OPTIMUM DESIGN OF EXPERIMENTS in FOUR-STAGE NESTED VARIANCE–COMPONENTS MODELS

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$\boxed{\textbf{OUTLINE}}$

- Motivating Example
- Nested Variance Components Model – Design issues related to estimation of variance components
- Discussion of the 4-stage model
- A brief overview of the results for 2-stage and 3-stage models
- What is our approach?
  - Consider a suitably restricted class of designs
  - Obtain locally optimum designs by complete search (for small N)
  - Obtain DESIGN MEASURES for large sample sizes
  - For practical use, select a design based on prior knowledge about design parameters and cost information
- Summary Remarks
- Future Work

PIGMENT PASTE EXAMPLE – BHH (1978)

- A batch process is used in the manufacture of a pigment paste. A characteristic of interest to the quality control personnel is the *moisture content* of the product.

- Past information suggests that, the moisture content varies about a mean of approximately 25 units with a standard deviation of approximately 6 units (1 unit = 0.001%). According to the standards of the company, this variability is regarded as excessive.

- A batch of pigment paste consists of approximately 80 drums of material. The standard procedure for taking a sample consisted of

  (1) randomly select five drums of the material from the batch,

  (2) taking a certain amount of material from each selected drum with a sampling tube designed to obtain representative material from all the layers in the drum,

  (3) thoroughly mixing the five portions of the material, and

  (4) taking a sample from the aggregate mixture which is then sent out to the laboratory for testing.

$\boxed{\textbf{PIGMENT PASTE EXAMPLE – BHH (1978)}}$

- Apart from the analytical test variation, which should be small if the laboratory apparatus is under control, two other sources of variation in the moisture content y may be identified:

  (a) the variation from batch to batch of material, and

  (b) the chemical sampling variation within a batch.

- In order to study these sources, 15 batches of material were randomly taken and sampled twice, by the process described above, yielding 30 samples.
- Each sample was then split into two parts to produce information about the analytical test variation (error).
- These 60 subsamples were introduced into the stream of routine analysis at the analytical laboratory.

MODEL FOR PIGMENT PASTE EXAMPLE

In this study the factors batch and chemical sampling are regarded as random, so the model for the response y for batch i, sample j and replicate k is

$$y_{ijk} = \mu + \alpha_i + \beta_{ij} + \epsilon_{ijk}$$

where $i = 1$, 2,. . . , 15, $b = 1,\ 2$ and $k = 1,\ 2$.

The effects α_i, β_{ij} and ϵ_{ijk} are assumed to be independent random variables with zero means and variances σ_α^2. σ_β^2 and σ_ϵ^2 respectively.

The analysis of variance (ANOVA) estimates for the variance components are

$$\hat{\sigma}_\epsilon^2 = 0.9167, \qquad \hat{\sigma}_\beta^2 = 28.5333, \qquad \hat{\sigma}_\alpha^2 = 7.1280.$$

- As expected, the variability introduced by the testing process at the laboratory, or random error, is in fact small. This component of variance is unlikely to be of the greatest interest to the investigator.
- However, in this particular design, it is the quantity estimated most precisely. It has 30 degrees of freedom compared to 14 and 15 for the other two parameters.

ANALYSIS OF VARIANCE for PIGMENT PASTE EXAMPLE

Source	Degrees of Freedom	Sum of Squares	Mean Square	Expected Mean Square
Batch	14	1210.9333	86.49524	$\sigma_\epsilon^2 + 2\sigma_\beta^2 + 4\sigma_\alpha^2$
Sample(Batch)	15	869.7500	57.98333	$\sigma_\epsilon^2 + 2\sigma_\beta^2$
Error	30	27.5000	0.91667	σ_ϵ^2

Parameter	ANOVA Estimate	Standard Error
σ_ϵ	0.9167	0.2366
σ_β	28.5333	10.5869
σ_α	7.2180	9.7313

- Need designs that allow efficient estimation of all the variance components of interest.

DESIGNS FOR k-STAGE NESTED MODELS

2-STAGE NESTED MODEL: Hammersley (1949), Crump (1954), Anderson (1960, 1961, 1975), Anderson & Crump (1967), Thompson & Anderson (1975), and others.

3-STAGE NESTED MODEL: Prairie (1961, 1962), Anderson R. L & Bancroft (1952), Calvin & Miller (1961), Goldsmith (1969), Goldsmith & Gaylor (1970), Delgado& Iyer (1999)

4-STAGE NESTED MODEL: Delgado (1997, Ph.D thesis, Colorado State University)

FOUR–STAGE NESTED VARIANCE COMPONENTS MODEL

$$y_{ijkl} = \mu + \alpha_i + \beta_{ij} + \gamma_{ijk} + \epsilon_{ijkl}$$

$i = 1,\ 2, \ldots, a,$ $\qquad$ $j = 1,\ 2, \ldots, b_i$

$k = 1,\ 2, \ldots, c_{ij},$ $\qquad$ $l = 1,\ 2, \ldots, n_{ijk}$

$b_* = \sum_i b_i,$ $\qquad$ $c_{**} = \sum_i \sum_j c_{ij}$

$N = \sum_i \sum_j \sum_k n_{ijk}$

$\alpha_i \sim N(0, \sigma^2_\alpha),$ $\qquad$ $\beta_{ij} \sim N(0, \sigma^2_\beta)$

$\gamma_{ijk} \sim N(0, \sigma^2_\gamma),$ $\qquad$ $\epsilon_{ijk} \sim N(0, \sigma^2_\epsilon)$

FOUR–STAGE NESTED VARIANCE COMPONENTS MODEL

A product is manufactured using BATCHes of raw material.

Each batch of raw material will last for several DAYs.

Large numbers of PARTs are made each day.

Multiple MEASUREMENTs may be made on each selected part.

- **Batch Variability**
- **Day to day variability**
- **Part to part variability**
- **Measurement variability**

1. Select a BATCHES
2. From batch i select b_i DAYS
3. From day ij, select c_{ij} PARTS
4. Finally, on part ijk, make n_{ijk} MEASUREMENTS
5. Analyze the data and estimate the variance components.

$\boxed{\textbf{THE FOUR–STAGE NESTED MODEL}}$

$$\mathbf{y} = \mathbf{1}_N \mu + \mathbf{Z}_3 \boldsymbol{\alpha} + \mathbf{Z}_2 \boldsymbol{\beta} + \mathbf{Z}_1 \boldsymbol{\gamma} + \mathbf{Z}_0 \boldsymbol{\epsilon}$$

where

- $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\epsilon}$ are the vectors of the random effects α_i, β_{ij}, γ_{ijk} and ϵ_{ijk}, respectively, in lexicographic order.
- The incidence matrices are $\mathbf{Z}_0 = \mathbf{I}_N$, $\mathbf{Z}_1 = \{_d \mathbf{1}_{n_{ijk}}\}_{i,j,k}$, $\mathbf{Z}_2 = \{_d \mathbf{1}_{n_{ij*}}\}_{i,j}$ and $\mathbf{Z}_3 = \{_d \mathbf{1}_{n_{i**}}\}_i$.

$$\mathrm{E}(\mathbf{y}) = \mu \mathbf{1}_N$$

$$\boldsymbol{\Sigma} = \mathrm{Var}(\mathbf{y}) = \sigma^2_\alpha \, \mathbf{V}_3 + \sigma^2_\beta \, \mathbf{V}_2 + \sigma^2_\gamma \, \mathbf{V}_1 + \sigma^2_\epsilon \, \mathbf{V}_0.$$

$$\mathbf{V}_0 = \mathbf{Z}_0 \mathbf{Z}_0' = \mathbf{I}_N, \qquad \mathbf{V}_1 = \mathbf{Z}_1 \mathbf{Z}_1' = \{_d \, \mathbf{J}_{n_{ijk}} \}_{i,j,k},$$

$$\mathbf{V}_2 = \mathbf{Z}_2 \mathbf{Z}_2' = \{_d \, \mathbf{J}_{n_{ij*}} \}_{i,j}, \qquad \mathbf{V}_3 = \mathbf{Z}_3 \mathbf{Z}_3' = \{_d \, \mathbf{J}_{n_{i**}} \}_i$$

$\boxed{\textbf{NOTATION}}$

$$\boldsymbol{\sigma}^2 = \begin{bmatrix} \sigma_\epsilon^2 \\ \sigma_\gamma^2 \\ \sigma_\beta^2 \\ \sigma_\alpha^2 \end{bmatrix} \qquad \mathbf{s} = \begin{bmatrix} \mathbf{y}'\mathbf{A}_0\mathbf{y} \\ \mathbf{y}'\mathbf{A}_1\mathbf{y} \\ \mathbf{y}'\mathbf{A}_2\mathbf{y} \\ \mathbf{y}'\mathbf{A}_3\mathbf{y} \end{bmatrix}$$

The matrices of the quadratic forms are

$$\mathbf{A}_0 = \mathbf{C}_0 - \mathbf{C}_{abc} = \mathbf{I}_N - \left\{ {}_d\, \frac{1}{n_{ijk}} \mathbf{J}_{n_{ijk}} \right\}_{i,j,k},$$

$$\mathbf{A}_1 = \mathbf{C}_{abc} - \mathbf{C}_{ab} = \left\{ {}_d\, \frac{1}{n_{ijk}} \mathbf{J}_{n_{ijk}} \right\}_{i,j,k} - \left\{ {}_d \frac{1}{n_{ij*}} \mathbf{J}_{n_{ij*}} \right\}_{i,j}$$

$$\mathbf{A}_2 = \mathbf{C}_{ab} - \mathbf{C}_a = \left\{ {}_d \frac{1}{n_{ij*}} \mathbf{J}_{n_{ij*}} \right\}_{i,j} - \left\{ {}_d\, \frac{1}{n_{i**}} \mathbf{J}_{n_{i**}} \right\}_i$$

$$\mathbf{A}_3 = \mathbf{C}_a - \mathbf{C}_\mu = \left\{ {}_d\, \frac{1}{n_{i**}} \mathbf{J}_{n_{i**}} \right\}_i - \frac{1}{N}\, \mathbf{J}_N.$$

ANALYSIS OF VARIANCE

Source	Degrees of Freedom	Sum of Squares	Expected Sum of Squares
A	$a-1$	$\mathbf{y}'\mathbf{A}_3\mathbf{y}$	$h_7\sigma_\epsilon^2 + h_8\sigma_\gamma^2 + h_9\sigma_\beta^2 + h_{10}\sigma_\alpha^2$
B	$b_* - a$	$\mathbf{y}'\mathbf{A}_2\mathbf{y}$	$h_4\sigma_\epsilon^2 + h_5\sigma_\gamma^2 + h_6\sigma_\beta^2$
C	$c_{**} - b_*$	$\mathbf{y}'\mathbf{A}_1\mathbf{y}$	$h_2\sigma_\epsilon^2 + h_3\sigma_\gamma^2$
Error	$N - c_{**}$	$\mathbf{y}'\mathbf{A}_0\mathbf{y}$	$h_1\sigma_\epsilon^2$

For a balanced sampling plan, the degrees of freedom are

$$a-1, a(b-1), ab(c-1), abc(n-1)$$

respectively. Note that $N = abcn =$ total number of measurements.

Example: If $a = 4, b = 3, c = 2, n = 2$, then the degrees of freedom are, respectively, 3, 8, 12, 24. Thus, balanced plans tend to use more resources for estimating variance components at the higher levels of nesting.

