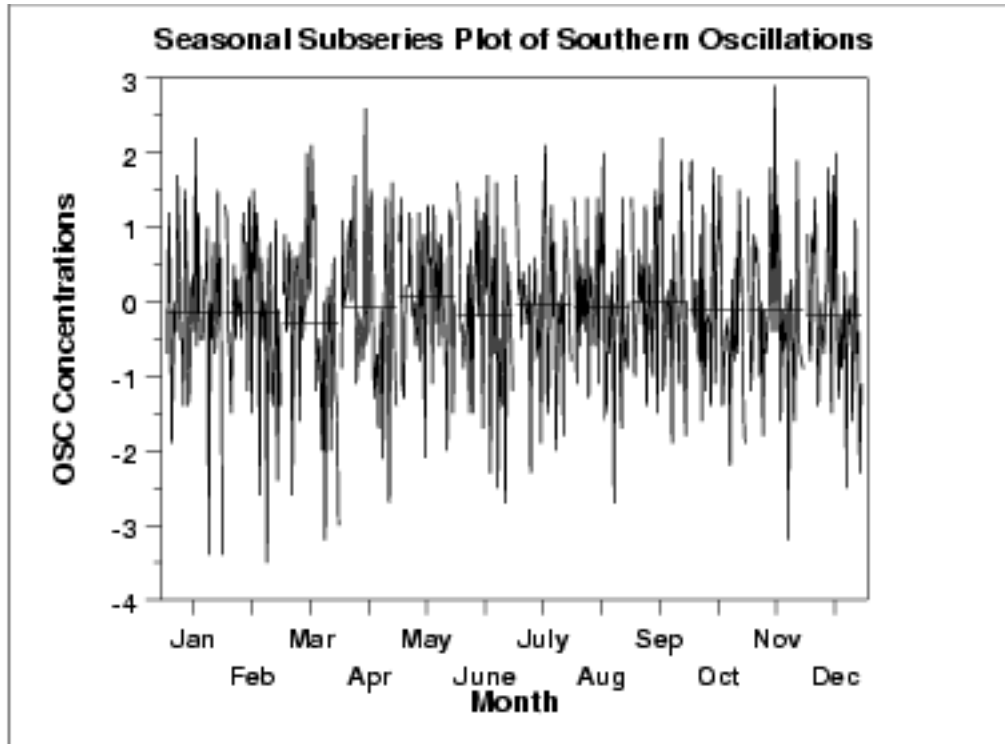
The following plots are from a [data set of southern oscillations](#) for predicting el nino.

*Run
Sequence
Plot*



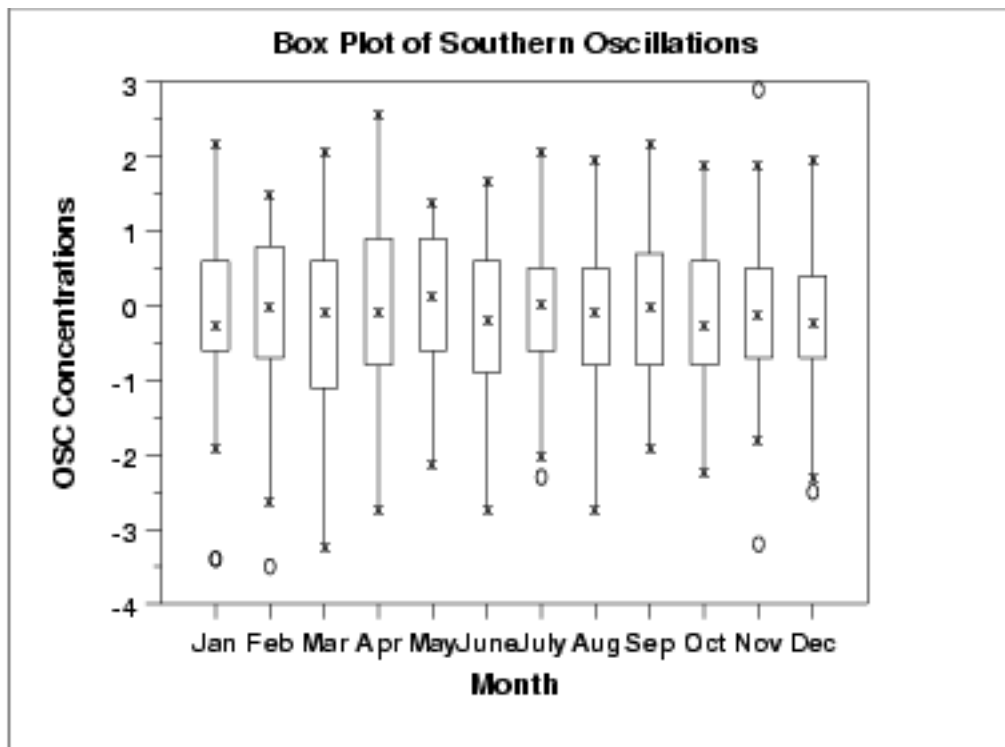
No obvious periodic patterns are apparent in the run sequence plot.

*Seasonal
Subseries
Plot*



The means for each month are relatively close and show no obvious pattern.

Box Plot



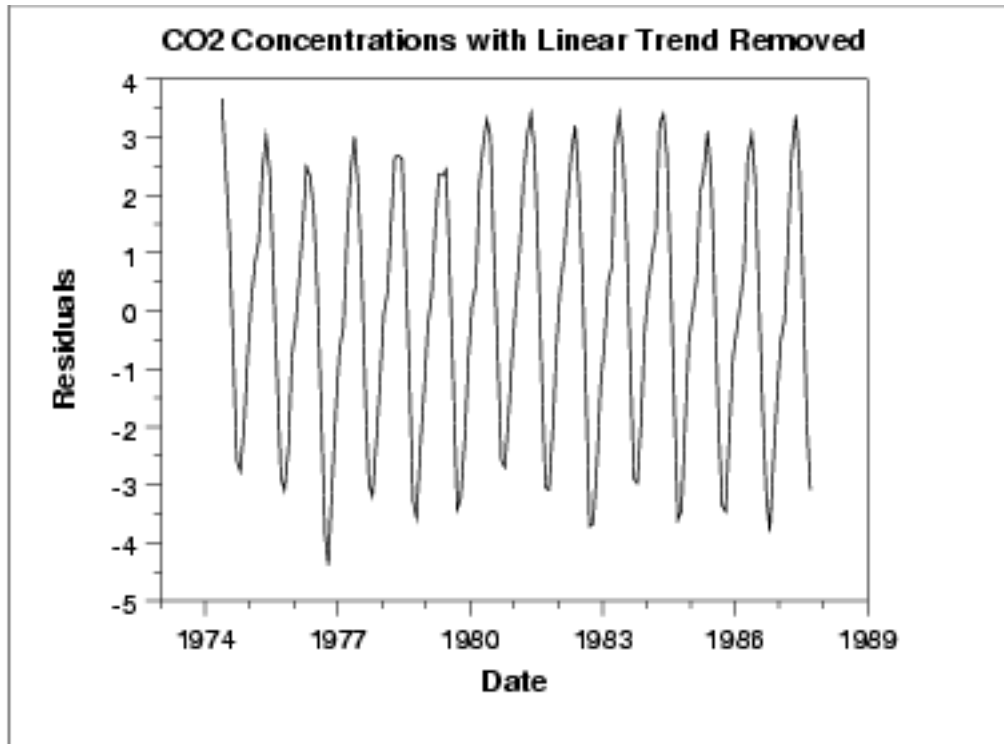
As with the seasonal subseries plot, no obvious seasonal pattern is apparent.

Due to the rather large number of observations, the box plot shows the difference between months better than the seasonal subseries plot.

*Example
with
Seasonality*

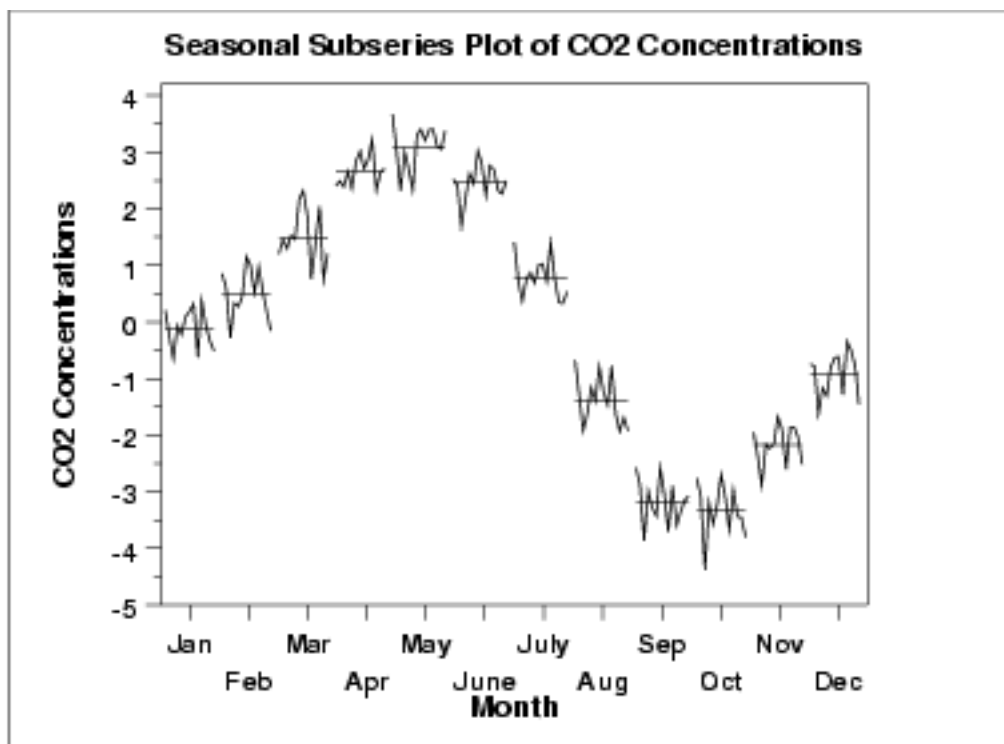
The following plots are from a [data set of monthly CO2 concentrations](#). A [linear trend](#) has been removed from these data.

*Run
Sequence
Plot*



This plot shows periodic behavior. However, it is difficult to determine the nature of the seasonality from this plot.

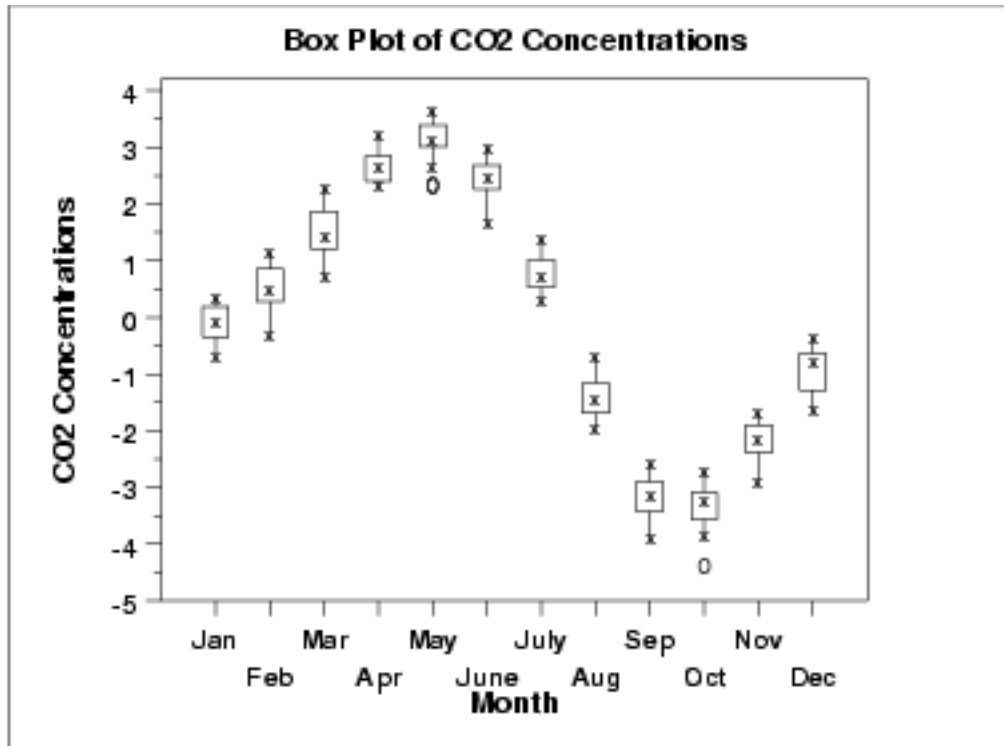
*Seasonal
Subseries
Plot*



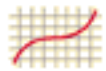
The seasonal subseries plot shows the seasonal pattern more clearly. In

this case, the CO₂ concentrations are at a minimum in September and October. From there, steadily the concentrations increase until June and then begin declining until September.

Box Plot



As with the seasonal subseries plot, the seasonal pattern is quite evident in the box plot.



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6.4.4.3. [Seasonality](#)

6.4.4.3.1. Seasonal Subseries Plot

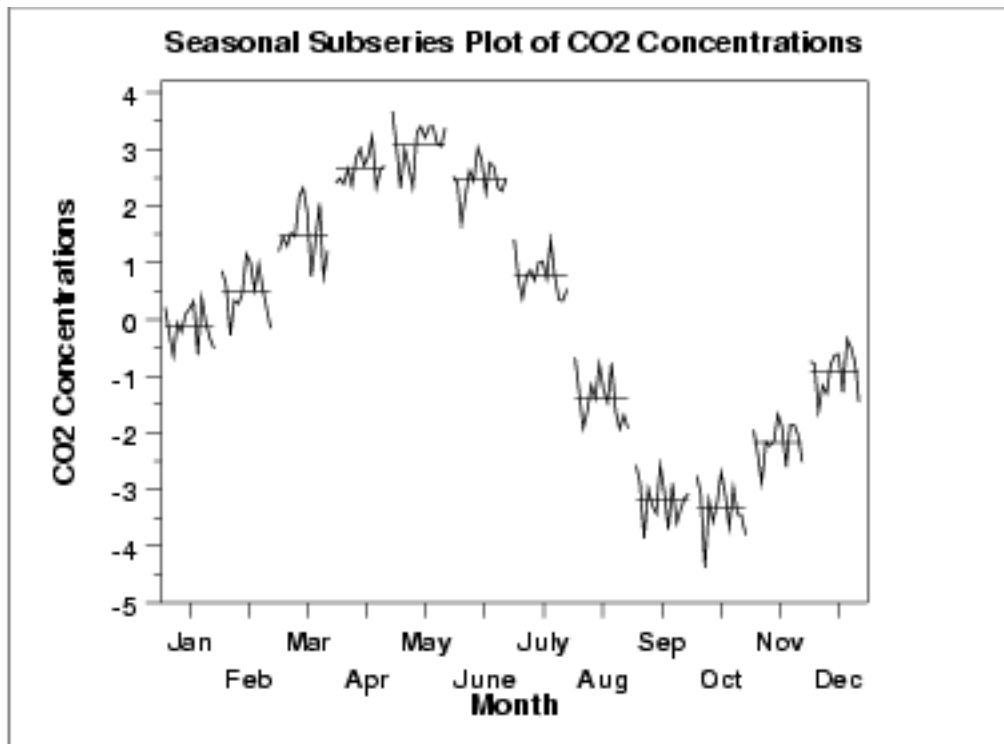
Purpose

Seasonal subseries plots ([Cleveland 1993](#)) are a tool for detecting seasonality in a time series.

This plot is only useful if the period of the seasonality is already known. In many cases, this will in fact be known. For example, monthly data typically has a period of 12.

If the period is not known, an [autocorrelation plot](#) or [spectral plot](#) can be used to determine it.

Sample Plot



This seasonal subseries plot containing monthly data of CO₂ concentrations reveals a strong seasonality pattern. The CO₂ concentrations peak in May, steadily decrease through September, and then begin rising again until the May peak.

This plot allows you to detect both between group and within group patterns.

If there is a large number of observations, then a [box plot](#) may be preferable.

Definition

Seasonal subseries plots are formed by

Vertical axis: Response variable

Horizontal axis: Time ordered by season. For example, with monthly data, all the January values are plotted (in chronological order), then all the February values, and so on.

In addition, a reference line is drawn at the group means.

The user must specify the length of the seasonal pattern before generating this plot. In most cases, the analyst will know this from the context of the problem and data collection.

Questions

The seasonal subseries plot can provide answers to the following questions:

1. Do the data exhibit a seasonal pattern?
2. What is the nature of the seasonality?
3. Is there a within-group pattern (e.g., do January and July exhibit similar patterns)?
4. Are there any outliers once seasonality has been accounted for?

Importance

It is important to know when analyzing a time series if there is a significant seasonality effect. The seasonal subseries plot is an excellent tool for determining if there is a seasonal pattern.

Related Techniques

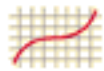
[Box Plot](#)

[Run Sequence Plot](#)

[Autocorrelation Plot](#)

Software

Seasonal subseries plots are available in a few general purpose statistical software programs. They are available in [Dataplot](#). It may possible to write macros to generate this plot in most statistical software programs that do not provide it directly.



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6.4.4.4. Common Approaches to Univariate Time Series

There are a number of approaches to modeling time series. We outline a few of the most common approaches below.

*Trend,
Seasonal,
Residual
Decompositions*

One approach is to decompose the time series into a trend, seasonal, and residual component.

[Triple exponential smoothing](#) is an example of this approach. Another example, called seasonal *loess*, is based on [locally weighted least squares](#) and is discussed by [Cleveland \(1993\)](#). We do not discuss seasonal *loess* in this handbook.

*Frequency
Based Methods*

Another approach, commonly used in scientific and engineering applications, is to analyze the series in the frequency domain. An example of this approach in modeling a sinusoidal type data set is shown in the [beam deflection case study](#). The [spectral plot](#) is the primary tool for the frequency analysis of time series.

Detailed discussions of frequency-based methods are included in [Bloomfield \(1976\)](#), [Jenkins and Watts \(1968\)](#), and [Chatfield \(1996\)](#).

Autoregressive (AR) Models

A common approach for modeling univariate time series is the autoregressive (AR) model:

$$X_t = \delta + \phi_1 X_{t-1} + \phi_2 X_{t-2} + \dots + \phi_p X_{t-p} + A_t$$

where X_t is the time series, A_t is white noise, and

$$\delta = \left(1 - \sum_{i=1}^p \phi_i\right) \mu$$

with μ denoting the process mean.

An autoregressive model is simply a [linear regression](#) of the current value of the series against one or more prior values of the series. The value of p is called the order of the AR model.

AR models can be analyzed with one of various methods, including [standard linear least squares techniques](#). They also have a straightforward interpretation.

Moving Average (MA) Models

Another common approach for modeling univariate time series models is the moving average (MA) model:

$$X_t = \mu + A_t - \theta_1 A_{t-1} - \theta_2 A_{t-2} - \dots - \theta_q A_{t-q}$$

where X_t is the time series, μ is the mean of the series, A_{t-i} are white noise, and $\theta_1, \dots, \theta_q$ are the parameters of the model. The value of q is called the order of the MA model.

That is, a moving average model is conceptually a [linear regression](#) of the current value of the series against the white noise or random shocks of one or more prior values of the series. The random shocks at each point are assumed to come from the same distribution, typically a normal distribution, with location at zero and constant scale. The distinction in this model is that these random shocks are propagated to future values of the time series. Fitting the MA estimates is more complicated than with AR models because the error terms are not observable. This means that iterative non-linear fitting procedures need to be used in place of linear least squares. MA models also have a less obvious interpretation than AR models.

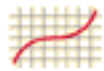
Sometimes the [ACF](#) and [PACF](#) will suggest that a MA model would be a better model choice and sometimes both AR and MA terms should be used in the same model (see [Section 6.4.4.5](#)).

Note, however, that the error terms *after* the model is fit should be independent and follow the standard [assumptions for a univariate process](#).

*Box-Jenkins
Approach*

Box and Jenkins popularized an approach that combines the moving average and the autoregressive approaches in the book "[*Time Series Analysis: Forecasting and Control*](#)" (Box, Jenkins, and Reinsel, 1994).

Although both autoregressive and moving average approaches were already known (and were originally investigated by Yule), the contribution of Box and Jenkins was in developing a systematic methodology for identifying and estimating models that could incorporate both approaches. This makes Box-Jenkins models a powerful class of models. The next several sections will discuss these models in detail.



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6.4.4.5. Box-Jenkins Models

Box-Jenkins Approach

The Box-Jenkins ARMA model is a combination of the [AR](#) and [MA](#) models (described on the [previous page](#)):

$$X_t = \delta + \phi_1 X_{t-1} + \phi_2 X_{t-2} + \dots + \phi_p X_{t-p} + A_t - \theta_1 A_{t-1} - \theta_2 A_{t-2} - \dots - \theta_q A_{t-q}$$

where the terms in the equation have the same meaning as given for the AR and MA model.

Comments

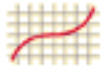
on

Box-Jenkins Model

A couple of notes on this model.

1. The Box-Jenkins model assumes that the time series is [stationary](#). Box and Jenkins recommend differencing non-stationary series one or more times to achieve stationarity. Doing so produces an ARIMA model, with the "I" standing for "Integrated".
2. Some formulations transform the series by subtracting the mean of the series from each data point. This yields a series with a mean of zero. Whether you need to do this or not is dependent on the software you use to estimate the model.
3. Box-Jenkins models can be extended to include [seasonal](#) autoregressive and seasonal moving average terms. Although this complicates the notation and mathematics of the model, the underlying concepts for seasonal autoregressive and seasonal moving average terms are similar to the non-seasonal autoregressive and moving average terms.
4. The most general Box-Jenkins model includes difference operators, autoregressive terms, moving average terms, seasonal difference operators, seasonal autoregressive terms, and seasonal moving average terms. As with modeling in general, however, only necessary terms should be included in the model. Those interested in the mathematical details can consult [Box, Jenkins and Reisel \(1994\)](#), [Chatfield \(1996\)](#), or [Brockwell and Davis \(2002\)](#).

<i>Stages in Box-Jenkins Modeling</i>	<p>There are three primary stages in building a Box-Jenkins time series model.</p> <ol style="list-style-type: none">1. Model Identification2. Model Estimation3. Model Validation
<i>Remarks</i>	<p>The following remarks regarding Box-Jenkins models should be noted.</p> <ol style="list-style-type: none">1. Box-Jenkins models are quite flexible due to the inclusion of both autoregressive and moving average terms.2. Based on the Wold decomposition theorem (not discussed in the Handbook), a stationary process can be approximated by an ARMA model. In practice, finding that approximation may not be easy.3. Chatfield (1996) recommends decomposition methods for series in which the trend and seasonal components are dominant.4. Building good ARIMA models generally requires more experience than commonly used statistical methods such as regression.
<i>Sufficiently Long Series Required</i>	<p>Typically, effective fitting of Box-Jenkins models requires at least a moderately long series. Chatfield (1996) recommends at least 50 observations. Many others would recommend at least 100 observations.</p>



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6.4.4.6. Box-Jenkins Model Identification

Stationarity and Seasonality

The first step in developing a Box-Jenkins model is to determine if the series is [stationary](#) and if there is any significant [seasonality](#) that needs to be modeled.

Detecting stationarity

Stationarity can be assessed from a [run sequence plot](#). The run sequence plot should show constant location and scale. It can also be detected from an [autocorrelation plot](#). Specifically, non-stationarity is often indicated by an autocorrelation plot with very slow decay.

Detecting seasonality

Seasonality (or periodicity) can usually be assessed from an [autocorrelation plot](#), a [seasonal subseries plot](#), or a [spectral plot](#).

Differencing to achieve stationarity

Box and Jenkins recommend the differencing approach to achieve stationarity. However, fitting a curve and subtracting the fitted values from the original data can also be used in the context of Box-Jenkins models.

Seasonal differencing

At the model identification stage, our goal is to detect seasonality, if it exists, and to identify the order for the seasonal autoregressive and seasonal moving average terms. For many series, the period is known and a single seasonality term is sufficient. For example, for monthly data we would typically include either a seasonal AR 12 term or a seasonal MA 12 term. For Box-Jenkins models, we do not explicitly remove seasonality before fitting the model. Instead, we include the order of the seasonal terms in the model specification to the ARIMA estimation software. However, it may be helpful to apply a seasonal difference to the data and regenerate the autocorrelation and partial autocorrelation plots. This may help in the model identification of the non-seasonal component of the model. In some cases, the seasonal differencing may remove most or all of the seasonality effect.

Identify p and q Once stationarity and seasonality have been addressed, the next step is to identify the order (i.e., the p and q) of the autoregressive and moving average terms.

Autocorrelation and Partial Autocorrelation Plots The primary tools for doing this are the [autocorrelation plot](#) and the [partial autocorrelation plot](#). The sample autocorrelation plot and the sample partial autocorrelation plot are compared to the theoretical behavior of these plots when the order is known.

Order of Autoregressive Process (p) Specifically, for an AR(1) process, the sample autocorrelation function should have an exponentially decreasing appearance. However, higher-order AR processes are often a mixture of exponentially decreasing and damped sinusoidal components.

For higher-order autoregressive processes, the sample autocorrelation needs to be supplemented with a partial autocorrelation plot. The partial autocorrelation of an AR(p) process becomes zero at lag $p+1$ and greater, so we examine the sample partial autocorrelation function to see if there is evidence of a departure from zero. This is usually determined by placing a 95% confidence interval on the sample partial autocorrelation plot (most software programs that generate sample autocorrelation plots will also plot this confidence interval). If the software program does not generate the confidence band, it is approximately $\pm 2/\sqrt{N}$, with N denoting the sample size.

Order of Moving Average Process (q) The autocorrelation function of a MA(q) process becomes zero at lag $q+1$ and greater, so we examine the sample autocorrelation function to see where it essentially becomes zero. We do this by placing the 95% confidence interval for the sample autocorrelation function on the sample autocorrelation plot. Most software that can generate the autocorrelation plot can also generate this confidence interval.

The sample partial autocorrelation function is generally not helpful for identifying the order of the moving average process.

Shape of Autocorrelation Function

The following table summarizes how we use the sample autocorrelation function for model identification.

SHAPE	INDICATED MODEL
Exponential, decaying to zero	Autoregressive model. Use the partial autocorrelation plot to identify the order of the autoregressive model.
Alternating positive and negative, decaying to zero	Autoregressive model. Use the partial autocorrelation plot to help identify the order.
One or more spikes, rest are essentially zero	Moving average model, order identified by where plot becomes zero.
Decay, starting after a few lags	Mixed autoregressive and moving average model.
All zero or close to zero	Data is essentially random.
High values at fixed intervals	Include seasonal autoregressive term.
No decay to zero	Series is not stationary.

Mixed Models Difficult to Identify

In practice, the sample autocorrelation and partial autocorrelation functions are random variables and will not give the same picture as the theoretical functions. This makes the model identification more difficult. In particular, mixed models can be particularly difficult to identify.

Although experience is helpful, developing good models using these sample plots can involve much trial and error. For this reason, in recent years information-based criteria such as FPE (Final Prediction Error) and AIC (Aikake Information Criterion) and others have been preferred and used. These techniques can help automate the model identification process. These techniques require computer software to use. Fortunately, these techniques are available in many commercial statistical software programs that provide ARIMA modeling capabilities.

For additional information on these techniques, see [Brockwell and Davis \(1987, 2002\)](#).

Examples

We show a typical series of plots for performing the initial model identification for

1. the [southern oscillations](#) data and
2. the [CO₂ monthly concentrations](#) data.

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SEMATECH

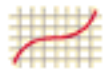
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6.4.4.6. [Box-Jenkins Model Identification](#)

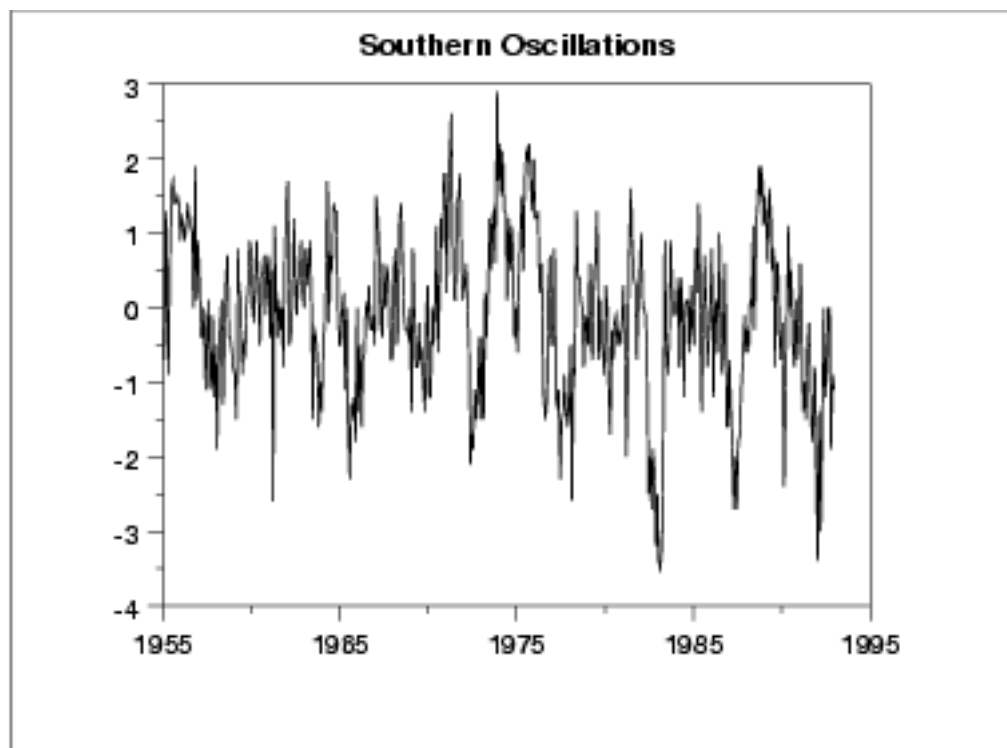
6.4.4.6.1. Model Identification for Southern Oscillations Data

*Example for
Southern
Oscillations*

We show typical series of plots for the initial model identification stages of Box-Jenkins modeling for two different examples.

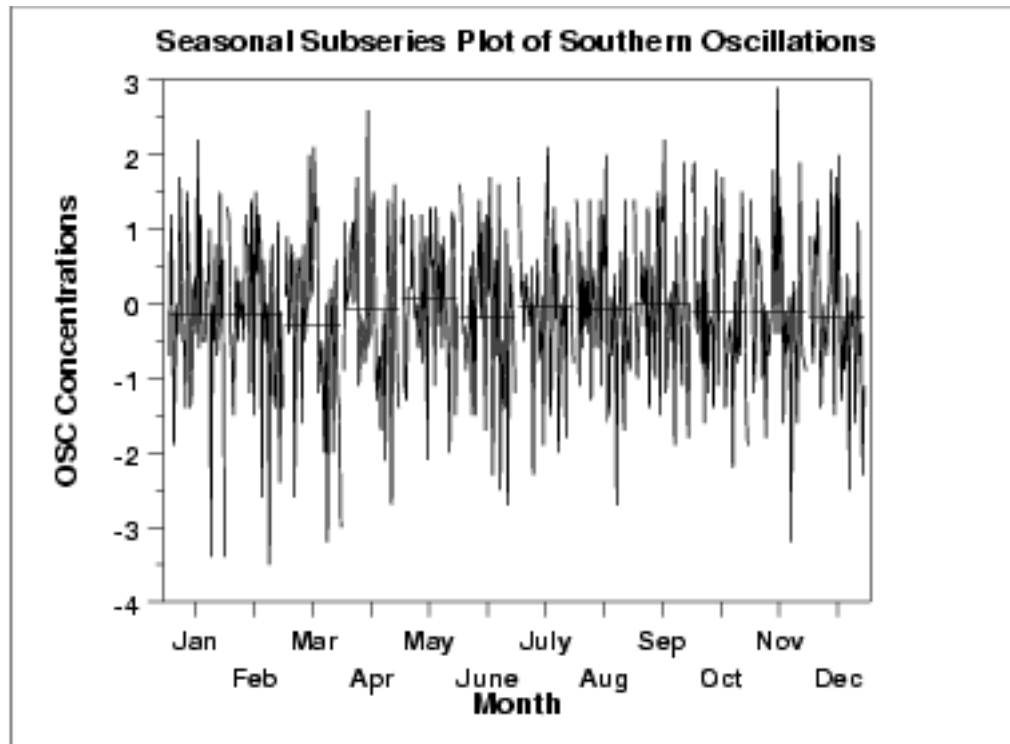
The first example is for the [southern oscillations](#) data set. We start with the run sequence plot and seasonal subseries plot to determine if we need to address stationarity and seasonality.

*Run Sequence
Plot*



The run sequence plot indicates stationarity.

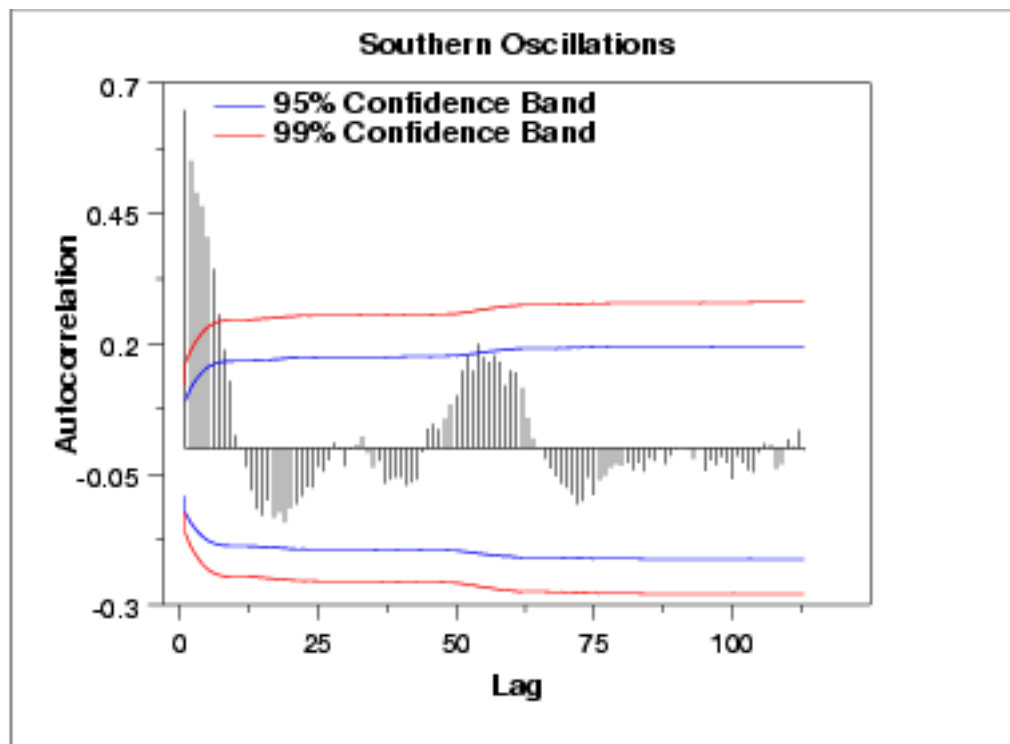
*Seasonal
Subseries Plot*



The seasonal subseries plot indicates that there is no significant seasonality.