$\boxed{\textbf{METHOD OF MOMENTS ESTIMATOR OF } \boldsymbol{\sigma}^2}$

$$E(\mathbf{s}) = \begin{bmatrix} E\left(\mathbf{y}'\mathbf{A}_0\mathbf{y}\right) \\ E\left(\mathbf{y}'\mathbf{A}_1\mathbf{y}\right) \\ E\left(\mathbf{y}'\mathbf{A}_2\mathbf{y}\right) \\ E\left(\mathbf{y}'\mathbf{A}_3\mathbf{y}\right) \end{bmatrix} = \mathbf{H}\boldsymbol{\sigma}^2$$

$$\mathbf{H} = \begin{bmatrix} h_1 & 0 & 0 & 0 \\ h_2 & h_3 & 0 & 0 \\ h_4 & h_5 & h_6 & 0 \\ h_7 & h_8 & h_9 & h_{10} \end{bmatrix} = \begin{bmatrix} N - c_{**} & 0 & 0 & 0 \\ c_{**} - b_* & N - k_6 & 0 & 0 \\ b_* - a & k_6 - k_5 & N - k_4 & 0 \\ a - 1 & k_5 - k_3 & k_4 - k_2 & N - k_1 \end{bmatrix}$$

METHOD OF MOMENTS ESTIMATOR OF $\boldsymbol{\sigma}^2$ (*continued*)

The estimator of $\boldsymbol{\sigma}^2$ is given by $\mathbf{H}^{-1}\mathbf{s}$, or equivalently, by

$$\begin{bmatrix} \hat{\sigma}^2_\epsilon \\ \hat{\sigma}^2_\gamma \\ \hat{\sigma}^2_\beta \\ \hat{\sigma}^2_\alpha \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -\frac{1}{\lambda_1} & \frac{1}{\lambda_1} & 0 & 0 \\ \frac{\lambda_2-\lambda_1}{\lambda_1\lambda_3} & -\frac{\lambda_2}{\lambda_1\lambda_3} & \frac{1}{\lambda_3} & 0 \\ \frac{\lambda_3(\lambda_4-\lambda_1)+\lambda_5(\lambda_1-\lambda_2)}{\lambda_1\lambda_3\lambda_6} & \frac{\lambda_2\lambda_5-\lambda_3\lambda_4}{\lambda_1\lambda_3\lambda_6} & -\frac{\lambda_5}{\lambda_3\lambda_6} & \frac{1}{\lambda_6} \end{bmatrix} \begin{bmatrix} \text{MSE} \\ \text{MSC} \\ \text{MSB} \\ \text{MSA} \end{bmatrix}$$

$$\begin{array}{ll} \lambda_1 = (N-k_6)/(c_{**}-b_*) & \lambda_2 = (k_6-k_5)/(b_*-a) \\ \lambda_3 = (N-k_4)/(b_*-a) & \lambda_4 = (k_5-k_3)/(a-1) \\ \lambda_5 = (k_4-k_2)/(a-1) \text{ and} & \lambda_6 = (N-k_1)/(a-1) \end{array}$$

- MSA, MSB, MSC and MSE are the usual mean squares of the analysis of variance.

METHOD OF MOMENTS ESTIMATOR OF $\boldsymbol{\sigma}^2$ (*continued*)

$$k_1 = \frac{\sum_i n_{i**}^2}{N} \qquad k_2 = \frac{\sum_i \sum_j n_{ij*}^2}{N}$$

$$k_3 = \frac{\sum_i \sum_j \sum_k n_{ijk}^2}{N} \qquad k_4 = \frac{\sum_i \sum_j n_{ij*}^2}{n_{i**}}$$

$$k_5 = \frac{\sum_i \sum_j \sum_k n_{ijk}^2}{n_{i**}} \qquad k_6 = \frac{\sum_i \sum_j \sum_k n_{ijk}^2}{n_{ij*}}.$$

- Necessary conditions for $\boldsymbol{\sigma}^2$ to be estimable are:

$$\begin{array}{ll} N - c_{**} \neq 0 & N - k_6 \neq 0 \\ N - k_4 \neq 0 \text{ and} & N - k_1 \neq 0 \end{array}$$

- These, in turn, imply that $N \neq c_{**}$, $c_{**} \neq b_*$, $b_* \neq a$, and $a \neq 1$.
- These conditions show that there should be some degree of replication at each level of nesting. For instance, $a > 1$ means that the first level factor A must be replicated at least twice.

$\boxed{\textbf{THE VARIANCE MATRIX OF } \hat{\boldsymbol{\sigma}}^2}$

Define the following vector of quadratic forms:

$$\mathbf{T} = \begin{bmatrix} \mathbf{y}'\mathbf{C}_0\mathbf{y} \\ \mathbf{y}'\mathbf{C}_{abc}\mathbf{y} \\ \mathbf{y}'\mathbf{C}_{ab}\mathbf{y} \\ \mathbf{y}'\mathbf{C}_{a}\mathbf{y} \\ \mathbf{y}'\mathbf{C}_{\mu}\mathbf{y} \end{bmatrix}$$

where, recall

$$\mathbf{A}_0 = \mathbf{C}_0 - \mathbf{C}_{abc} = \mathbf{I}_N - \left\{ {}_d \, \frac{1}{n_{ijk}} \mathbf{J}_{n_{ijk}} \right\}_{i,j,k},$$

$$\mathbf{A}_1 = \mathbf{C}_{abc} - \mathbf{C}_{ab} = \left\{ {}_d \, \frac{1}{n_{ijk}} \mathbf{J}_{n_{ijk}} \right\}_{i,j,k} - \left\{ {}_d \frac{1}{n_{ij*}} \mathbf{J}_{n_{ij*}} \right\}_{i,j}$$

$$\mathbf{A}_2 = \mathbf{C}_{ab} - \mathbf{C}_{a} = \left\{ {}_d \frac{1}{n_{ij*}} \mathbf{J}_{n_{ij*}} \right\}_{i,j} - \left\{ {}_d \, \frac{1}{n_{i**}} \mathbf{J}_{n_{i**}} \right\}_{i}$$

$$\mathbf{A}_3 = \mathbf{C}_{a} - \mathbf{C}_{\mu} = \left\{ {}_d \, \frac{1}{n_{i**}} \mathbf{J}_{n_{i**}} \right\}_{i} - \frac{1}{N} \, \mathbf{J}_N.$$

$\boxed{\textbf{THE VARIANCE MATRIX OF } \hat{\boldsymbol{\sigma}}^2}$

$$\text{Let} \quad \mathbf{G} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{bmatrix}. \qquad \text{Recall} \quad \mathbf{T} = \begin{bmatrix} \mathbf{y}'\mathbf{C}_0\mathbf{y} \\ \mathbf{y}'\mathbf{C}_{abc}\mathbf{y} \\ \mathbf{y}'\mathbf{C}_{ab}\mathbf{y} \\ \mathbf{y}'\mathbf{C}_a\mathbf{y} \\ \mathbf{y}'\mathbf{C}_\mu\mathbf{y} \end{bmatrix}$$

Therefore $\boxed{\boldsymbol{s} = \boldsymbol{G}\,\boldsymbol{T}}$

The vector $\hat{\boldsymbol{\sigma}}^2$ may be expressed as $\boxed{\hat{\boldsymbol{\sigma}}^2 = \mathbf{H}^{-1}\mathbf{G}\mathbf{T}.}$

$$\mathbf{V} = \mathrm{Var}(\hat{\boldsymbol{\sigma}}^2) = \mathbf{H}^{-1}\mathbf{G}\ \mathrm{Var}(\mathbf{T})\ (\mathbf{H}^{-1}\mathbf{G})'$$

The symmetric matrix $\mathrm{Var}(\mathbf{T})$ is given by

$$\mathrm{Var}(\mathbf{T}) = \{_m\ 2\mathrm{Tr}(\mathbf{C}_i\boldsymbol{\Sigma}\mathbf{C}_{i'}\boldsymbol{\Sigma}) + 4\mu^2\mathbf{1}'\mathbf{C}_i\boldsymbol{\Sigma}\mathbf{C}_{i'}\mathbf{1}\ \}_{i,i'}$$

THE VARIANCE MATRIX OF $\hat{\boldsymbol{\sigma}}^2$ (*continued*)

The individual elements of $\mathrm{Var}(\mathbf{T})$ are

$$
\begin{aligned}
V_{55} &= 2\sigma_\epsilon^4(k_1\,\rho_3 + k_2\,\rho_2 + k_3\,\rho_1 + 1)^2, \\
V_{44} &= 2\sigma_\epsilon^4(Nk_1\,\rho_3^2 + k_{22}\,\rho_2^2 + k_{21}\,\rho_1^2 + a + 2Nk_2\,\rho_3\,\rho_2 + 2Nk_3\,\rho_3\,\rho_1 \\
&\quad +2N\,\rho_3 + 2k_{20}\,\rho_2\,\rho_1 + 2k_4\,\rho_2 + 2k_5\,\rho_1), \\
V_{45} &= 2\sigma_\epsilon^4(k_7\,\rho_3^2 + k_{13}\,\rho_2^2 + k_{14}\,\rho_1^2 + N + 2k_{23}\,\rho_3\,\rho_2 + 2k_{24}\,\rho_3\,\rho_1 \\
&\quad +2Nk_1\,\rho_3 + 2k_{17}\,\rho_2\,\rho_1 + 2Nk_2\,\rho_2 + 2Nk_3\,\rho_1)/N, \\
V_{33} &= V_{44} + 2\sigma_\epsilon^4[(Nk_2 - k_{22})\,\rho_2^2 + (k_{19} - k_{21})\,\rho_1^2 + (b_* - a) \\
&\quad +2(Nk_3 - k_{20})\,\rho_2\,\rho_1 + 2(N - k_4)\,\rho_2 + 2(k_6 - k_5)\,\rho_1], \\
V_{34} &= V_{44} + 2\sigma_\epsilon^4[(k_{12} - k_{22})\,\rho_2^2 + (k_{18} - k_{21})\,\rho_1^2 + 2(k_{16} - k_{20})\,\rho_2\,\rho_1], \\
V_{35} &= V_{45} + 2\sigma_\epsilon^4[(k_8 - k_{13})\,\rho_2^2 + (k_{15} - k_{14})\,\rho_1^2 + 2(k_{25} - k_{17})\,\rho_2\,\rho_1)]/N, \\
V_{22} &= V_{33} + 2\sigma_\epsilon^4[(Nk_3 - k_{19})\,\rho_1^2 + (c_{**} - b_*) + 2(N - k_6)\,\rho_1], \\
V_{23} &= V_{33} + 2\sigma_\epsilon^4(k_{11} - k_{19})\,\rho_1^2, \\
V_{24} &= V_{34} + 2\sigma_\epsilon^4(k_{10} - k_{18})\,\rho_1^2.
\end{aligned}
$$

THE VARIANCE MATRIX OF $\hat{\boldsymbol{\sigma}}^2$ (*continued*)

$$
\begin{aligned}
V_{25} &= V_{35} + 2\sigma_\epsilon^4 \left(\frac{k_9 - k_{15}}{N} \right) \rho_3^2, \\
V_{11} &= 2N\sigma_\epsilon^4 (k_1\, \rho_3^2 + k_2\, \rho_2^2 + k_3\, \rho_1^2 + 1 + 2k_2\, \rho_3\, \rho_2 + 2k_3\, \rho_3\, \rho_1 \\
&\quad +2\, \rho_3 + 2k_3\, \rho_2\, \rho_1 + 2\, \rho_2 + 2\, \rho_1), \\
V_{12} &= 2\sigma_\epsilon^4 (Nk_1\, \rho_3^2 + Nk_2\, \rho_2^2 + Nk_3\, \rho_1^2 + c_{**} + 2Nk_2\, \rho_3\, \rho_2 + 2Nk_3\, \rho_3\, \rho_1 \\
&\quad +2N\, \rho_3 + 2Nk_3\, \rho_2\, \rho_1 + 2N\, \rho_2 + 2N\, \rho_1), \\
V_{13} &= 2\sigma_\epsilon^4 (Nk_1\, \rho_3^2 + Nk_2\, \rho_2^2 + k_{11}\, \rho_1^2 + b_* + 2Nk_2\, \rho_3\, \rho_2 + 2Nk_3\, \rho_3\, \rho_1 \\
&\quad +2N\, \rho_3 + 2Nk_3\, \rho_2\, \rho_1 + 2N\, \rho_2 + 2k_6\, \rho_1), \\
V_{14} &= 2\sigma_\epsilon^4 (Nk_1\, \rho_3^2 + k_{12}\, \rho_2^2 + k_{10}\, \rho_1^2 + a + 2Nk_2\, \rho_3\, \rho_2 + 2Nk_3\, \rho_3\, \rho_1 \\
&\quad +2N\, \rho_3 + 2k_{16}\, \rho_2\, \rho_1 + 2k_4\, \rho_2 + 2k_5\, \rho_1), \text{ and} \\
V_{15} &= 2\sigma_\epsilon^4 (k_7\, \rho_3^2 + k_8\, \rho_2^2 + k_9\, \rho_1^2 + N + 2k_{23}\, \rho_3\, \rho_2 + 2k_{24}\, \rho_3\, \rho_1 \\
&\quad +2Nk_1\, \rho_1 + 2k_{25}\, \rho_2\, \rho_1 + 2Nk_2\, \rho_2 + 2Nk_3\, \rho_1)/N.
\end{aligned}
$$

where

$$\boxed{\rho_1 = \sigma_\gamma^2/\sigma_\epsilon^2,\ \rho_2 = \sigma_\beta^2/\sigma_\epsilon^2 \text{ and } \rho_3 = \sigma_\alpha^2/\sigma_\epsilon^2.}$$

and ...

THE VARIANCE MATRIX OF $\hat{\boldsymbol{\sigma}}^2$ (*continued*)

$$k_1 = \frac{\sum_i n_{i**}^2}{N}, \qquad k_2 = \frac{\sum_i \sum_j n_{ij*}^2}{N},$$

$$k_3 = \frac{\sum_i \sum_j \sum_k n_{ijk}^2}{N}, \qquad k_4 = \frac{\sum_i \sum_j n_{ij*}^2}{n_{i**}}$$

$$k_5 = \frac{\sum_i \sum_j \sum_k n_{ijk}^2}{n_{i**}}, \qquad k_6 = \frac{\sum_i \sum_j \sum_k n_{ijk}^2}{n_{ij*}},$$

$$k_7 = \sum_i n_{i**}^3, \qquad k_8 = \sum_i \sum_j n_{ij*}^3,$$

$$k_9 = \sum_i \sum_j \sum_k n_{ijk}^3, \qquad k_{10} = \sum_i \frac{\sum_j \sum_k n_{ijk}^3}{n_{i**}},$$

$$k_{11} = \sum_i \sum_j \frac{\sum_k n_{ijk}^3}{n_{ij*}}, \qquad k_{12} = \sum_i \frac{\sum_j n_{ij*}^3}{n_{i**}},$$

$$k_{13} = \sum_i \frac{(\sum_j n_{ij*}^2)^2}{n_{i**}}, \qquad k_{14} = \sum_i \frac{(\sum_j \sum_k n_{ijk}^2)^2}{n_{i**}},$$

THE VARIANCE MATRIX OF $\hat{\boldsymbol{\sigma}}^2$ (*continued*)

$$k_{15} = \sum_i \sum_j \frac{(\sum_k n_{ijk}^2)^2}{n_{ij*}}, \qquad k_{16} = \sum_i \frac{\sum_j n_{ij*}\,(\sum_k n_{ijk}^2)}{n_{i**}},$$

$$k_{17} = \sum_i \frac{(\sum_j n_{ij*}^2)(\sum_j \sum_k n_{ijk}^2)}{n_{i**}}, \qquad k_{18} = \sum_i \frac{\sum_j (\sum_k n_{ijk}^2)^2 / n_{ij*}}{n_{i**}},$$

$$k_{19} = \sum_i \sum_j \frac{(\sum_k n_{ijk}^2)^2}{n_{ij*}^2}, \qquad k_{20} = \sum_i \frac{(\sum_j n_{ij*}^2)(\sum_j \sum_k n_{ijk}^2)}{n_{i**}^2},$$

$$k_{21} = \sum_i \frac{(\sum_j \sum_k n_{ijk}^2)^2}{n_{i**}^2}, \qquad k_{22} = \sum_i \frac{(\sum_j n_{ij*}^2)^2}{n_{i**}^2},$$

$$k_{23} = \sum_i n_{i**} \left(\sum_j n_{ij*}^2 \right), \qquad k_{24} = \sum_i n_{i**} \left(\sum_j \sum_k n_{ijk}^2 \right),$$

and $$k_{25} = \sum_i \sum_j n_{ij*} \left(\sum_k n_{ijk}^2 \right).$$ *See* Mahamunulu (1963)

DESIGN CRITERIA

The optimal allocation of experimental resources in variance components models is done by minimizing some function of $\mathrm{Var}(\hat{\boldsymbol{\sigma}}^2)$. Several criteria have been proposed. Some of the common criteria are

- D–*optimality*: a design is D-optimal if it maximizes the determinant of the information matrix, i.e. if it minimizes the determinant of the variance–covariance matrix of the variance estimators. This determinant is often called the generalized variance.
- A–*optimality*: an A–Optimal design is that which minimizes the sum (or average) of the variances of the parameters of interest.
- A_s–*optimality*: A third criterion, called the adjusted or scaled trace criterion has been proposed for the design of variance components models (Prairie, Gaylor). This criterion seeks to minimize the trace of the scaled or adjusted variance–covariance matrix of the estimators

$$\mathbf{V}_s = \left\{ m \, \frac{\mathrm{Cov}(\hat{\sigma}_i^2, \hat{\sigma}_j^2)}{\sigma_i^2 \, \sigma_j^2} \right\}_{i,j}$$

DESIGN CRITERIA

- It should be noted that $\mathbf{V}_s$ is simply the variance–covariance matrix of the estimators $\mathbf{V}$ with each element scaled by the size of the variance components involved in the computation of the element.
- In this sense $\mathbf{V}_s$ may be viewed as a generalized coefficient of variation matrix and the trace of this matrix as an average of the squared coefficients of variation.
- We will denote a design that arises from this criterion as an A_s–optimal design.

OPTIMIZATION PROBLEM

Given N, find a design with this total sample size such that the corresponding design constants $a, \{a_i\}, \{b_{ij}\}, \{n_{ijk}\}$ minimize the chosen optimality criterion for a given value of ρ_1, ρ_2, ρ_3.

NONLINEAR DESIGN PROBLEM

- The objective functions in the optimum design problem for variance components involve the unknown model parameters ρ_1, ρ_2, ρ_3.

- **Some approaches:** Bayesian, Multi-stage, Minimax, ...

- A key step is the determination of locally optimal designs.

- In principle, given locally optimal designs for a GRID of parameter values, GOOD DESIGNS for practical use may be determined in a straightforward manner.

- One could use numerical optimization (exchange algorithms) of an optimality criterion over the space of all allowable designs

- We chose to consider restricted classes of designs and attempt to find optimum designs in this class. We believe this approach allows us to get some insight into when and why certain design configurations turn out to be optimal.

BACKGROUND

- STAGGERED DESIGNS were introduced for estimation of variance components in a 3-stage or higher order nested model – Anderson 1960, Bainbridge 1963.
- The idea was to have more or less equal numbers of degrees of freedom for each level of the hierarchy. This generally requires IMBALANCE in the sampling plan.
- Most of the early work used ANOVA ESTIMATORS for variance components.
- Also, most of the early work concentrated on optimum designs for individual variance components or an individual ratio of variance components – i.e., single parameter optimum designs.

  The main results are by Crump 1954; Anderson 1960, 1961; Bainbridge 1963; Bush and Anderson 1963; Anderson and Crump 1967.

$\boxed{\textbf{BACKGROUND – MULTIPLE PARAMETERS}}$

- Goldsmith 1969; Goldsmith and Gaylor 1970 – a suitable scalar function of the variance matrix of the estimators is minimized (D, A, A_s criteria).
- Some authors have considered the asymptotic variance matrix of the MLEs or REMLs to study optimum designs for variance components – Muse 1974; Muse and Anderson 1978; Muse et al. 1982.
- Anderson (1975), Khuri and Sahai (1985) – give a comprehensive survey of designs for variance components.

$\boxed{\textbf{TWO-STAGE NESTED MODEL}}$

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$
$$i = 1,\, 2, \ldots,\, a,\;\; j = 1,\, 2, \ldots,\, n_i,\;\; N = \textstyle\sum_{i=1}^{a} n_i$$

Parameters of interest:

$$\mu,\, \sigma_\alpha^2,\, \sigma_\epsilon^2,\, \rho = \sigma_\alpha^2 / \sigma_\epsilon^2$$

ANALYSIS OF VARIANCE

Source	Degrees of Freedom	Mean Squares	Expected Mean Square
A	$a-1$	MSA	$\lambda\, \sigma_\alpha^2 + \sigma_\epsilon^2$
Error	$N-a$	MSE	σ_ϵ^2

$$\lambda = (N - k_1)/(a-1), \qquad k_1 = \textstyle\sum_i^a n_i^2 / N$$

$\boxed{\textbf{ANOVA ESTIMATORS}}$

OLSE of μ

$$\hat{\mu} = \overline{y}_{**}$$

ANOVA estimators

$$\hat{\sigma}^2_\alpha = \frac{\text{MSA} - \text{MSE}}{\lambda} \qquad\qquad \hat{\sigma}^2_\epsilon = \text{MSE}$$

$$\tilde{\rho} = (\text{MSA} - \text{MSB})/(\lambda\ \text{MSB})$$

The estimator $\tilde{\rho}$ is biased. An unbiased estimator is (**Crump (1954)**)

$$\hat{\rho} = \frac{1}{\lambda}\left[\frac{N-a-2}{N-a}\frac{\text{MSA}}{\text{MSE}} - 1\right]$$

Hammersley (1949)

- Obtained approximate optimum designs for estimating σ_α^2.
- Showed $\mathrm{Var}(\hat{\sigma}_\alpha^2)$ would be minimized by allocating an equal number of observations
$$n = \frac{N\rho + N + 1}{N\rho + 2}$$
to each class.
- Since n is not always an integer, he suggested that the closest integer should be taken.

Crump (1954)

- Proposed optimum designs for σ_α^2, σ_ϵ^2, and $\rho = \sigma_\alpha^2/\sigma_\epsilon^2$, for a fixed total number of observations N, and costs proportional to N; see also Anderson & Crump 1967.
- Optimum designs depend on the unknown value $\rho = \sigma_\alpha^2/\sigma_\epsilon^2$.
- Optimum design for one parameter is not necessarily optimum for another parameter.

$\boxed{\textbf{CRUMP's SOLUTION for } \sigma_\alpha^2}$

1. For the optimal number $a = a_\alpha$ of first stage classes, use

$$\boxed{a_\alpha = \frac{N(N\rho + 2)}{N(\rho + 1) + 1}}$$

   if it is an integer. Then, for fixed N, $\mathrm{Var}(\hat{\sigma}_\alpha^2)$ is minimized if

$$N = (n+1)a_{n+1} + na_n,$$

   where $a_{n+1} + a_n = a$; i.e. $n_i = n + 1$ for $i = 1, 2, \ldots, a_{n+1}$ and $n_i = n$ for $i = a_{n+1} + 1, 2, \ldots, a$. This design is referred to as (a_{n+1}, a_n) design by Thompson (1975).

2. If a_α is not an integer, select the bracketing integers and compute $\mathrm{Var}(\hat{\sigma}_\alpha^2)$ for each case, using the (a_{n+1}, a_n) allocation. Whichever variance is smaller, compute the variance for the next adjacent integral value. Continue this process until the smallest variance is obtained.

3. If one of the adjacent integers produces a balanced plan, then use this value for a.

Note that the optimal number of first stage levels depends on the unknown value of ρ.