Since the above plots show that this series does not exhibit any significant non-stationarity or seasonality, we generate the autocorrelation and partial autocorrelation plots of the raw data.

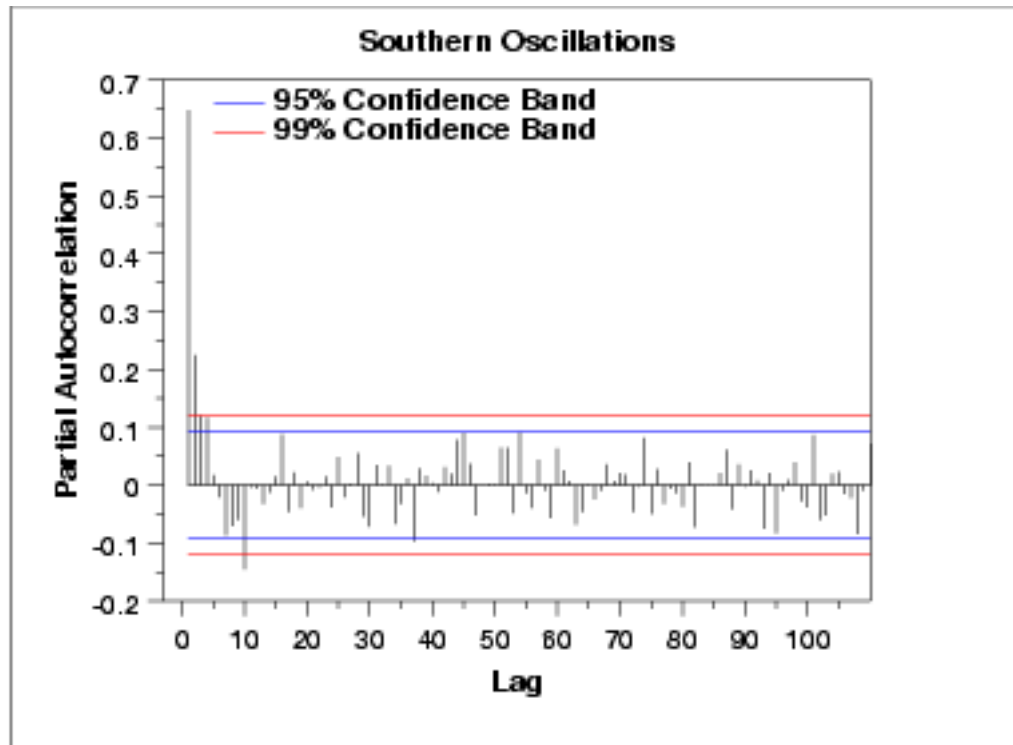
*Autocorrelation
Plot*



The autocorrelation plot shows a mixture of exponentially decaying

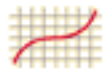
and damped sinusoidal components. This indicates that an autoregressive model, with order greater than one, may be appropriate for these data. The partial autocorrelation plot should be examined to determine the order.

*Partial
Autocorrelation
Plot*



The partial autocorrelation plot suggests that an AR(2) model might be appropriate.

In summary, our initial attempt would be to fit an AR(2) model with no seasonal terms and no differencing or trend removal. Model validation should be performed before accepting this as a final model.



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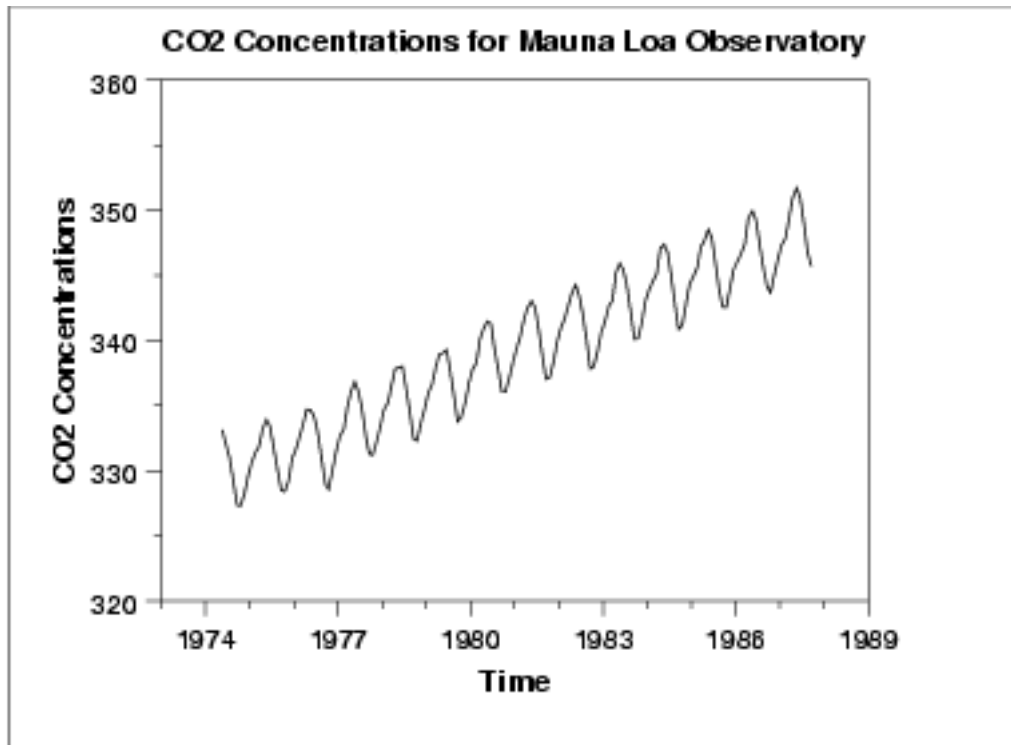
6.4.4.6. [Box-Jenkins Model Identification](#)

6.4.4.6.2. Model Identification for the CO₂ Concentrations Data

*Example for
Monthly CO₂
Concentrations*

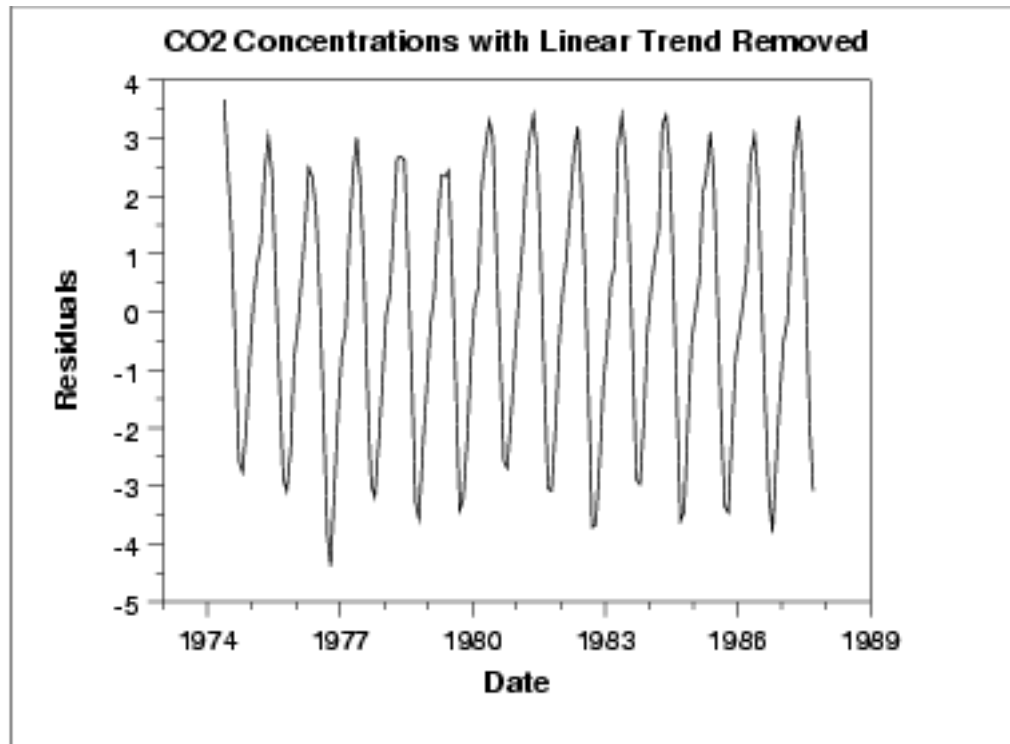
The second example is for the [monthly CO₂ concentrations](#) data set. As before, we start with the run sequence plot to check for stationarity.

*Run Sequence
Plot*



The initial run sequence plot of the data indicates a rising trend. A visual inspection of this plot indicates that a simple linear fit should be sufficient to remove this upward trend.

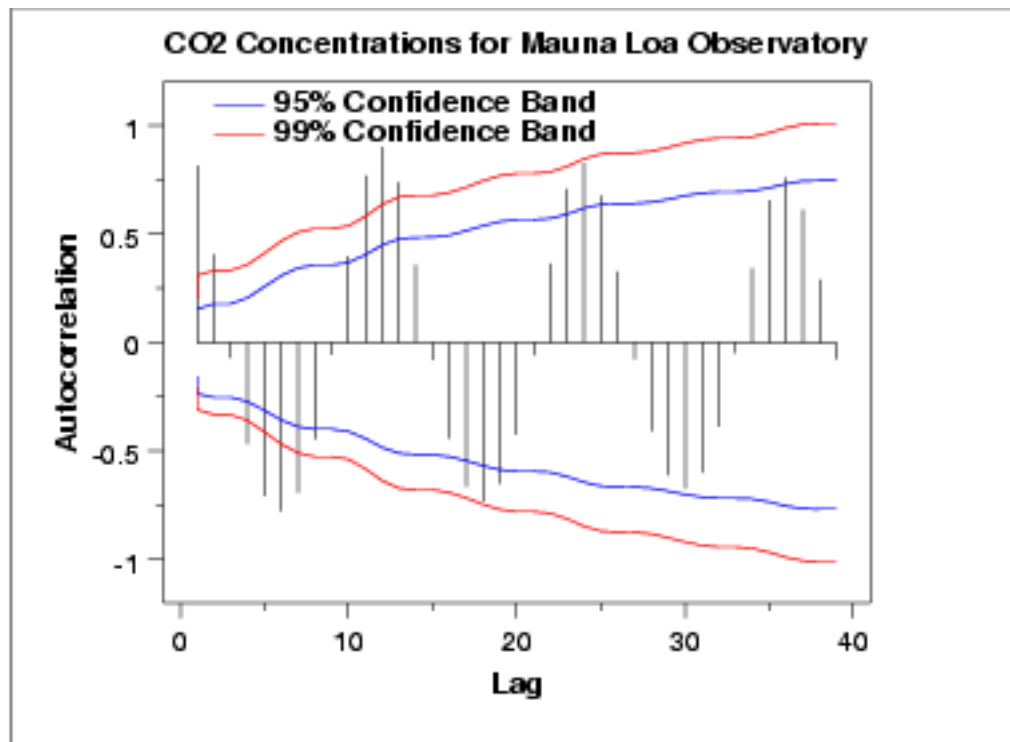
Linear Trend Removed



This plot contains the residuals from a linear fit to the original data. After removing the linear trend, the run sequence plot indicates that the data have a constant location and variance, which implies stationarity.

However, the plot does show seasonality. We generate an autocorrelation plot to help determine the period followed by a seasonal subseries plot.

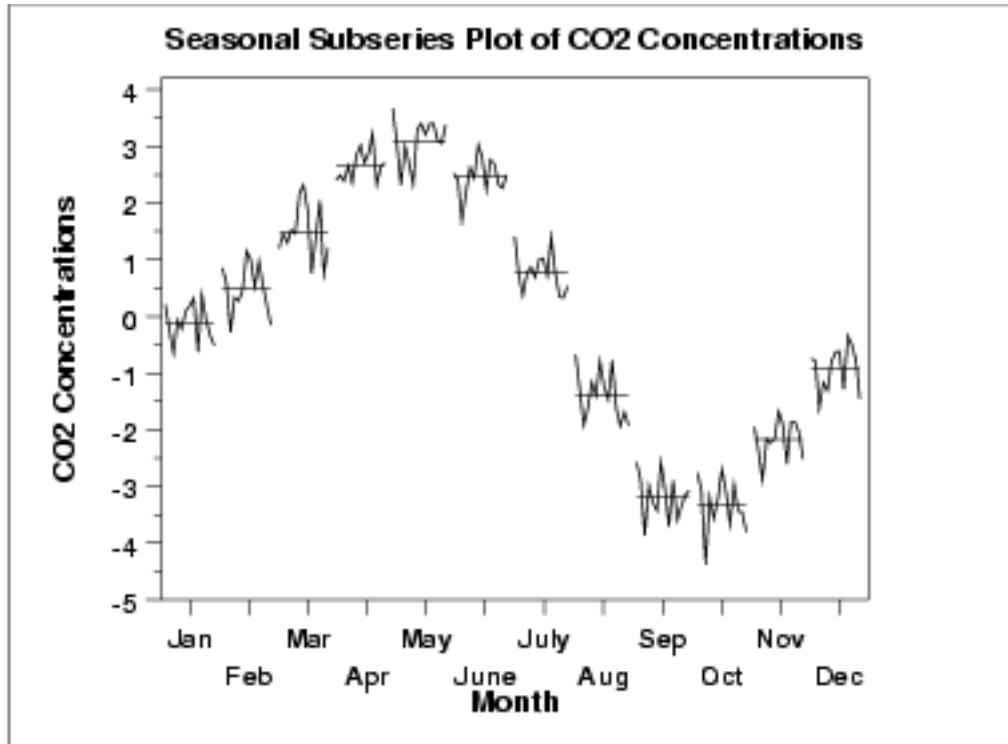
Autocorrelation Plot



The autocorrelation plot shows an alternating pattern of positive and negative spikes. It also shows a repeating pattern every 12 lags, which indicates a seasonality effect.

The two connected lines on the autocorrelation plot are 95% and 99% confidence intervals for statistical significance of the autocorrelations.

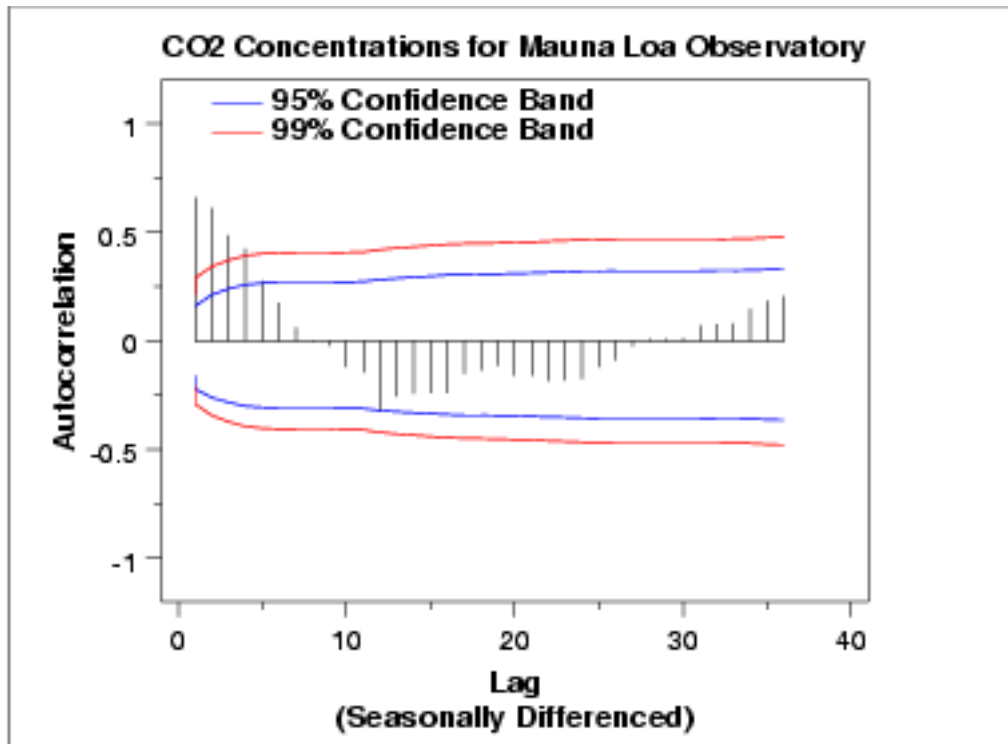
*Seasonal
Subseries Plot*



A significant seasonal pattern is obvious in this plot, so we need to include seasonal terms in fitting a Box-Jenkins model. Since this is monthly data, we would typically include either a lag 12 seasonal autoregressive and/or moving average term.

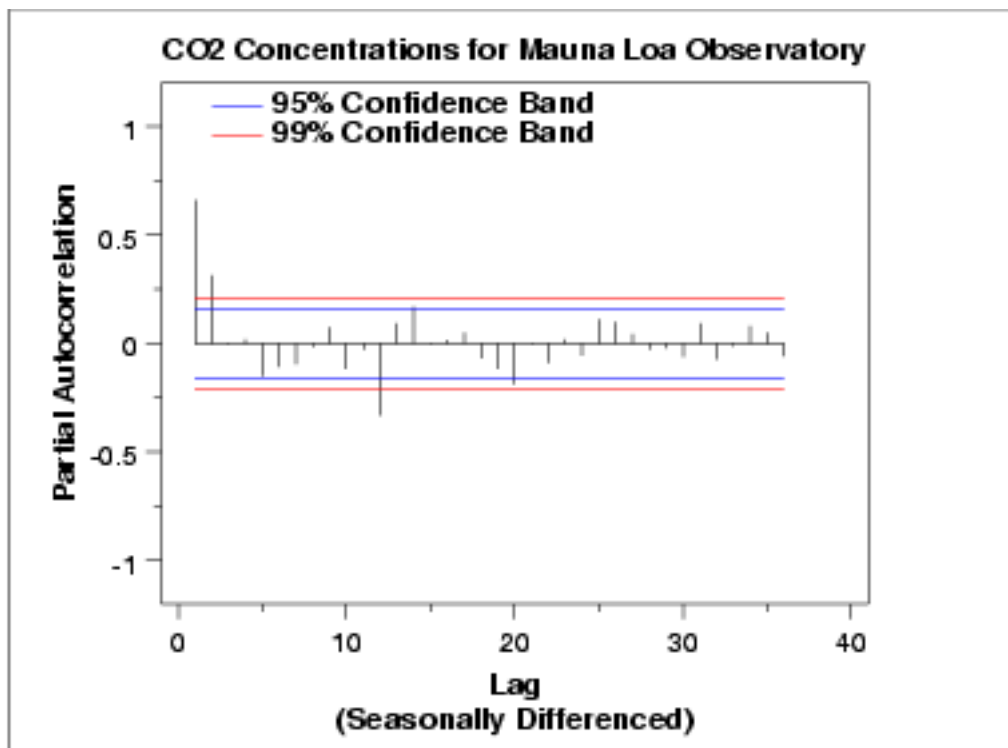
To help identify the non-seasonal components, we will take a seasonal difference of 12 and generate the autocorrelation plot on the seasonally differenced data.

*Autocorrelation
Plot for
Seasonally
Differenced
Data*



This autocorrelation plot shows a mixture of exponential decay and a damped sinusoidal pattern. This indicates that an AR model, with order greater than one, may be appropriate. We generate a partial autocorrelation plot to help identify the order.

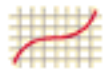
*Partial
Autocorrelation
Plot of
Seasonally
Differenced
Data*



The partial autocorrelation plot suggests that an AR(2) model might be appropriate since the partial autocorrelation becomes zero after the second lag. The lag 12 is also significant, indicating some

remaining seasonality.

In summary, our initial attempt would be to fit an AR(2) model with a seasonal AR(12) term on the data with a linear trend line removed. We could try the model both with and without seasonal differencing applied. Model validation should be performed before accepting this as a final model.



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6.4.4.6. [Box-Jenkins Model Identification](#)

6.4.4.6.3. Partial Autocorrelation Plot

Purpose:
Model
Identification
for
Box-Jenkins
Models

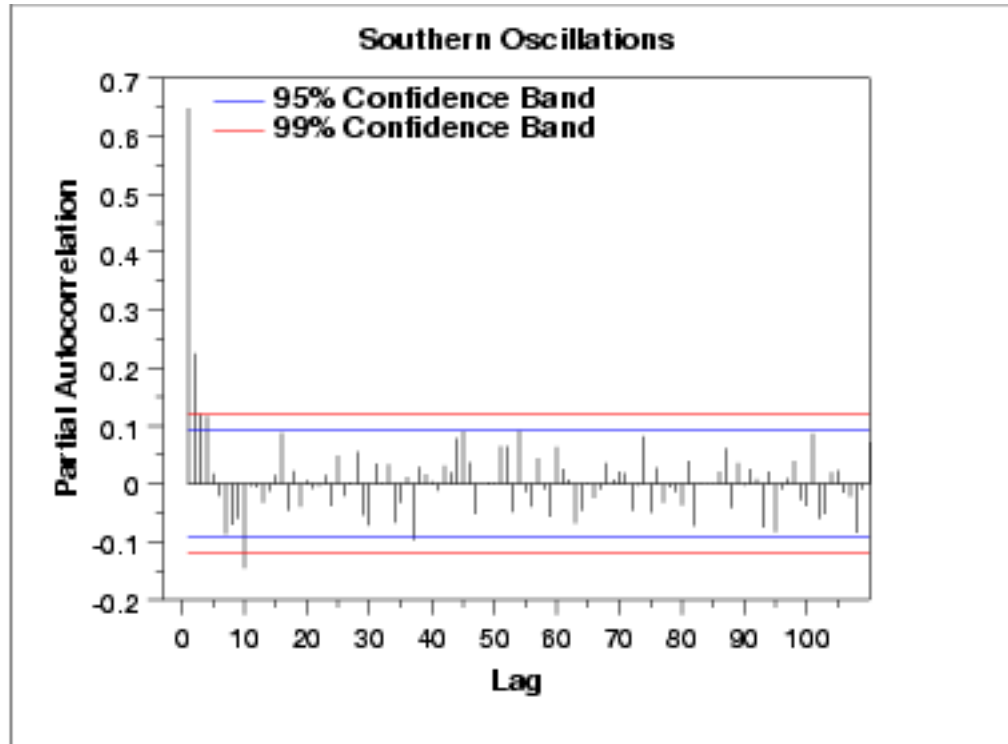
Partial autocorrelation plots ([Box and Jenkins, pp. 64-65, 1970](#)) are a commonly used tool for model identification in Box-Jenkins models.

The partial autocorrelation at lag k is the autocorrelation between X_t and X_{t-k} that is not accounted for by lags 1 through $k-1$.

There are algorithms, not discussed here, for computing the partial autocorrelation based on the sample autocorrelations. See ([Box, Jenkins, and Reinsel 1970](#)) or ([Brockwell, 1991](#)) for the mathematical details.

Specifically, partial autocorrelations are useful in identifying the order of an [autoregressive model](#). The partial autocorrelation of an AR(p) process is zero at lag $p+1$ and greater. If the sample autocorrelation plot indicates that an AR model may be appropriate, then the sample partial autocorrelation plot is examined to help identify the order. We look for the point on the plot where the partial autocorrelations essentially become zero. Placing a 95% confidence interval for statistical significance is helpful for this purpose.

The approximate 95% confidence interval for the partial autocorrelations are at $\pm 2/\sqrt{N}$.

Sample Plot

This partial autocorrelation plot shows clear statistical significance for lags 1 and 2 (lag 0 is always 1). The next few lags are at the borderline of statistical significance. If the autocorrelation plot indicates that an AR model is appropriate, we could start our modeling with an AR(2) model. We might compare this with an AR(3) model.

Definition

Partial autocorrelation plots are formed by

Vertical axis: Partial autocorrelation coefficient at lag h .

Horizontal axis: Time lag h ($h = 0, 1, 2, 3, \dots$).

In addition, 95% confidence interval bands are typically included on the plot.

Questions

The partial autocorrelation plot can help provide answers to the following questions:

1. Is an AR model appropriate for the data?
2. If an AR model is appropriate, what order should we use?

Related Techniques

[Autocorrelation Plot](#)

[Run Sequence Plot](#)

[Spectral Plot](#)

Case Study

The partial autocorrelation plot is demonstrated in the [Negiz data case study](#).

Software

Partial autocorrelation plots are available in many general purpose statistical software programs including [Dataplot](#).

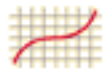


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6.4.4.7. Box-Jenkins Model Estimation

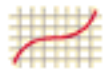
Use Software Estimating the parameters for the Box-Jenkins models is a quite complicated non-linear estimation problem. For this reason, the parameter estimation should be left to a high quality software program that fits Box-Jenkins models. Fortunately, many commercial statistical software programs now fit Box-Jenkins models.

Approaches The main approaches to fitting Box-Jenkins models are [non-linear least squares](#) and maximum likelihood estimation.

Maximum likelihood estimation is generally the preferred technique. The likelihood equations for the full Box-Jenkins model are complicated and are not included here. See ([Brockwell and Davis, 1991](#)) for the mathematical details.

Sample Output for Model Estimation The [Negiz case study](#) shows an example of the Box-Jenkins model-fitting output using the Dataplot software. The two examples later in this section show sample output from the SEMPLOTT software.

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6.4.4.8. Box-Jenkins Model Diagnostics

*Assumptions
for a Stable
Univariate
Process*

Model diagnostics for Box-Jenkins models is similar to model validation for [non-linear least squares fitting](#).

That is, the error term A_t is assumed to follow the [assumptions for a stationary univariate process](#). The residuals should be white noise (or independent when their distributions are normal) drawings from a fixed distribution with a constant mean and variance. If the Box-Jenkins model is a good model for the data, the residuals should satisfy these assumptions.

If these assumptions are not satisfied, we need to fit a more appropriate model. That is, we go back to the model identification step and try to develop a better model. Hopefully the analysis of the residuals can provide some clues as to a more appropriate model.

*4-Plot of
Residuals*

As discussed in the EDA chapter, one way to assess if the residuals from the Box-Jenkins model follow the assumptions is to generate a [4-plot](#) of the residuals and an [autocorrelation plot](#) of the residuals. One could also look at the value of the Box-Ljung ([1978](#)) statistic.

An example of analyzing the residuals from a Box-Jenkins model is given in the [Negiz data case study](#).

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6.4.4. [Univariate Time Series Models](#)

6.4.4.9. Example of Univariate Box-Jenkins Analysis

*Example
with the
SEMPLOT
Software*

A computer software package is needed to do a Box-Jenkins time series analysis. The computer output on this page will illustrate sample output from a Box-Jenkins analysis using the [SEMSTAT](#) statistical software program. It analyzes the series F data set in the Box, Jenkins and Reinsel text.

The [graph](#) of the data and the resulting forecasts after fitting a model are portrayed below.

Output from other software programs will be similar, but not identical.

*Model
Identification
Section*

With the SEMSTAT program, you start by entering a valid file name or you can select a file extension to search for files of particular interest. In this program, if you press the enter key, ALL file names in the directory are displayed.

Enter FILESPEC or EXTENSION (1-3 letters): To quit, press F10.

? bookf.bj

MAX MIN MEAN VARIANCE NO. DATA

80.0000 23.0000 51.7086 141.8238 70

Do you wish to make transformations? y/n n

Input order of difference or 0: 0

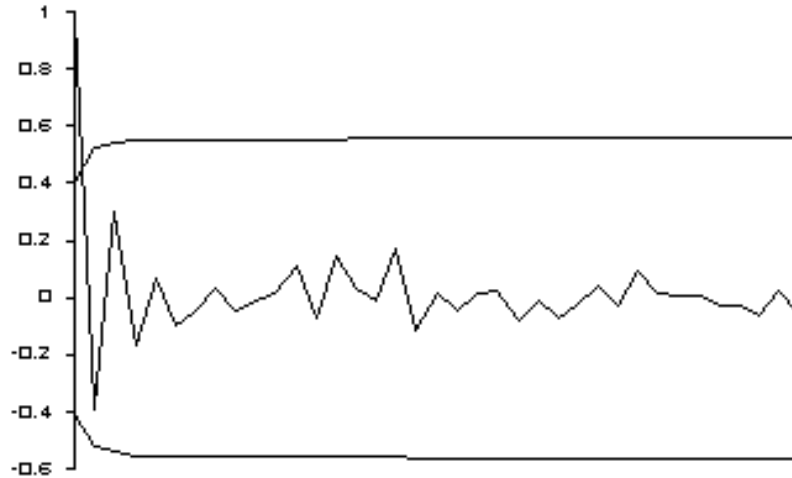
Input period of seasonality (2-12) or 0: 0

Time Series: bookf.bj. Regular difference: 0 Seasonal Difference: 0

Autocorrelation Function for the first 35 lags

0	1.0000	12	-0.0688	24	-0.0731
1	-0.3899	13	0.1480	25	-0.0195
2	0.3044	14	0.0358	26	0.0415
3	-0.1656	15	-0.0067	27	-0.0221
4	0.0707	16	0.1730	28	0.0889
5	-0.0970	17	-0.7013	29	0.0162
6	-0.0471	18	0.0200	30	0.0039
7	0.0354	19	-0.0473	31	0.0046
8	-0.0435	20	0.0161	32	-0.0248
9	-0.0048	21	0.0223	33	-0.0259
10	0.0144	22	-0.0787	34	-0.0629
11	0.1099	23	-0.0096	35	0.0261

Auto Correlation Function
with 95% Confidence Limits



*Model
Fitting
Section*

Enter FILESPEC or EXTENSION (1-3 letters): To quit, press F10.

? bookf.bj

MAX MIN MEAN VARIANCE NO. DATA

80.0000 23.0000 51.7086 141.8238 70

Do you wish to make transformations? y/n n

Input order of difference or 0: 0

Input NUMBER of AR terms: 2

Input NUMBER of MA terms: 0

Input period of seasonality (2-12) or 0: 0

***** OUTPUT SECTION *****

AR estimates with Standard Errors

Phi 1 : -0.3397 0.1224

Phi 2 : 0.1904 0.1223

Original Variance : 141.8238

Residual Variance : 110.8236

Coefficient of Determination: 21.8582

***** Test on randomness of Residuals *****

The Chi-Square value = 11.7034

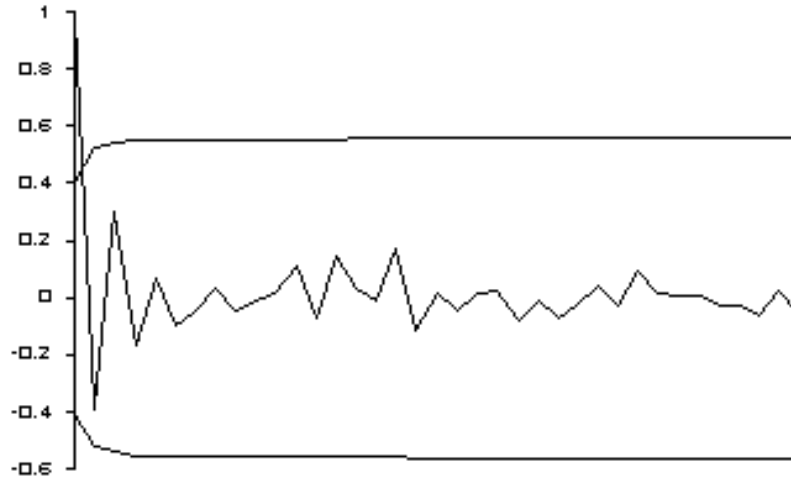
with degrees of freedom = 23

The 95th percentile = 35.16596

Hypothesis of randomness accepted.

Press any key to proceed to the forecasting section.

Auto Correlation Function
with 95% Confidence Limits



Forecasting Section

FORECASTING SECTION

Defaults are obtained by pressing the enter key, without input.

Default for number of periods ahead from last period = 6.

Default for the confidence band around the forecast = 90%.

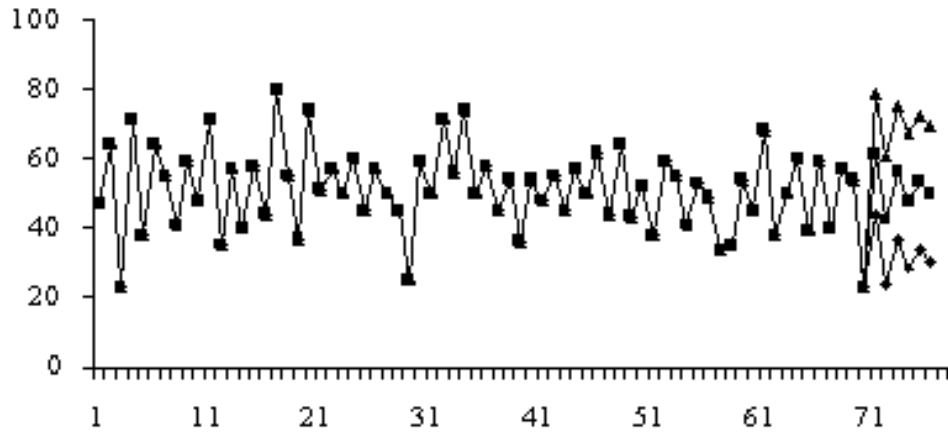
How many periods ahead to forecast? (9999 to quit...):

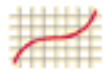
Enter confidence level for the forecast limits :

90 Percent Confidence limits

Next	Lower	Forecast	Upper
71	43.8734	61.1930	78.5706
72	24.0239	42.3156	60.6074
73	36.9575	56.0006	75.0438
74	28.4916	47.7573	67.0229
75	33.7942	53.1634	72.5326
76	30.3487	49.7573	69.1658

Series F with forecasts and 90% confidence limits





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6.4.4.10. Box-Jenkins Analysis on Seasonal Data

Example with the SEMPLOT Software for a Seasonal Time Series

A computer software package is needed to do a Box-Jenkins time series analysis for seasonal data. The computer output on this page will illustrate sample output from a Box-Jenkins analysis using the [SEMSTAT](#) statistical software program. It analyzes the series G data set in the Box, Jenkins and Reinsel text.