$\boxed{\textbf{CRUMP's SOLUTION for } \rho = \sigma_\alpha^2/\sigma_\epsilon^2}$

1. For the optimal number $a = a_\rho$ of first stage classes, use

$$a_\rho = 1 + \frac{(N-5)(N\rho+1)}{2N\rho + N - 3}$$

   if it is an integer. Use the (a_{n+1}, a_n) allocation for the second level nesting.

2. If a_ρ is not an integer, select the bracketing integers and compute $\mathrm{Var}(\hat{\sigma}_\rho^2)$ for each case, using the (a_{n+1}, a_n) allocation. Whichever variance is smaller, compute the variance for the next adjacent integral value. Continue this process until the smallest variance is obtained.

3. If one of the adjacent integers produces a balanced plan, then use this value for a.

Note that the optimal number of first stage levels depends on the unknown value of ρ.

COMMENTS on CRUMP's SOLUTIONS

- Crump studied the loss in efficiency due to the use of an incorrect value of ρ and found that it to be generally less than 10% if $1/2 < \rho_1/\rho_0 < 2$, where ρ_0 is the true value of the parameter ρ and ρ_1 is the incorrect value used in the determination of the optimal number of classes. The percentage loss in efficiency becomes quite large as ρ_1 departs more from ρ_0.

- For a large total sample size N, Crump observed that

$$\frac{a_\alpha}{a_\rho} \to \frac{1+2\rho}{1+\rho}.$$

  So an optimal allocation requires more classes to estimate σ_α^2 than to estimate ρ when N is large.

- Since $\rho = \sigma_\alpha^2/\sigma_\epsilon^2$, a good estimate of ρ is dependent more on obtaining a better estimate of σ_ϵ^2 than of σ_α^2; hence, fewer first stage classes are required for $\hat{\rho}$.

OPTIMUM ESTIMATION OF MULTIPLE PARAMETERS

- When a sampling plan is designed to be optimal for one parameter, how good is it for other parameters? Crump examined this question.
- He concluded that a single criterion is needed if several parameters are of interest simultaneously. This criterion should involve the precision of all of the parameters of interest.
- Thompson & Anderson studied the simultaneous problem of design selection and estimation procedure to estimate the variance components in the two-stage model, using minimum mean square error (MSE) as the criterion.

  In their work they considered truncated ANOVA estimators (i.e. $\sigma_\alpha^2 \geq 0$), maximum likelihood (ML) and modified ML estimators of the parameters of interest.

  Exact values of the MSE were calculated for balanced designs and compared to Crump's (a_1, a_2) design. Several MSE's for unbalanced designs were obtained through simulations.

MULTIPLE PARAMETERS (*continued*)

For balanced designs, Thompson & Anderson concluded that the modified ML estimators are superior and that for these estimators the optimal design is less sensitive to ρ than designs based on minimizing the usual ANOVA estimators.

Generally, the Anderson–Crump allocation is close to the optimal allocation using the modified ML estimators.

When ρ is large, maximum likelihood provides estimators of σ_α^2 with smaller MSE than the other procedures for the design (a_1, a_2). This is the optimal design for large ρ.

THREE–STAGE NESTED MODEL

$$y_{ijk} = \mu + \alpha_i + \beta_{ij} + \epsilon_{ijk}$$

$i = 1,\ 2, \ldots,\ a,$ $\quad j = 1,\ 2, \ldots,\ b_i$

$k = 1,\ 2, \ldots,\ n_{ij},$ $\quad b_* = \sum_{i=1}^{a} b_i$

$n_{i*} = \sum_{j=1}^{b_i} n_{ij},$ $\quad N = \sum_{i=1}^{a} \sum_{j=1}^{b_i} n_{ij}$

$\alpha_i \sim N(0, \sigma_\alpha^2),$ $\quad \beta_{ij} \sim N(0, \sigma_\beta^2)$

$\epsilon_{ijk} \sim N(0, \sigma_\epsilon^2)$

$\boxed{\textbf{ANALYSIS OF VARIANCE}}$

Source	Degrees of Freedom	Mean Squares	Expected Mean Square
A	$a-1$	MSA	$\lambda_1\,\sigma_\alpha^2 + \lambda_2\,\sigma_\beta^2 + \sigma_\epsilon^2$
B	$b_* - a$	MSB	$\lambda_3\sigma_\beta^2 + \sigma_\epsilon^2$
Error	$N - b_*$	MSE	σ_ϵ^2

$$\lambda_1 = \frac{N-k_1}{a-1}, \quad \lambda_2 = \frac{k_2-k_3}{a-1}, \quad \text{and} \quad \lambda_3 = \frac{N-k_2}{b_*-a}$$

$$k_1 = \frac{\sum_{i=1}^a n_{i*}^2}{N}, \quad k_2 = \sum_{i=1}^a \frac{\sum_{j=1}^{b_i} n_{ij}^2}{N} \quad \text{and} \quad k_3 = \frac{\sum_{i=1}^a \sum_{j=1}^{b_i} n_{ij}^2}{N}.$$

$\boxed{\textbf{ANOVA ESTIMATORS}}$

OLSE

$$\hat{\mu} = \overline{y}_{***}$$

ANOVA estimators

$$\hat{\sigma}_{\epsilon}^2 = \mathrm{MSE}$$

$$\hat{\sigma}_{\beta}^2 = \frac{\mathrm{MSB(A)} - \mathrm{MSE}}{\lambda_3}$$

and

$$\hat{\sigma}_{\alpha}^2 = \frac{\lambda_3 \mathrm{MSA} - \lambda_2 \mathrm{MSB} - (\lambda_3 - \lambda_2)\, \mathrm{MSE}}{\lambda_1 \lambda_3}$$

$$k_1 = \frac{\sum_{i=1}^{a} n_{i*}^2}{N}, \quad k_2 = \sum_{i=1}^{a} \frac{\sum_{j=1}^{b_i} n_{ij}^2}{N} \quad \text{and} \quad k_3 = \frac{\sum_{i=1}^{a} \sum_{j=1}^{b_i} n_{ij}^2}{N}.$$

PRAIRIE's RESULTS FOR INDIVIDUAL PARAMETERS (1961, 1962)

Cost proportional to N (the total number of observations)

Optimal estimation of μ:

Select a design that has one observation in each of N first stage classes.

Optimal estimation of σ_ϵ^2:

Select a design with all N observations in a single second stage class within a single first stage class.

Optimal estimation of σ_β^2:

Choose $a = 1$ and proceed as suggested by Crump for the second and third stage allocation.

PRAIRIE's RESULTS (*continued*)

Optimal estimation of σ_α^2:

Start with a balanced design in which $b_* = N$ and then use Crump's allocation with $\sigma_\beta^2 + \sigma_\epsilon^2$ substituted for σ_β^2. This procedure is suggested assuming a balanced design would be optimal.

Optimal estimation of $\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_\epsilon^2$:

Select a design with $a = b_* = N$.

For optimal estimation of $\rho = \sigma_\alpha^2/(\sigma_\beta^2 + \sigma_\epsilon^2)$:

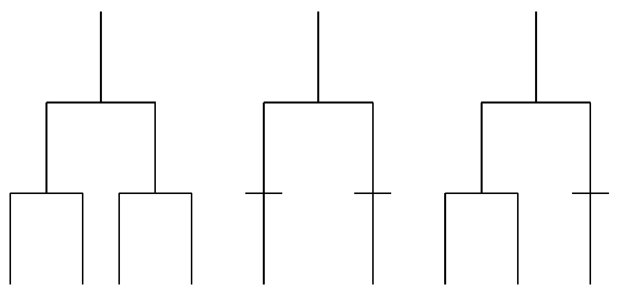
Set $b_* = N$ and then use Crump's allocation of ρ.

DESIGNS FOR ESTIMATING MULTIPLE PARAMETERS

- Prairie studied several **staggered designs** previously presented by Anderson and Bancroft 1952; Anderson 1960; Calvin and Miller (1961).
- The first design presented was the so called Anderson–design which consisted of $a/2$ configurations of type-1 and $a/2$ configurations of type-2 in the **figure** below.
- For these designs, the degrees of freedom for the first, second and third stage sums of squares are $a-1$, a and a, respectively.

Configurations used in Prairie's designs

Stage	Structure Number 1	2	3
1			
2			
3			



PRAIRIE's DESIGNS (*continued*)

For assignments of degrees of freedom other than $a-1$, a, a where balance cannot be achieved, Prairie proposed a specific procedure for constructing a design, called the **$\mathbf{D_2}$-design**. Suppose the required degrees of freedom are df_1, df_2, df_3, respectively, for MSA, MSB, and MSE.

$$\boxed{a = 1 + df_1\textbf{,}\ b_* = 1 + df_1 + df_2\textbf{, and } N = 1 + df_1 + df_2 + df_3\textbf{.}}$$

1. The number of first stage classes is a. Write
$$\frac{b_*}{a} = q_2 + \frac{r_2}{a}, \qquad \text{for } 0 \leq r_2 < a.$$
To each first stage class assign q_2 second stage classes and then one extra second level class to each of the r_2 first stage classes.

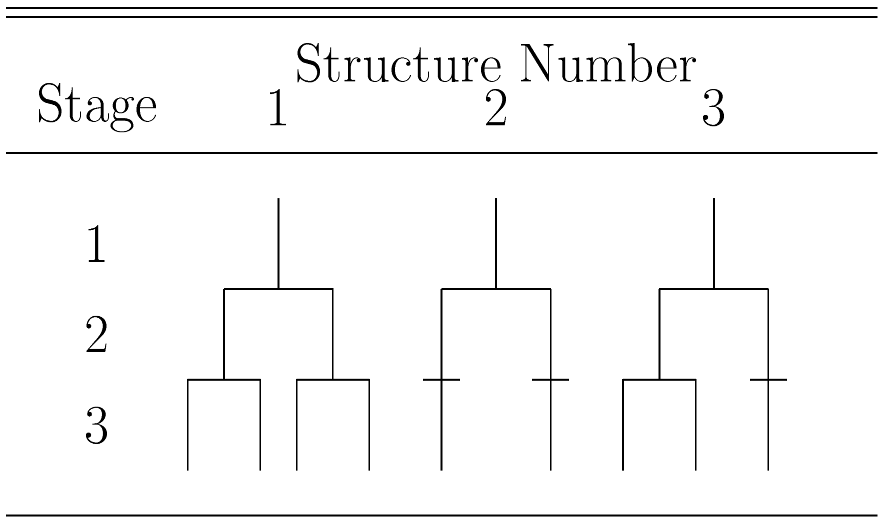
2. Write
$$\frac{N}{a} = q_1 + \frac{r_1}{a}, \qquad \text{for } 0 \leqslant r_1 < a$$
and assign $q_1 + 1$ observations to each of r_1 first stage classes and q_1 observations to the remaining $a - r_1$ first stage classes.

3. Within each first stage class, assign the observations to the second stage class as equally as possible.

PRAIRIE's DESIGNS (*continued*)

For the assignment of degrees of freedom $a-1$, a, a this procedure will produce designs that consist of a configurations of the Type 3 shown in the figure below.

Configurations used in Prairie's designs



PRAIRIE's DESIGNS (*continued*)

$\boldsymbol{D}_1$-Designs:

A third group of designs proposed are the $\boldsymbol{D}_1$-**designs**. These are constructed by dividing the first stage into groups and then assigning the second and third stages so that balance is maintained in each group.

Suppose the degrees of freedom specified are df_1, df_2, df_3. Then a k-group $\boldsymbol{D}_1$-**design** exists if the following equations have positive integer solutions.

$$\begin{aligned} a_1 + \ldots + a_k &= 1 + df_1 \\ a_1 b_1 + \ldots + a_k b_k &= 1 + df_1 + df_2 \\ a_1 b_1 c_1 + \ldots + a_k b_k c_k &= 1 + df_1 + df_2 + df_3 \end{aligned}$$

$\boxed{\textbf{EXAMPLES of } D_1\textbf{-Designs:}}$

Suppose the required degrees of freedom are 23, 8, 16, respectively, for the three stages.

- For $k = 2$, we have the following solution:

$$a_1 = 16, a_2 = 8, b_1 = 1, b_2 = 2, c_1 = 1, c_2 = 2.$$

- Another solution for $k = 2$ is:

$$a_1 = 16, a_2 = 8, b_1 = 1, b_2 = 2, c_1 = 2, c_2 = 1.$$

- For $k = 3$, the following are a subset of all solutions:

$$a_1 = 16, a_2 = 4, a_3 = 4, b_1 = 1, b_2 = 3, b_3 = 1, c_1 = 1, c_2 = 2, c_3 = 2$$

$$a_1 = 16, a_2 = 4, a_3 = 4, b_1 = 1, b_2 = 3, b_3 = 1, c_1 = 1, c_2 = 1, c_3 = 1$$

$$a_1 = 12, a_2 = 8, a_3 = 4, b_1 = 1, b_2 = 2, b_3 = 1, c_1 = 3, c_2 = 1, c_3 = 1$$

$$a_1 = 12, a_2 = 8, a_3 = 4, b_1 = 1, b_2 = 2, b_3 = 1, c_1 = 2, c_2 = 3, c_3 = 2$$

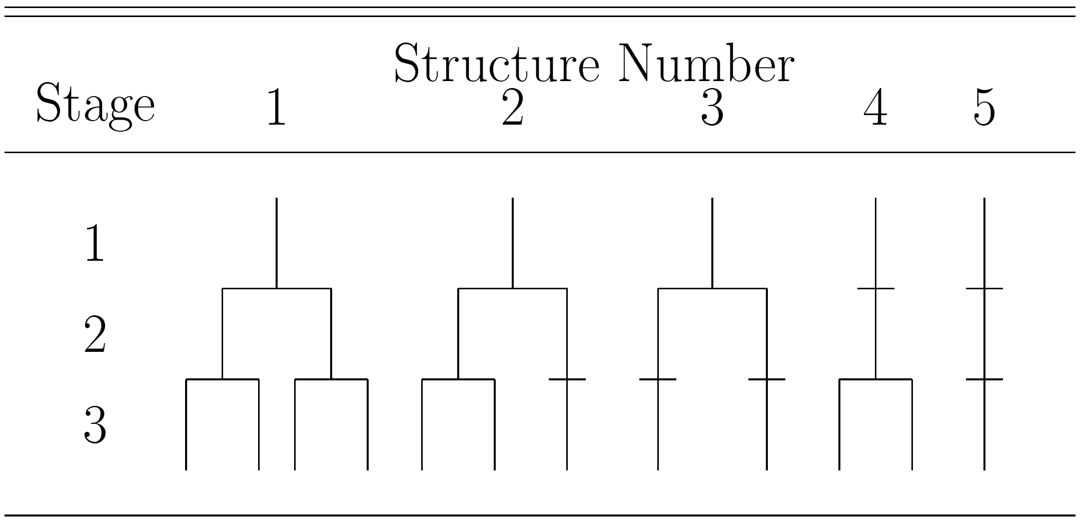
$$a_1 = 12, a_2 = 8, a_3 = 4, b_1 = 1, b_2 = 2, b_3 = 1, c_1 = 1, c_2 = 3, c_3 = 6$$

PRAIRIE's CONCLUSIONS

- Prairie considered a sample of size $N = 48$ with eight different assignments of degrees of freedom.
- For each df assignment, D_1, D_2 and Anderson-designs (whenever possible) were constructed.
- The variances of the ANOVA estimators of the variance components were compared for several values of $\rho_1 = \sigma_\alpha^2/\sigma_\epsilon^2$ and $\rho_2 = \sigma_\beta^2/\sigma_\epsilon^2$.
- Prairie reported that the manner in which the degrees of freedom are assigned to the sources of variation, as well as the true values of the variance components have a large effect on the optimality of a design.
- Prairie concluded that no single design is best for estimating all the variance components. However, STAGGERED DESIGNs appeared to be a good compromise.

GOLDSMITH's RESULTS (1969, 1970)

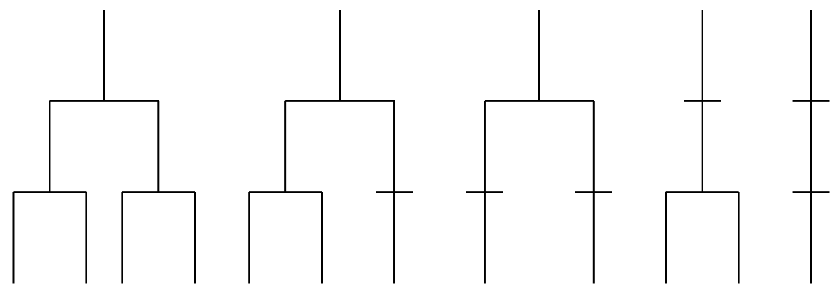
- Designs for the three-stage nested model based on the use of no more than three of the five fundamental structures shown in the figure below were proposed by Goldsmith 1969; Goldsmith and Gaylor 1970.
- The graphs in the figure are all the structures in a three–stage nested design in which each level can split into one or two sublevels.



GOLDSMITH's RESULTS (1969, 1970) *(continued)*

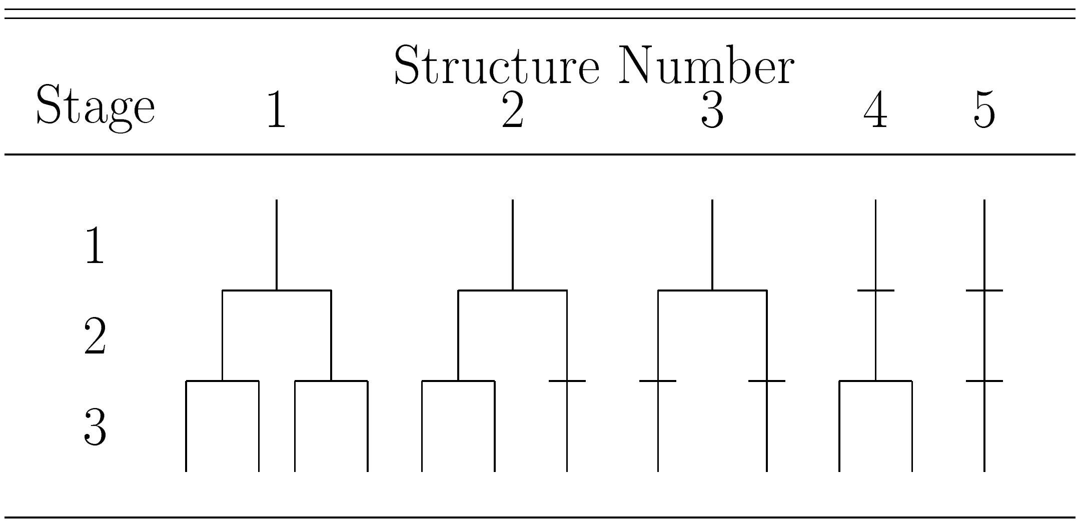
- A particular design will consist of r_i replicates of the ith structure, such that $4r_1 + 3r_2 + 2r_3 + 2r_4 + r_5 = N$.
- This design will be referred to by the vector $(r_1, r_2, r_3, r_4, r_5)$. For example, the design $(2, 0, 1, 1, 0)$ indicates that the experiment would be run with two replicates of the structure 1 and one replicate of each of the structures 3 and 4.

Stage	Structure Number 1	2	3	4	5
1					
2					
3					



RESULTS OF GOLDSMITH & GAYLOR 1970

- For a sample of size 12, there are 61 different GOLDSMITH/GAYLOR designs which allow the ANOVA estimation of all three variance components.
- Each of these 61 designs was replicated r times, $r = 1(1)10$, producing designs for sample size that range from $N = 12(12)120$.
- For instance if $r = 3$ and the design $(2, 0, 1, 1, 0)$ is used, the experimental plan will be $(6, 0, 3, 3, 0)$ or six replicates of structure 1 and three of structures 3 and 4. The total number of observations N is then 36.



Configurations used in Goldsmith's designs

$\boxed{\textbf{RESULTS OF GOLDSMITH \& GAYLOR } (\textit{continued})}$

- Optimum designs were determined for samples of size $12r$, $r = 1(1)10$ and forty-nine variance component configurations $(1, \rho_1, \rho_2)$ formed by setting $\rho_1 = 2^k$ and $\rho_2 = 2^m$, where $k = -3(1)3$ and $m = -3(1)3$.
- The criteria used to compare the designs were the **trace** (total variance) and the generalized variance (**determinant**) of the variance-covariance matrix of the ANOVA estimators of the variance components. A proposed third criterion was the **trace of the scaled variance–covariance matrix** with elements given by

$$\frac{\mathrm{Cov}(\hat{\sigma}_i^2, \hat{\sigma}_j^2)}{\sigma_i^2\, \sigma_j^2}.$$

This is the called the adjusted or **scaled trace criterion**.

RESULTS OF GOLDSMITH & GAYLOR (*continued*)

- Goldsmith & Gaylor found that the sample size is critical to the choice of an optimum design. This is especially true when the sample size is small. Small changes in the variance components values tended to shift the optimum designs from one configuration to another, especially for $r = 1, 2, 3$ (i.e. for samples of sizes 12, 24 and 36, respectively).
- These changes are less pronounced in case of a large sample size. This is particularly true when the trace is used as criterion for the choice of design.

RESULTS OF GOLDSMITH & GAYLOR (*continued*)

- When both ρ_1 and ρ_2 are small, the balanced design was found to be optimum since it concentrates the sampling in the third stage.
- However, when ρ_1 is large, designs with the highest second-stage degrees of freedom are produced. On the other hand, if ρ_2 is large, then designs with a high first-stage sampling are selected.
- The determinant criterion was found to be insensitive to changes in sample size and variance component configuration. Hence Goldsmith and Gaylor recommend that this criterion should not be used when deciding the sampling plan.
- The scaled trace criterion is relatively insensitive to changes of the sample size and of ρ_2. However it is sensitive to variance component configuration only through changes of ρ_1.

$\boxed{\textbf{DELGADO (1997), DELGADO \& IYER (1999)}}$

Extended Goldsmith's work in several directions.

- Considered sample sizes other than $12r$ are considered. This led to the consideration of the class of all designs with at most two splits at each level that allow the estimation of all the variance components.
- By using this larger collection of designs, obtained designs with better properties than those proposed by Goldsmith and Gaylor.

  Example: $N = 24$, $\rho_1 = 4$ and $\rho_2 = 8$. Goldsmith and Gaylor suggest $r = 2$ replicates of the design $(0, 4, 0, 0, 0)$ for D-optimality. However if all 292 possible designs (rather than 61) in the more complete class are considered, then the design that minimizes the determinant is a single replicate of the design $(3, 4, 0, 0, 0)$, which was not one of the candidates considered by Gaylor and Goldsmith.

- This motivated consideration of the class of designs that consist of replicates of structures in which each level can be split into up to three sublevels (more generally, s sublevels). This class includes the two–split designs as a subclass.

$\boxed{\textbf{THE CLASS } C^*_{3,s}}$

- The class $\mathcal{C}^*_{3,s}$ is the collection of all three–stage nested designs $\mathcal{D}$ for which $b_i \leq s$ and $n_{ij} \leq s$ for $i = 1, 2, \ldots, a$ and $j = 1, 2, \ldots, b_i$.
- **ATOMS:** Designs in $\mathcal{C}^*_{3,s}$ for which $a = 1$ will be called the atoms of $\mathcal{C}^*_{3,s}$.
- The collection of all atoms in $\mathcal{C}^*_{3,s}$ will be denoted by $\mathcal{A}_{3,s}$.
- The number of elements in $\mathcal{A}_{3,s}$ by $p_3(s)$.
- We label the atoms in $\mathcal{C}^*_{3,s}$ by $A_1, A_2, \ldots, A_{p_3(s)}$.