The graph of the data and the resulting forecasts after fitting a model are portrayed below.

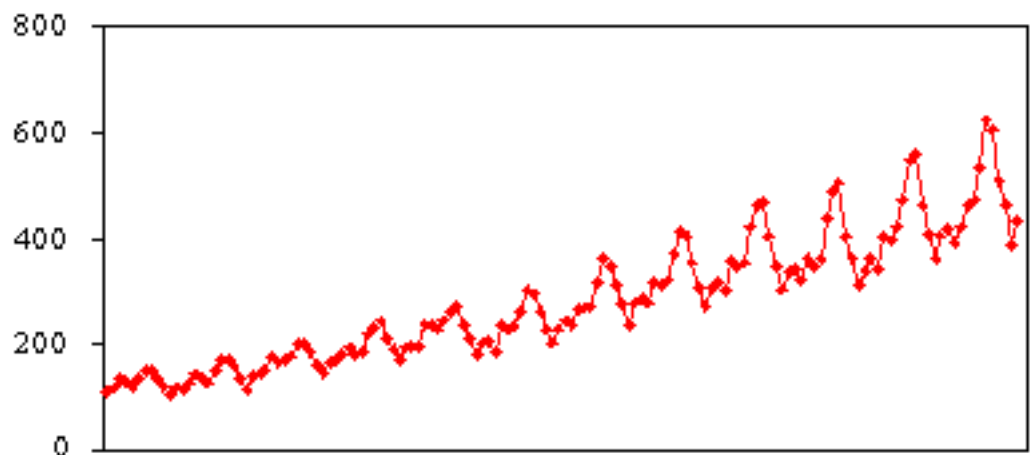
Model Identification Section

Enter FILESPEC or EXTENSION (1-3 letters):

To quit, press F10.

? bookg.bj

Series G of Box and Jenkins



144 observations

MAX	MIN	MEAN	VARIANCE	NO. DATA
622.0000	104.0000	280.2986	14391.9170	144

Do you wish to make transformations? y/n y

The following transformations are available:

- 1 Square root
- 2 Cube root
- 3 Natural log
- 4 Natural log log
- 5 Common log
- 6 Exponentiation
- 7 Reciprocal
- 8 Square root of Reciprocal
- 9 Normalizing $(X-\bar{X})/\text{Standard deviation}$
- 10 Coding $(X-\text{Constant 1})/\text{Constant 2}$

Enter your selection, by number: 3

Statistics of Transformed series:

Mean: 5.542 Variance 0.195

Input order of difference or 0: 1

Input period of seasonality (2-12) or 0: 12

Input order of seasonal difference or 0: 0

Statistics of Differenced series:

Mean: 0.009 Variance 0.011

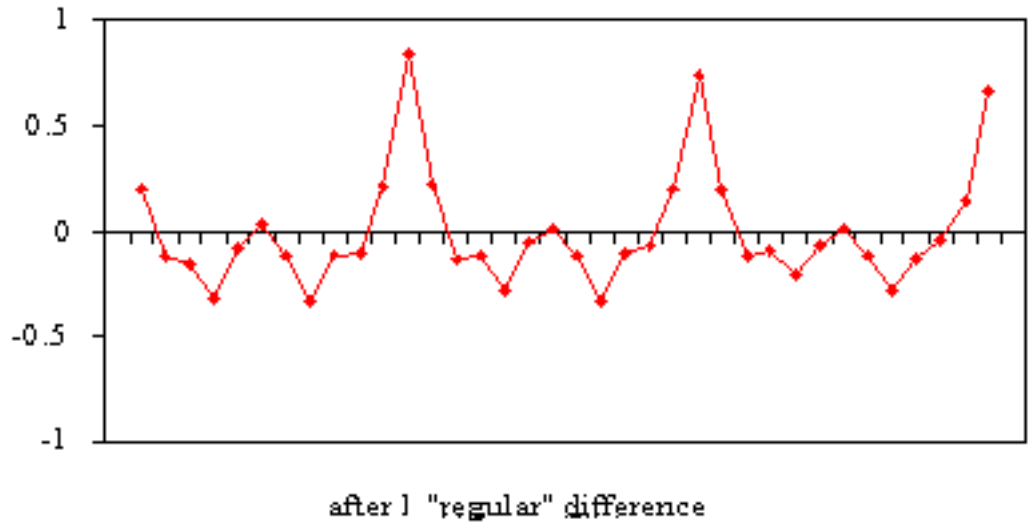
Time Series: bookg.bj.

Regular difference: 1 Seasonal Difference: 0

Autocorrelation Function for the first 36 lags

1	0.19975	13	0.21509	25	0.19726
2	-0.12010	14	-0.13955	26	-0.12388
3	-0.15077	15	-0.11600	27	-0.10270
4	-0.32207	16	-0.27894	28	-0.21099
5	-0.08397	17	-0.05171	29	-0.06536
6	0.02578	18	0.01246	30	0.01573
7	-0.11096	19	-0.11436	31	-0.11537
8	-0.33672	20	-0.33717	32	-0.28926
9	-0.11559	21	-0.10739	33	-0.12688
10	-0.10927	22	-0.07521	34	-0.04071
11	0.20585	23	0.19948	35	0.14741
12	0.84143	24	0.73692	36	0.65744

Autocorrelation Function of Series G



Analyzing Autocorrelation Plot for Seasonality

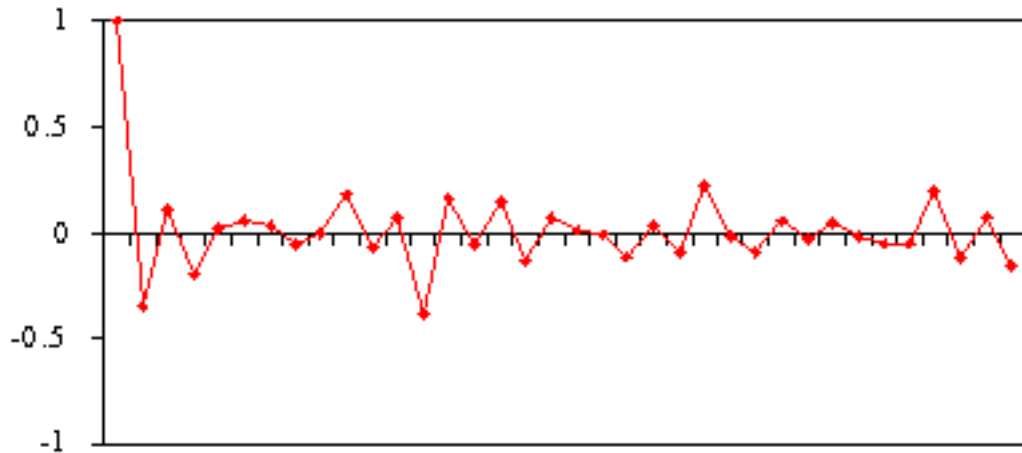
If you observe very large autocorrelations at lags spaced n periods apart, for example at lags 12 and 24, then there is evidence of periodicity. That effect should be removed, since the objective of the identification stage is to reduce the autocorrelations throughout. So if simple differencing was not enough, try seasonal differencing at a selected period. In the above case, the period is 12. It could, of course, be any value, such as 4 or 6.

The number of seasonal terms is rarely more than 1. If you know the shape of your forecast function, or you wish to assign a particular shape to the forecast function, you can select the appropriate number of terms for seasonal AR or seasonal MA models.

The book by Box and Jenkins, *Time Series Analysis Forecasting and Control* (the later edition is Box, Jenkins and Reinsel, 1994) has a discussion on these forecast functions on pages 326 - 328. Again, if you have only a faint notion, but you do know that there was a trend upwards before differencing, pick a seasonal MA term and see what comes out in the diagnostics.

The results after taking a seasonal difference look good!

Autocorrelation of Series G



after 1 "regular" and 1 "seasonal" difference

Model Fitting Section

Now we can proceed to the estimation, diagnostics and forecasting routines. The following program is again executed from a menu and issues the following flow of output:

Enter FILESPEC or EXTENSION (1-3 letters):

To quit press F10.

? bookg.bj

MAX	MIN	MEAN	VARIANCE	NO. DATA
622.0000	104.0000	280.2986	14391.9170	144

Do you wish to make
transformations? y/n

y (we selected a square root
transformation because a closer
inspection of the plot revealed
increasing variances over time)

Statistics of Transformed series:

Mean: 5.542	Variance 0.195
-------------	----------------

Input order of difference or 0: 1

Input NUMBER of AR terms: Blank defaults to 0

Input NUMBER of MA terms: 1

Input period of seasonality (2-12) or
0: 12

Input order of seasonal difference or
0: 1

Input NUMBER of seasonal AR
terms: Blank defaults to 0

Input NUMBER of seasonal MA
terms: 1

Statistics of Differenced series:

Mean:	0.000	Variance	0.002
Pass 1 SS:		0.1894	
Pass 2 SS:		0.1821	
Pass 3 SS:		0.1819	

Estimation is finished after 3 Marquardt iterations.

Output Section

MA estimates with Standard Errors

Theta 1 : 0.3765 0.0811

Seasonal MA estimates with Standard Errors

Theta 1 : 0.5677 0.0775

Original Variance	:	0.0021
Residual Variance (MSE)	:	0.0014
Coefficient of Determination	:	33.9383

AIC criteria $\ln(\text{SSE})+2k/n$: -1.4959

BIC criteria $\ln(\text{SSE})+\ln(n)k/n$: -1.1865

$k = p + q + P + Q + d + sD =$ number of estimates + order of regular difference + product of period of seasonality and seasonal difference.

n is the total number of observations.

In this problem k and n are: 15 144

***** Test on randomness of Residuals *****

The Box-Ljung value	=	28.4219
The Box-Pierce value	=	24.0967
with degrees of freedom	=	30
The 95th percentile	=	43.76809

Hypothesis of randomness accepted.

Forecasting Section

Defaults are obtained by pressing the enter key, without input.

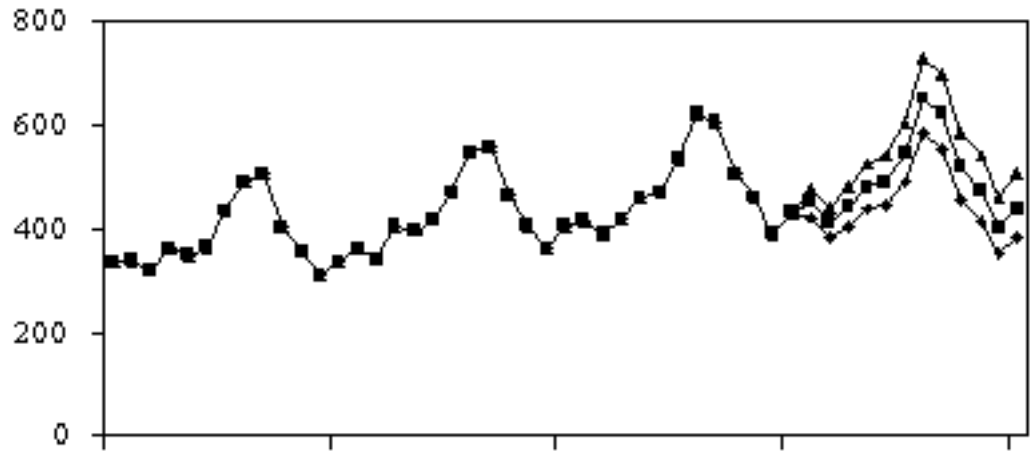
Default for number of periods ahead from last period = 6.

Default for the confidence band around the forecast = 90%.

Next Period	Lower	Forecast	Upper
145	423.4257	450.1975	478.6620
146	382.9274	411.6180	442.4583
147	407.2839	441.9742	479.6191
148	437.8781	479.2293	524.4855
149	444.3902	490.1471	540.6153
150	491.0981	545.5740	606.0927
151	583.6627	652.7856	730.0948
152	553.5620	623.0632	701.2905
153	458.0291	518.6510	587.2965

154	417.4242	475.3956	541.4181
155	350.7556	401.6725	459.9805
156	382.3264	440.1473	506.7128

Last 36 points of Series G



with 12 Forecasts and a 90% CI



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6.4.5. Multivariate Time Series Models

If each time series observation is a vector of numbers, you can model them using a multivariate form of the Box-Jenkins model

The multivariate form of the Box-Jenkins univariate models is sometimes called the ARMAV model, for AutoRegressive Moving Average Vector or simply vector ARMA process.

The ARMAV model for a stationary multivariate time series, with a zero mean vector, represented by

$$\mathbf{x}_t = (x_{1t}, x_{2t}, \dots, x_{nt})^T \quad -\infty < t < \infty$$

is of the form

$$\begin{aligned} \mathbf{x}_t = & \phi_1 \mathbf{x}_{t-1} + \phi_2 \mathbf{x}_{t-2} + \dots + \phi_p \mathbf{x}_{t-p} + \mathbf{a}_t \\ & - \theta_1 \mathbf{a}_{t-1} - \theta_2 \mathbf{a}_{t-2} - \dots - \theta_q \mathbf{a}_{t-q} \end{aligned}$$

where

- \mathbf{x}_t and \mathbf{a}_t are $n \times 1$ column vectors with \mathbf{a}_t representing multivariate white noise
- $\phi_k = \{\phi_{k,jj}\}$, $k = 1, 2, \dots, p$
- $\theta_k = \{\theta_{k,jj}\}$, $k = 1, 2, \dots, q$

are $n \times n$ matrices for autoregressive and moving average parameters

- $E[\mathbf{a}_t] = \mathbf{0}$
- $E(\mathbf{a}_t \mathbf{a}'_{t-k}) = \mathbf{0} \quad k \neq 0$
- $E(\mathbf{a}_t \mathbf{a}'_{t-k}) = \Sigma_a \quad k = 0$

where Σ_a is the dispersion or covariance matrix of \mathbf{a}_t

As an example, for a bivariate series with $n = 2$, $p = 2$, and $q = 1$, the ARMAV(2,1) model is:

$$\begin{aligned} \begin{pmatrix} x_{1t} \\ x_{2t} \end{pmatrix} = & \begin{pmatrix} \phi_{1.11} & \phi_{1.12} \\ \phi_{1.21} & \phi_{1.22} \end{pmatrix} \begin{pmatrix} x_{1t-1} \\ x_{2t-1} \end{pmatrix} + \\ & \begin{pmatrix} \phi_{2.11} & \phi_{2.12} \\ \phi_{2.21} & \phi_{2.22} \end{pmatrix} \begin{pmatrix} x_{1t-2} \\ x_{2t-2} \end{pmatrix} \\ + & \begin{pmatrix} a_{1t} \\ a_{2t} \end{pmatrix} - \begin{pmatrix} \theta_{1.11} & \theta_{1.12} \\ \theta_{1.21} & \theta_{1.22} \end{pmatrix} \begin{pmatrix} a_{1t-1} \\ a_{2t-1} \end{pmatrix} \end{aligned}$$

with

$$\mathbf{a}_t = \begin{pmatrix} a_{1t} \\ a_{2t} \end{pmatrix}$$

Estimation of parameters and covariance matrix difficult

The estimation of the matrix parameters and [covariance matrix](#) is complicated and very difficult without computer software. The estimation of the Moving Average matrices is especially an ordeal. If we opt to ignore the MA component(s) we are left with the ARV model given by:

$$\mathbf{x}_t = \phi_1 \mathbf{x}_{t-1} + \phi_2 \mathbf{x}_{t-2} + \dots + \phi_p \mathbf{x}_{t-p} + \mathbf{a}_t$$

where

- \mathbf{x}_t is a vector of observations, $\mathbf{x}_{1t}, \mathbf{x}_{2t}, \dots, \mathbf{x}_{nt}$ at time t
- \mathbf{a}_t is a vector of white noise, $\mathbf{a}_{1t}, \mathbf{a}_{2t}, \dots, \mathbf{a}_{nt}$ at time t
- $\phi_k = \{\phi_{k,jj}\}$, $k = 1, 2, \dots, p$
is a $n \times n$ matrix of autoregressive parameters
- $E[\mathbf{a}_t] = \mathbf{0}$
- $E(\mathbf{a}_t \mathbf{a}'_{t-k}) = \mathbf{0} \quad k \neq 0$
- $E(\mathbf{a}_t \mathbf{a}'_{t-k}) = \Sigma_a \quad k = 0$

where $\Sigma_a = E[\mathbf{a}_t \mathbf{a}'_t]$ is the dispersion or covariance matrix

A model with p autoregressive matrix parameters is an ARV(p) model or a vector AR model.

The parameter matrices may be estimated by multivariate least squares, but there are other methods such as maximum likelihood estimation.

Interesting properties of parameter matrices

There are a few interesting properties associated with the phi or AR parameter matrices. Consider the following example for a bivariate series with $n=2$, $p=2$, and $q=0$. The ARMAV(2,0) model is:

$$\begin{pmatrix} x_t \\ y_t \end{pmatrix} = \begin{pmatrix} \phi_{1.11} & \phi_{1.12} \\ \phi_{1.21} & \phi_{1.22} \end{pmatrix} \begin{pmatrix} x_{t-1} \\ y_{t-1} \end{pmatrix} + \begin{pmatrix} \phi_{2.11} & \phi_{2.12} \\ \phi_{2.21} & \phi_{2.22} \end{pmatrix} \begin{pmatrix} x_{t-2} \\ y_{t-2} \end{pmatrix} + \begin{pmatrix} a_{1t} \\ a_{2t} \end{pmatrix}$$

Without loss of generality, assume that the X series is input and the Y series are output and that the mean vector = (0,0).

Therefore, transform the observation by subtracting their respective averages.

Diagonal terms of Phi matrix

The diagonal terms of each Phi matrix are the scalar estimates for each series, in this case:

$$\begin{aligned} &\phi_{1.11}, \phi_{2.11} \text{ for the input series } X, \\ &\phi_{1.22}, \phi_{2.22} \text{ for the output series } Y. \end{aligned}$$

Transfer mechanism

The lower off-diagonal elements represent the influence of the input on the output.

This is called the "transfer" mechanism or transfer-function model as discussed by Box and Jenkins in Chapter 11. The ϕ terms here correspond to their δ terms.

The upper off-diagonal terms represent the influence of the output on the input.

Feedback

This is called "feedback". The presence of feedback can also be seen as a high value for a coefficient in the correlation matrix of the residuals. A "true" transfer model exists when there is no feedback.

This can be seen by expressing the matrix form into scalar form:

$$\begin{aligned} x_t &= \phi_{1.11}x_{t-1} + \phi_{2.11}x_{t-2} + \phi_{1.12}y_{t-1} + \phi_{2.12}y_{t-2} + a_{1t} \\ y_t &= \phi_{1.22}x_{t-1} + \phi_{2.22}y_{t-2} + \phi_{1.21}x_{t-1} + \phi_{2.21}x_{t-2} + a_{2t} \end{aligned}$$

Delay

Finally, delay or "dead" time can be measured by studying the lower off-diagonal elements again.

If, for example, $\phi_{1.21}$ is non-significant, the delay is 1 time period.

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6.4.5. [Multivariate Time Series Models](#)

6.4.5.1. Example of Multivariate Time Series Analysis

A multivariate Box-Jenkins example

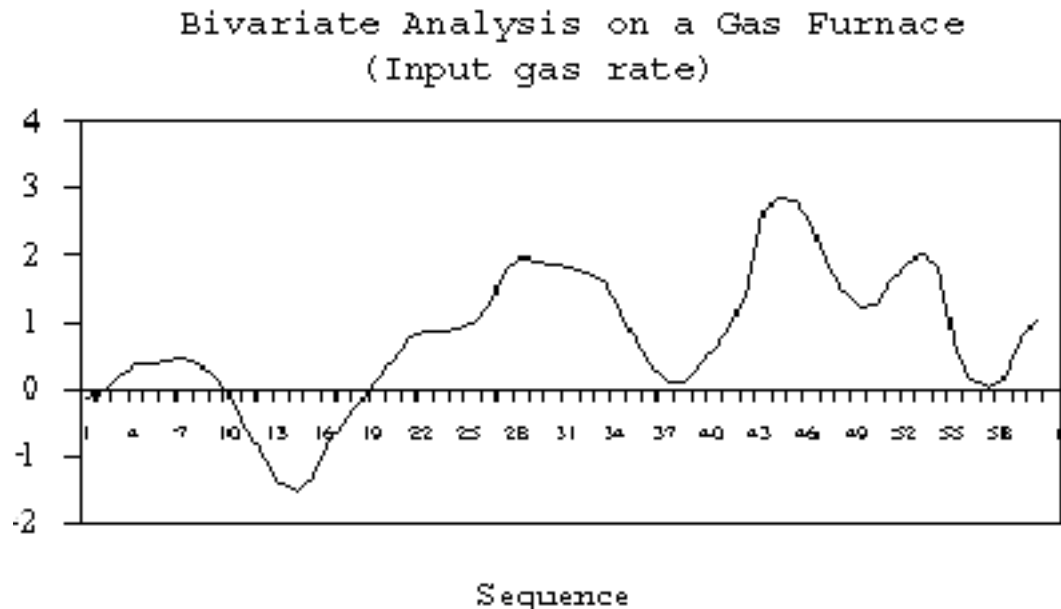
As an example, we will analyze the gas furnace data from the Box-Jenkins textbook. In this gas furnace, air and methane were combined in order to obtain a mixture of gases which contained CO₂ (carbon dioxide). The methane gas feedrate constituted the input series and followed the process

$$\text{Methane Gas Input Feed} = .60 - .04 X(t)$$

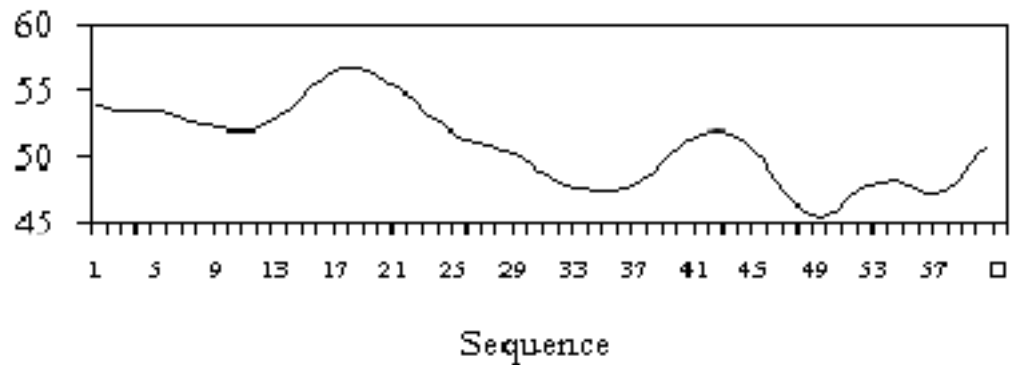
the CO₂ concentration was the output, $Y(t)$. In this experiment 296 successive pairs of observations (X_t, Y_t) were read off from the continuous records at 9-second intervals. For the example described below, the first 60 pairs were used. It was decided to fit a bivariate model as described in the previous section and to study the results.

Plots of input and output series

The plots of the input and output series are displayed below.



Bivariate Analysis of a Gas Furnace
(Outlet Gas in % CO)



From a suitable Box-Jenkins software package, we select the routine for multivariate time series analysis. Typical output information and prompts for input information will look as follows:

SEMPLOT
output

MULTIVARIATE AUTOREGRESSION

Enter FILESPEC **GAS.BJ**

Explanation of Input

How many series? : 2 *the input and the output series*
Which order? : 2 *this means that we consider times*
t-1 and t-2 in the model , which is
a special case of the general [ARV](#)
model

<u>SERIES</u>	<u>MAX</u>	<u>MIN</u>	<u>MEAN</u>	<u>VARIANCE</u>
1	56.8000	45.6000	50.8650	9.0375
2	2.8340	-1.5200	0.7673	1.0565

NUMBER OF OBSERVATIONS: 60 .

THESE WILL BE MEAN CORRECTED. *so we don't have to*
fit the means

OPTION TO TRANSFORM DATA

Transformations? : y/N

OPTION TO DETREND DATA

Seasonal adjusting? : y/N

FITTING ORDER: 2

OUTPUT SECTION

the notation of the output follows the notation of the previous section

MATRIX FORM OF ESTIMATES

$$\begin{array}{cc} \phi_1 & \\ 1.2265 & 0.2295 \\ -0.0755 & 1.6823 \\ \phi_2 & \\ -0.4095 & -0.8057 \\ 0.0442 & -0.8589 \end{array}$$

	Estimate	Std. Err	t value	Prob(t)
Con 1	-0.0337	0.0154	-2.1884	0.9673
Con 2	0.003	0.0342	0.0914	0.0725
ϕ 1.11	1.2265	0.0417	29.4033	> .9999
ϕ 1.12	0.2295	0.0530	4.3306	0.9999
ϕ 1.21	-0.0755	0.0926	-0.8150	0.5816
ϕ 1.22	1.6823	0.1177	14.2963	> .9999
ϕ 2.11	-0.4095	0.0354	-11.5633	> .9999
ϕ 2.12	-0.8057	0.0714	-11.2891	> .9999
ϕ 2.21	0.0442	0.0786	0.5617	0.4235
ϕ 2.22	-0.8589	0.1585	-5.4194	> .9999

Statistics on the Residuals

MEANS

-0.0000 0.0000

COVARIANCE MATRIX

0.01307	-0.00118
-0.00118	0.06444

CORRELATION MATRIX

1.0000	-0.0407
-0.0407	1.0000

<u>SERIES</u>	<u>ORIGINAL VARIANCE</u>	<u>RESIDUAL VARIANCE</u>	<u>COEFFICIENT OF DETERMINATION</u>
1	9.03746	0.01307	99.85542
2	1.05651	0.06444	93.90084

This illustrates excellent univariate fits for the individual series.

This portion of the computer output lists the results of testing for independence (randomness) of each of the series.

Theoretical Chi-Square Value:

The 95th percentile = 35.16595

for degrees of freedom = 23

Test on randomness of Residuals for Series: 1

The Box-Ljung value = 20.7039 Both Box-Ljung and
Box-Pierce

The Box-Pierce value = 16.7785 tests for randomness of
residuals

Hypothesis of randomness accepted. using the chi-square test on
the

sum of the squared residuals.

Test on randomness of Residuals for Series: 2

The Box-Ljung value = 16.9871 For example, $16.98 < 35.17$

The Box-Pierce value = 13.3958 and $13.40 < 35.17$

Hypothesis of randomness accepted.

FORECASTING SECTION

The forecasting method is an extension of the model and follows the theory outlined in the previous section. Based on the estimated variances and number

of forecasts we can compute the forecasts and their confidence limits.

The user, in this software, is able to choose how many forecasts to obtain, and at what confidence levels.

Defaults are obtained by pressing the enter key, without input.

Default for number of periods ahead from last period = 6.

Default for the confidence band around the forecast = 90%.

How many periods ahead to forecast? 6

Enter confidence level for the forecast limits : .90:

SERIES: 1

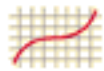
90 Percent Confidence limits

Next Period	Lower	Forecast	Upper
61	51.0534	51.2415	51.4295
62	50.9955	51.3053	51.6151
63	50.5882	50.9641	51.3400
64	49.8146	50.4561	51.0976
65	48.7431	49.9886	51.2341
66	47.6727	49.6864	51.7001

SERIES: 2

90 Percent Confidence limits

Next Period	Lower	Forecast	Upper
61	0.8142	1.2319	1.6495
62	0.4777	1.2957	2.1136
63	0.0868	1.2437	2.4005
64	-0.2661	1.1300	2.5260
65	-0.5321	1.0066	2.5453
66	-0.7010	0.9096	2.5202

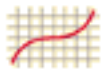


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6.5. Tutorials

*Tutorial
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6.5.1. What do we mean by "Normal" data?

The Normal distribution model

"Normal" data are data that are drawn (come from) a population that has a normal distribution. This distribution is inarguably the most important and the most frequently used distribution in both the theory and application of statistics. If X is a normal random variable, then the probability distribution of X is

Normal probability distribution

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \quad -\infty < x < \infty$$

Parameters of normal distribution

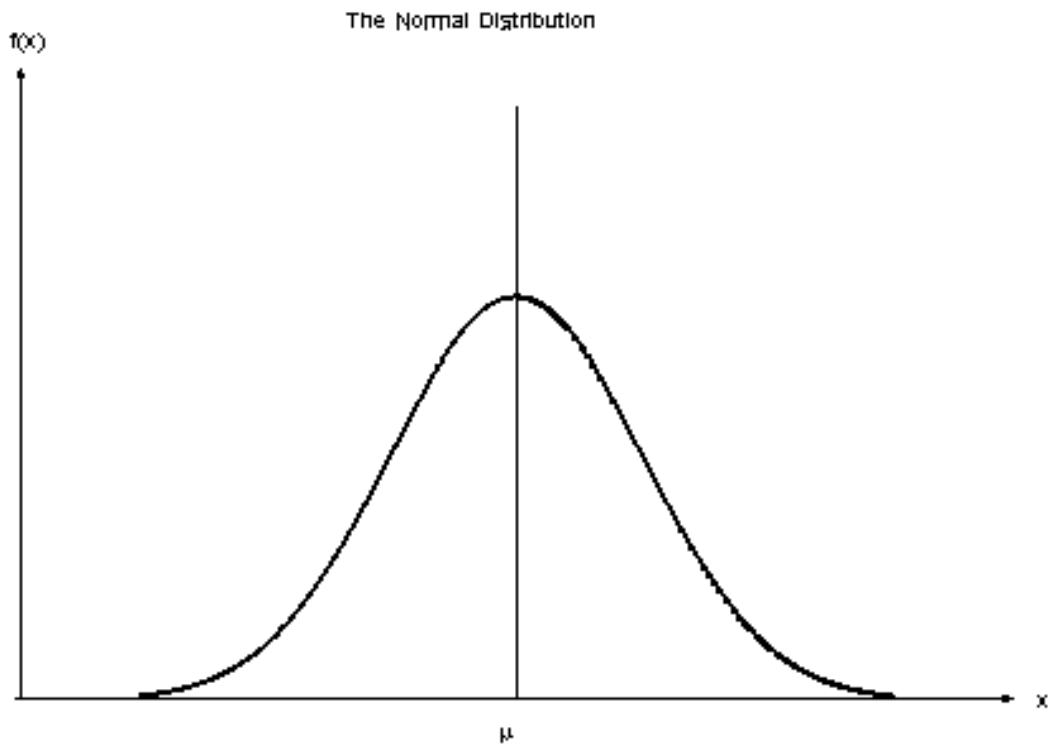
The parameters of the normal distribution are the mean μ and the standard deviation σ (or the variance σ^2). A special notation is employed to indicate that X is normally distributed with these parameters, namely

$$X \sim N(\mu, \sigma) \text{ or } X \sim N(\mu, \sigma^2).$$

Shape is symmetric and unimodal

The shape of the normal distribution is symmetric and unimodal. It is called the *bell-shaped* or *Gaussian* distribution after its inventor, Gauss (although De Moivre also deserves credit).

The visual appearance is given below.



Property of probability distributions is that area under curve equals one

A property of a special class of non-negative functions, called probability distributions, is that the area under the curve equals unity. One finds the area under any portion of the curve by integrating the distribution between the specified limits. The area under the bell-shaped curve of the normal distribution can be shown to be equal to 1, and therefore the normal distribution is a probability distribution.

Interpretation of σ

There is a simple interpretation of σ

68.27% of the population fall between $\mu \pm 1 \sigma$

95.45% of the population fall between $\mu \pm 2 \sigma$

99.73% of the population fall between $\mu \pm 3 \sigma$

The cumulative normal distribution

The cumulative normal distribution is defined as the probability that the normal variate is less than or equal to some value v , or

$$P\{X \leq v\} = F(v) = \int_{-\infty}^v \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} dx$$

Unfortunately this integral cannot be evaluated in closed form and one has to resort to numerical methods. But even so, tables for all possible values of μ and σ would be required. A change of variables rescues the situation. We let

$$z = \frac{x - \mu}{\sigma}$$

Now the evaluation can be made independently of μ and σ ; that is,

$$P\{X \leq v\} = P\left\{z \leq \frac{v - \mu}{\sigma}\right\} = \Phi\left(\frac{v - \mu}{\sigma}\right)$$

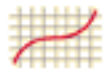
where $\Phi(\cdot)$ is the cumulative distribution function of the *standard normal distribution* ($\mu = 0$, $\sigma = 1$).

$$\phi(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}}$$

*Tables for the
cumulative
standard
normal
distribution*

Tables of the cumulative standard normal distribution are given in every statistics textbook and in the [handbook](#). A rich variety of approximations can be found in the literature on numerical methods.

For example, if $\mu = 0$ and $\sigma = 1$ then the area under the curve from $\mu - 1\sigma$ to $\mu + 1\sigma$ is the area from 0 - 1 to 0 + 1, which is 0.6827. Since most standard normal tables give area to the left of the lookup value, they will have for $z = 1$ an area of .8413 and for $z = -1$ an area of .1587. By subtraction we obtain the area between -1 and +1 to be .8413 - .1587 = .6826.



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6.5.2. What to do when data are non-normal

Often it is possible to transform non-normal data into approximately normal data

Non-normality is a way of life, since no characteristic (height, weight, etc.) will have *exactly* a normal distribution. One strategy to make non-normal data resemble normal data is by using a transformation. There is no dearth of transformations in statistics; the issue is which one to select for the situation at hand. Unfortunately, the choice of the "best" transformation is generally not obvious.

This was recognized in 1964 by [G.E.P. Box and D.R. Cox](#). They wrote a paper in which a useful family of power transformations was suggested. These transformations are defined only for positive data values. This should not pose any problem because a constant can always be added if the set of observations contains one or more negative values.

The Box-Cox power transformations are given by

The Box-Cox Transformation

$$x(\lambda) = \frac{(x^\lambda - 1)}{\lambda} \quad \lambda \neq 0$$

$$x(\lambda) = \ln(x) \quad \lambda = 0$$

Given the vector of data observations $\mathbf{x} = x_1, x_2, \dots, x_n$, one way to select the power λ is to use the λ that maximizes the logarithm of the likelihood function

The logarithm of the likelihood function

$$f(\mathbf{x}, \lambda) = -\frac{n}{2} \ln \left[\sum_{i=1}^n \frac{(x_i(\lambda) - \bar{x}(\lambda))^2}{n} \right] + (\lambda - 1) \sum_{i=1}^n \ln(x_i)$$

where

$$\bar{x}(\lambda) = \frac{1}{n} \sum_{i=1}^n x_i(\lambda)$$

is the arithmetic mean of the transformed data.