THE NUMBER OF ATOMS IN THE CLASS $C^*_{3,s}$

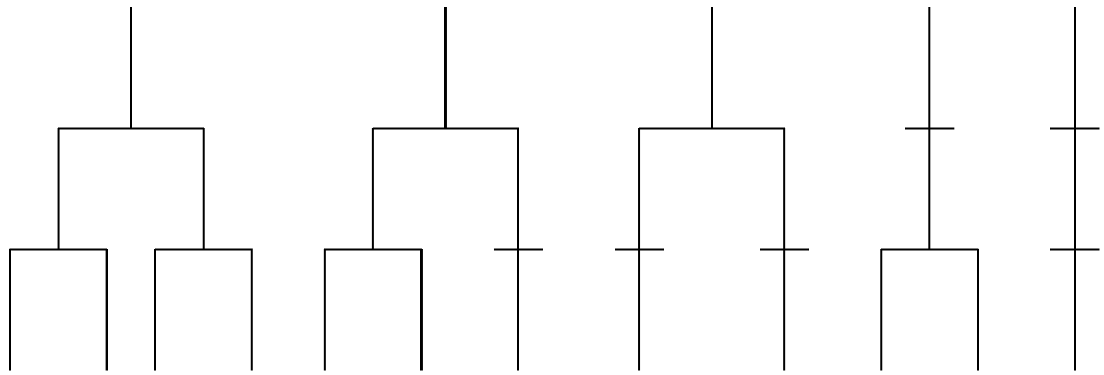
The number of atoms in $\mathcal{C}^*_{3,s}$ is given by

$$p_3(s) = \sum_{i=s}^{2s-1} \binom{i}{s-1}$$

s	1	2	3	4	5	6
$p_3(s)$	1	5	19	69	251	923

ATOMS IN THE CLASS $C^*_{3,2}$

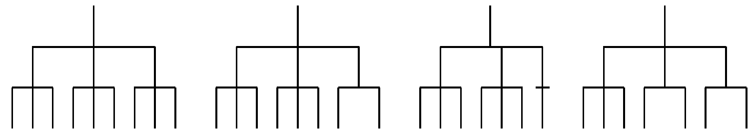
Stage	Atom Number 1	2	3	4	5
1					
2					
3					

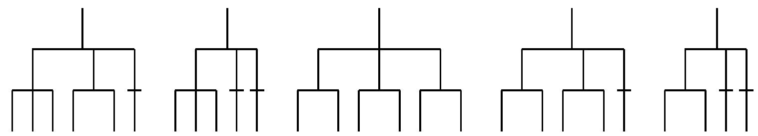


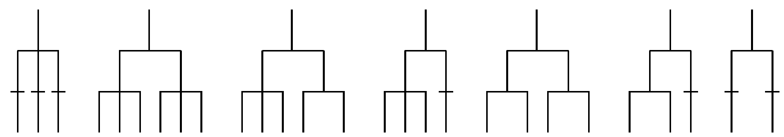
	1	2	3	4	5
b_i	2	2	2	1	1
n_{ij}	2,2	2,1	1,1	2	1
$n_{i.}$	4	3	2	2	1

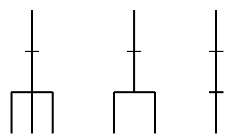
ATOMS IN THE CLASS $C^*_{3,3}$

Atom Number

Stage	1	2	3	4
1 2 3				
b_i	3	3	3	3
n_{ij}	3,3,3	3,3,2	3,3,1	3,2,2
$n_{i.}$	9	8	7	7

	5	6	7	8	9
1 2 3					
b_i	3	3	3	3	3
n_{ij}	3,2,1	3,1,1	2,2,2	2,2,1	2,1,1
$n_{i.}$	6	5	6	5	4

	10	11	12	13	14	15	16
1 2 3							
b_i	3	2	2	2	2	2	2
n_{ij}	1,1,1	3,3	3,2	3,1	2,2	2,1	1,1
$n_{i.}$	3	6	5	4	4	3	2

	17	18	19
1 2 3			
b_i	1	1	1
n_{ij}	3	2	1
$n_{i.}$	3	2	1

DESIGNS IN THE CLASS $C^*_{3,s}$

- Any given design $\mathcal{D}$ in $\mathcal{C}^*_{3,s}$ is the union of atoms in $\mathcal{A}_{3,s}$, where each atom may occur 0, 1 or more times. If r_l is the number of times atom A_l occurs in $\mathcal{D}$, then $\mathcal{D}$ is completely determined by the pattern vector $(r_1, \ldots, r_{p_3(s)})$.
- Only a subset of designs in $\mathcal{C}^*_{3,s}$ correspond to a given sample size N.
- Not all designs in this class will allow the estimation of all the variance components in the model. For example in $\mathcal{C}^*_{3,2}$, the variance components σ^2_β and σ^2_ϵ are not estimable if the design $(0, 0, 0, 0, N)$ is used.
- As a consequence, we consider only the subset of $\mathcal{C}^*_{3,s}$ such that all the model parameters are estimable.

$\boxed{\textbf{THE CLASS } C_{3,s,k}(N)}$

The class $\mathcal{C}_{3,s,k}(N)$ of three–stage nested designs is the collection all N–observation designs in $\mathcal{C}^*_{3,s}$ such that

(i) at most k distinct atoms occur in $\mathcal{D}$ and

(ii) all the variance components in the model are estimable.

If $(r_1, \ldots, r_{p_3(s)})$ is the pattern vector of $\mathcal{D}$, then r_l must be zero for all but at most k values of $l = 1,\ 2, \ldots,\ p_3(s)$.

$\boxed{\textbf{DESIGNS IN THE CLASS } C_{3,s,k}(N)}$

- The class of designs under consideration is completely determined by s, k, and N.
- $\mathcal{C}_{3,2,k}(N) \subseteq \mathcal{C}_{3,3,k}(N) \subseteq \mathcal{C}_{3,4,k}(N) \subseteq \ldots.$
- $\mathcal{C}_{3,s,1}(N) \subseteq \mathcal{C}_{3,s,2}(N) \subseteq \mathcal{C}_{3,s,3}(N) \subseteq \ldots.$
- The larger s is and the larger k is, the larger is the class $C_{3,s,k}(N)$. Hence, searching for optimum designs in the class $C_{3,s,k}(N)$, with large s and large k gives a better chance for finding the "true" optimal design. However, from the point of view of computational feasibility, there is a question as to the largest practical values for s and k.
- The classes proposed by Prairie (1961) or by Goldsmith (1969, 1970) are subsets of $\mathcal{C}_{3,2,3}(N)$.

NUMBER OF DESIGNS IN THE CLASS $C_{3,2,3}(N)$

The cardinality $t_{3,2,3}(N)$ of $\mathcal{C}_{3,2,3}(N)$ is

$$t_{3,2,3}(N) = \frac{83}{9} - \frac{109}{24}(N+2) + \frac{55}{96}(N+2)^2 + \frac{(-1)^N}{8}\left[11 - 3(N+2) + \frac{1}{4}(N+2)^2\right] + \frac{4}{9}\cos(2N\pi/3) + \frac{3}{8}\cos(N\pi/2)$$

N	20	40	60	80	100
$t_{3,2,3}(N)$	195	870	2029	3670	5795

N	120	140	160	180	200
$t_{3,2,3}(N)$	8404	11495	15070	19129	23670

NUMBER OF DESIGNS IN THE CLASS $C_{3,3,3}(N)$

The cardinality $t_{3,3,3}(N)$ of $\mathcal{C}_{3,3,3}(N)$ is given by the recurrence relation

$$\begin{aligned}
t(N) = 4\,t(N-1) - 10\,t(N-2) - 19\,t(N-3) - 30\,t(N-4) \\
- 41\,t(N-5) - 49\,t(N-6) - 51\,t(N-7) - 44\,t(N-8) \\
- 26\,t(N-9) + 3\,t(N-10) + 40\,t(N-11) + 80\,t(N-12) \\
+ 116\,t(N-13) + 141\,t(N-14) + 149\,t(N-15) + 137\,t(N-16) \\
+ 105\,t(N-17) + 57\,t(N-18) - 57\,t(N-20) - 105\,t(N-21) \\
- 137\,t(N-22) - 149\,t(N-23) - 141\,t(N-24) - 116\,t(N-25) \\
- 80\,t(N-26) - 40\,t(N-27) - 3\,t(N-28) + 26\,t(N-29) \\
+ 44\,t(N-30) + 51\,t(N-31) + 49\,t(N-32) + 41\,t(N-33) \\
+ 30\,t(N-34) + 19\,t(N-35) + 10\,t(N-36) + 4\,t(N-37) + t(N-38)
\end{aligned}$$

with initial conditions ... (*next slide)*

NUMBER OF DESIGNS IN THE CLASS $C_{3,3,3}(N)$ (*continued*)

$$
\begin{array}{llll}
t(1)=0, & t(2)=0, & t(3)=0, & t(4)=2, \\
t(5)=9, & t(6)=24, & t(7)=49, & t(8)=91, \\
t(9)=150, & t(10)=232, & t(11)=338, & t(12)=467, \\
t(13)=619, & t(14)=788, & t(15)=977, & t(16)=1192, \\
t(17)=1410, & t(18)=1657, & t(19)=1909, & t(20)=2239, \\
t(21)=2464, & t(22)=2881, & t(23)=3133, & t(24)=3605, \\
t(25)=3866, & t(26)=4451, & t(27)=4628, & t(28)=5358, \\
t(29)=5503, & t(30)=6371, & t(31)=6435, & t(32)=7404, \\
t(33)=7472, & t(34)=8590, & t(35)=8541, & t(36)=9889, \\
t(37)=9670 & \text{and} \quad t(38)=11159. & &
\end{array}
$$

- A complete search for optimum designs in this class is feasible for fairly large sample sizes, up to around $N = 200$.
- A `FORTRAN` program is available for finding optimum designs with the class $\mathcal{C}_{3,2,3}(N)$ or $\mathcal{C}_{3,3,3}(N)$ for a given sample size and assumed prior values of ρ_1 and ρ_2, the variance ratios.
- When complete search becomes impractical, we have large sample results.

$\boxed{\textbf{THE CLASS } \mathcal{C}^*_{4,s}}$

We define a class of designs constructed using staggered structures. Complete search will be performed within this class to find locally optimal designs.

- The class $\mathcal{C}^*_{4,s}$ is the collection of all four stage nested designs in which $a \leq s$, $b_i \leq s$, $c_{ij} \leq s$ and $n_{ijk} \leq s$ for $i = 1, 2, \ldots, a$, $j = 1, 2, \ldots, b_i$, and $k = 1, \ldots, c_{ij}$.
- Designs in $\mathcal{C}^*_{4,s}$ for which $a = 1$ are called the atoms of $\mathcal{C}^*_{4,s}$.
- The collection of these atoms will be denoted by $\mathcal{A}_{4,s}$ and the number of elements in $\mathcal{A}_{4,s}$ by $p_4(s)$.
- We label the atoms in $\mathcal{A}_{4,s}$ by $A_1, A_2, \ldots, A_{p_4(s)}$.