Confidence bound for λ

In addition, a confidence bound (based on the [likelihood ratio](#) statistic) can be constructed for λ as follows: A set of λ values that represent an approximate $100(1-\alpha)\%$ confidence bound for λ is formed from those λ that satisfy

$$f(\mathbf{x}, \lambda) \geq f(\mathbf{x}, \hat{\lambda}) - .5 \chi_{.1}^2$$

where $\hat{\lambda}$ denotes the maximum likelihood estimator for λ and $\chi_{.1}^2$ is the upper $100\alpha(1-\alpha)$ percentile of the chi-square distribution with 1 degree of freedom.

Example of the Box-Cox scheme

To illustrate the procedure, we used the data from Johnson and Wichern's textbook (Prentice Hall 1988), Example 4.14. The observations are microwave radiation measurements.

Sample data

```
.15 .09 .18 .10 .05 .12 .08
.05 .08 .10 .07 .02 .01 .10
.10 .10 .02 .10 .01 .40 .10
.05 .03 .05 .15 .10 .15 .09
.08 .18 .10 .20 .11 .30 .02
.20 .20 .30 .30 .40 .30 .05
```

Table of log-likelihood values for various values of λ

The values of the log-likelihood function obtained by varying λ from -2.0 to 2.0 are given below.

λ	LLF	λ	LLF	λ	LLF
-2.0	7.1146	-0.6	89.0587	0.7	103.0322
-1.9	14.1877	-0.5	92.7855	0.8	101.3254
-1.8	21.1356	-0.4	96.0974	0.9	99.3403
-1.7	27.9468	-0.3	98.9722	1.0	97.1030
-1.6	34.6082	-0.2	101.3923	1.1	94.6372
-1.5	41.1054	-0.1	103.3457	1.2	91.9643
-1.4	47.4229	0.0	104.8276	1.3	89.1034
-1.3	53.5432	0.1	105.8406	1.4	86.0714
-1.2	59.4474	0.2	106.3947	1.5	82.8832
-1.1	65.1147	0.3	106.5069	1.6	79.5521
-0.9	75.6471	0.4	106.1994	1.7	76.0896
-0.8	80.4625	0.5	105.4985	1.8	72.5061
-0.7	84.9421	0.6	104.4330	1.9	68.8106

This table shows that $\lambda = .3$ maximizes the log-likelihood function (LLF). This becomes 0.28 if a second digit of accuracy is calculated.

The Box-Cox transform is also discussed in Chapter 1 under the [Box Cox Linearity Plot](#) and the [Box Cox Normality Plot](#). The Box-Cox normality plot discussion provides a graphical method for choosing λ to transform a data set to normality. The criterion used to choose λ for the Box-Cox linearity plot is the value of λ that maximizes the correlation between the transformed x-values and the y-values when making a normal probability plot of the (transformed) data.



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6.5.3. Elements of Matrix Algebra

Elementary Matrix Algebra

Basic definitions and operations of matrix algebra - needed for multivariate analysis

Vectors and matrices are arrays of numbers. The algebra for symbolic operations on them is different from the algebra for operations on scalars, or single numbers. For example there is no division in matrix algebra, although there is an operation called "multiplying by an inverse". It is possible to express the exact equivalent of matrix algebra equations in terms of scalar algebra expressions, but the results look rather messy.

It can be said that the matrix algebra notation is shorthand for the corresponding scalar longhand.

Vectors

A *vector* is a column of numbers

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_p \end{bmatrix}$$

The scalars a_i are the elements of vector \mathbf{a} .

Transpose

The *transpose* of \mathbf{a} , denoted by \mathbf{a}' , is the row arrangement of the elements of \mathbf{a} .

$$\mathbf{a}' = [a_1 \quad a_2 \quad \cdots \quad a_p]$$

Sum of two vectors

The **sum of two vectors** (say, a and b) is the vector of sums of corresponding elements.

$$\mathbf{a} + \mathbf{b} = \begin{bmatrix} a_1 + b_1 \\ a_2 + b_2 \\ \vdots \\ a_p + b_p \end{bmatrix}$$

The difference of two vectors is the vector of differences of corresponding elements.

Product of $a'b$

The **product $a'b$** is a scalar formed by

$$\mathbf{a}'\mathbf{b} = [a_1b_1 + a_2b_2 + \cdots + a_pb_p]$$

which may be written in shortcut notation as

$$c = \sum_{i=1}^p a_i b_i$$

where a_i and b_i are the i th elements of vector \mathbf{a} and \mathbf{b} , respectively.

Product of ab'

The **product ab'** is a *square matrix*

$$\mathbf{ab}' = \begin{bmatrix} a_1b_1 & a_1b_2 & \cdots & a_1b_p \\ a_2b_1 & a_2b_2 & \cdots & a_2b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_pb_1 & a_pb_2 & \cdots & a_pb_p \end{bmatrix}$$

Product of scalar times a vector

The product of a scalar k , times a vector \mathbf{a} is k times each element of \mathbf{a}

$$k\mathbf{a} = \mathbf{a}k = \begin{bmatrix} ka_1 \\ ka_2 \\ \vdots \\ ka_p \end{bmatrix}$$

A matrix is a rectangular table of numbers

A matrix is a rectangular table of numbers, with p rows and n columns. It is also referred to as an array of n column vectors of length p . Thus

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{p1} & a_{p2} & \cdots & a_{pn} \end{bmatrix}$$

is a p by n matrix. The typical element of \mathbf{A} is a_{ij} , denoting the element of row i and column j .

Matrix addition and subtraction

Matrices are **added and subtracted** on an element-by-element basis. Thus

$$\mathbf{A} + \mathbf{B} = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} & \cdots & a_{1n} + b_{1n} \\ a_{21} + b_{21} & a_{22} + b_{22} & \cdots & a_{2n} + b_{2n} \\ \vdots & \vdots & & \vdots \\ a_{p1} + b_{p1} & a_{p2} + b_{p2} & \cdots & a_{pn} + b_{pn} \end{bmatrix}$$

Matrix multiplication

Matrix **multiplication** involves the computation of the sum of the products of elements from a row of the first matrix (the premultiplier on the left) and a column of the second matrix (the postmultiplier on the right). This sum of products is computed for every combination of rows and columns. For example, if **A** is a 2 x 3 matrix and **B** is a 3 x 2 matrix, the product **AB** is

$$\mathbf{AB} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} & a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} \\ a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} & a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} \end{bmatrix}$$

Thus, the product is a 2 x 2 matrix. This came about as follows: The number of columns of **A** must be equal to the number of rows of **B**. In this case this is 3. If they are not equal, multiplication is impossible. If they are equal, then the number of rows of the product **AB** is equal to the number of rows of **A** and the number of columns is equal to the number of columns of **B**.

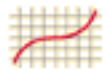
Example of 3x2 matrix multiplied by a 2x3

It follows that the result of the product **BA** is a 3 x 3 matrix

$$\mathbf{BA} = \begin{bmatrix} b_{11}a_{11} + b_{12}a_{21} & b_{11}a_{12} + b_{12}a_{22} & b_{11}a_{13} + b_{12}a_{23} \\ b_{21}a_{11} + b_{22}a_{21} & b_{21}a_{12} + b_{22}a_{22} & b_{21}a_{13} + b_{22}a_{23} \\ b_{31}a_{11} + b_{32}a_{21} & b_{31}a_{12} + b_{32}a_{22} & b_{31}a_{13} + b_{32}a_{23} \end{bmatrix}$$

General case for matrix multiplication

In general, if **A** is a $k \times p$ matrix and **B** is a $p \times n$ matrix, the product **AB** is a $k \times n$ matrix. If $k = n$, then the product **BA** can also be formed. We say that matrices conform for the operations of addition, subtraction or multiplication when their respective orders (numbers of row and columns) are such as to permit the operations. Matrices that do not conform for addition or subtraction cannot be added or subtracted. Matrices that do not conform for multiplication cannot be multiplied.



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6.5.3. [Elements of Matrix Algebra](#)

6.5.3.1. Numerical Examples

Numerical examples of matrix operations

Numerical examples of the matrix operations described on the [previous page](#) are given here to clarify these operations.

Sample matrices If

$$\mathbf{A} = \begin{bmatrix} 5 & 6 \\ 3 & 7 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 3 & 2 \\ 1 & 5 \end{bmatrix}$$

then

Matrix addition, subtraction, and multiplication

$$\mathbf{A} + \mathbf{B} = \begin{bmatrix} 8 & 8 \\ 4 & 12 \end{bmatrix} \quad \text{and} \quad \mathbf{A} - \mathbf{B} = \begin{bmatrix} 2 & 4 \\ 2 & 2 \end{bmatrix}$$

and

$$\mathbf{AB} = \begin{bmatrix} 21 & 40 \\ 16 & 41 \end{bmatrix} \quad \text{and} \quad \mathbf{BA} = \begin{bmatrix} 21 & 32 \\ 20 & 41 \end{bmatrix}$$

*Multiply matrix
by a scalar*

To multiply a matrix by a given scalar, each element of the matrix is multiplied by that scalar

$$2\mathbf{A} = \begin{bmatrix} 10 & 12 \\ 6 & 14 \end{bmatrix} \quad \text{and} \quad .5\mathbf{B} = \begin{bmatrix} 1.5 & 1.0 \\ 0.5 & 2.5 \end{bmatrix}$$

*Pre-multiplying
matrix by
transpose of a
vector*

Pre-multiplying a $p \times n$ matrix by the transpose of a p -element vector yields a n -element transpose

$$\mathbf{c}' = \mathbf{a}'\mathbf{B} = \begin{bmatrix} a_1 & a_2 \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix}' = \begin{bmatrix} c_1 & c_2 & c_3 \end{bmatrix}$$

*Post-multiplying
matrix by vector*

Post-multiplying a $p \times n$ matrix by an n -element vector yields an n -element vector

$$\mathbf{c} = \mathbf{B}\mathbf{A} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

Quadratic form

It is not possible to pre-multiply a matrix by a column vector, nor to post-multiply a matrix by a row vector. The matrix product $\mathbf{a}'\mathbf{B}\mathbf{a}$ yields a scalar and is called a quadratic form. Note that \mathbf{B} must be a square matrix if $\mathbf{a}'\mathbf{B}\mathbf{a}$ is to conform to multiplication. Here is an example of a quadratic form

$$\mathbf{a}'\mathbf{B}\mathbf{a} = \begin{bmatrix} 2 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 11 & 7 \end{bmatrix} \begin{bmatrix} 2 \\ 3 \end{bmatrix} = 43$$

Inverting a matrix

The matrix analog of division involves an operation called *inverting a matrix*. Only square matrices can be inverted. Inversion is a tedious numerical procedure and it is best performed by computers. There are many ways to invert a matrix, but ultimately whichever method is selected by a program is immaterial. If you wish to try one method by hand, a very popular numerical method is the Gauss-Jordan method.

Identity matrix

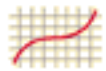
To augment the notion of the inverse of a matrix, \mathbf{A}^{-1} (\mathbf{A} inverse) we notice the following relation

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{A} \mathbf{A}^{-1} = \mathbf{I}$$

\mathbf{I} is a matrix of form

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

\mathbf{I} is called the identity matrix and is a special case of a *diagonal* matrix. Any matrix that has zeros in all of the off-diagonal positions is a diagonal matrix.



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6.5.3. [Elements of Matrix Algebra](#)

6.5.3.2. Determinant and Eigenstructure

A matrix determinant is difficult to define but a very useful number

Unfortunately, not every square matrix has an inverse (although most do). Associated with any square matrix is a single number that represents a unique function of the numbers in the matrix. This scalar function of a square matrix is called the *determinant*. *The determinant of a matrix \mathbf{A} is denoted by $|\mathbf{A}|$.* A formal definition for the determinant of a square matrix $\mathbf{A} = (a_{ij})$ is somewhat beyond the scope of this Handbook. Consult any good linear algebra textbook if you are interested in the mathematical details.

Singular matrix

As is the case of inversion of a square matrix, calculation of the determinant is tedious and computer assistance is needed for practical calculations. If the determinant of the (square) matrix is exactly zero, the matrix is said to be *singular* and it has no inverse.

Determinant of variance-covariance matrix

Of great interest in statistics is the determinant of a square symmetric matrix \mathbf{D} whose diagonal elements are sample variances and whose off-diagonal elements are sample covariances. Symmetry means that the matrix and its transpose are identical (i.e., $\mathbf{A} = \mathbf{A}'$). An example is

$$\mathbf{D} = \begin{bmatrix} s_1^2 & s_1 s_2 r_{12} & \cdots & s_1 s_p r_{1p} \\ s_2 s_1 r_{21} & s_2^2 & \cdots & s_2 s_p r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ s_p s_1 r_{p1} & s_p s_2 r_{p2} & \cdots & s_p^2 \end{bmatrix}$$

where s_1 and s_2 are sample standard deviations and r_{ij} is the sample correlation.

\mathbf{D} is the *sample variance-covariance matrix* for observations of a multivariate vector of p elements. The determinant of \mathbf{D} , in this case, is sometimes called the *generalized variance*.

Characteristic equation

In addition to a determinant and possibly an inverse, every square matrix has associated with it a *characteristic equation*. The characteristic equation of a matrix is formed by subtracting some particular value, usually denoted by the greek letter λ (lambda), from each diagonal element of the matrix, such that the determinant of the resulting matrix is equal to zero. For example, the characteristic equation of a second order (2 x 2) matrix \mathbf{A} may be written as

Definition of the characteristic equation for 2x2 matrix

$$|\mathbf{A} - \lambda\mathbf{I}| = \begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = 0$$

Eigenvalues of a matrix

For a matrix of order p , there may be as many as p different values for λ that will satisfy the equation. These different values are called the eigenvalues of the matrix.

Eigenvectors of a matrix

Associated with each eigenvalue is a vector, \mathbf{v} , called the *eigenvector*. The eigenvector satisfies the equation

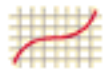
$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

Eigenstructure of a matrix

If the complete set of eigenvalues is arranged in the diagonal positions of a diagonal matrix \mathbf{V} , the following relationship holds

$$\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{L}$$

This equation specifies the complete *eigenstructure* of \mathbf{A} . Eigenstructures and the associated theory figure heavily in multivariate procedures and the numerical evaluation of \mathbf{L} and \mathbf{V} is a central computing problem.



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6.5.4. Elements of Multivariate Analysis

Multivariate analysis

Multivariate analysis is a branch of statistics concerned with the analysis of multiple measurements, made on one or several samples of individuals. For example, we may wish to measure length, width and weight of a product.

Multiple measurement, or observation, as row or column vector

A multiple measurement or observation may be expressed as

$$\mathbf{x} = [4 \ 2 \ 0.6]$$

referring to the physical properties of length, width and weight, respectively. It is customary to denote multivariate quantities with bold letters. The collection of measurements on \mathbf{x} is called a vector. In this case it is a row vector. We could have written \mathbf{x} as a column vector.

$$\mathbf{x} = \begin{bmatrix} 4 \\ 2 \\ 0.6 \end{bmatrix}$$

Matrix to represent more than one multiple measurement

If we take several such measurements, we record them in a rectangular array of numbers. For example, the \mathbf{X} matrix below represents 5 observations, on each of three variables.

$$\mathbf{X} = \begin{bmatrix} 4.0 & 2.0 & .60 \\ 4.2 & 2.1 & .59 \\ 3.9 & 2.0 & .58 \\ 4.3 & 2.1 & .62 \\ 4.1 & 2.2 & .63 \end{bmatrix}$$

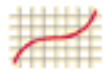
By convention, rows typically represent observations and columns represent variables

In this case the number of rows, ($n = 5$), is the number of observations, and the number of columns, ($p = 3$), is the number of variables that are measured. The rectangular array is an assembly of n row vectors of length p . This array is called a matrix, or, more specifically, a n by p matrix. Its name is \mathbf{X} . The names of matrices are usually written in bold, uppercase letters, as in [Section 6.5.3](#). We could just as well have written \mathbf{X} as a p (variables) by n (measurements) matrix as follows:

$$\mathbf{X} = \begin{bmatrix} 4.0 & 4.2 & 3.9 & 4.3 & 4.1 \\ 2.0 & 2.1 & 2.0 & 2.1 & 2.2 \\ .60 & .59 & .58 & .62 & .63 \end{bmatrix}$$

Definition of Transpose

A matrix with rows and columns exchanged in this manner is called the transpose of the original matrix.



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6.5.4. [Elements of Multivariate Analysis](#)

6.5.4.1. Mean Vector and Covariance Matrix

The first step in analyzing multivariate data is computing the mean vector and the variance-covariance matrix.

Sample data matrix

Consider the following matrix:

$$\mathbf{X} = \begin{bmatrix} 4.0 & 2.0 & .60 \\ 4.2 & 2.1 & .59 \\ 3.9 & 2.0 & .58 \\ 4.3 & 2.1 & .62 \\ 4.1 & 2.2 & .63 \end{bmatrix}$$

The set of 5 observations, measuring 3 variables, can be described by its *mean vector* and *variance-covariance matrix*. The three variables, from left to right are length, width, and height of a certain object, for example. Each row vector \mathbf{X}_i is another observation of the three variables (or components).

Definition of mean vector and variance-covariance matrix

The mean vector consists of the [means](#) of each variable and the variance-covariance matrix consists of the [variances](#) of the variables along the main diagonal and the covariances between each pair of variables in the other matrix positions.

The formula for computing the covariance of the variables X and Y is

$$COV = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{n - 1}$$

with \bar{X} and \bar{Y} denoting the means of X and Y , respectively.

*Mean vector
and
variance-
covariance
matrix for
sample data
matrix*

The results are:

$$\bar{\mathbf{x}} = [4.10 \quad 2.08 \quad .604]$$

$$\mathbf{S} = \begin{bmatrix} 0.025 & 0.0075 & 0.00175 \\ 0.0075 & 0.0070 & 0.00135 \\ 0.00175 & 0.00135 & 0.00043 \end{bmatrix}$$

where the mean vector contains the arithmetic averages of the three variables and the (unbiased) variance-covariance matrix \mathbf{S} is calculated by

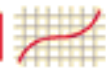
$$\mathbf{S} = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{X}_i - \bar{\mathbf{X}})(\mathbf{X}_i - \bar{\mathbf{X}})'$$

where $n = 5$ for this example.

Thus, 0.025 is the variance of the length variable, 0.0075 is the covariance between the length and the width variables, 0.00175 is the covariance between the length and the height variables, 0.007 is the variance of the width variable, 0.00135 is the covariance between the width and height variables and .00043 is the variance of the height variable.

*Centroid,
dispersion
matrix*

The mean vector is often referred to as the *centroid* and the variance-covariance matrix as the *dispersion* or dispersion matrix. Also, the terms variance-covariance matrix and covariance matrix are used interchangeably.



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6.5.4.2. The Multivariate Normal Distribution

Multivariate normal model

When multivariate data are analyzed, the multivariate normal model is the most commonly used model.

The multivariate normal distribution model extends the univariate [normal distribution model](#) to fit vector observations.

Definition of multivariate normal distribution

A p -dimensional vector of random variables

$$\mathbf{X} = X_1, X_2, \dots, X_p \quad -\infty < X_i < \infty, i = 1, \dots, p$$

is said to have a multivariate normal distribution if its density function $f(\mathbf{X})$ is of the form

$$\begin{aligned} f(\mathbf{X}) &= f(X_1, X_2, \dots, X_p) \\ &= \left(\frac{1}{2\pi}\right)^{p/2} |\Sigma|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{X} - \mathbf{m})' \Sigma^{-1} (\mathbf{X} - \mathbf{m})\right\} \end{aligned}$$

where $\mathbf{m} = (m_1, \dots, m_p)$ is the vector of means and Σ is the variance-covariance matrix of the multivariate normal distribution. The shortcut notation for this density is

$$\mathbf{X} = N_p(\mathbf{m}, \Sigma)$$

Univariate normal distribution

When $p = 1$, the one-dimensional vector $\mathbf{X} = X_1$ has the normal distribution with mean m and variance σ^2

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-m)^2/(2\sigma^2)} \quad -\infty < x < \infty$$

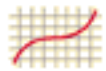
*Bivariate
normal
distribution*

When $p = 2$, $\mathbf{X} = (X_1, X_2)$ has the bivariate normal distribution with a two-dimensional vector of means, $\mathbf{m} = (m_1, m_2)$ and covariance matrix

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix}$$

The correlation between the two random variables is given by

$$\rho = \frac{\sigma_{21}}{\sigma_1 \sigma_2}$$



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6.5.4.3. Hotelling's T squared

Hotelling's T^2 distribution

A multivariate method that is the multivariate counterpart of Student's- t and which also forms the basis for certain multivariate control charts is based on Hotelling's T^2 distribution, which was introduced by [Hotelling \(1947\)](#).

Univariate t -test for mean

Recall, from [Section 1.3.5.2](#),

$$t = \frac{\bar{x} - \mu}{s/\sqrt{n}}$$

has a t distribution provided that X is normally distributed, and can be used as long as X doesn't differ greatly from a normal distribution. If we wanted to test the hypothesis that $\mu = \mu_0$, we would then have

$$t = \frac{\bar{x} - \mu_0}{s/\sqrt{n}}$$

so that

$$\begin{aligned} t^2 &= (\bar{x} - \mu_0)^2 / (s^2/n) \\ &= n(\bar{x} - \mu_0)(s^2)^{-1}(\bar{x} - \mu_0) \end{aligned}$$

Generalize to p variables

When t^2 is generalized to p variables it becomes

$$T^2 = n(\bar{\mathbf{x}} - \boldsymbol{\mu}_0)S^{-1}(\bar{\mathbf{x}} - \boldsymbol{\mu}_0)$$

with

$$\bar{\mathbf{x}} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_p \end{bmatrix} \quad \boldsymbol{\mu}_0 = \begin{bmatrix} \mu_1^0 \\ \mu_2^0 \\ \vdots \\ \mu_p^0 \end{bmatrix}$$

S^{-1} is the inverse of the sample variance-covariance matrix, S , and n is the sample size upon which each \bar{x}_i , $i = 1, 2, \dots, p$, is based. (The

diagonal elements of S are the variances and the off-diagonal elements are the covariances for the p variables. This is discussed further in [Section 6.5.4.3.1.](#))

Distribution of T^2

It is well known that when $\mu = \mu_0$

$$T^2 \sim \frac{p(n-1)}{n-p} F_{(p, n-p)}$$

with $F_{(p, n-p)}$ representing the [F distribution](#) with p degrees of freedom for the numerator and $n - p$ for the denominator. Thus, if μ were specified to be μ_0 , this could be tested by taking a single p -variate sample of size n , then computing T^2 and comparing it with

$$\frac{p(n-1)}{n-p} F_{\alpha(p, n-p)}$$

for a suitably chosen α .

Result does not apply directly to multivariate Shewhart-type charts

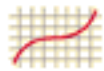
Although this result applies to hypothesis testing, it does not apply directly to multivariate Shewhart-type charts (for which there is no μ_0), although the result might be used as an approximation when a large sample is used and data are in subgroups, with the upper control limit (UCL) of a chart based on the approximation.

Three-sigma limits from univariate control chart

When a univariate control chart is used for Phase I (analysis of historical data), and subsequently for Phase II (real-time process monitoring), the general form of the control limits is the same for each phase, although this need not be the case. Specifically, three-sigma limits are used in the univariate case, which skirts the relevant distribution theory for each Phase.

Selection of different control limit forms for each Phase

Three-sigma units are generally not used with multivariate charts, however, which makes the selection of different control limit forms for each Phase (based on the relevant distribution theory), a natural choice.



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6.5.4.3.1. T² Chart for Subgroup Averages -- Phase I

Estimate μ with $\bar{\bar{x}}$

Since μ is generally unknown, it is necessary to estimate μ analogous to the way that μ is estimated when an \bar{X} chart is used. Specifically, when there are rational subgroups, μ is estimated by $\bar{\bar{x}}$, with

$$\bar{\bar{x}} = \begin{bmatrix} \bar{\bar{x}}_1 \\ \bar{\bar{x}}_2 \\ \vdots \\ \bar{\bar{x}}_p \end{bmatrix}$$

Obtaining the $\bar{\bar{x}}_i$

Each $\bar{\bar{x}}_i$, $i = 1, 2, \dots, p$, is obtained the same way as with an \bar{X} chart, namely, by taking k subgroups of size n and computing

$$\bar{\bar{x}}_i = \left(\frac{1}{k}\right) \sum_{l=1}^k \bar{x}_{il}$$

Here \bar{x}_{il} is used to denote the average for the l th subgroup of the i th variable. That is,

$$\bar{x}_{il} = \sum_{r=1}^n x_{ilr}$$

with x_{ilr} denoting the r th observation (out of n) for the i th variable in the l th subgroup.

Estimating the variances and covariances

The variances and covariances are similarly averaged over the subgroups. Specifically, the s_{ij} elements of the variance-covariance matrix S are obtained as

$$s_{ij} = \left(\frac{1}{k}\right) \sum_{l=1}^k s_{ijl}$$

with s_{ijl} for $i \neq j$ denoting the sample covariance between variables X_i and X_j for the l th subgroup, and s_{ij} for $i = j$ denotes the sample variance of X_i . The variances $s_{ii}^2 (= s_{iil})$ for subgroup l and for variables $i = 1, 2, \dots, p$ are computed as

$$\frac{1}{n-1} \sum_{r=1}^n (x_{ilr} - \bar{x}_{il})^2.$$

Similarly, the covariances s_{ijl} between variables X_i and X_j for subgroup l are computed as

$$\frac{1}{n-1} \sum_{r=1}^n (x_{ilr} - \bar{x}_{il})(x_{jlr} - \bar{x}_{jl}).$$

Compare T^2 against control values

As with an \bar{X} chart (or any other chart), the k subgroups would be tested for control by computing k values of T^2 and comparing each against the UCL. If any value falls above the UCL (there is no lower control limit), the corresponding subgroup would be investigated.

Formula for plotted T^2 values

Thus, one would plot

$$T_j^2 = n(\bar{x}^{(j)} - \bar{\bar{x}})' S_p^{-1} (\bar{x}^{(j)} - \bar{\bar{x}})$$

for the j th subgroup ($j = 1, 2, \dots, k$), with $\bar{\bar{x}}$ denoting a vector with p elements that contains the subgroup averages for each of the p characteristics for the j th subgroup. (S_p^{-1} is the inverse matrix of the "pooled" variance-covariance matrix, S_p , which is obtained by averaging the subgroup variance-covariance matrices over the k subgroups.)

Formula for the upper control limit

Each of the k values of T_j^2 given in the equation above would be compared with

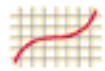
$$UCL = \left(\frac{kn p - kp - np + p}{kn - k - p + 1}\right) F_{\alpha, (p, kn - k - p + 1)}$$

*Lower
control limits*

A lower control limit is generally not used in multivariate control chart applications, although some control chart methods do utilize a LCL. Although a small value for T_j^2 might seem desirable, a value that is very small would likely indicate a problem of some type as we would not expect every element of $\bar{\mathbf{x}}^{(j)}$ to be virtually equal to every element in $\bar{\mathbf{x}}$.

*Delete
out-of-control
points once
cause
discovered
and corrected*

As with any Phase I control chart procedure, if there are any points that plot above the UCL and can be identified as corresponding to out-of-control conditions that have been corrected, the point(s) should be deleted and the UCL recomputed. The remaining points would then be compared with the new UCL and the process continued as long as necessary, remembering that points should be deleted only if their correspondence with out-of-control conditions can be identified and the cause(s) of the condition(s) were removed.



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6.5.4.3.2. T^2 Chart for Subgroup Averages -- Phase II

Phase II requires recomputing S_p and $\bar{\bar{x}}$ and different control limits

Determining the UCL that is to be subsequently applied to *future* subgroups entails recomputing, if necessary, S_p and $\bar{\bar{x}}$, and using a constant and an F -value that are different from the form given [for the Phase I control limits](#). The form is different because different distribution theory is involved since future subgroups are assumed to be independent of the "current" set of subgroups that is used in calculating S_p and $\bar{\bar{x}}$. (The same thing happens with \bar{X} charts; the problem is simply ignored through the use of 3-sigma limits, although a different approach should be used when there is a small number of subgroups -- and the necessary theory has been worked out.)

Illustration

To illustrate, assume that a subgroups had been discarded (with possibly $a = 0$) so that $k - a$ subgroups are used in obtaining S_p and $\bar{\bar{x}}$. We shall let these two values be represented by S_p^* and $\bar{\bar{x}}^*$ to distinguish them from the original values, S_p and $\bar{\bar{x}}$, before any subgroups are deleted. Future values to be plotted on the multivariate chart would then be obtained from

$$n(\bar{\bar{x}}^{(future)} - \bar{\bar{x}}^*)'(S_p^*)^{-1}(\bar{\bar{x}}^{(future)} - \bar{\bar{x}}^*)$$

with $\bar{\bar{x}}^{(future)}$ denoting an arbitrary vector containing the averages for the p characteristics for a single subgroup obtained in the future. Each of these future values would be plotted on the multivariate chart and compared with

*Phase II
control
limits*

$$UCL = \left(\frac{p(k-a+1)(n-1)}{(k-a)n - k + a - p + 1} \right) F_{\alpha, (p, (k-a)n - k + a - p + 1)}$$

with a denoting the number of the original subgroups that are deleted before computing S_p^* and $\bar{\bar{x}}^*$. Notice that the equation for the control limits for Phase II given here does *not* reduce to [the equation for the control limits for Phase I](#) when $a = 0$, nor should we expect it to since the Phase I UCL is used when testing for control of the entire *set* of subgroups that is used in computing S_p and $\bar{\bar{x}}$.

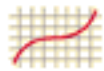
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6.5.4.3.3. Chart for Individual Observations -- Phase I

Multivariate individual control charts

Control charts for multivariate individual observations can be constructed, just as charts can be constructed for [univariate individual observations](#).

Constructing the control chart

Assume there are m historical multivariate observations to be tested for control, so that $Q_j, j = 1, 2, \dots, m$ are computed, with

$$Q_j = (x - \bar{x}_m)' S_m^{-1} (x - \bar{x}_m)$$

Control limits

Each value of Q_j is compared against control limits of

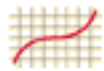
$$LCL = \left(\frac{(m-1)^2}{m} \right) B \left(1 - \frac{\alpha}{2}, \frac{p}{2}, \frac{m-p-1}{2} \right)$$

$$UCL = \left(\frac{(m-1)^2}{m} \right) B \left(\frac{\alpha}{2}, \frac{p}{2}, \frac{m-p-1}{2} \right)$$

with $B(\cdot)$ denoting the [beta distribution](#) with parameters $p/2$ and $(m-p-1)/2$. These limits are due to Tracy, Young and Mason (1992). Note that a LCL is stated, unlike the other multivariate control chart procedures given in this section. Although interest will generally be centered at the UCL, a value of Q below the LCL should also be investigated, as this could signal problems in data recording.

Delete points if special cause(s) are identified and corrected

As in the case when subgroups are used, if any points plot outside these control limits and special cause(s) that were subsequently removed can be identified, the point(s) would be deleted and the control limits recomputed, making the appropriate adjustments on the degrees of freedom, and re-testing the remaining points against the new limits.



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6.5.4.3.4. Chart for Individual Observations -- Phase II

*Control
limits*

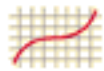
In Phase II, each value of Q_j would be plotted against the UCL of

$$\frac{p(m+1)(m-1)}{m^2 - mp} F_{\alpha, (p, m-p)}$$

with, as before, p denoting the number of characteristics.

*Further
Information*

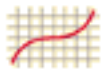
The control limit expressions given in this section and the immediately preceding sections are given in [Ryan \(2000, Chapter 9\)](#).

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6.5.4.3.5. Charts for Controlling Multivariate Variability

No satisfactory charts for multivariate variability

Unfortunately, there are no charts for controlling multivariate variability, with either subgroups or individual observations, that are simple, easy-to-understand and implement, and statistically defensible. Methods based on the generalized variance have been proposed for subgroup data, but such methods have been criticized by [Ryan \(2000, Section 9.4\)](#) and some references cited therein. For individual observations, the multivariate analogue of a univariate moving range chart might be considered as an estimator of the variance-covariance matrix for Phase I, although the distribution of the estimator is unknown.

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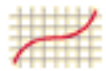
6.5.4.3.6. Constructing Multivariate Charts

Multivariate control charts not commonly available in statistical software

Although control charts were originally constructed and maintained by hand, it would be extremely impractical to try to do that with the chart procedures that were presented in Sections 6.5.4.3.1-6.5.4.3.4.

Unfortunately, the well-known statistical software packages do not have capability for the four procedures just outlined. However, [Dataplot](#), which is used for case studies and tutorials throughout this e-Handbook, does have that capability.

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6.5.5. Principal Components

Dimension reduction tool

A Multivariate Analysis problem could start out with a substantial number of correlated variables. **Principal Component Analysis** is a dimension-reduction tool that can be used advantageously in such situations. Principal component analysis aims at reducing a large set of variables to a small set that still contains most of the information in the large set.

Principal factors

The technique of principal component analysis enables us to create and use a reduced set of variables, which are called *principal factors*. A reduced set is much easier to analyze and interpret. To study a data set that results in the estimation of roughly 500 parameters may be difficult, but if we could reduce these to 5 it would certainly make our day. We will show in what follows how to achieve substantial dimension reduction.

Inverse transformation not possible

While these principal factors represent or replace one or more of the original variables, it should be noted that they are not just a one-to-one transformation, so inverse transformations are not possible.

Original data matrix

To shed a light on the structure of principal components analysis, let us consider a multivariate data matrix \mathbf{X} , with n rows and p columns. The p elements of each row are scores or measurements on a subject such as height, weight and age.

Linear function that maximizes variance

Next, *standardize* the \mathbf{X} matrix so that each column mean is 0 and each column variance is 1. Call this matrix \mathbf{Z} . Each column is a vector variable, z_i , $i = 1, \dots, p$. The main idea behind principal component analysis is to derive a linear function \mathbf{y} for each of the vector variables z_i . This linear function possesses an extremely important property; namely, its variance is maximized.

Linear function is component of z

This linear function is referred to as a component of z . To illustrate the computation of a single element for the j th y vector, consider the product $y = z v'$ where v' is a column vector of V and V is a $p \times p$ coefficient matrix that carries the p -element variable z into the derived n -element variable y . V is known as the eigen vector matrix. The dimension of z is $1 \times p$, the dimension of v' is $p \times 1$. The scalar algebra for the component score for the i th individual of $y_j, j = 1, \dots, p$ is:

$$y_{ji} = v'_{1i}z_{1i} + v'_{2i}z_{2i} + \dots + v'_{pi}z_{pi}$$

This becomes in matrix notation for all of the y :

$$Y = ZV$$

Mean and dispersion matrix of y

The mean of y is $m_y = V'm_z = 0$, because $m_z = 0$.

The dispersion matrix of y is

$$D_y = V'D_zV = V'RV$$

R is correlation matrix

Now, it can be shown that the dispersion matrix D_z of a standardized variable is a correlation matrix. Thus R is the correlation matrix for z .

Number of parameters to estimate increases rapidly as p increases

At this juncture you may be tempted to say: "so what?". To answer this let us look at the intercorrelations among the elements of a vector variable. The number of parameters to be estimated for a p -element variable is

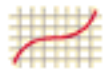
- p means
- p variances
- $(p^2 - p)/2$ covariances
- for a total of $2p + (p^2 - p)/2$ parameters.

So

- If $p = 2$, there are 5 parameters
- If $p = 10$, there are 65 parameters
- If $p = 30$, there are 495 parameters

Uncorrelated variables require no covariance estimation

All these parameters must be estimated and interpreted. That is a herculean task, to say the least. Now, if we could transform the data so that we obtain a vector of uncorrelated variables, life becomes much more bearable, since there are no covariances.



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6.5.5. [Principal Components](#)

6.5.5.1. Properties of Principal Components

Orthogonalizing Transformations

Transformation from \mathbf{z} to \mathbf{y}

The equation $\mathbf{y} = \mathbf{V}'\mathbf{z}$ represents a transformation, where \mathbf{y} is the transformed variable, \mathbf{z} is the original standardized variable and \mathbf{V} is the premultiplier to go from \mathbf{z} to \mathbf{y} .

Orthogonal transformations simplify things

To produce a transformation vector for \mathbf{y} for which the elements are uncorrelated is the same as saying that we want \mathbf{V} such that \mathbf{D}_y is a diagonal matrix. That is, all the off-diagonal elements of \mathbf{D}_y must be zero. This is called an *orthogonalizing transformation*.

Infinite number of values for \mathbf{V}

There are an infinite number of values for \mathbf{V} that will produce a diagonal \mathbf{D}_y for any correlation matrix \mathbf{R} . Thus the mathematical problem "find a unique \mathbf{V} such that \mathbf{D}_y is diagonal" cannot be solved as it stands. A number of famous statisticians such as Karl Pearson and Harold Hotelling pondered this problem and suggested a "variance maximizing" solution.

Principal components maximize variance of the transformed elements, one by one

Hotelling (1933) derived the "principal components" solution. It proceeds as follows: for the first principal component, which will be the first element of \mathbf{y} and be defined by the coefficients in the first column of \mathbf{V} , (denoted by \mathbf{v}_1), we want a solution such that the variance of \mathbf{y}_1 will be maximized.

Constrain \mathbf{v} to generate a unique solution

The constraint on the numbers in \mathbf{v}_1 is that the sum of the squares of the coefficients equals 1. Expressed mathematically, we wish to maximize

$$\frac{1}{N} \sum_{i=1}^M y_{1i}^2$$

where

$$y_{1i} = \mathbf{v}_1' \mathbf{z}_i$$

and $\mathbf{v}_1' \mathbf{v}_1 = 1$ (this is called "normalizing " \mathbf{v}_1).

Computation of first principal component from \mathbf{R} and \mathbf{v}_1

Substituting the middle equation in the first yields

$$\frac{1}{N} \sum_{i=1}^M y_{1i}^2 = \mathbf{v}_1' \mathbf{R} \mathbf{v}_1$$

where \mathbf{R} is the correlation matrix of \mathbf{Z} , which, in turn, is the standardized matrix of \mathbf{X} , the original data matrix. Therefore, we want to maximize $\mathbf{v}_1' \mathbf{R} \mathbf{v}_1$ subject to $\mathbf{v}_1' \mathbf{v}_1 = 1$.

The eigenstructure

Lagrange multiplier approach

Let

$$\phi_1 = \mathbf{v}_1' \mathbf{R} \mathbf{v}_1 - \lambda_1 (\mathbf{v}_1' \mathbf{v}_1 - 1)$$

>

introducing the restriction on \mathbf{v}_1 via the Lagrange multiplier approach. It can be shown ([T.W. Anderson, 1958, page 347](#), theorem 8) that the vector of partial derivatives is

$$\frac{\partial \phi_1}{\partial \mathbf{v}_1} = 2\mathbf{R} \mathbf{v}_1 - 2\lambda_1 \mathbf{v}_1$$

and setting this equal to zero, dividing out 2 and factoring gives

$$(\mathbf{R} - \lambda_1 \mathbf{I})\mathbf{v}_1 = 0$$

This is known as "the problem of the eigenstructure of \mathbf{R} ".

*Set of p
homogeneous
equations*

The partial differentiation resulted in a set of p homogeneous equations, which may be written in matrix form as follows

$$\begin{bmatrix} (1-\lambda_i) & r_{12} & \cdots & r_{1p} \\ r_{21} & (1-\lambda_i) & \cdots & r_{2p} \\ \vdots & \vdots & & \vdots \\ r_{p1} & r_{p2} & \cdots & (1-\lambda_i) \end{bmatrix} \begin{bmatrix} v_{1i} \\ v_{2i} \\ \vdots \\ v_{pi} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The characteristic equation

*Characteristic
equation of \mathbf{R} is
a polynomial of
degree p*

The characteristic equation of \mathbf{R} is a polynomial of degree p , which is obtained by expanding the determinant of

$$|\mathbf{R} - \lambda \mathbf{I}| = \begin{vmatrix} r_{11} - \lambda & & \cdots & r_{1p} \\ r_{21} & r_{22} - \lambda & \cdots & r_{2p} \\ \vdots & \vdots & & \vdots \\ r_{p1} & r_{p2} & \cdots & r_{pp} - \lambda \end{vmatrix} = 0$$

and solving for the roots $\lambda_j, j = 1, 2, \dots, p$.

*Largest
eigenvalue*

Specifically, the largest eigenvalue, λ_1 , and its associated vector, \mathbf{v}_1 , are required. Solving for this eigenvalue and vector is another mammoth numerical task that can realistically only be performed by a computer. In general, software is involved and the algorithms are complex.

*Remainig p
eigenvalues*

After obtaining the first eigenvalue, the process is repeated until all p eigenvalues are computed.

Full eigenstructure of \mathbf{R}

To succinctly define the full eigenstructure of \mathbf{R} , we introduce another matrix \mathbf{L} , which is a diagonal matrix with λ_j in the j th position on the diagonal. Then the full eigenstructure of \mathbf{R} is given as

$$\mathbf{R}\mathbf{V} = \mathbf{V}\mathbf{L}$$

where

$$\mathbf{V}'\mathbf{V} = \mathbf{V}\mathbf{V}' = \mathbf{I}$$

and

$$\mathbf{V}'\mathbf{R}\mathbf{V} = \mathbf{L} = \mathbf{D}_y$$

Principal Factors

Scale to zero means and unit variances

It was mentioned before that it is helpful to scale any transformation \mathbf{y} of a vector variable \mathbf{z} so that its elements have zero means and unit variances. Such a standardized transformation is called a *factoring* of \mathbf{z} , or of \mathbf{R} , and each linear component of the transformation is called a factor.

Deriving unit variances for principal components

Now, the principal components already have zero means, but their variances are not 1; in fact, they are the eigenvalues, comprising the diagonal elements of \mathbf{L} . It is possible to derive the principal factor with unit variance from the principal component as follows

$$f_i = \frac{y_i}{\sqrt{\lambda}}$$

or for all factors:

$$\mathbf{f} = \mathbf{L}^{-1/2}\mathbf{y}$$

substituting $\mathbf{V}'\mathbf{z}$ for \mathbf{y} we have

$$\mathbf{f} = \mathbf{L}^{-1/2}\mathbf{V}'\mathbf{z} = \mathbf{B}'\mathbf{z}$$

where

$$\mathbf{B} = \mathbf{V}\mathbf{L}^{-1/2}$$

B matrix

The matrix \mathbf{B} is then the matrix of *factor score coefficients* for principal factors.

How many Eigenvalues?

Dimensionality of the set of factor scores The number of eigenvalues, N , used in the final set determines the dimensionality of the set of factor scores. For example, if the original test consisted of 8 measurements on 100 subjects, and we extract 2 eigenvalues, the set of factor scores is a matrix of 100 rows by 2 columns.

Eigenvalues greater than unity Each column or principal factor should represent a number of original variables. Kaiser (1966) suggested a rule-of-thumb that takes as a value for N , the number of eigenvalues larger than unity.

Factor Structure

Factor structure matrix S The primary interpretative device in principal components is the factor structure, computed as

$$\mathbf{S} = \mathbf{V}\mathbf{L}^{1/2}$$

S is a matrix whose elements are the correlations between the principal components and the variables. If we retain, for example, two eigenvalues, meaning that there are two principal components, then the S matrix consists of two columns and p (number of variables) rows.

Table showing relation between variables and principal components

	Principal Component	
Variable	1	2
1	r_{11}	r_{12}
2	r_{21}	r_{22}
3	r_{31}	r_{32}
4	r_{41}	r_{42}

The r_{ij} are the correlation coefficients between variable i and principal component j , where i ranges from 1 to 4 and j from 1 to 2.

The communality SS' is the source of the "explained" correlations among the variables. Its diagonal is called "the communality".

Rotation

Factor analysis If this correlation matrix, i.e., the factor structure matrix, does not help much in the interpretation, it is possible to rotate the axis of the principal components. This may result in the polarization of the correlation coefficients. Some practitioners refer to rotation after generating the factor structure as *factor analysis*.

Varimax rotation

A popular scheme for rotation was suggested by Henry Kaiser in 1958. He produced a method for orthogonal rotation of factors, called the varimax rotation, which cleans up the factors as follows:

for each factor, high loadings (correlations) will result for a few variables; the rest will be near zero.

Example

The following computer output from a principal component analysis on a 4-variable data set, followed by varimax rotation of the factor structure, will illustrate his point.

Variable	Before Rotation		After Rotation	
	Factor 1	Factor 2	Factor 1	Factor 2
1	.853	-.989	.997	.058
2	.634	.762	.089	.987
3	.858	-.498	.989	.076
4	.633	.736	.103	.965

Communality*Formula for communality statistic*

A measure of how well the selected factors (principal components) "explain" the variance of each of the variables is given by a statistic called *communality*. This is defined by

$$h_k^2 = \sum_{i=1}^k S_{ki}^2$$

Explanation of communality statistic

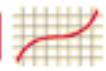
That is: the square of the correlation of variable k with factor i gives the part of the variance accounted for by that factor. The sum of these squares for n factors is the communality, or explained variance for that variable (row).

Roadmap to solve the V matrix

*Main steps to
obtaining
eigenstructure
for a
correlation
matrix*

In summary, here are the main steps to obtain the eigenstructure for a correlation matrix.

1. Compute \mathbf{R} , the correlation matrix of the original data. \mathbf{R} is also the correlation matrix of the standardized data.
2. Obtain the characteristic equation of \mathbf{R} which is a polynomial of degree p (the number of variables), obtained from expanding the determinant of $|\mathbf{R}-\lambda \mathbf{I}| = 0$ and solving for the roots λ_i , that is: $\lambda_1, \lambda_2, \dots, \lambda_p$.
3. Then solve for the columns of the \mathbf{V} matrix, ($\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_p$). The roots, λ_i , are called the *eigenvalues* (or latent values). The columns of \mathbf{V} are called the *eigenvectors*.



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6.5.5. [Principal Components](#)

6.5.5.2. Numerical Example

*Calculation
of principal
components
example*

A **numerical example** may clarify the mechanics of principal component analysis.

*Sample data
set*

Let us analyze the following 3-variate dataset with 10 observations. Each observation consists of 3 measurements on a wafer: thickness, horizontal displacement and vertical displacement.

$$X = \begin{bmatrix} 7 & 4 & 3 \\ 4 & 1 & 8 \\ 6 & 3 & 5 \\ 8 & 6 & 1 \\ 8 & 5 & 7 \\ 7 & 2 & 9 \\ 5 & 3 & 3 \\ 9 & 5 & 8 \\ 7 & 4 & 5 \\ 8 & 2 & 2 \end{bmatrix}$$

Compute the correlation matrix First compute the correlation matrix

$$R = \begin{bmatrix} 1.00 & .67 & -.10 \\ .67 & 1.00 & -.29 \\ -.10 & -.29 & 1.00 \end{bmatrix}$$

Solve for the roots of \mathbf{R} Next solve for the roots of \mathbf{R} , using software

	λ value	proportion
1	1.769	.590
2	.927	.899
3	.304	1.000

Notice that

- Each eigenvalue satisfies $|\mathbf{R} - \lambda \mathbf{I}| = 0$.
- The sum of the eigenvalues = $3 = p$, which is equal to the trace of \mathbf{R} (i.e., the sum of the main diagonal elements).
- The determinant of \mathbf{R} is the product of the eigenvalues.
- The product is $\lambda_1 \times \lambda_2 \times \lambda_3 = .499$.

Compute the first column of the \mathbf{V} matrix Substituting the first eigenvalue of 1.769 and \mathbf{R} in the appropriate equation we obtain

$$\begin{bmatrix} -.769 & .67 & -.10 \\ .67 & -.769 & -.29 \\ -.10 & -.29 & -.769 \end{bmatrix} \cdot \begin{bmatrix} v_{11} \\ v_{21} \\ v_{31} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

This is the matrix expression for 3 homogeneous equations with 3 unknowns and yields the first column of \mathbf{V} : .64 .69 -.34 (again, a computerized solution is indispensable).

Compute the remaining columns of the V matrix

Repeating this procedure for the other 2 eigenvalues yields the matrix **V**

$$\mathbf{V} = \begin{bmatrix} .64 & .38 & -.66 \\ .69 & .10 & .72 \\ -.34 & .91 & .20 \end{bmatrix}$$

Notice that if you multiply **V** by its transpose, the result is an identity matrix, $\mathbf{V}'\mathbf{V}=\mathbf{I}$.

Compute the L^{1/2} matrix

Now form the matrix $\mathbf{L}^{1/2}$, which is a diagonal matrix whose elements are the square roots of the eigenvalues of **R**. Then obtain **S**, the factor structure, using $\mathbf{S} = \mathbf{V} \mathbf{L}^{1/2}$

$$\begin{bmatrix} .64 & .38 & -.66 \\ .69 & .10 & .72 \\ -.34 & .91 & .20 \end{bmatrix} \begin{bmatrix} 1.33 & 0 & 0 \\ 0 & .96 & 0 \\ 0 & 0 & .55 \end{bmatrix} = \begin{bmatrix} .85 & .37 & -.37 \\ .91 & .10 & .40 \\ -.45 & .88 & .11 \end{bmatrix}$$

So, for example, .91 is the correlation between variable 2 and the first principal component.

Compute the communality

Next compute the communality, using the first two eigenvalues only

$$\mathbf{SS}' = \begin{bmatrix} .85 & .37 \\ .91 & .09 \\ -.45 & .88 \end{bmatrix} \begin{bmatrix} .85 & .91 & -.45 \\ .37 & .09 & .88 \end{bmatrix} = \begin{bmatrix} .8662 & .8140 & -.0606 \\ .8140 & .8420 & -.3321 \\ -.0606 & -.3321 & .9876 \end{bmatrix}$$

Diagonal elements report how much of the variability is explained

Communality consists of the diagonal elements.

var	
1	.8662
2	.8420
3	.9876

This means that the first two principal components "explain" 86.62% of the first variable, 84.20 % of the second variable, and 98.76% of the third.

Compute the coefficient matrix

The coefficient matrix, **B**, is formed using the reciprocals of the diagonals of $\mathbf{L}^{1/2}$

$$\mathbf{B} = \mathbf{V}\mathbf{L}^{-1/2} = \begin{bmatrix} .48 & .40 & -.18 \\ .52 & .10 & 1.31 \\ -.26 & .95 & .37 \end{bmatrix}$$

Compute the principal factors

Finally, we can compute the factor scores from \mathbf{ZB} , where **Z** is **X** converted to standard score form. These columns are the *principal factors*.

$$\mathbf{F} = \mathbf{ZB} = \begin{bmatrix} .41 & -.69 & .06 \\ -2.11 & .07 & .63 \\ -.46 & -.32 & .30 \\ 1.62 & -1.00 & .70 \\ .70 & 1.09 & .65 \\ -.86 & 1.32 & -.85 \\ -.60 & -1.31 & .86 \\ .94 & 1.72 & -.04 \\ .22 & .03 & .34 \\ .15 & -.91 & -2.65 \end{bmatrix}$$

Principal factors control chart

These factors can be plotted against the indices, which could be times. If time is used, *the resulting plot is an example of a principal factors control chart.*

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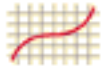
6.6. Case Studies in Process Monitoring

*Detailed,
Realistic
Examples*

The general points of the first five sections are illustrated in this section using data from physical science and engineering applications. Each example is presented step-by-step in the text, and is often cross-linked with the relevant sections of the chapter describing the analysis in general. Each analysis can also be repeated using a worksheet linked to the appropriate Dataplot macros. The worksheet is also linked to the step-by-step analysis presented in the text for easy reference.

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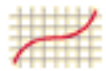
6.6.1. Lithography Process

*Lithography
Process*

This case study illustrates the use of control charts in analyzing a lithography process.

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2. [Graphical Representation of the Data](#)
3. [Subgroup Analysis](#)
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6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

6.6.1. [Lithography Process](#)

6.6.1.1. Background and Data

Case Study for SPC in Batch Processing Environment

Semiconductor processing creates multiple sources of variability to monitor

One of the assumptions in using classical Shewhart SPC charts is that the only source of variation is from part to part (or within subgroup variation). This is the case for most continuous processing situations. However, many of today's processing situations have different sources of variation. The semiconductor industry is one of the areas where the processing creates multiple sources of variation.

In semiconductor processing, the basic experimental unit is a silicon wafer. Operations are performed on the wafer, but individual wafers can be grouped multiple ways. In the diffusion area, up to 150 wafers are processed in one time in a diffusion tube. In the etch area, single wafers are processed individually. In the lithography area, the light exposure is done on sub-areas of the wafer. There are many times during the production of a computer chip where the experimental unit varies and thus there are different sources of variation in this batch processing environment.

THE following is a case study of a lithography process. Five sites are measured on each wafer, three wafers are measured in a cassette (typically a grouping of 24 - 25 wafers) and thirty cassettes of wafers are used in the study. The width of a line is the measurement under study. There are two line width variables. The first is the original data and the second has been cleaned up somewhat. This case study uses the raw data. The entire data table is 450 rows long with six columns.

Case study
data: wafer
line width
measurements

			Raw		Cleaned
	Cassette	Wafer	Line	Sequence	Line
		Site	Width		Width
	=====				
1	1	Top	3.199275	1	3.197275
1	1	Lef	2.253081	2	2.249081
1	1	Cen	2.074308	3	2.068308
1	1	Rgt	2.418206	4	2.410206
1	1	Bot	2.393732	5	2.383732
1	2	Top	2.654947	6	2.642947
1	2	Lef	2.003234	7	1.989234
1	2	Cen	1.861268	8	1.845268
1	2	Rgt	2.136102	9	2.118102
1	2	Bot	1.976495	10	1.956495
1	3	Top	2.887053	11	2.865053
1	3	Lef	2.061239	12	2.037239
1	3	Cen	1.625191	13	1.599191
1	3	Rgt	2.304313	14	2.276313
1	3	Bot	2.233187	15	2.203187
2	1	Top	3.160233	16	3.128233
2	1	Lef	2.518913	17	2.484913
2	1	Cen	2.072211	18	2.036211
2	1	Rgt	2.287210	19	2.249210
2	1	Bot	2.120452	20	2.080452
2	2	Top	2.063058	21	2.021058
2	2	Lef	2.217220	22	2.173220
2	2	Cen	1.472945	23	1.426945
2	2	Rgt	1.684581	24	1.636581
2	2	Bot	1.900688	25	1.850688
2	3	Top	2.346254	26	2.294254
2	3	Lef	2.172825	27	2.118825
2	3	Cen	1.536538	28	1.480538
2	3	Rgt	1.966630	29	1.908630
2	3	Bot	2.251576	30	2.191576
3	1	Top	2.198141	31	2.136141
3	1	Lef	1.728784	32	1.664784
3	1	Cen	1.357348	33	1.291348
3	1	Rgt	1.673159	34	1.605159
3	1	Bot	1.429586	35	1.359586
3	2	Top	2.231291	36	2.159291
3	2	Lef	1.561993	37	1.487993
3	2	Cen	1.520104	38	1.444104
3	2	Rgt	2.066068	39	1.988068

6.6.1.1. Background and Data

3	2	Bot	1.777603	40	1.697603
3	3	Top	2.244736	41	2.162736
3	3	Lef	1.745877	42	1.661877
3	3	Cen	1.366895	43	1.280895
3	3	Rgt	1.615229	44	1.527229
3	3	Bot	1.540863	45	1.450863
4	1	Top	2.929037	46	2.837037
4	1	Lef	2.035900	47	1.941900
4	1	Cen	1.786147	48	1.690147
4	1	Rgt	1.980323	49	1.882323
4	1	Bot	2.162919	50	2.062919
4	2	Top	2.855798	51	2.753798
4	2	Lef	2.104193	52	2.000193
4	2	Cen	1.919507	53	1.813507
4	2	Rgt	2.019415	54	1.911415
4	2	Bot	2.228705	55	2.118705
4	3	Top	3.219292	56	3.107292
4	3	Lef	2.900430	57	2.786430
4	3	Cen	2.171262	58	2.055262
4	3	Rgt	3.041250	59	2.923250
4	3	Bot	3.188804	60	3.068804
5	1	Top	3.051234	61	2.929234
5	1	Lef	2.506230	62	2.382230
5	1	Cen	1.950486	63	1.824486
5	1	Rgt	2.467719	64	2.339719
5	1	Bot	2.581881	65	2.451881
5	2	Top	3.857221	66	3.725221
5	2	Lef	3.347343	67	3.213343
5	2	Cen	2.533870	68	2.397870
5	2	Rgt	3.190375	69	3.052375
5	2	Bot	3.362746	70	3.222746
5	3	Top	3.690306	71	3.548306
5	3	Lef	3.401584	72	3.257584
5	3	Cen	2.963117	73	2.817117
5	3	Rgt	2.945828	74	2.797828
5	3	Bot	3.466115	75	3.316115
6	1	Top	2.938241	76	2.786241
6	1	Lef	2.526568	77	2.372568
6	1	Cen	1.941370	78	1.785370
6	1	Rgt	2.765849	79	2.607849
6	1	Bot	2.382781	80	2.222781
6	2	Top	3.219665	81	3.057665
6	2	Lef	2.296011	82	2.132011
6	2	Cen	2.256196	83	2.090196
6	2	Rgt	2.645933	84	2.477933
6	2	Bot	2.422187	85	2.252187

6.6.1.1. Background and Data

6	3	Top	3.180348	86	3.008348
6	3	Lef	2.849264	87	2.675264
6	3	Cen	1.601288	88	1.425288
6	3	Rgt	2.810051	89	2.632051
6	3	Bot	2.902980	90	2.722980
7	1	Top	2.169679	91	1.987679
7	1	Lef	2.026506	92	1.842506
7	1	Cen	1.671804	93	1.485804
7	1	Rgt	1.660760	94	1.472760
7	1	Bot	2.314734	95	2.124734
7	2	Top	2.912838	96	2.720838
7	2	Lef	2.323665	97	2.129665
7	2	Cen	1.854223	98	1.658223
7	2	Rgt	2.391240	99	2.19324
7	2	Bot	2.196071	100	1.996071
7	3	Top	3.318517	101	3.116517
7	3	Lef	2.702735	102	2.498735
7	3	Cen	1.959008	103	1.753008
7	3	Rgt	2.512517	104	2.304517
7	3	Bot	2.827469	105	2.617469
8	1	Top	1.958022	106	1.746022
8	1	Lef	1.360106	107	1.146106
8	1	Cen	0.971193	108	0.755193
8	1	Rgt	1.947857	109	1.729857
8	1	Bot	1.643580	110	1.42358
8	2	Top	2.357633	111	2.135633
8	2	Lef	1.757725	112	1.533725
8	2	Cen	1.165886	113	0.939886
8	2	Rgt	2.231143	114	2.003143
8	2	Bot	1.311626	115	1.081626
8	3	Top	2.421686	116	2.189686
8	3	Lef	1.993855	117	1.759855
8	3	Cen	1.402543	118	1.166543
8	3	Rgt	2.008543	119	1.770543
8	3	Bot	2.139370	120	1.899370
9	1	Top	2.190676	121	1.948676
9	1	Lef	2.287483	122	2.043483
9	1	Cen	1.698943	123	1.452943
9	1	Rgt	1.925731	124	1.677731
9	1	Bot	2.057440	125	1.807440
9	2	Top	2.353597	126	2.101597
9	2	Lef	1.796236	127	1.542236
9	2	Cen	1.241040	128	0.985040
9	2	Rgt	1.677429	129	1.419429
9	2	Bot	1.845041	130	1.585041
9	3	Top	2.012669	131	1.750669

6.6.1.1. Background and Data

9	3	Lef	1.523769	132	1.259769
9	3	Cen	0.790789	133	0.524789
9	3	Rgt	2.001942	134	1.733942
9	3	Bot	1.350051	135	1.080051
10	1	Top	2.825749	136	2.553749
10	1	Lef	2.502445	137	2.228445
10	1	Cen	1.938239	138	1.662239
10	1	Rgt	2.349497	139	2.071497
10	1	Bot	2.310817	140	2.030817
10	2	Top	3.074576	141	2.792576
10	2	Lef	2.057821	142	1.773821
10	2	Cen	1.793617	143	1.507617
10	2	Rgt	1.862251	144	1.574251
10	2	Bot	1.956753	145	1.666753
10	3	Top	3.072840	146	2.780840
10	3	Lef	2.291035	147	1.997035
10	3	Cen	1.873878	148	1.577878
10	3	Rgt	2.475640	149	2.177640
10	3	Bot	2.021472	150	1.721472
11	1	Top	3.228835	151	2.926835
11	1	Lef	2.719495	152	2.415495
11	1	Cen	2.207198	153	1.901198
11	1	Rgt	2.391608	154	2.083608
11	1	Bot	2.525587	155	2.215587
11	2	Top	2.891103	156	2.579103
11	2	Lef	2.738007	157	2.424007
11	2	Cen	1.668337	158	1.352337
11	2	Rgt	2.496426	159	2.178426
11	2	Bot	2.417926	160	2.097926
11	3	Top	3.541799	161	3.219799
11	3	Lef	3.058768	162	2.734768
11	3	Cen	2.187061	163	1.861061
11	3	Rgt	2.790261	164	2.462261
11	3	Bot	3.279238	165	2.949238
12	1	Top	2.347662	166	2.015662
12	1	Lef	1.383336	167	1.049336
12	1	Cen	1.187168	168	0.851168
12	1	Rgt	1.693292	169	1.355292
12	1	Bot	1.664072	170	1.324072
12	2	Top	2.385320	171	2.043320
12	2	Lef	1.607784	172	1.263784
12	2	Cen	1.230307	173	0.884307
12	2	Rgt	1.945423	174	1.597423
12	2	Bot	1.907580	175	1.557580
12	3	Top	2.691576	176	2.339576
12	3	Lef	1.938755	177	1.584755

6.6.1.1. Background and Data

12	3	Cen	1.275409	178	0.919409
12	3	Rgt	1.777315	179	1.419315
12	3	Bot	2.146161	180	1.786161
13	1	Top	3.218655	181	2.856655
13	1	Lef	2.912180	182	2.548180
13	1	Cen	2.336436	183	1.970436
13	1	Rgt	2.956036	184	2.588036
13	1	Bot	2.423235	185	2.053235
13	2	Top	3.302224	186	2.930224
13	2	Lef	2.808816	187	2.434816
13	2	Cen	2.340386	188	1.964386
13	2	Rgt	2.795120	189	2.417120
13	2	Bot	2.865800	190	2.485800
13	3	Top	2.992217	191	2.610217
13	3	Lef	2.952106	192	2.568106
13	3	Cen	2.149299	193	1.763299
13	3	Rgt	2.448046	194	2.060046
13	3	Bot	2.507733	195	2.117733
14	1	Top	3.530112	196	3.138112
14	1	Lef	2.940489	197	2.546489
14	1	Cen	2.598357	198	2.202357
14	1	Rgt	2.905165	199	2.507165
14	1	Bot	2.692078	200	2.292078
14	2	Top	3.764270	201	3.362270
14	2	Lef	3.465960	202	3.061960
14	2	Cen	2.458628	203	2.052628
14	2	Rgt	3.141132	204	2.733132
14	2	Bot	2.816526	205	2.406526
14	3	Top	3.217614	206	2.805614
14	3	Lef	2.758171	207	2.344171
14	3	Cen	2.345921	208	1.929921
14	3	Rgt	2.773653	209	2.355653
14	3	Bot	3.109704	210	2.689704
15	1	Top	2.177593	211	1.755593
15	1	Lef	1.511781	212	1.087781
15	1	Cen	0.746546	213	0.320546
15	1	Rgt	1.491730	214	1.063730
15	1	Bot	1.268580	215	0.838580
15	2	Top	2.433994	216	2.001994
15	2	Lef	2.045667	217	1.611667
15	2	Cen	1.612699	218	1.176699
15	2	Rgt	2.082860	219	1.644860
15	2	Bot	1.887341	220	1.447341
15	3	Top	1.923003	221	1.481003
15	3	Lef	2.124461	222	1.680461
15	3	Cen	1.945048	223	1.499048

6.6.1.1. Background and Data

15	3	Rgt	2.210698	224	1.762698
15	3	Bot	1.985225	225	1.535225
16	1	Top	3.131536	226	2.679536
16	1	Lef	2.405975	227	1.951975
16	1	Cen	2.206320	228	1.750320
16	1	Rgt	3.012211	229	2.554211
16	1	Bot	2.628723	230	2.168723
16	2	Top	2.802486	231	2.340486
16	2	Lef	2.185010	232	1.721010
16	2	Cen	2.161802	233	1.695802
16	2	Rgt	2.102560	234	1.634560
16	2	Bot	1.961968	235	1.491968
16	3	Top	3.330183	236	2.858183
16	3	Lef	2.464046	237	1.990046
16	3	Cen	1.687408	238	1.211408
16	3	Rgt	2.043322	239	1.565322
16	3	Bot	2.570657	240	2.090657
17	1	Top	3.352633	241	2.870633
17	1	Lef	2.691645	242	2.207645
17	1	Cen	1.942410	243	1.456410
17	1	Rgt	2.366055	244	1.878055
17	1	Bot	2.500987	245	2.010987
17	2	Top	2.886284	246	2.394284
17	2	Lef	2.292503	247	1.798503
17	2	Cen	1.627562	248	1.131562
17	2	Rgt	2.415076	249	1.917076
17	2	Bot	2.086134	250	1.586134
17	3	Top	2.554848	251	2.052848
17	3	Lef	1.755843	252	1.251843
17	3	Cen	1.510124	253	1.004124
17	3	Rgt	2.257347	254	1.749347
17	3	Bot	1.958592	255	1.448592
18	1	Top	2.622733	256	2.110733
18	1	Lef	2.321079	257	1.807079
18	1	Cen	1.169269	258	0.653269
18	1	Rgt	1.921457	259	1.403457
18	1	Bot	2.176377	260	1.656377
18	2	Top	3.313367	261	2.791367
18	2	Lef	2.559725	262	2.035725
18	2	Cen	2.404662	263	1.878662
18	2	Rgt	2.405249	264	1.877249
18	2	Bot	2.535618	265	2.005618
18	3	Top	3.067851	266	2.535851
18	3	Lef	2.490359	267	1.956359
18	3	Cen	2.079477	268	1.543477
18	3	Rgt	2.669512	269	2.131512

6.6.1.1. Background and Data

18	3	Bot	2.105103	270	1.565103
19	1	Top	4.293889	271	3.751889
19	1	Lef	3.888826	272	3.344826
19	1	Cen	2.960655	273	2.414655
19	1	Rgt	3.618864	274	3.070864
19	1	Bot	3.562480	275	3.012480
19	2	Top	3.451872	276	2.899872
19	2	Lef	3.285934	277	2.731934
19	2	Cen	2.638294	278	2.082294
19	2	Rgt	2.918810	279	2.360810
19	2	Bot	3.076231	280	2.516231
19	3	Top	3.879683	281	3.317683
19	3	Lef	3.342026	282	2.778026
19	3	Cen	3.382833	283	2.816833
19	3	Rgt	3.491666	284	2.923666
19	3	Bot	3.617621	285	3.047621
20	1	Top	2.329987	286	1.757987
20	1	Lef	2.400277	287	1.826277
20	1	Cen	2.033941	288	1.457941
20	1	Rgt	2.544367	289	1.966367
20	1	Bot	2.493079	290	1.913079
20	2	Top	2.862084	291	2.280084
20	2	Lef	2.404703	292	1.820703
20	2	Cen	1.648662	293	1.062662
20	2	Rgt	2.115465	294	1.527465
20	2	Bot	2.633930	295	2.043930
20	3	Top	3.305211	296	2.713211
20	3	Lef	2.194991	297	1.600991
20	3	Cen	1.620963	298	1.024963
20	3	Rgt	2.322678	299	1.724678
20	3	Bot	2.818449	300	2.218449
21	1	Top	2.712915	301	2.110915
21	1	Lef	2.389121	302	1.785121
21	1	Cen	1.575833	303	0.969833
21	1	Rgt	1.870484	304	1.262484
21	1	Bot	2.203262	305	1.593262
21	2	Top	2.607972	306	1.995972
21	2	Lef	2.177747	307	1.563747
21	2	Cen	1.246016	308	0.630016
21	2	Rgt	1.663096	309	1.045096
21	2	Bot	1.843187	310	1.223187
21	3	Top	2.277813	311	1.655813
21	3	Lef	1.764940	312	1.140940
21	3	Cen	1.358137	313	0.732137
21	3	Rgt	2.065713	314	1.437713
21	3	Bot	1.885897	315	1.255897