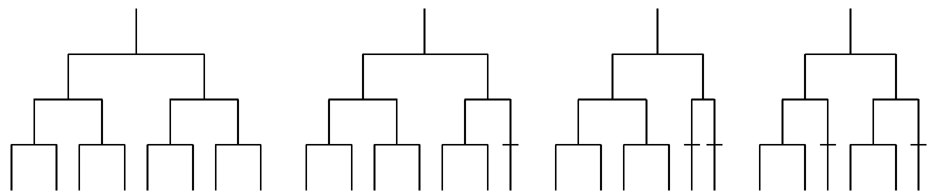
NUMBER OF ATOMS IN $\mathcal{A}_{4,s}$

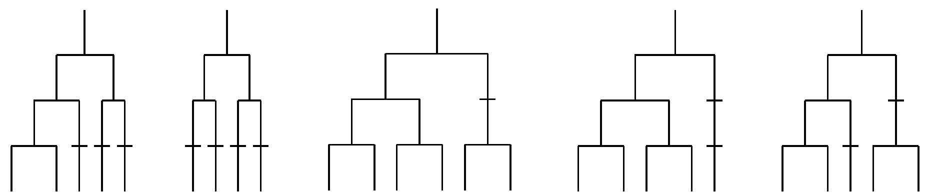
- A recurrence relation exists.
- For $s = 2, 3, 4, 5, 6, 7, 8, 9, 10$, the number of atoms in $\mathcal{A}_{4,s}$ is given by

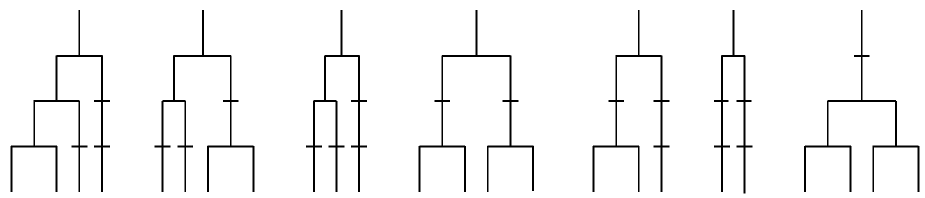
$$
\begin{aligned}
&p_4(2) = 20\\
&p_4(3) = 1539\\
&p_4(4) = 1088429\\
&p_4(5) = 8809549055\\
&p_4(6) = 878487565272239\\
&p_4(7) = 111958259424776262 6695\\
&p_4(8) = 18709083803797153776767847374\\
&p_4(9) = 4186904993091626163441378607213472999\\
&p_4(10) = 12774039515000779353945535626120067642635015377
\end{aligned}
$$

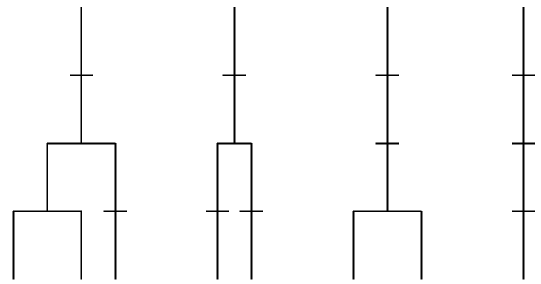
$\boxed{\textbf{ATOMS IN } \mathcal{A}_{4,2}}$

- The number of atoms in class $\mathcal{A}_{4,3}$ is $p_4(3) = 1539$ which gives rise to too large a number of designs of size N even for moderate N.
- Hence in this work we restrict ourselves to designs for which $s = 2$.
- The 20 atoms in $\mathcal{A}_{4,2}$ are . . ..

Stage	Atom 1	2	3	4
1 2 3 4				
b_i	2	2	2	2
c_{ij}	2,2	2,2	2,2	2,2
n_{ijk}	2,2,2,2	2,2,2,1	2,2,1,1	2,1,2,1

	5	6	7	8	9
1 2 3 4					
b_i	2	2	2	2	2
c_{ij}	2,2	2,2	2,1	2,1	2,1
n_{ijk}	2,1,1,1	1,1,1,1	2,2,2	2,2,1	2,1,2

	10	11	12	13	14	15	16
1 2 3 4							
b_i	2	2	2	2	2	2	1
c_{ij}	2,1	2,1	2,1	1,1	1,1	1,1	2
n_{ijk}	2,1,1	1,1,2	1,1,1	2,2	2,1	1,1	2,2

Stage	Atom 17	Atom 18	Atom 19	Atom 20
1				
2				
3				
4				
b_i	1	1	1	1
c_{ij}	2	2	1	1
n_{ijk}	2,1	1,1	2	1

$\boxed{\textbf{THE CLASS } \mathcal{C}_{4,s,k}(N)}$

- Any given design $\mathcal{D}$ in $\mathcal{C}^*_{4,s}$ consists of the union of atoms in $\mathcal{A}_{4,s}$, where each atom may occur 0, 1 or more times.
- If $r_\alpha(\mathcal{D})$ is the number of times atom A_α occurs in $\mathcal{D}$, then the design is completely determined by the pattern vector $\mathbf{r} = (r_1, r_2, \ldots, r_{p_4(s)})'$.
- We now characterize a subclass of $\mathcal{C}^*_{4,s}$ of designs restricted by
  (1) the number of atoms in $\mathcal{D}$,
  (2) the sample size and
  (3) the requirement that all variance components are estimable as follows

Definition: The class $\mathcal{C}_{4,s,k}(N)$ of four stage nested designs is the collection of all N–observation designs in $\mathcal{C}^*_{4,s}$ such that

(i) at most k distinct atoms occur in the design $\mathcal{D}$ and

(ii) all the variance components in the model are estimable.

If $(r_1, \ldots, r_{p_4(s)})$ is the pattern vector of a design $\mathcal{D}$, then r_α must be zero for all but at most k values of $\alpha = 1, 2, \ldots, p_4(s)$.
Thus, the proposed class is completely determined by s, k, and N.

$\boxed{\textbf{NUMBER OF DESIGNS IN } \mathcal{C}_{4,2,3}}$

Suppose that the sample size of a four–stage nested model is greater or equal to 9. The cardinality $t_{4,2,3}(N)$ of $\mathcal{C}_{4,2,3}(N)$ is then given by the recurrence relation[1]

$$\begin{gathered}
t(N) = t(N-46) + 4\,t(N-45) + 13\,t(N-44) + 32\,t(N-43) + \\
69\,t(N-42) + 129\,t(N-41) + 218\,t(N-40) + 332\,t(N-39) + \\
461\,t(N-38) + 580\,t(N-37) + 656\,t(N-36) + 649\,t(N-35) + \\
522\,t(N-34) + 255\,t(N-33) - 151\,t(N-32) - 657\,t(N-31) - \\
1200\,t(N-30) - 1685\,t(N-29) - 2021\,t(N-28) - 2121\,t(N-27) - \\
1943\,t(N-26) - 1485\,t(N-25) - 805\,t(N-24) + 805\,t(N-22) + \\
1485\,t(N-21) + 1943\,t(N-20) + 2121\,t(N-19) + 2021\,t(N-18) + \\
1685\,t(N-17) + 1200\,t(N-16) + 657\,t(N-15) + 151\,t(N-14) - \\
255\,t(N-13) - 522\,t(N-12) - 649\,t(N-11) - 656\,t(N-10) - \\
580\,t(N-9) - 461\,t(N-8) - 332\,t(N-7) - 218\,t(N-6) - \\
129\,t(N-5) - 69\,t(N-4) - 32\,t(N-3) - 13\,t(N-2) - 4\,t(N-1)
\end{gathered}$$

[1]For the sake of simplicity, we have dropped the subindex $(4,2)$ from the terms.

NUMBER OF DESIGNS IN $\mathcal{C}_{4,2,3}$ INITIAL CONDITIONS

Initial conditions are given by

$$
\begin{array}{llll}
t(1) = 0, & t(2) = 0, & t(3) = 0, & t(4) = 2, \\
t(5) = 8, & t(6) = 24, & t(7) = 54, & t(8) = 115, \\
t(9) = 197, & t(10) = 331, & t(11) = 468, & t(12) = 683, \\
t(13) = 846, & t(14) = 1156, & t(15) = 1305, & t(16) = 1744, \\
t(17) = 1848, & t(18) = 2459, & t(19) = 2483, & t(20) = 3328, \\
t(21) = 3171, & t(22) = 4333, & t(23) = 4025, & t(24) = 5364, \\
t(25) = 4955, & t(26) = 6692, & t(27) = 5856, & t(28) = 7995, \\
t(29) = 7015, & t(30) = 9493, & t(31) = 8208, & t(32) = 11100, \\
t(33) = 9417, & t(34) = 12867, & t(35) = 10843, & t(36) = 14664, \\
t(37) = 12273, & t(38) = 16708, & t(39) = 13822, & t(40) = 18801, \\
t(41) = 15431, & t(42) = 21112, & t(43) = 17149, & t(44) = 23431, \\
 & t(45) = 19037, & t(46) = 25836. &
\end{array}
$$

For $N < 9$ the cardinalities are $t(1) = 0$, $t(2) = 0$, $t(3) = 0$, $t(4) = 0$, $t(5) = 5$, $t(6) = 21$, $t(7) = 53$ and $t(8) = 114$

FINDING OPTIMAL DESIGNS IN $\mathcal{C}_{4,2,3}(N)$

- For sample sizes N around 200, the number of designs in $\mathcal{C}_{4,2,3}(N)$ is not too large, so a complete search for optimal designs in this class is feasible.
- We have a `FORTRAN` program that can be used to search for optimal designs in class $\mathcal{C}_{4,2,3}(N)$ for a given sample size and assumed prior values of ρ_1, ρ_2 and ρ_3.
- For larger sample sizes a complete search is impractical. Hence we separately investigate optimal designs for large sample sizes.

SMALL SAMPLE DESIGNS

- Optimal designs were obtained for small sample sizes upto $N = 120$. Comparisons between these designs and the large sample designs (to be discussed later) indicate that optimal designs in $\mathcal{C}_{4,2,3}(120)$ are almost as efficient as the corresponding asymptotic designs.
- If A_s-optimal designs are considered, then atoms 16 through 20 are not used for any of the the prior variance configurations that were tested. These atoms do not contribute any information to the estimation of the second stage variance σ_β^2.
- Other atoms that do not contribute to the estimation, either of σ_α^2, σ_γ^2 or σ_ϵ^2 are A_6, A_{12}, A_{13}, A_{14} and A_{15}. These atoms tend to be combined with others that have a large number of replicates of the different levels of the model.

$\boldsymbol{A_s}$-OPTIMUM DESIGNS IN $\mathcal{C}_{4,2,3}(48)$

			Atom													
ρ_1	ρ_2	ρ_3	1	3	4	5	6	8	10	11	12	15	18	Det(**V**)	Tr(**V**)	Tr($\mathbf{V}_s$)
0.1	0.1	0.1	6	-	-	-	-	-	-	-	-	-	-	0.000E+0	2.818E-1	1.993E+1
		0.5	6	-	-	-	-	-	-	-	-	-	-	1.000E-4	4.418E-1	1.584E+1
		1.0	6	-	-	-	-	-	-	-	-	-	-	2.000E-4	8.218E-1	1.559E+1
		2.0	6	-	-	-	-	-	-	-	-	-	-	5.000E-4	2.182E+0	1.549E+1
		5.0	6	-	-	-	-	-	-	-	-	-	-	2.900E-3	1.106E+1	1.543E+1
	0.5	0.1	6	-	-	-	-	-	-	-	-	-	-	1.000E-4	5.458E-1	2.441E+1
		0.5	6	-	-	-	-	-	-	-	-	-	-	3.000E-4	7.698E-1	1.059E+1
		1.0	6	-	-	-	-	-	-	-	-	-	-	8.000E-4	1.230E+0	9.917E+0
		2.0	6	-	-	-	-	-	-	-	-	-	-	2.500E-3	2.750E+0	9.669E+0
		5.0	6	-	-	-	-	-	-	-	-	-	-	1.240E-2	1.211E+1	9.549E+0
	1.0	0.1	4	-	-	-	-	-	-	-	-	8	-	1.000E-3	1.091E+0	4.310E+1
		0.5	6	-	-	-	-	-	-	-	-	-	-	1.500E-3	1.412E+0	1.142E+1
		1.0	6	-	-	-	-	-	-	-	-	-	-	3.100E-3	1.972E+0	9.975E+0
		2.0	6	-	-	-	-	-	-	-	-	-	-	7.900E-3	3.692E+0	9.483E+0
		5.0	6	-	-	-	-	-	-	-	-	-	-	3.600E-2	1.365E+1	9.261E+0
	2.0	0.1	2	-	-	-	-	-	-	-	-	16	-	1.690E-2	2.382E+0	8.630E+1
		0.5	6	-	-	-	-	-	-	-	-	-	-	9.600E-3	3.472E+0	1.473E+1
		1.0	6	-	-	-	-	-	-	-	-	-	-	1.630E-2	4.232E+0	1.090E+1
		2.0	6	-	-	-	-	-	-	-	-	-	-	3.500E-2	6.352E+0	9.714E+0
		5.0	6	-	-	-	-	-	-	-	-	-	-	1.334E-1	1.751E+1	9.234E+0
	5.0	0.1	1	-	-	-	-	-	-	-	-	20	-	8.325E-1	7.671E+0	2.644E+2
		0.5	4	-	-	-	-	-	-	-	-	8	-	2.256E-1	1.214E+1	3.084E+1
		1.0	6	-	-	-	-	-	-	-	-	-	-	2.495E-1	1.721E+1	1.621E+1
		2.0	6	-	-	-	-	-	-	-	-	-	-	4.049E-1	2.053E+1	1.129E+1
		5.0	6	-	-	-	-	-	-	-	-	-	-	1.096E+0	3.529E+1	9.572E+0
0.5	0.1	0.1	4	-	-	-	4	-	-	-	-	-	-	2.000E-4	6.063E-1	2.626E+1
		0.5	6	-	-	-	-	-	-	-	-	-	-	4.000E-4	7.185E-1	1.814E+1
		1.0	6	-	-	-	-	-	-	-	-	-	-	1.100E-3	1.139E+0	1.771E+1
		2.0	6	-	-	-	-	-	-	-	-	-	-	3.500E-3	2.579E+0	1.754E+1
		5.0	6	-	-	-	-	-	-	-	-	-	-	1.870E-2	1.170E+1	1.745E+1
	0.5	0.1	2	-	-	-	8	-	-	-	-	-	-	1.400E-3	1.114E+0	2.101E+1
		0.5	4	-	-	-	4	-	-	-	-	-	-	2.200E-3	1.117E+0	4.094E+0