6.6.1.1. Background and Data

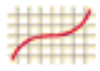
22	1	Top	3.126184	316	2.494184
22	1	Lef	2.843505	317	2.209505
22	1	Cen	2.041466	318	1.405466
22	1	Rgt	2.816967	319	2.178967
22	1	Bot	2.635127	320	1.995127
22	2	Top	3.049442	321	2.407442
22	2	Lef	2.446904	322	1.802904
22	2	Cen	1.793442	323	1.147442
22	2	Rgt	2.676519	324	2.028519
22	2	Bot	2.187865	325	1.537865
22	3	Top	2.758416	326	2.106416
22	3	Lef	2.405744	327	1.751744
22	3	Cen	1.580387	328	0.924387
22	3	Rgt	2.508542	329	1.850542
22	3	Bot	2.574564	330	1.914564
23	1	Top	3.294288	331	2.632288
23	1	Lef	2.641762	332	1.977762
23	1	Cen	2.105774	333	1.439774
23	1	Rgt	2.655097	334	1.987097
23	1	Bot	2.622482	335	1.952482
23	2	Top	4.066631	336	3.394631
23	2	Lef	3.389733	337	2.715733
23	2	Cen	2.993666	338	2.317666
23	2	Rgt	3.613128	339	2.935128
23	2	Bot	3.213809	340	2.533809
23	3	Top	3.369665	341	2.687665
23	3	Lef	2.566891	342	1.882891
23	3	Cen	2.289899	343	1.603899
23	3	Rgt	2.517418	344	1.829418
23	3	Bot	2.862723	345	2.172723
24	1	Top	4.212664	346	3.520664
24	1	Lef	3.068342	347	2.374342
24	1	Cen	2.872188	348	2.176188
24	1	Rgt	3.040890	349	2.342890
24	1	Bot	3.376318	350	2.676318
24	2	Top	3.223384	351	2.521384
24	2	Lef	2.552726	352	1.848726
24	2	Cen	2.447344	353	1.741344
24	2	Rgt	3.011574	354	2.303574
24	2	Bot	2.711774	355	2.001774
24	3	Top	3.359505	356	2.647505
24	3	Lef	2.800742	357	2.086742
24	3	Cen	2.043396	358	1.327396
24	3	Rgt	2.929792	359	2.211792
24	3	Bot	2.935356	360	2.215356
25	1	Top	2.724871	361	2.002871

6.6.1.1. Background and Data

25	1	Lef	2.239013	362	1.515013
25	1	Cen	2.341512	363	1.615512
25	1	Rgt	2.263617	364	1.535617
25	1	Bot	2.062748	365	1.332748
25	2	Top	3.658082	366	2.926082
25	2	Lef	3.093268	367	2.359268
25	2	Cen	2.429341	368	1.693341
25	2	Rgt	2.538365	369	1.800365
25	2	Bot	3.161795	370	2.421795
25	3	Top	3.178246	371	2.436246
25	3	Lef	2.498102	372	1.754102
25	3	Cen	2.445810	373	1.699810
25	3	Rgt	2.231248	374	1.483248
25	3	Bot	2.302298	375	1.552298
26	1	Top	3.320688	376	2.568688
26	1	Lef	2.861800	377	2.107800
26	1	Cen	2.238258	378	1.482258
26	1	Rgt	3.122050	379	2.364050
26	1	Bot	3.160876	380	2.400876
26	2	Top	3.873888	381	3.111888
26	2	Lef	3.166345	382	2.402345
26	2	Cen	2.645267	383	1.879267
26	2	Rgt	3.309867	384	2.541867
26	2	Bot	3.542882	385	2.772882
26	3	Top	2.586453	386	1.814453
26	3	Lef	2.120604	387	1.346604
26	3	Cen	2.180847	388	1.404847
26	3	Rgt	2.480888	389	1.702888
26	3	Bot	1.938037	390	1.158037
27	1	Top	4.710718	391	3.928718
27	1	Lef	4.082083	392	3.298083
27	1	Cen	3.533026	393	2.747026
27	1	Rgt	4.269929	394	3.481929
27	1	Bot	4.038166	395	3.248166
27	2	Top	4.237233	396	3.445233
27	2	Lef	4.171702	397	3.377702
27	2	Cen	3.04394	398	2.247940
27	2	Rgt	3.91296	399	3.114960
27	2	Bot	3.714229	400	2.914229
27	3	Top	5.168668	401	4.366668
27	3	Lef	4.823275	402	4.019275
27	3	Cen	3.764272	403	2.958272
27	3	Rgt	4.396897	404	3.588897
27	3	Bot	4.442094	405	3.632094
28	1	Top	3.972279	406	3.160279
28	1	Lef	3.883295	407	3.069295

6.6.1.1. Background and Data

28	1	Cen	3.045145	408	2.229145
28	1	Rgt	3.51459	409	2.696590
28	1	Bot	3.575446	410	2.755446
28	2	Top	3.024903	411	2.202903
28	2	Lef	3.099192	412	2.275192
28	2	Cen	2.048139	413	1.222139
28	2	Rgt	2.927978	414	2.099978
28	2	Bot	3.15257	415	2.322570
28	3	Top	3.55806	416	2.726060
28	3	Lef	3.176292	417	2.342292
28	3	Cen	2.852873	418	2.016873
28	3	Rgt	3.026064	419	2.188064
28	3	Bot	3.071975	420	2.231975
29	1	Top	3.496634	421	2.654634
29	1	Lef	3.087091	422	2.243091
29	1	Cen	2.517673	423	1.671673
29	1	Rgt	2.547344	424	1.699344
29	1	Bot	2.971948	425	2.121948
29	2	Top	3.371306	426	2.519306
29	2	Lef	2.175046	427	1.321046
29	2	Cen	1.940111	428	1.084111
29	2	Rgt	2.932408	429	2.074408
29	2	Bot	2.428069	430	1.568069
29	3	Top	2.941041	431	2.079041
29	3	Lef	2.294009	432	1.430009
29	3	Cen	2.025674	433	1.159674
29	3	Rgt	2.21154	434	1.343540
29	3	Bot	2.459684	435	1.589684
30	1	Top	2.86467	436	1.992670
30	1	Lef	2.695163	437	1.821163
30	1	Cen	2.229518	438	1.353518
30	1	Rgt	1.940917	439	1.062917
30	1	Bot	2.547318	440	1.667318
30	2	Top	3.537562	441	2.655562
30	2	Lef	3.311361	442	2.427361
30	2	Cen	2.767771	443	1.881771
30	2	Rgt	3.388622	444	2.500622
30	2	Bot	3.542701	445	2.652701
30	3	Top	3.184652	446	2.292652
30	3	Lef	2.620947	447	1.726947
30	3	Cen	2.697619	448	1.801619
30	3	Rgt	2.860684	449	1.962684
30	3	Bot	2.758571	450	1.858571



6. [Process or Product Monitoring and Control](#)

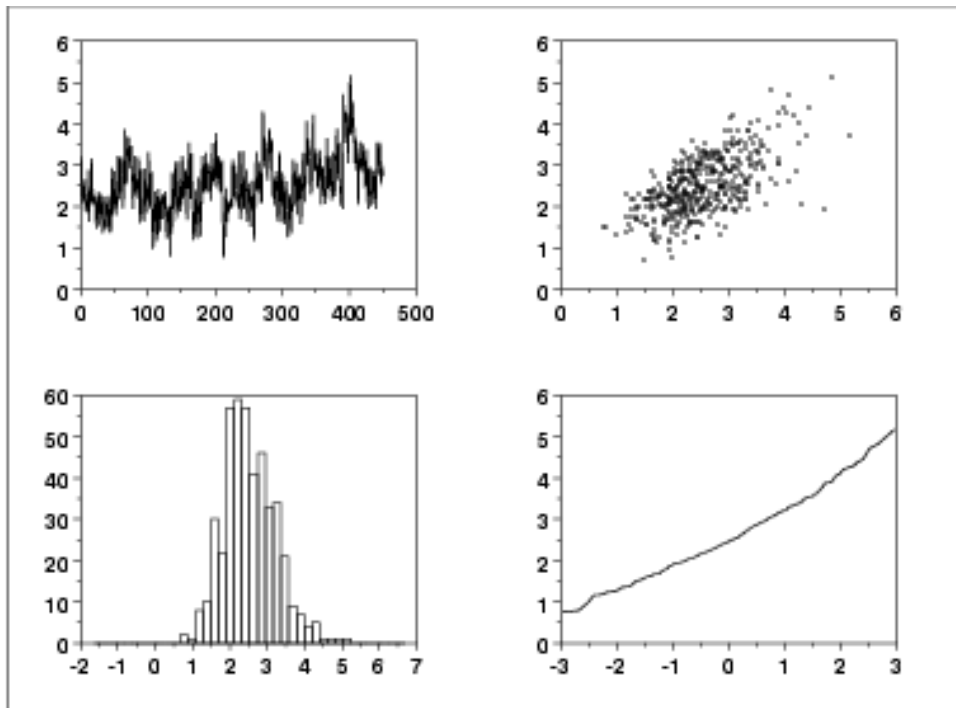
6.6. [Case Studies in Process Monitoring](#)

6.6.1. [Lithography Process](#)

6.6.1.2. Graphical Representation of the Data

The first step in analyzing the data is to generate some simple plots of the response and then of the response versus the various factors.

4-Plot of Data



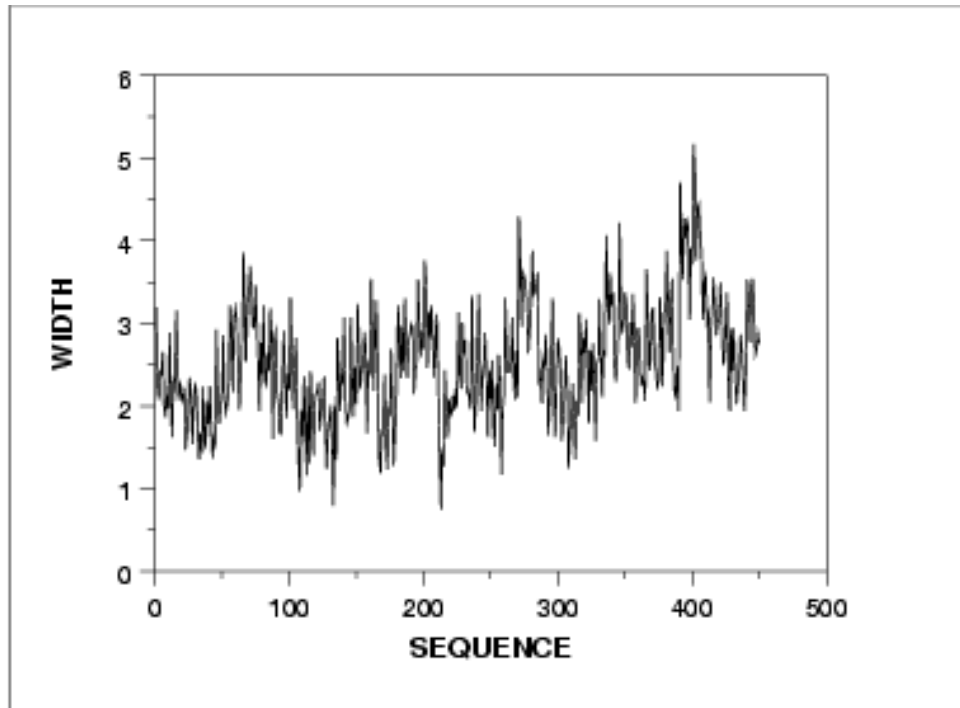
Interpretation This [4-plot](#) shows the following.

1. The [run sequence plot](#) (upper left) indicates that the location and scale are not constant over time. This indicates that the three factors do in fact have an effect of some kind.
2. The [lag plot](#) (upper right) indicates that there is some mild autocorrelation in the data. This is not unexpected as the data are grouped in a logical order of the three factors (i.e., not randomly) and the run sequence plot indicates that there are factor effects.
3. The [histogram](#) (lower left) shows that most of the data fall between 1 and 5, with the center of the data at about 2.2.

4. Due to the non-constant location and scale and autocorrelation in the data, distributional inferences from the [normal probability plot](#) (lower right) are not meaningful.

The run sequence plot is shown at full size to show greater detail. In addition, a numerical summary of the data is generated.

*Run
Sequence
Plot of Data*



*Numerical
Summary*

SUMMARY

NUMBER OF OBSERVATIONS = 450

```

*****
*          LOCATION MEASURES          *          DISPERSION MEASURES          *
*          *          *          *          *          *          *          *
* MIDRANGE      =  0.2957607E+01 * RANGE          =  0.4422122E+01
* MEAN          =  0.2532284E+01 * STAND. DEV.  =  0.6937559E+00
* MIDMEAN      =  0.2393183E+01 * AV. AB. DEV. =  0.5482042E+00
* MEDIAN        =  0.2453337E+01 * MINIMUM      =  0.7465460E+00
*              =                    * LOWER QUART. =  0.2046285E+01
*              =                    * LOWER HINGE  =  0.2048139E+01
*              =                    * UPPER HINGE  =  0.2971948E+01
*              =                    * UPPER QUART. =  0.2987150E+01
*****

```

6.6.1.2. Graphical Representation of the Data

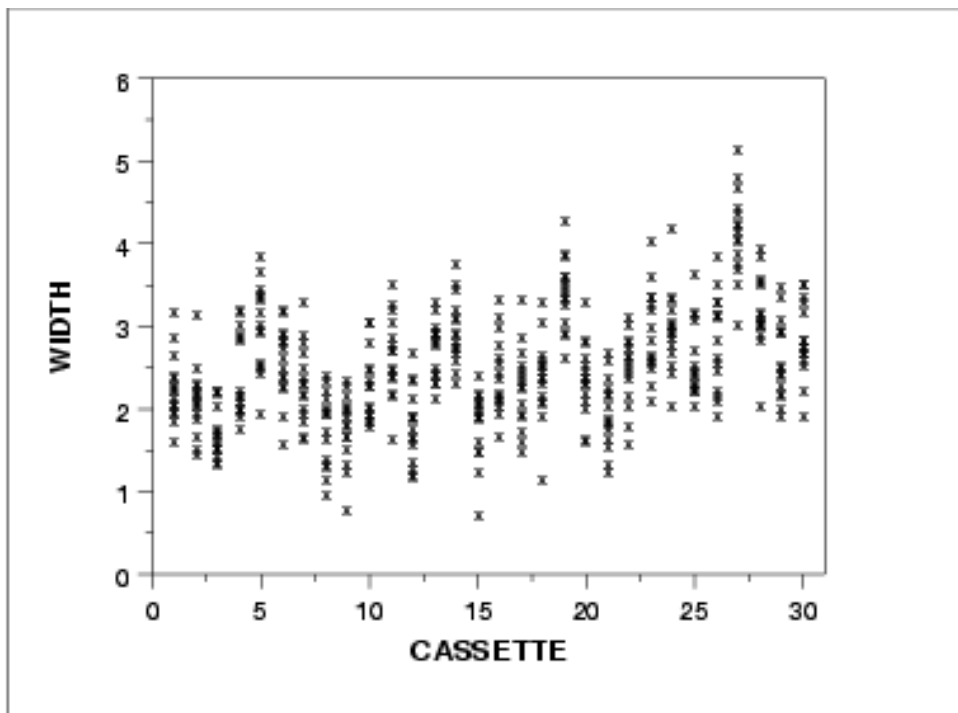
```
*
*
*          =          *   MAXIMUM          =   0.5168668E+01
*
*****
*          RANDOMNESS MEASURES          *          DISTRIBUTIONAL MEASURES
*
*****
*   AUTO COEF   =   0.6072572E+00   *   ST. 3RD MOM.   =   0.4527434E+00
*
*          =   0.0000000E+00   *   ST. 4TH MOM.   =   0.3382735E+01
*
*          =   0.0000000E+00   *   ST. WILK-SHA   =   0.6957975E+01
*
*          =          *   UNIFORM PPCC   =   0.9681802E+00
*
*          =          *   NORMAL   PPCC   =   0.9935199E+00
*
*          =          *   TUK   - .5 PPCC   =   0.8528156E+00
*
*          =          *   CAUCHY   PPCC   =   0.5245036E+00
*
*****
```

This summary generates a variety of statistics. In this case, we are primarily interested in the mean and standard deviation. From this summary, we see that the mean is 2.53 and the standard deviation is 0.69.

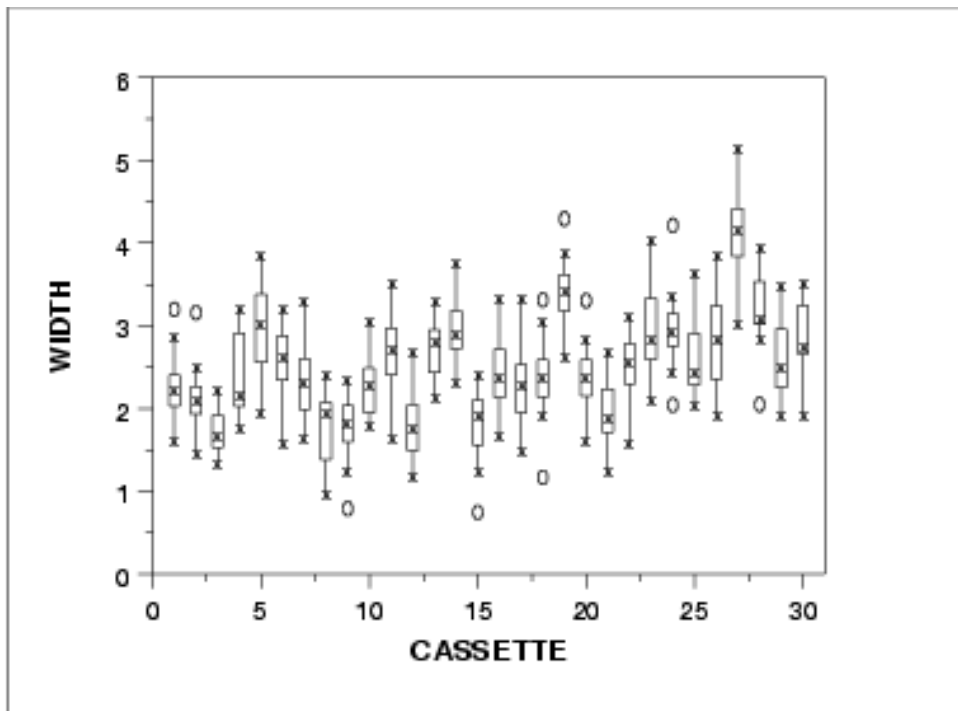
*Plot response
against
individual
factors*

The next step is to plot the response against each individual factor. For comparison, we generate both a [scatter plot](#) and a [box plot](#) of the data. The scatter plot shows more detail. However, comparisons are usually easier to see with the box plot, particularly as the number of data points and groups become larger.

*Scatter plot
of width
versus
cassette*



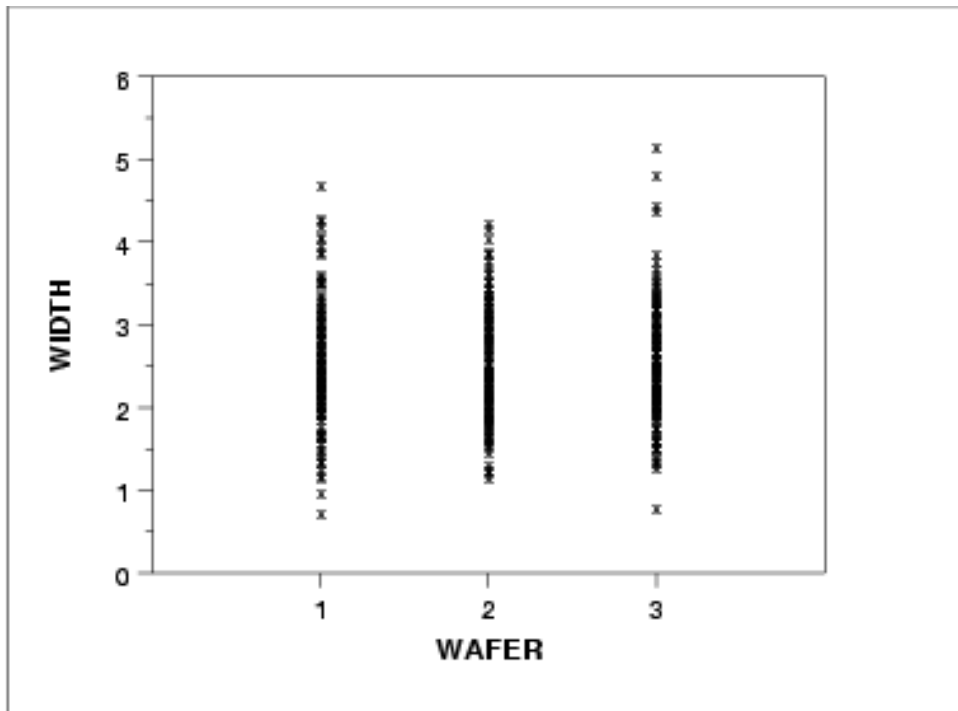
*Box plot of
width versus
cassette*



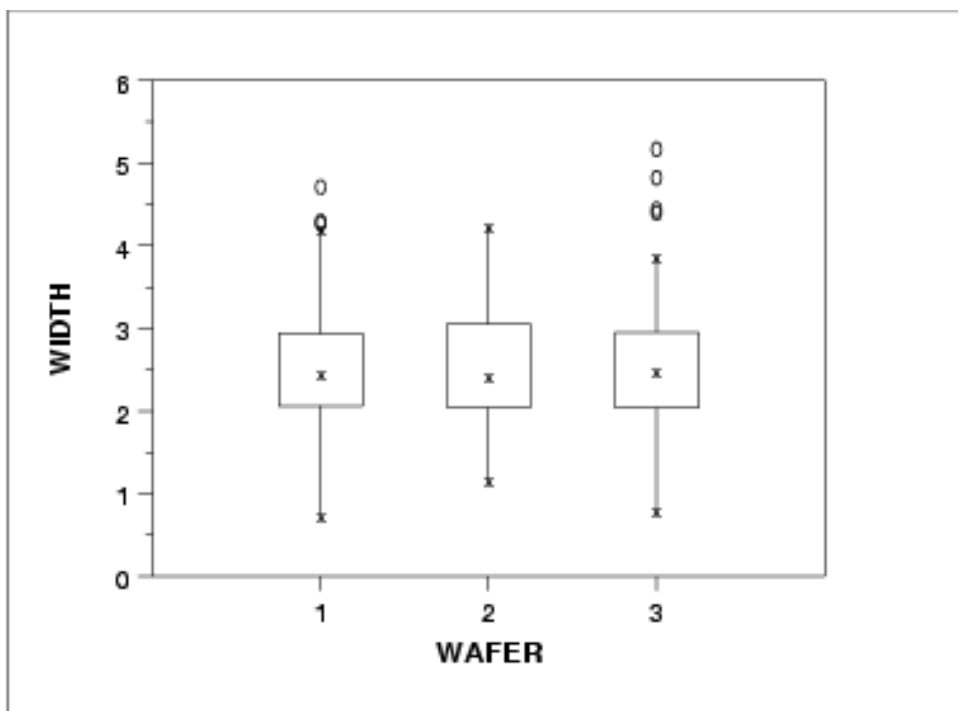
Interpretation We can make the following conclusions based on the above scatter and box plots.

1. There is considerable variation in the location for the various cassettes. The medians vary from about 1.7 to 4.
2. There is also some variation in the scale.
3. There are a number of outliers.

Scatter plot of width versus wafer



Box plot of width versus wafer

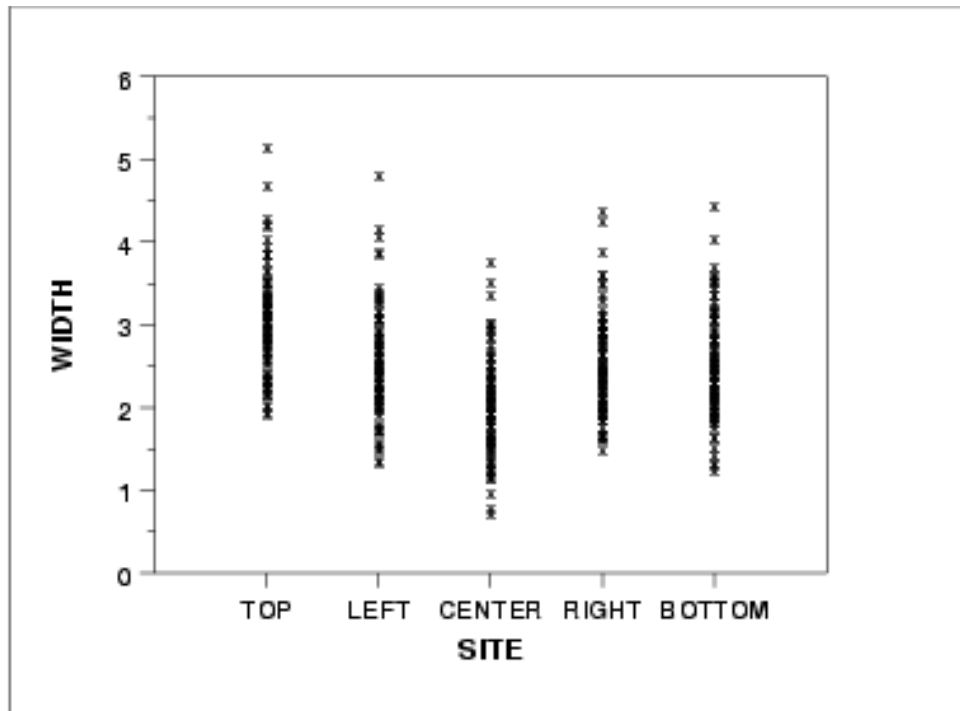


Interpretation

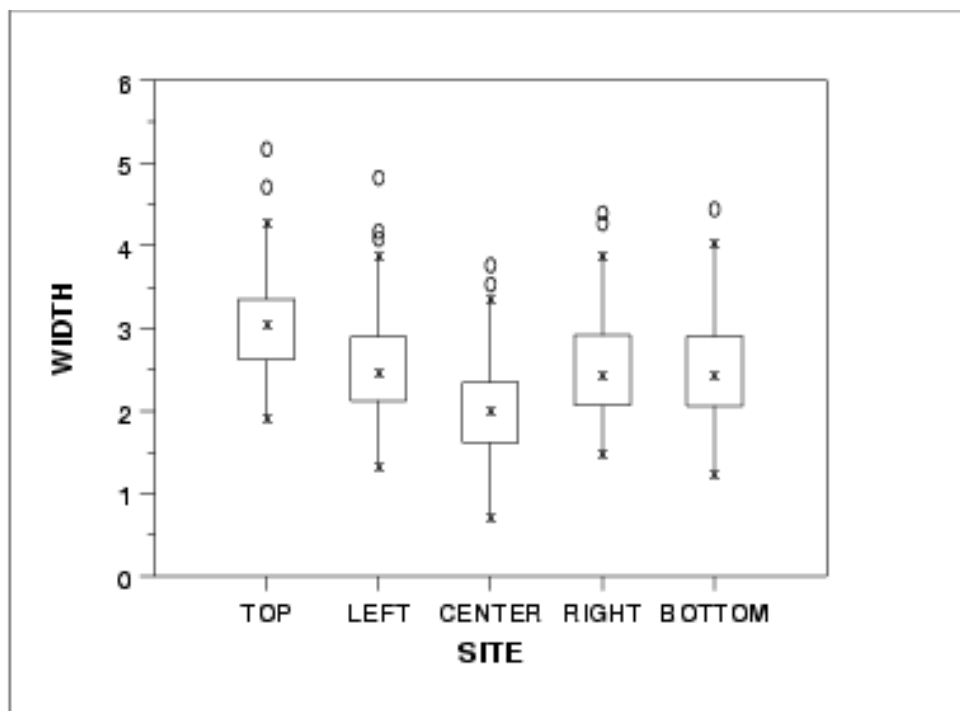
We can make the following conclusions based on the above scatter and box plots.

1. The locations for the 3 wafers are relatively constant.
2. The scales for the 3 wafers are relatively constant.
3. There are a few outliers on the high side.
4. It is reasonable to treat the wafer factor as homogeneous.

Scatter plot of width versus site



Box plot of width versus site



Interpretation

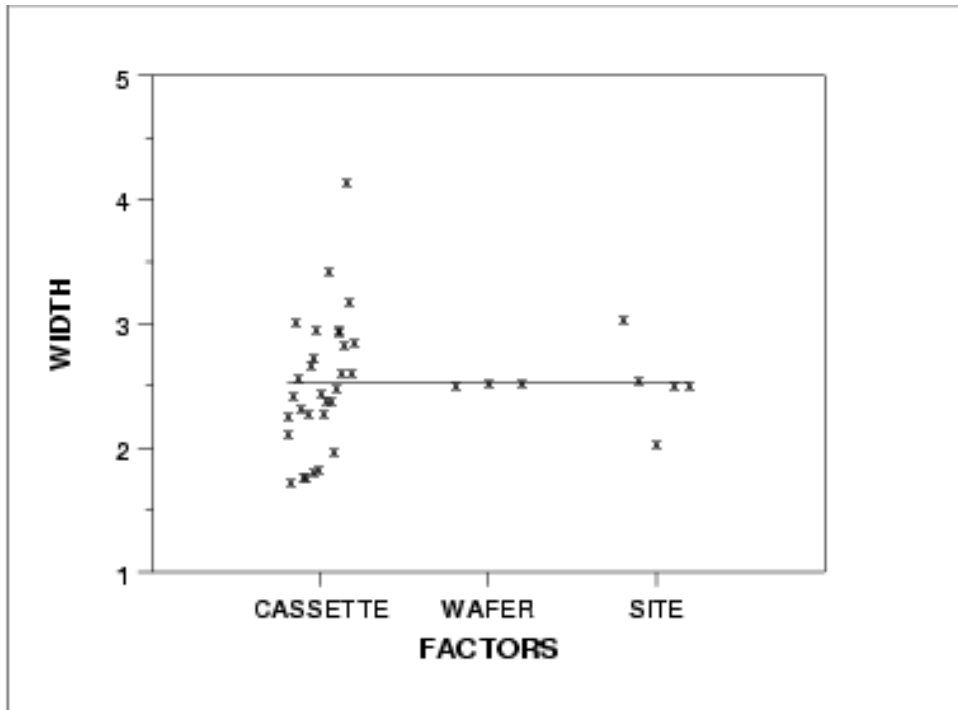
We can make the following conclusions based on the above scatter and box plots.

1. There is some variation in location based on site. The center site in particular has a lower median.
2. The scales are relatively constant across sites.
3. There are a few outliers.

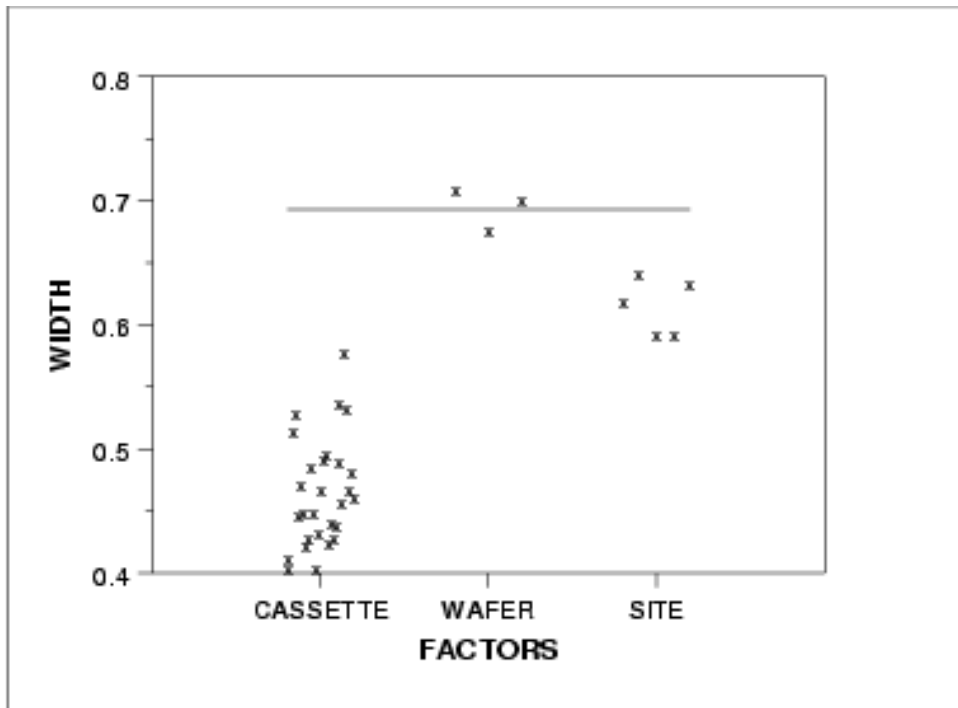
*Dex mean
and sd plots*

We can use the [dex mean plot](#) and the [dex standard deviation plot](#) to show the factor means and standard deviations together for better comparison.

*Dex mean
plot*



Dex sd plot



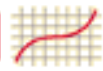
Summary

The above graphs show that there are differences between the lots and the sites.

There are various ways we can create subgroups of this dataset: each lot could be a subgroup, each wafer could be a subgroup, or each site measured could be a subgroup (with only one data value in each subgroup).

Recall that for a classical Shewhart Means chart, the average within subgroup standard deviation is used to calculate the control limits for the Means chart. However, on the means chart you are monitoring the subgroup mean-to-mean variation. There is no problem if you are in a continuous processing situation - this becomes an issue if you are operating in a batch processing environment.

We will look at various control charts based on different subgroupings [next](#).



6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

6.6.1. [Lithography Process](#)

6.6.1.3. Subgroup Analysis

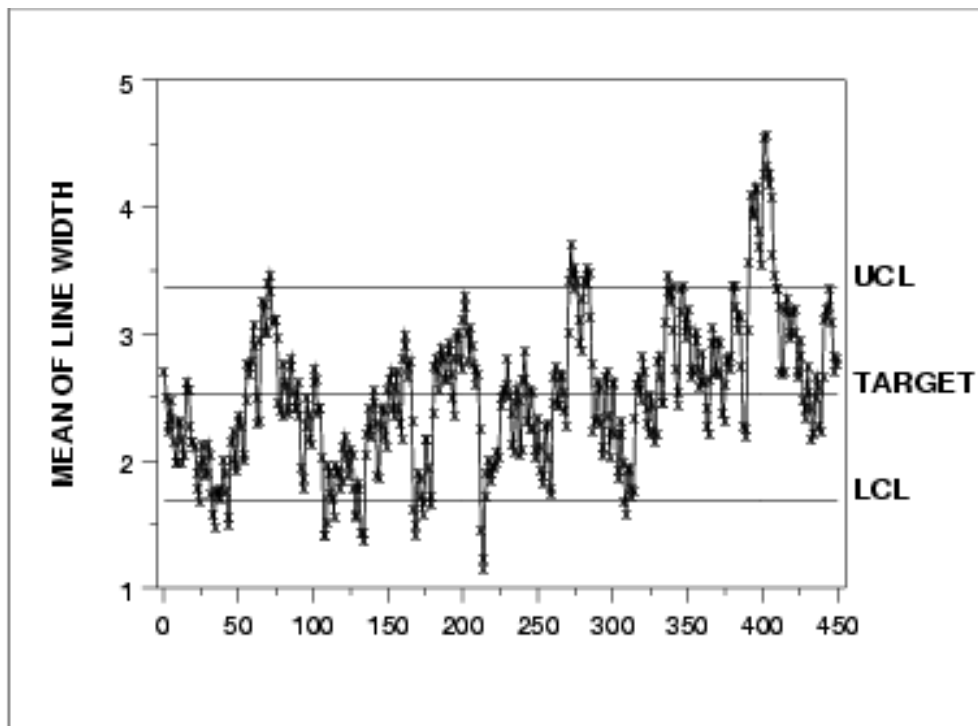
Control charts for subgroups

The resulting classical [Shewhart control charts](#) for each possible subgroup are shown below.

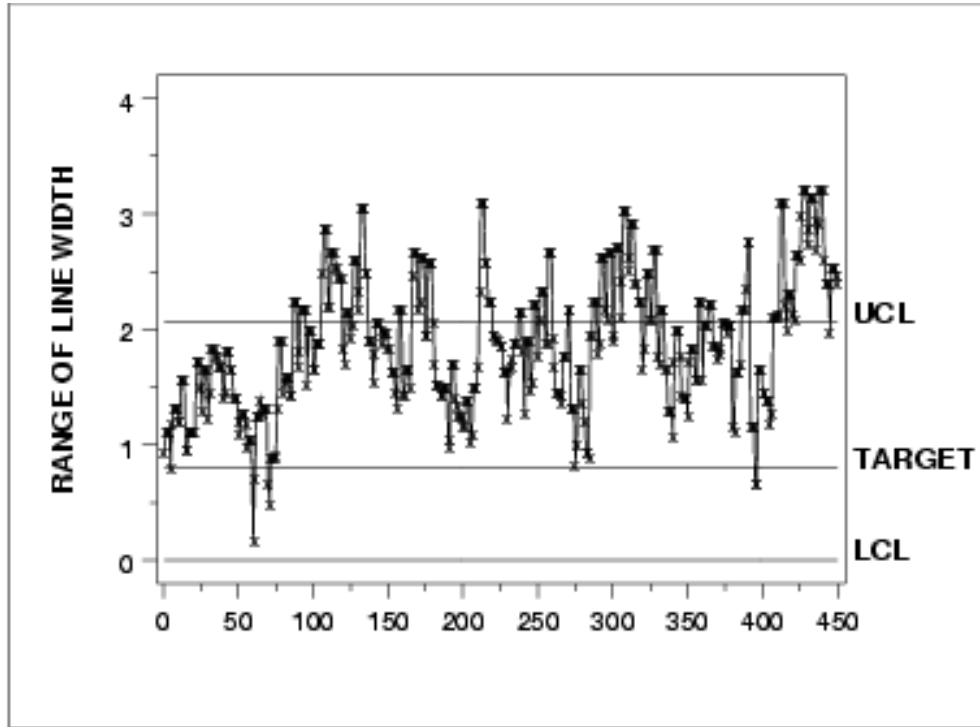
Site as subgroup

The first pair of control charts use the site as the subgroup. However, since site has a subgroup size of one we use the control charts for [individual measurements](#). A moving average and a moving range chart are shown.

Moving average control chart



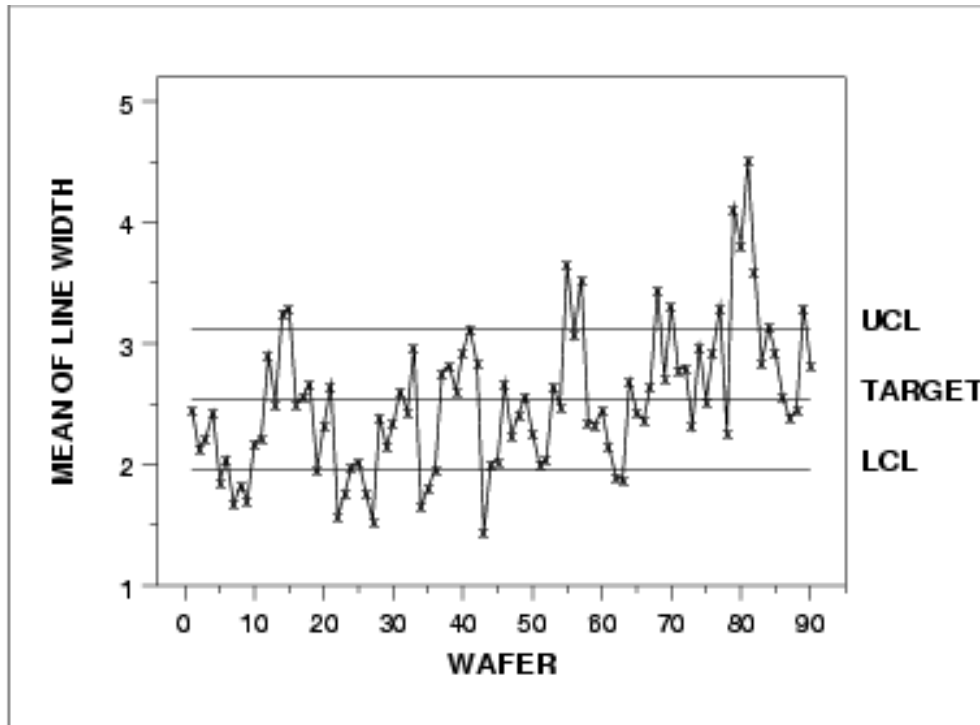
*Moving
range control
chart*



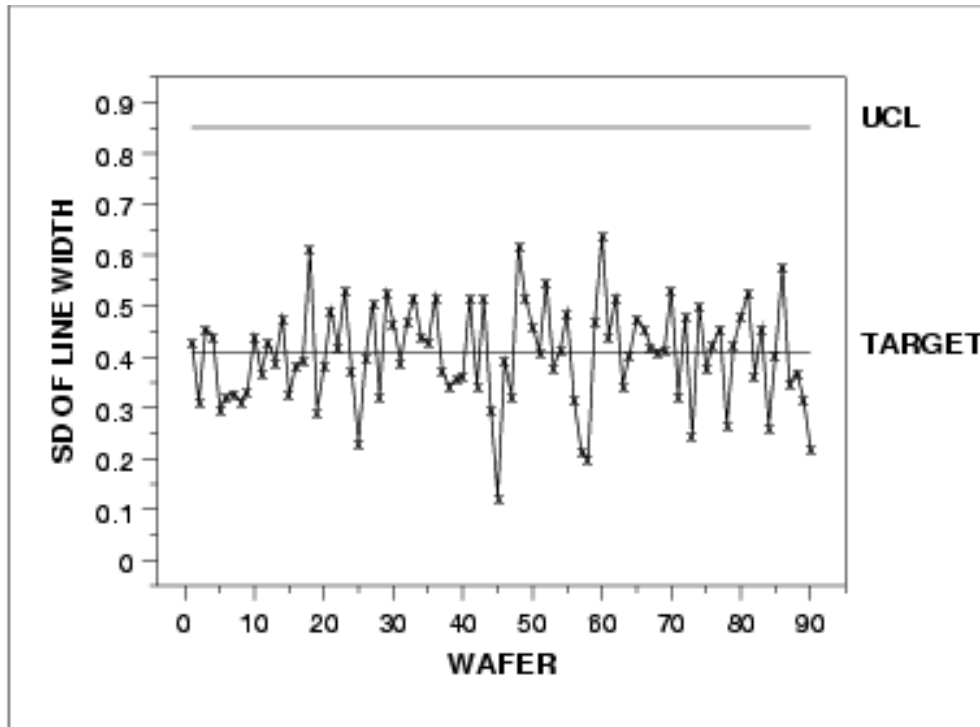
*Wafer as
subgroup*

The next pair of control charts use the wafer as the subgroup. In this case, that results in a subgroup size of 5. A mean and a standard deviation control chart are shown.

*Mean control
chart*



*SD control
chart*

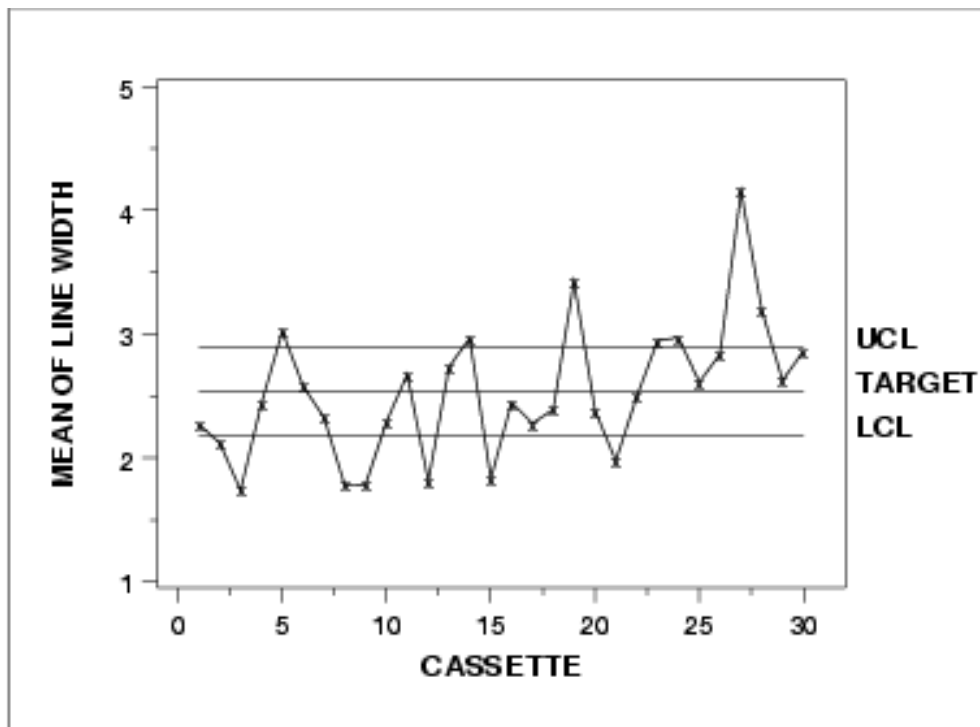


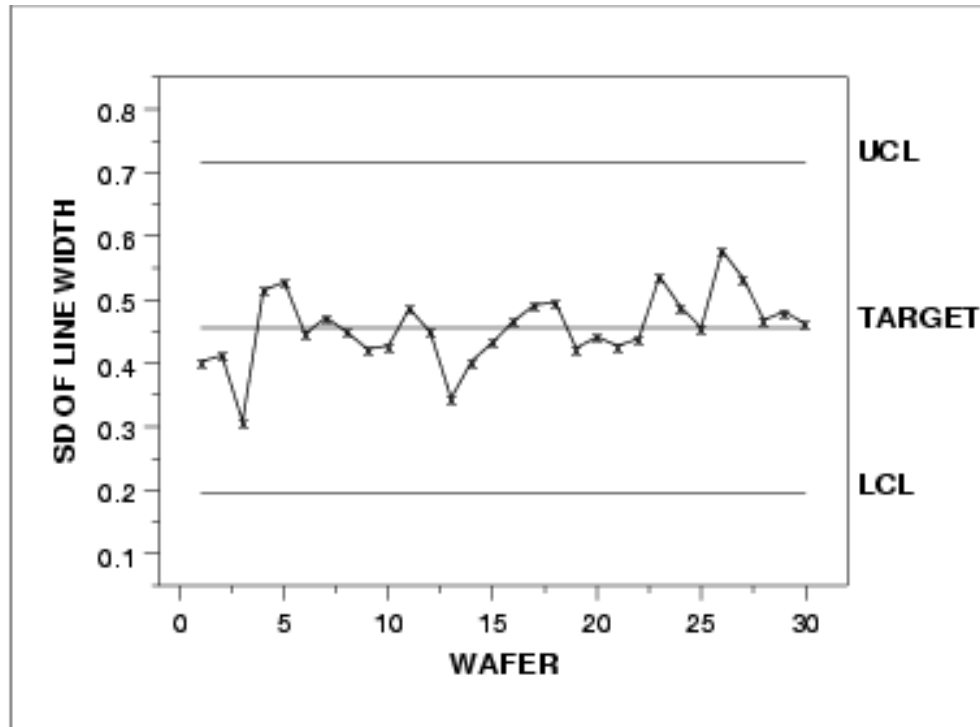
Note that there is no LCL here because of the small subgroup size.

*Cassette as
subgroup*

The next pair of control charts use the cassette as the subgroup. In this case, that results in a subgroup size of 15. A mean and a standard deviation control chart are shown.

*Mean control
chart*



SD control chart*Interpretation*

Which of these subgroupings of the data is correct? As you can see, each subgrouping produces a different chart. Part of the answer lies in the manufacturing requirements for this process. Another aspect that can be statistically determined is the magnitude of each of the sources of variation. In order to understand our data structure and how much variation each of our sources contribute, we need to perform a variance component analysis. The variance component analysis for this data set is shown below.

Component of variance table

Component	Variance Component Estimate
Cassette	0.2645
Wafer	0.0500
Site	0.1755

Equating mean squares with expected values

If your software does not generate the variance components directly, they can be computed from a standard analysis of variance output by [equating means squares \(MSS\) to expected mean squares \(EMS\)](#).

JMP ANOVA output

Below we show SAS JMP 4 output for this dataset that gives the SS, MSS, and components of variance (the model entered into JMP is a nested, random factors model). The EMS table contains the coefficients needed to write the equations setting MSS values equal to their EMS's. This is further described below.

Tests wrt Random Effects

Source	SS	MS Num	DF Num	F Ratio	Prob > F
Cassette&Random	127.403	4.3932	29	10.3285	<.0001
Wafer[Cassette]&Random	25.5209	0.42535	60	2.4237	<.0001
Site[Cassette,Wafer]&Random	63.1786	0.1755	360	.	.

Expected Mean Squares

The Mean Square per row by the Variance Component per column

EMS

	Intercept	Cassette&Random	Wafer[Cassette]&Random	Site[Cassette,Wafer]&Random
Intercept	0	0	0	0
Cassette&Random	0	15	5	1
Wafer[Cassette]&Random	0	0	5	1
Site[Cassette,Wafer]&Random	0	0	0	1

plus 1.0 times Residual Error Variance

Variance Component Estimates

Component	Var Comp Est	Percent of Total
Cassette&Random	0.264524	53.986
Wafer[Cassette]&Random	0.04997	10.198
Site[Cassette,Wafer]&Random	0.175496	35.816
Total	0.48999	100.000

These estimates based on equating Mean Squares to Expected Value.

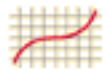
Variance Components Estimation From the ANOVA table, labelled "Tests wrt to Random Effects" in the JMP output, we can make the following variance component calculations:

$$4.3932 = (3*5)*\text{Var}(\text{cassettes}) + 5*\text{Var}(\text{wafer}) + \text{Var}(\text{site})$$

$$0.42535 = 5*\text{Var}(\text{wafer}) + \text{Var}(\text{site})$$

$$0.1755 = \text{Var}(\text{site})$$

Solving these equations we obtain the variance component estimates 0.2645, 0.04997 and 0.1755 for cassettes, wafers and sites, respectively.



6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

6.6.1. [Lithography Process](#)

6.6.1.4. Shewhart Control Chart

Choosing the right control charts to monitor the process

The largest source of variation in this data is the lot-to-lot variation. So, using classical Shewhart methods, if we specify our subgroup to be anything other than lot, we will be ignoring the known lot-to-lot variation and could get out-of-control points that already have a known, assignable cause - the data comes from different lots. However, in the lithography processing area the measurements of most interest are the site level measurements, not the lot means. How can we get around this seeming contradiction?

Chart sources of variation separately

One solution is to chart the important sources of variation separately. We would then be able to monitor the variation of our process and truly understand where the variation is coming from and if it changes. For this dataset, this approach would require having two sets of control charts, one for the individual site measurements and the other for the lot means. This would double the number of charts necessary for this process (we would have 4 charts for line width instead of 2).

Chart only most important source of variation

Another solution would be to have one chart on the largest source of variation. This would mean we would have one set of charts that monitor the lot-to-lot variation. From a manufacturing standpoint, this would be unacceptable.

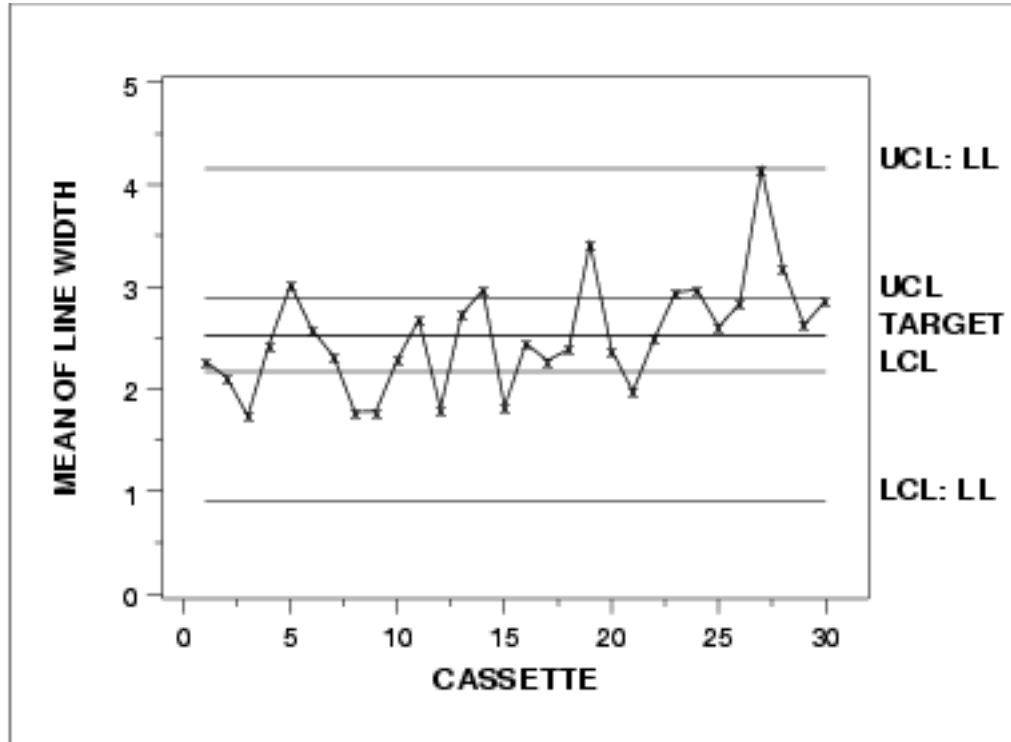
Use boxplot type chart

We could create a non-standard chart that would plot all the individual data values and group them together in a [boxplot](#) type format by lot. The control limits could be generated to monitor the individual data values while the lot-to-lot variation would be monitored by the patterns of the groupings. This would take special programming and management intervention to implement non-standard charts in most floor shop control systems.

Alternate form for mean control chart

A commonly applied solution is the first option; have multiple charts on this process. When creating the control limits for the lot means, care must be taken to use the lot-to-lot variation instead of the within lot variation. The resulting control charts are: the standard individuals/moving range charts (as seen previously), and a control chart on the lot means that is different from the previous lot means chart. This new chart uses the lot-to-lot variation to calculate control limits instead of the average within-lot standard deviation. The accompanying standard deviation chart is the same as seen previously.

Mean control chart using lot-to-lot variation



The control limits labeled with "UCL" and "LCL" are the standard control limits. The control limits labeled with "UCL: LL" and "LCL: LL" are based on the lot-to-lot variation.



6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

6.6.1. [Lithography Process](#)

6.6.1.5. Work This Example Yourself

[View
Dataplot
Macro for
this Case
Study](#)

This page allows you to repeat the analysis outlined in the case study description on the previous page using [Dataplot](#). It is required that you have already [downloaded and installed](#) Dataplot and [configured your browser](#). to run Dataplot. Output from each analysis step below will be displayed in one or more of the Dataplot windows. The four main windows are the Output Window, the Graphics window, the Command History window, and the data sheet window. Across the top of the main windows there are menus for executing Dataplot commands. Across the bottom is a command entry window where commands can be typed in.

Data Analysis Steps	Results and Conclusions
<p><i>Click on the links below to start Dataplot and run this case study yourself. Each step may use results from previous steps, so please be patient. Wait until the software verifies that the current step is complete before clicking on the next step.</i></p>	<p><i>The links in this column will connect you with more detailed information about each analysis step from the case study description.</i></p>
<p>1. Invoke Dataplot and read data.</p> <p>1. Read in the data.</p>	<p>1. You have read 5 columns of numbers into Dataplot, variables CASSETTE, WAFER, SITE, WIDTH, and RUNSEQ.</p>
<p>2. Plot of the response variable</p> <p>1. Numerical summary of WIDTH.</p> <p>2. 4-Plot of WIDTH.</p>	<p>1. The summary shows the mean line width is 2.53 and the standard deviation of the line width is 0.69.</p> <p>2. The 4-plot shows non-constant location and scale and moderate autocorrelation.</p>

3. Run sequence plot of WIDTH.

3. The run sequence plot shows non-constant location and scale.

3. Generate scatter and box plots against individual factors.

1. Scatter plot of WIDTH versus CASSETTE.

1. The scatter plot shows considerable variation in location.

2. Box plot of WIDTH versus CASSETTE.

2. The box plot shows considerable variation in location and scale and the presence of some outliers.

3. Scatter plot of WIDTH versus WAFER.

3. The scatter plot shows minimal variation in location and scale.

4. Box plot of WIDTH versus WAFER.

4. The box plot shows minimal variation in location and scale. It also show some outliers.

5. Scatter plot of WIDTH versus SITE.

5. The scatter plot shows some variation in location.

6. Box plot of WIDTH versus SITE.

6. The box plot shows some variation in location. Scale seems relatively constant. Some outliers.

7. Dex mean plot of WIDTH versus CASSETTE, WAFER, and SITE.

7. The dex mean plot shows effects for CASSETTE and SITE, no effect for WAFER.

8. Dex sd plot of WIDTH versus CASSETTE, WAFER, and SITE.

8. The dex sd plot shows effects for CASSETTE and SITE, no effect for WAFER.

4. Subgroup analysis.

1. Generate a moving mean control chart.

2. Generate a moving range control chart.

3. Generate a mean control chart for WAFER.

4. Generate a sd control chart for WAFER.

5. Generate a mean control chart for CASSETTE.

6. Generate a sd control chart for CASSETTE.

7. Generate an analysis of variance. This is not currently implemented in DATAPLOT for nested datasets.

8. Generate a mean control chart using lot-to-lot variation.

1. The moving mean plot shows a large number of out-of-control points.

2. The moving range plot shows a large number of out-of-control points.

3. The mean control chart shows a large number of out-of-control points.

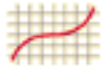
4. The sd control chart shows no out-of-control points.

5. The mean control chart shows a large number of out-of-control points.

6. The sd control chart shows no out-of-control points.

7. The analysis of variance and components of variance calculations show that cassette to cassette variation is 54% of the total and site to site variation is 36% of the total.

8. The mean control chart shows one point that is on the boundary of being out of control.

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6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

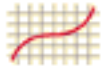
6.6.2. Aerosol Particle Size

*Box-Jenkins
Modeling of
Aerosol
Particle Size*

This case study illustrates the use of Box-Jenkins modeling with aerosol particle size data.

1. [Background and Data](#)
2. [Model Identification](#)
3. [Model Estimation](#)
4. [Model Validation](#)
5. [Work This Example Yourself](#)

[HOME](#)[TOOLS & AIDS](#)[SEARCH](#)[BACK](#)[NEXT](#)



6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

6.6.2. [Aerosol Particle Size](#)

6.6.2.1. Background and Data

Data Source The source of the data for this case study is Antuan Negiz who analyzed these data while he was a post-doc in the NIST Statistical Engineering Division from the Illinois Institute of Technology.

Data Collection These data were collected from an aerosol mini-spray dryer device. The purpose of this device is to convert a slurry stream into deposited particles in a drying chamber. The device injects the slurry at high speed. The slurry is pulverized as it enters the drying chamber when it comes into contact with a hot gas stream at low humidity. The liquid contained in the pulverized slurry particles is vaporized, then transferred to the hot gas stream leaving behind dried small-sized particles.

The response variable is particle size, which is collected equidistant in time. There are a variety of associated variables that may affect the injection process itself and hence the size and quality of the deposited particles. For this case study, we restrict our analysis to the response variable.

Applications Such deposition process operations have many applications from powdered laundry detergents at one extreme to ceramic molding at an important other extreme. In ceramic molding, the distribution and homogeneity of the particle sizes are particularly important because after the molds are baked and cured, the properties of the final molded ceramic product is strongly affected by the intermediate uniformity of the base ceramic particles, which in turn is directly reflective of the quality of the initial atomization process in the aerosol injection device.

*Aerosol
Particle Size
Dynamic
Modeling
and Control*

The data set consists of particle sizes collected over time. The basic distributional properties of this process are of interest in terms of distributional shape, constancy of size, and variation in size. In addition, this time series may be examined for autocorrelation structure to determine a prediction model of particle size as a function of time--such a model is frequently autoregressive in nature. Such a high-quality prediction equation would be essential as a first step in developing a predictor-corrective recursive feedback mechanism which would serve as the core in developing and implementing real-time dynamic corrective algorithms. The net effect of such algorithms is, of course, a particle size distribution that is much less variable, much more stable in nature, and of much higher quality. All of this results in final ceramic mold products that are more uniform and predictable across a wide range of important performance characteristics.

For the purposes of this case study, we restrict the analysis to determining an appropriate Box-Jenkins model of the particle size.

*Case study
data*

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6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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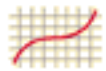
6.6.2.1. Background and Data

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6.6.2.1. Background and Data

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[6. Process or Product Monitoring and Control](#)

[6.6. Case Studies in Process Monitoring](#)

[6.6.2. Aerosol Particle Size](#)

6.6.2.2. Model Identification

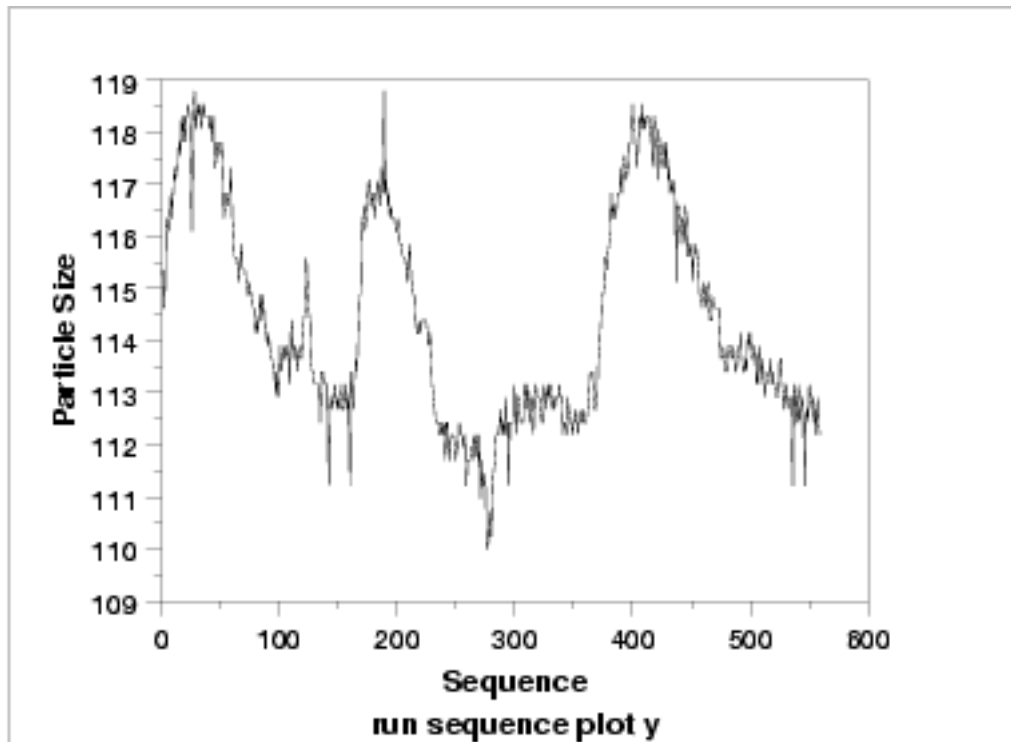
*Check for
Stationarity,
Outliers,
Seasonality*

The first step in the analysis is to generate a [run sequence plot](#) of the response variable. A run sequence plot can indicate [stationarity](#) (i.e., constant location and scale), the presence of outliers, and seasonal patterns.

Non-stationarity can often be removed by differencing the data or fitting some type of trend curve. We would then attempt to fit a Box-Jenkins model to the differenced data or to the residuals after fitting a trend curve.

Although Box-Jenkins models can estimate seasonal components, the analyst needs to specify the seasonal period (for example, 12 for monthly data). Seasonal components are common for economic time series. They are less common for engineering and scientific data.

*Run Sequence
Plot*



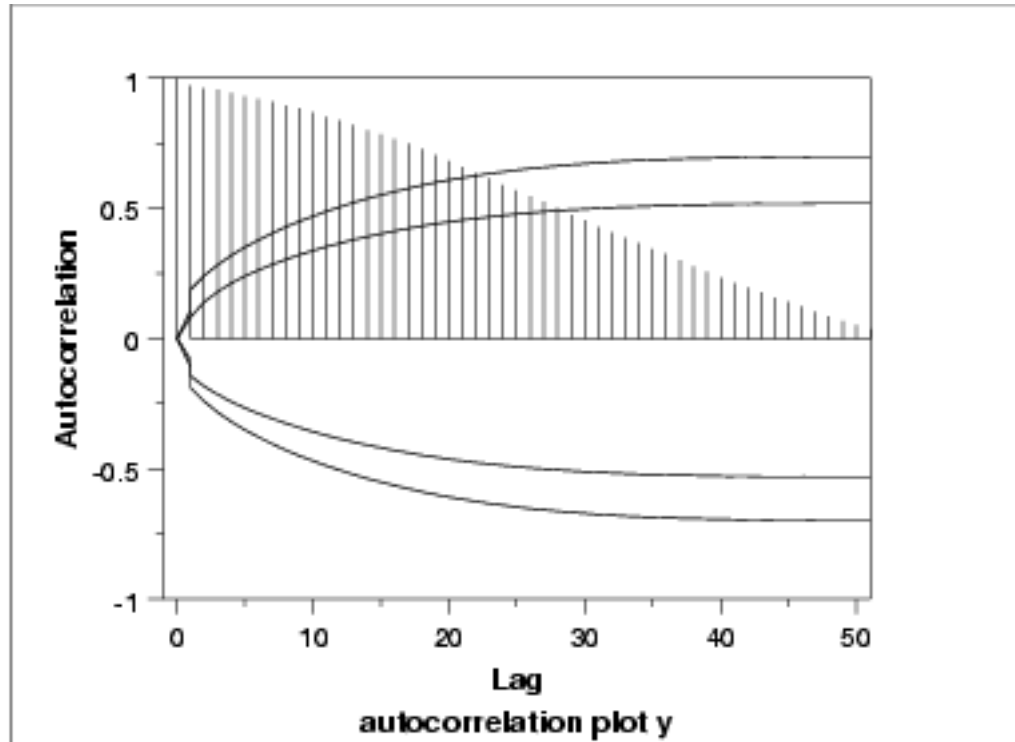
*Interpretation
of the Run
Sequence Plot*

We can make the following conclusions from the run sequence plot.

1. The data show strong and positive autocorrelation.
2. There does not seem to be a significant trend or any obvious seasonal pattern in the data.

The next step is to examine the sample autocorrelations using the [autocorrelation plot](#).

*Autocorrelation
Plot*

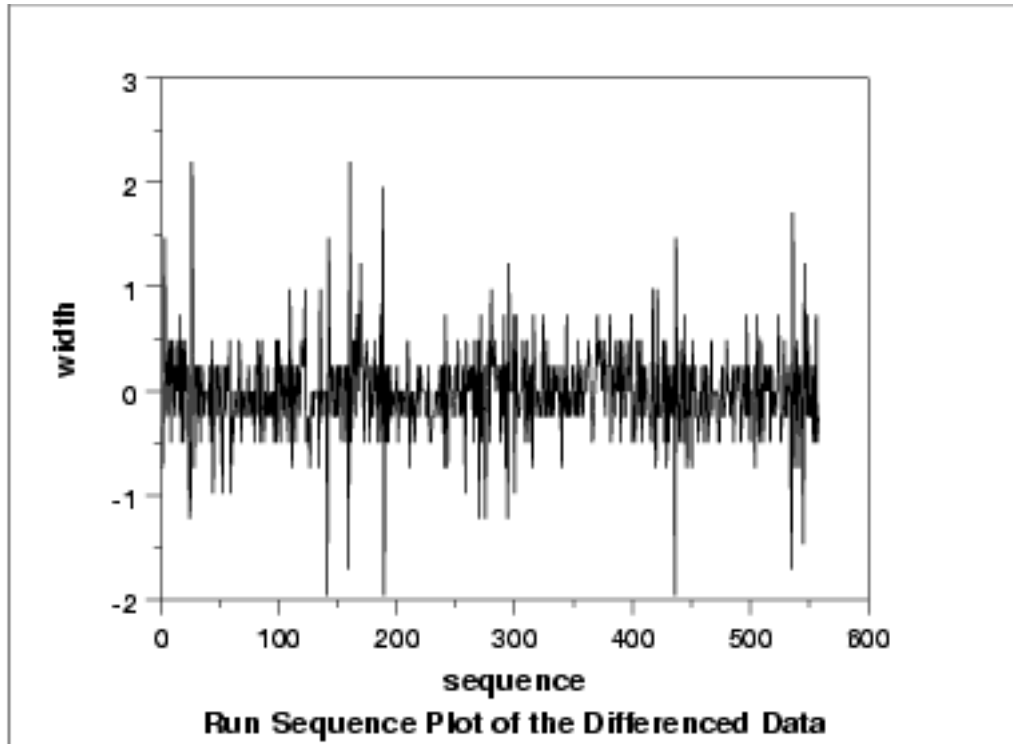


*Interpretation
of the
Autocorrelation
Plot*

The autocorrelation plot has a [95% confidence band](#), which is constructed based on the assumption that the process is a moving average process. The autocorrelation plot shows that the sample autocorrelations are very strong and positive and decay very slowly.

The autocorrelation plot indicates that the process is non-stationary and suggests an ARIMA model. The next step is to difference the data.

*Run Sequence
Plot of
Differenced
Data*

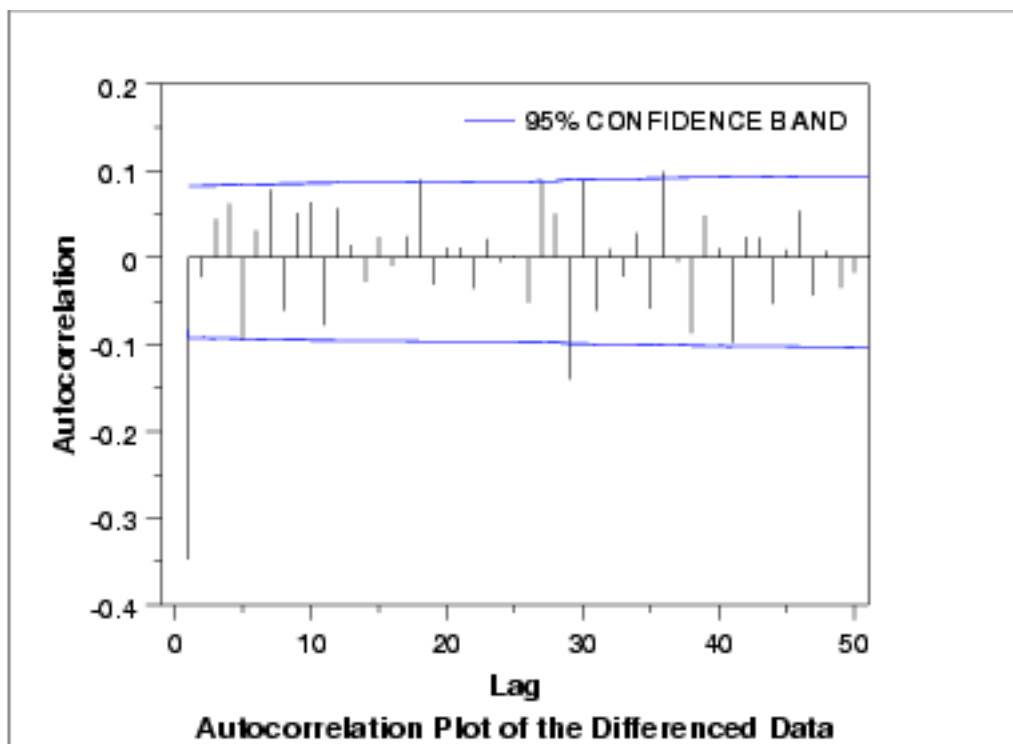


*Interpretation
of the Run
Sequence Plot*

The run sequence plot of the differenced data shows that the mean of the differenced data is around zero, with the differenced data less autocorrelated than the original data.

The next step is to examine the sample autocorrelations of the differenced data.

*Autocorrelation
Plot of the
Differenced
Data*

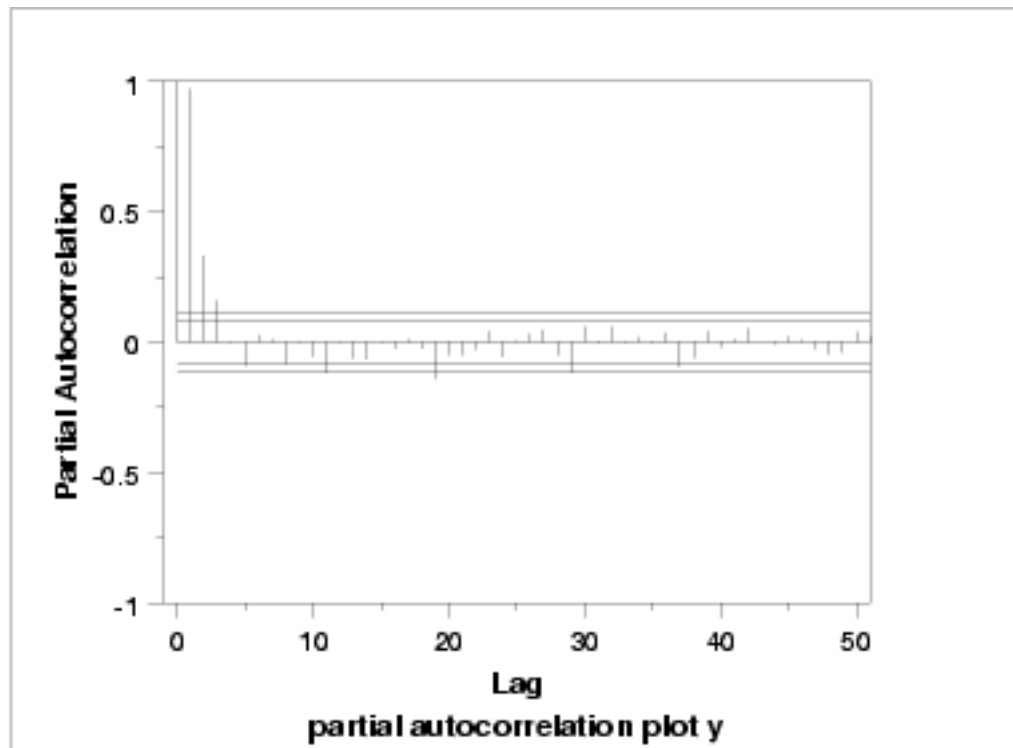


*Interpretation
of the
Autocorrelation
Plot of the
Differenced
Data*

The autocorrelation plot of the differenced data with a 95% confidence band shows that only the autocorrelation at lag 1 is significant. The autocorrelation plot together with run sequence of the differenced data suggest that the differenced data are stationary. Based on the autocorrelation plot, an MA(1) model is suggested for the differenced data.

To examine other possible models, we produce the partial autocorrelation plot of the differenced data.

*Partial
Autocorrelation
Plot of the
Differenced
Data*



*Interpretation
of the Partial
Autocorrelation
Plot of the
Differenced
Data*

The partial autocorrelation plot of the differenced data with 95% confidence bands shows that only the partial autocorrelations of the first and second lag are significant. This suggests an AR(2) model for the differenced data.

*Akaike
Information
Criterion (AIC
and AICC)*

Information-based criteria, such as the AIC or AICC (see [Brockwell and Davis \(2002\), pp. 171-174](#)), can be used to automate the choice of an appropriate model. When available, the AIC or AICC can be a useful tool for model identification.

Many software programs for time series analysis will generate the AIC or AICC for a broad range of models. At this time, Dataplot does not support this feature. However, based on the plots in this section, we will examine the ARIMA(2,1,0) and ARIMA(0,1,1) models in detail.

Note that whatever method is used for model identification, model diagnostics should be performed on the selected model.

6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

6.6.2. [Aerosol Particle Size](#)

6.6.2.3. Model Estimation

*Dataplot
ARMA
Output
for the
AR(2)
Model*

Based on the differenced data, Dataplot generated the following estimation output for the AR(2) model:

```
#####
# NONLINEAR LEAST SQUARES ESTIMATION FOR THE PARAMETERS OF #
# AN ARIMA MODEL USING BACKFORECASTS                        #
#####
```

SUMMARY OF INITIAL CONDITIONS

MODEL SPECIFICATION

FACTOR	(P	D	Q)	S
1	2	1	0	1

DEFAULT SCALING USED FOR ALL PARAMETERS.

```

                                                    ##STEP SIZE
FOR
                                                    #####PARAMETER
##APPROXIMATING
#####PARAMETER DESCRIPTION  STARTING VALUES
#####DERIVATIVE
INDEX #####TYPE  ##ORDER  ##FIXED  #####(PAR)
#####(STP)
    1  AR (FACTOR 1)          1      NO    0.10000000E+00
0.77167549E-06
    2  AR (FACTOR 1)          2      NO    0.10000000E+00
0.77168311E-06
    3      MU          ###      NO    0.00000000E+00
0.80630875E-06

NUMBER OF OBSERVATIONS          (N)   559
MAXIMUM NUMBER OF ITERATIONS ALLOWED          (MIT)
500
MAXIMUM NUMBER OF MODEL SUBROUTINE CALLS ALLOWED
1000

CONVERGENCE CRITERION FOR TEST BASED ON THE
FORECASTED RELATIVE CHANGE IN RESIDUAL SUM OF SQUARES (STOPSS)

```

6.6.2.3. Model Estimation

```

0.1000E-09
  MAXIMUM SCALED RELATIVE CHANGE IN THE PARAMETERS      (STOPP)
0.1489E-07

  MAXIMUM CHANGE ALLOWED IN THE PARAMETERS AT FIRST ITERATION (DELTA)
100.0
  RESIDUAL SUM OF SQUARES FOR INPUT PARAMETER VALUES
138.7
    (BACKFORECASTS INCLUDED)
  RESIDUAL STANDARD DEVIATION FOR INPUT PARAMETER VALUES      (RSD)
0.4999
  BASED ON DEGREES OF FREEDOM      559 -   1 -   3 =   555

  NONDEFAULT VALUES....

  AFCTOL.... V(31) =  0.2225074-307

##### RESIDUAL SUM OF SQUARES CONVERGENCE #####

ESTIMATES FROM LEAST SQUARES FIT (* FOR FIXED PARAMETER)
#####

          PARAMETER      STD DEV OF ###PAR/
#####APPROXIMATE
          ESTIMATES  #####PARAMETER  ####(SD      95 PERCENT
CONFIDENCE LIMITS
  TYPE ORD  ###(OF PAR)  #####ESTIMATES  ##(PAR)  #####LOWER
#####UPPER

  FACTOR 1
    AR 1 -0.40604575E+00  0.41885445E-01   -9.69 -0.47505616E+00
-0.33703534E+00
    AR 2 -0.16414479E+00  0.41836922E-01   -3.92 -0.23307525E+00
-0.95214321E-01
    MU ## -0.52091780E-02  0.11972592E-01   -0.44 -0.24935207E-01
0.14516851E-01

  NUMBER OF OBSERVATIONS      (N)   559
  RESIDUAL SUM OF SQUARES      109.2642
    (BACKFORECASTS INCLUDED)
  RESIDUAL STANDARD DEVIATION      0.4437031
  BASED ON DEGREES OF FREEDOM  559 -   1 -   3 =   555
  APPROXIMATE CONDITION NUMBER      3.498456

```

*Interpretation
of Output*

The first section of the output identifies the model and shows the starting values for the fit. This output is primarily useful for verifying that the model and starting values were correctly entered.

The section labeled "ESTIMATES FROM LEAST SQUARES FIT" gives the parameter estimates, standard errors from the estimates, and 95% confidence limits for the parameters. A confidence interval that contains zero indicates that the parameter is not statistically significant and could probably be dropped from the model.

The model for the differenced data, Y_t , is an AR(2) model:

$$Y_t = -0.406Y_{t-1} - 0.164Y_{t-2} - 0.00521$$

with $\sigma_{0.44}$.

It is often more convenient to express the model in terms of the original data, X_t , rather than the differenced data. From the definition of the difference, $Y_t = X_t - X_{t-1}$, we can make the appropriate substitutions into the above equation:

$$X_t - X_{t-1} = -0.406(X_{t-1} - X_{t-2}) - 0.164(X_{t-2} - X_{t-3}) - 0.00521$$

to arrive at the model in terms of the original series:

$$X_t = 0.594X_{t-1} + 0.242X_{t-2} + 0.164X_{t-3} - 0.00521$$

*Dataplot
ARMA
Output for
the MA(1)
Model*

Alternatively, based on the differenced data Dataplot generated the following estimation output for an MA(1) model:

```
#####
#  NONLINEAR LEAST SQUARES ESTIMATION FOR THE PARAMETERS OF #
#  AN ARIMA MODEL USING BACKFORECASTS                       #
#####
```

SUMMARY OF INITIAL CONDITIONS

MODEL SPECIFICATION

FACTOR	(P	D	Q)	S
1	0	1	1	1

DEFAULT SCALING USED FOR ALL PARAMETERS.

```

FOR
#####PARAMETER
##APPROXIMATING
#####PARAMETER DESCRIPTION STARTING VALUES
#####DERIVATIVE
INDEX #####TYPE ##ORDER ##FIXED #####(PAR)
#####STEP SIZE
```

```

#####(STP)

      1          MU      ###      NO      0.00000000E+00
0.20630657E-05
      2 MA (FACTOR 1)      1      NO      0.10000000E+00
0.34498203E-07

NUMBER OF OBSERVATIONS              (N)      559
MAXIMUM NUMBER OF ITERATIONS ALLOWED              (MIT)
500
MAXIMUM NUMBER OF MODEL SUBROUTINE CALLS ALLOWED
1000

CONVERGENCE CRITERION FOR TEST BASED ON THE
FORECASTED RELATIVE CHANGE IN RESIDUAL SUM OF SQUARES (STOPSS)
0.1000E-09
MAXIMUM SCALED RELATIVE CHANGE IN THE PARAMETERS              (STOPP)
0.1489E-07

MAXIMUM CHANGE ALLOWED IN THE PARAMETERS AT FIRST ITERATION (DELTA)
100.0
RESIDUAL SUM OF SQUARES FOR INPUT PARAMETER VALUES
120.0
      (BACKFORECASTS INCLUDED)
RESIDUAL STANDARD DEVIATION FOR INPUT PARAMETER VALUES              (RSD)
0.4645
BASED ON DEGREES OF FREEDOM              559 - 1 - 2 = 556

NONDEFAULT VALUES....

AFCTOL.... V(31) = 0.2225074-307

##### RESIDUAL SUM OF SQUARES CONVERGENCE #####

ESTIMATES FROM LEAST SQUARES FIT (* FOR FIXED PARAMETER)
#####

PARAMETER      STD DEV OF ###PAR/
#####APPROXIMATE
ESTIMATES      ####PARAMETER ####(SD      95 PERCENT
CONFIDENCE LIMITS
TYPE ORD      ###(OF PAR)      ####ESTIMATES ##(PAR)      #####LOWER
#####UPPER

FACTOR 1
MU ## -0.51160754E-02 0.11431230E-01 -0.45 -0.23950101E-01
0.13717950E-01
MA 1 0.39275694E+00 0.39028474E-01 10.06 0.32845386E+00
0.45706001E+00

NUMBER OF OBSERVATIONS              (N)      559
RESIDUAL SUM OF SQUARES              109.6880
      (BACKFORECASTS INCLUDED)
RESIDUAL STANDARD DEVIATION              0.4441628
BASED ON DEGREES OF FREEDOM 559 - 1 - 2 = 556
APPROXIMATE CONDITION NUMBER              3.414207

```

*Interpretation
of the Output*

The model for the differenced data, Y_t , is an ARIMA(0,1,1) model:

$$Y_t = a_t + 0.393a_{t-1} - 0.00511$$

with $\sigma_{0.44}$.

It is often more convenient to express the model in terms of the original data, X_t , rather than the differenced data. Making the appropriate substitutions into the above equation:

$$X_t - X_{t-1} = a_t - 0.393a_{t-1} - 0.00511$$

we arrive at the model in terms of the original series:

$$X_t = X_{t-1} + a_t - 0.393a_{t-1} - 0.00511$$

6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

6.6.2. [Aerosol Particle Size](#)

6.6.2.4. Model Validation

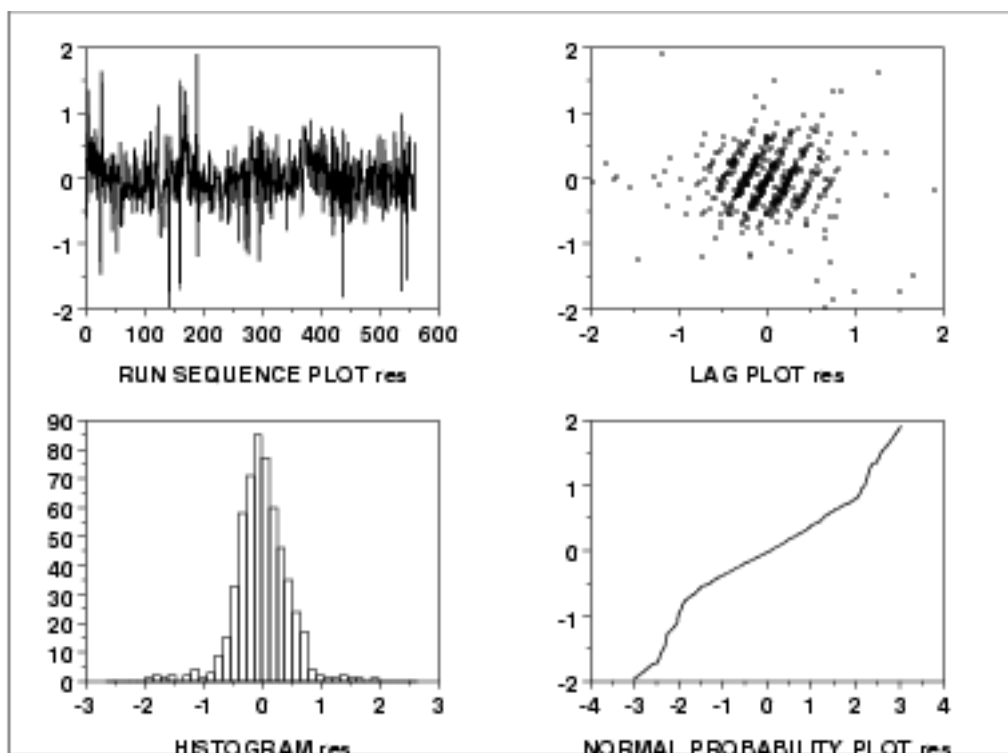
Residuals

After fitting the model, we should check whether the model is appropriate.

As with standard [non-linear least squares fitting](#), the primary tool for model diagnostic checking is residual analysis.

4-Plot of Residuals from ARIMA(2,1,0) Model

The [4-plot](#) is a convenient graphical technique for model validation in that it tests the assumptions for the residuals on a single graph.



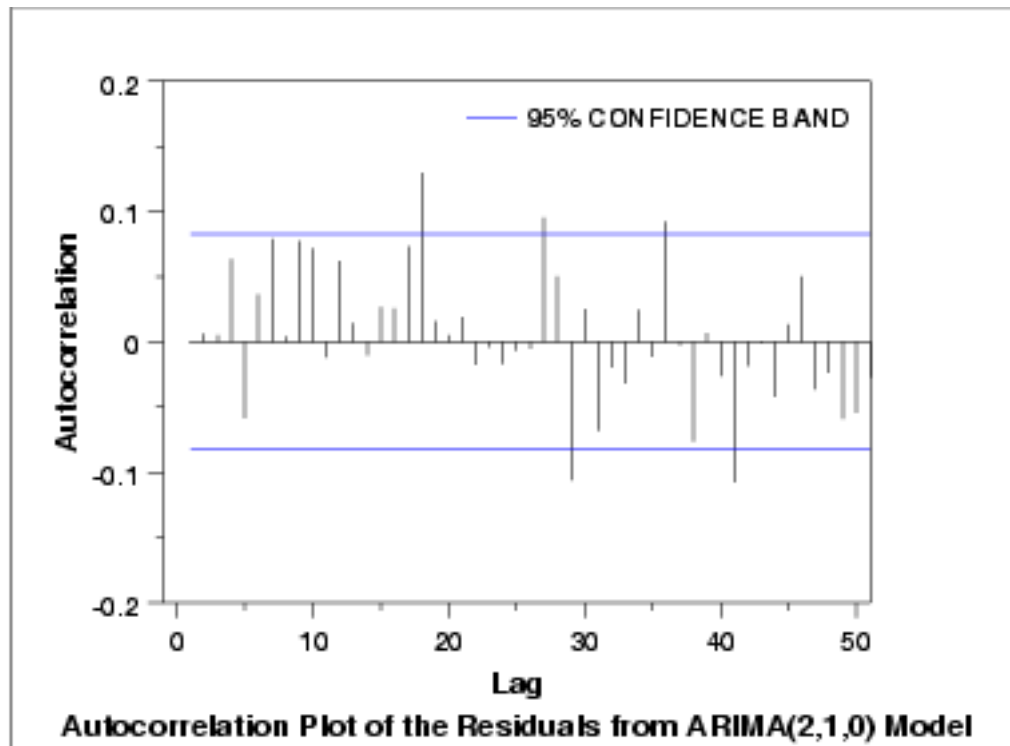
Interpretation of the 4-Plot

We can make the following conclusions based on the above 4-plot.

1. The [run sequence plot](#) shows that the residuals do not violate the assumption of constant location and scale. It also shows that most of the residuals are in the range (-1, 1).
2. The [lag plot](#) indicates that the residuals are not autocorrelated at lag 1.
3. The [histogram](#) and [normal probability plot](#) indicate that the normal distribution provides an adequate fit for this model.

Autocorrelation Plot of Residuals from ARIMA(2,1,0) Model

In addition, the [autocorrelation plot](#) of the residuals from the ARIMA(2,1,0) model was generated.



Interpretation of the Autocorrelation Plot

The autocorrelation plot shows that for the first 25 lags, all sample autocorrelations except those at lags 7 and 18 fall inside the 95% confidence bounds indicating the residuals appear to be random.

*Ljung-Box Test
for
Randomness
for the
ARIMA(2,1,0)
Model*

Instead of checking the autocorrelation of the residuals, portmanteau tests such as the test proposed by [Ljung and Box \(1978\)](#) can be used. In this example, the test of Ljung and Box indicates that the residuals are random at the 95% confidence level and thus the model is appropriate. Dataplot generated the following output for the Ljung-Box test.

LJUNG-BOX TEST FOR RANDOMNESS

1. STATISTICS:

NUMBER OF OBSERVATIONS	=	559
LAG TESTED	=	24
LAG 1 AUTOCORRELATION	=	-0.1012441E-02
LAG 2 AUTOCORRELATION	=	0.6160716E-02
LAG 3 AUTOCORRELATION	=	0.5182213E-02

LJUNG-BOX TEST STATISTIC	=	31.91066
--------------------------	---	----------

2. PERCENT POINTS OF THE REFERENCE CHI-SQUARE DISTRIBUTION
(REJECT HYPOTHESIS OF RANDOMNESS IF TEST STATISTIC VALUE
IS GREATER THAN PERCENT POINT VALUE)

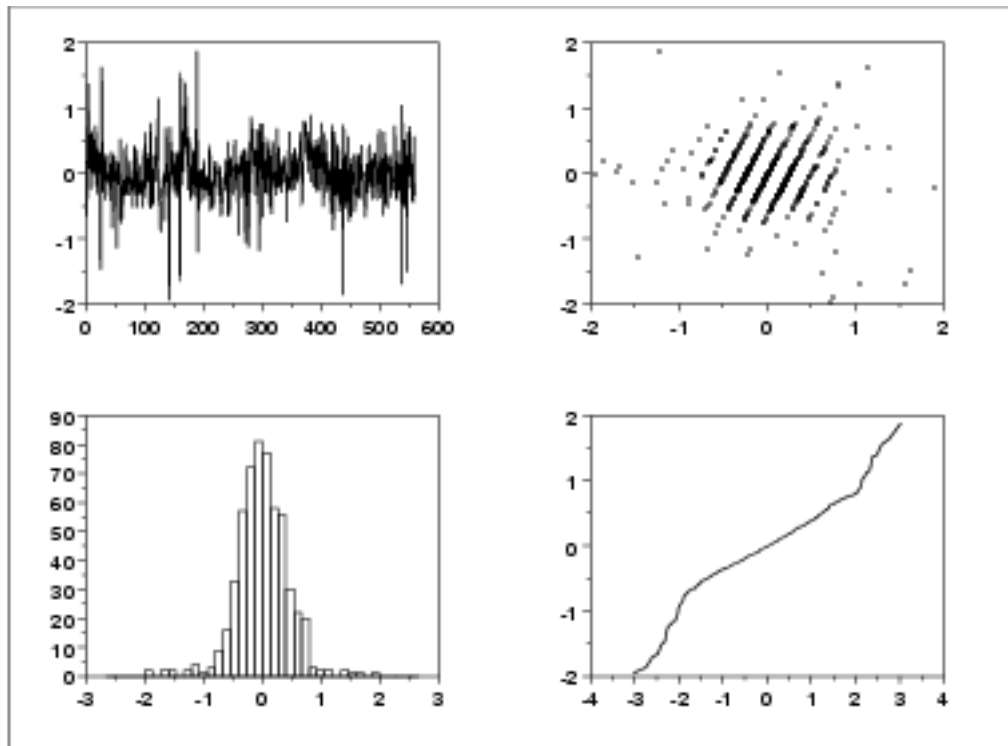
FOR LJUNG-BOX TEST STATISTIC

0	% POINT	=	0.
50	% POINT	=	23.33673
75	% POINT	=	28.24115
90	% POINT	=	33.19624
95	% POINT	=	36.41503
99	% POINT	=	42.97982

3. CONCLUSION (AT THE 5% LEVEL):
THE DATA ARE RANDOM.

*4-Plot of
Residuals from
ARIMA(0,1,1)
Model*

The [4-plot](#) is a convenient graphical technique for model validation in that it tests the assumptions for the residuals on a single graph.



*Interpretation
of the 4-Plot
from the
ARIMA(0,1,1)
Model*

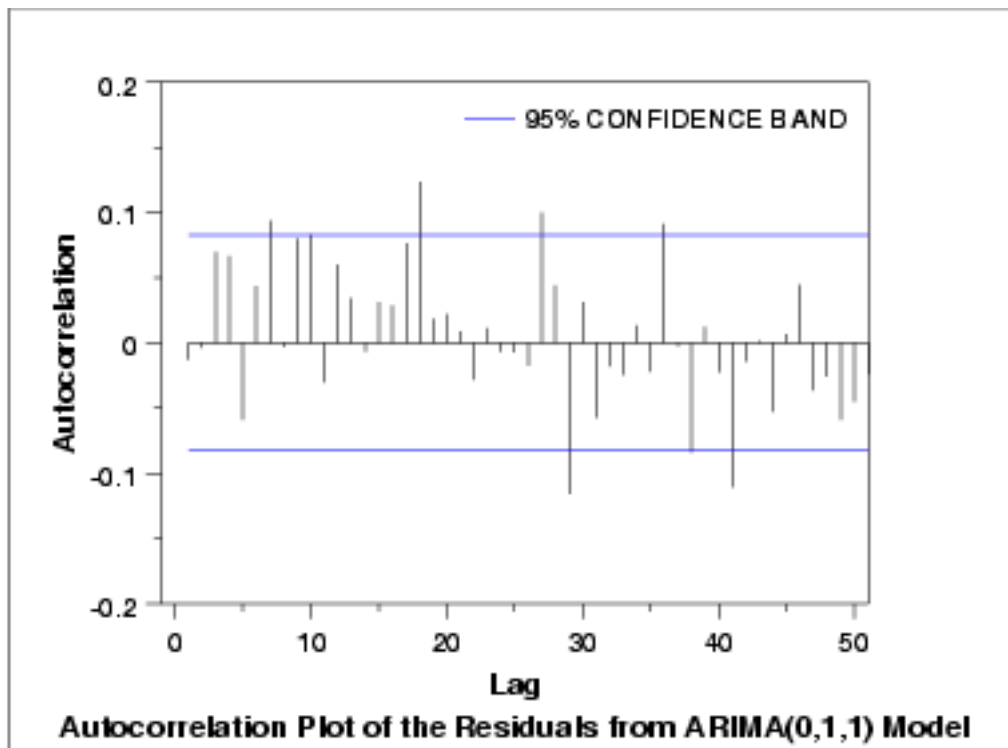
We can make the following conclusions based on the above 4-plot.

1. The [run sequence plot](#) shows that the residuals do not violate the assumption of constant location and scale. It also shows that most of the residuals are in the range (-1, 1).
2. The [lag plot](#) indicates that the residuals are not autocorrelated at lag 1.
3. The [histogram](#) and [normal probability plot](#) indicate that the normal distribution provides an adequate fit for this model.

This 4-plot of the residuals indicates that the fitted model is an adequate model for these data.

*Autocorrelation
Plot of
Residuals from
ARIMA(0,1,1)
Model*

The autocorrelation plot of the residuals from ARIMA(0,1,1) was generated.



*Interpretation
of the
Autocorrelation
Plot*

Similar to the result for the ARIMA(2,1,0) model, it shows that for the first 25 lags, all sample autocorrelations except those at lags 7 and 18 fall inside the 95% confidence bounds indicating the residuals appear to be random.

*Ljung-Box Test
for
Randomness of
the Residuals
for the
ARIMA(0,1,1)
Model*

The Ljung and Box test is also applied to the residuals from the ARIMA(0,1,1) model. The test indicates that the residuals are random at the 99% confidence level, but not at the 95% level.

Dataplot generated the following output for the Ljung-Box test.

LJUNG-BOX TEST FOR RANDOMNESS

1. STATISTICS:

NUMBER OF OBSERVATIONS	=	559
LAG TESTED	=	24
LAG 1 AUTOCORRELATION	=	-0.1280136E-01
LAG 2 AUTOCORRELATION	=	-0.3764571E-02
LAG 3 AUTOCORRELATION	=	0.7015200E-01

LJUNG-BOX TEST STATISTIC	=	38.76418
--------------------------	---	----------

2. PERCENT POINTS OF THE REFERENCE CHI-SQUARE DISTRIBUTION
(REJECT HYPOTHESIS OF RANDOMNESS IF TEST STATISTIC VALUE
IS GREATER THAN PERCENT POINT VALUE)

FOR LJUNG-BOX TEST STATISTIC

0	% POINT	=	0.
50	% POINT	=	23.33673
75	% POINT	=	28.24115
90	% POINT	=	33.19624
95	% POINT	=	36.41503

99 % POINT = 42.97982

3. CONCLUSION (AT THE 5% LEVEL):
THE DATA ARE NOT RANDOM.

Summary

Overall, the ARIMA(0,1,1) is an adequate model. However, the ARIMA(2,1,0) is a little better than the ARIMA(0,1,1).



6. [Process or Product Monitoring and Control](#)

6.6. [Case Studies in Process Monitoring](#)

6.6.2. [Aerosol Particle Size](#)

6.6.2.5. Work This Example Yourself

[View
Dataplot
Macro for
this Case
Study](#)

This page allows you to repeat the analysis outlined in the case study description on the previous page using [Dataplot](#). It is required that you have already [downloaded and installed](#) Dataplot and [configured your browser](#). to run Dataplot. Output from each analysis step below will be displayed in one or more of the Dataplot windows. The four main windows are the Output Window, the Graphics window, the Command History window, and the data sheet window. Across the top of the main windows there are menus for executing Dataplot commands. Across the bottom is a command entry window where commands can be typed in.

Data Analysis Steps

Results and Conclusions

Click on the links below to start Dataplot and run this case study yourself. Each step may use results from previous steps, so please be patient. Wait until the software verifies that the current step is complete before clicking on the next step.

The links in this column will connect you with more detailed information about each analysis step from the case study description.

1. Invoke Dataplot and read data.

[1. Read in the data.](#)

[1. You have read one column of numbers into Dataplot, variable Y.](#)

2. Model identification plots

[1. Run sequence plot of Y.](#)

[1. The run sequence plot shows that the data show strong and positive autocorrelation.](#)

[2. Autocorrelation plot of Y.](#)

[2. The autocorrelation plot indicates significant autocorrelation and that the data are not stationary.](#)

[3. Run sequence plot of the differenced data of Y.](#)

[3. The run sequence plot shows that the](#)

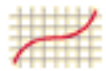
<p><u>4. Autocorrelation plot of the differenced data of Y.</u></p> <p><u>5. Partial autocorrelation plot of the differenced data of Y.</u></p>	<p><u>differenced data appear to be stationary and do not exhibit seasonality.</u></p> <p><u>4. The autocorrelation plot of the differenced data suggests an ARIMA(0,1,1) model may be appropriate.</u></p> <p><u>5. The partial autocorrelation plot suggests an ARIMA(2,1,0) model may be appropriate.</u></p>
<p>3. Estimate the model.</p> <p><u>1. ARIMA(2,1,0) fit of Y.</u></p> <p><u>2. ARIMA(0,1,1) fit of Y.</u></p>	<p><u>1. The ARMA fit generates parameter estimates for the ARIMA(2,1,0) model.</u></p> <p><u>2. The ARMA fit generates parameter estimates for the ARIMA(0,1,1) model.</u></p>
<p>4. Model validation.</p> <p><u>1. Generate a 4-plot of the residuals from the ARIMA(2,1,0) model.</u></p> <p><u>2. Generate an autocorrelation plot of the residuals from the ARIMA(2,1,0) model.</u></p> <p><u>3. Perform a Ljung-Box test of randomness for the residuals from the ARIMA(2,1,0) model.</u></p> <p><u>4. Generate a 4-plot of the residuals from the ARIMA(0,1,1) model.</u></p>	<p><u>1. The 4-plot shows that the assumptions for the residuals are satisfied.</u></p> <p><u>2. The autocorrelation plot of the residuals indicates that the residuals are random.</u></p> <p><u>3. The Ljung-Box test indicates that the residuals are random.</u></p> <p><u>4. The 4-plot shows that the assumptions for the residuals are satisfied.</u></p>

5. Generate an autocorrelation plot of the residuals from the ARIMA(0,1,1) model.

6. Perform a Ljung-Box test of randomness for the residuals from the ARIMA(0,1,1) model.

5. The autocorrelation plot of the residuals indicates that the residuals are random.

6. The Ljung-Box test indicates that the residuals are not random at the 95% level, but are random at the 99% level.



6. [Process or Product Monitoring and Control](#)

6.7. References

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