continued on next page

continued from previous page

ρ_1	ρ_2	ρ_3	1	3	4	5	6	8	10	11	12	15	18	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
		1.0	4	-	-	-	4	-	-	-	-	-	-	4.900E-3	1.519E+0	3.264E+0
		2.0	5	-	-	-	2	-	-	-	-	-	-	1.230E-2	2.993E+0	2.953E+0
		5.0	5	-	-	-	2	-	-	-	-	-	-	5.900E-2	1.155E+1	2.807E+0
	1.0	0.1	-	-	-	-	7	-	-	5	-	-	-	9.400E-3	1.987E+0	3.531E+1
		0.5	3	-	-	-	6	-	-	-	-	-	-	8.700E-3	1.736E+0	4.420E+0
		1.0	-	8	-	-	-	-	-	-	-	-	-	1.420E-2	2.227E+0	2.915E+0
		2.0	-	8	-	-	-	-	-	-	-	-	-	3.350E-2	3.577E+0	2.375E+0
		5.0	3	4	-	-	-	-	-	-	-	-	-	1.384E-1	1.266E+1	2.136E+0
	2.0	0.1	-	-	-	-	1	-	-	3	-	16	-	2.273E-1	4.706E+0	6.915E+1
		0.5	2	-	-	-	3	-	-	-	-	10	-	7.510E-2	3.323E+0	6.580E+0
		1.0	3	-	-	-	4	-	-	-	-	4	-	7.850E-2	3.944E+0	3.541E+0
		2.0	-	8	-	-	-	-	-	-	-	-	-	1.246E-1	5.910E+0	2.431E+0
		5.0	1	5	-	-	-	2	-	-	-	-	-	4.441E-1	1.483E+1	1.971E+0
	5.0	0.1	-	-	-	-	-	-	1	-	-	22	-	2.482E+1	1.507E+1	2.196E+2
		0.5	-	2	-	-	-	-	-	1	-	16	-	2.011E+0	9.252E+0	1.558E+1
		1.0	-	4	-	-	-	-	-	-	-	12	-	1.406E+0	1.070E+1	6.611E+0
		2.0	-	6	-	-	-	-	-	-	-	6	-	1.502E+0	1.473E+1	3.540E+0
		5.0	-	-	-	-	-	9	-	-	1	-	-	2.931E+0	2.706E+1	2.150E+0
1.0	0.1	0.1	1	-	-	-	10	-	-	-	-	-	-	2.900E-3	1.687E+0	4.392E+1
		0.5	1	-	-	-	10	-	-	-	-	-	-	7.800E-3	1.825E+0	3.167E+1
		1.0	1	-	-	-	10	-	-	-	-	-	-	1.720E-2	2.092E+0	3.113E+1
		2.0	1	-	-	-	10	-	-	-	-	-	-	4.740E-2	2.943E+0	3.093E+1
		5.0	1	-	-	-	10	-	-	-	-	-	-	2.273E-1	8.023E+0	3.085E+1
	0.5	0.1	1	-	-	-	10	-	-	-	-	-	-	9.600E-3	1.987E+0	2.737E+1
		0.5	2	-	-	-	8	-	-	-	-	-	-	1.270E-2	1.733E+0	4.619E+0
		1.0	-	4	-	-	6	-	-	-	-	-	-	2.520E-2	2.080E+0	3.600E+0
		2.0	-	4	-	-	6	-	-	-	-	-	-	6.270E-2	3.110E+0	3.255E+0
		5.0	-	6	-	-	3	-	-	-	-	-	-	2.216E-1	9.704E+0	3.091E+0
	1.0	0.1	-	-	-	-	10	-	-	2	-	-	-	5.790E-2	3.570E+0	4.336E+1
		0.5	-	-	4	-	6	-	-	-	-	-	-	3.450E-2	2.368E+0	4.443E+0
		1.0	-	4	-	-	6	-	-	-	-	-	-	6.100E-2	2.739E+0	2.739E+0
		2.0	-	6	-	-	3	-	-	-	-	-	-	1.117E-1	4.052E+0	2.154E+0
		5.0	-	6	-	-	3	-	-	-	-	-	-	4.471E-1	1.099E+1	1.900E+0
	2.0	0.1	-	-	-	-	1	-	-	2	-	18	-	1.173E+0	7.868E+0	8.149E+1

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ρ_1	ρ_2	ρ_3	1	3	4	5	6	8	10	11	12	15	18	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
		0.5	-	-	-	-	5	-	-	6	-	2	-	2.038E-1	4.168E+0	6.259E+0
		1.0	-	-	-	4	2	-	-	5	-	-	-	2.238E-1	4.511E+0	3.084E+0
		2.0	-	4	-	-	4	-	-	2	-	-	-	3.983E-1	5.993E+0	2.034E+0
		5.0	-	6	-	-	3	-	-	-	-	-	-	1.238E+0	1.411E+1	1.573E+0
	5.0	0.1	-	-	-	-	-	-	-	1	-	22	-	8.115E+1	2.621E+1	2.379E+2
		0.5	-	-	-	-	1	-	-	4	-	14	-	5.941E+0	1.144E+1	1.468E+1
		1.0	-	-	-	-	2	-	-	6	-	8	-	3.867E+0	1.157E+1	5.695E+0
		2.0	-	-	-	-	3	-	-	9	-	-	-	3.569E+0	1.393E+1	2.821E+0
		5.0	-	-	-	-	4	4	3	-	-	-	-	8.195E+0	2.506E+1	1.680E+0
2.0	0.1	0.1	1	-	-	-	10	-	-	-	-	-	-	2.910E-2	2.649E+0	9.384E+1
		0.5	-	2	-	-	9	-	-	-	-	-	-	6.200E-2	2.830E+0	6.783E+1
		1.0	-	2	-	-	9	-	-	-	-	-	-	1.192E-1	3.146E+0	6.678E+1
		2.0	-	2	-	-	9	-	-	-	-	-	-	2.892E-1	4.088E+0	6.643E+1
		5.0	-	2	-	-	9	-	-	-	-	-	-	1.244E+0	9.376E+0	6.628E+1
	0.5	0.1	-	-	-	-	11	-	-	1	-	-	-	2.504E-1	6.096E+0	4.653E+1
		0.5	-	2	-	-	9	-	-	-	-	-	-	1.314E-1	3.274E+0	7.025E+0
		1.0	-	2	-	-	9	-	-	-	-	-	-	2.337E-1	3.633E+0	5.456E+0
		2.0	-	2	-	-	9	-	-	-	-	-	-	5.258E-1	4.660E+0	4.961E+0
		5.0	-	4	-	-	6	-	-	-	-	-	-	1.340E+0	1.074E+1	4.745E+0
	1.0	0.1	-	-	-	-	11	-	-	1	-	-	-	5.788E-1	6.686E+0	6.506E+1
		0.5	1	-	-	-	10	-	-	-	-	-	-	2.859E-1	3.978E+0	5.795E+0
		1.0	-	4	-	-	6	-	-	-	-	-	-	3.027E-1	4.183E+0	3.418E+0
		2.0	-	4	-	-	6	-	-	-	-	-	-	6.289E-1	5.458E+0	2.617E+0
		5.0	-	4	-	-	6	-	-	-	-	-	-	2.315E+0	1.205E+1	2.300E+0
	2.0	0.1	-	-	-	-	4	-	-	1	-	14	-	5.206E+0	1.058E+1	1.181E+2
		0.5	-	-	-	-	7	-	-	4	-	2	-	1.102E+0	6.183E+0	7.677E+0
		1.0	-	-	-	-	6	-	-	6	-	-	-	1.181E+0	6.500E+0	3.438E+0
		2.0	-	-	-	8	2	-	-	-	-	-	-	1.639E+0	7.757E+0	2.127E+0
		5.0	-	-	-	8	2	-	-	-	-	-	-	5.256E+0	1.486E+1	1.607E+0
	5.0	0.1	-	-	-	-	-	-	-	1	-	22	-	3.063E+2	4.775E+1	2.998E+2
		0.5	-	-	-	-	1	-	-	3	-	16	-	3.094E+1	1.763E+1	1.660E+1
		1.0	-	-	-	-	2	-	-	5	-	10	-	1.601E+1	1.556E+1	5.960E+0
		2.0	-	-	-	-	3	-	-	7	-	4	-	1.450E+1	1.690E+1	2.726E+0
		5.0	-	-	-	-	3	-	-	9	-	-	-	2.722E+1	2.501E+1	1.512E+0

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ρ_1	ρ_2	ρ_3	1	3	4	5	6	8	10	11	12	15	18	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
5.0	0.1	0.1	-	-	-	1	10	-	-	-	1	-	-	5.581E+0	1.055E+1	3.506E+2
		0.5	-	1	-	-	10	-	-	-	-	-	1	4.621E+0	8.935E+0	2.598E+2
		1.0	-	1	-	-	10	-	-	-	-	-	1	7.064E+0	9.378E+0	2.563E+2
		2.0	-	1	-	-	10	-	-	-	-	-	1	1.351E+1	1.055E+1	2.553E+2
		5.0	-	1	-	-	10	-	-	-	-	-	1	4.537E+1	1.632E+1	2.549E+2
	0.5	0.1	-	-	-	-	11	-	-	1	-	-	-	9.065E+0	1.136E+1	1.342E+2
		0.5	-	2	-	-	9	-	-	-	-	-	-	3.935E+0	8.930E+0	1.933E+1
		1.0	-	2	-	-	9	-	-	-	-	-	-	5.853E+0	9.449E+0	1.499E+1
		2.0	-	2	-	-	9	-	-	-	-	-	-	1.083E+1	1.079E+1	1.372E+1
		5.0	-	2	-	-	9	-	-	-	-	-	-	3.487E+1	1.729E+1	1.325E+1
	1.0	0.1	-	-	-	-	11	-	-	1	-	-	-	1.499E+1	1.235E+1	1.602E+2
		0.5	-	2	-	-	9	-	-	-	-	-	-	6.390E+0	1.004E+1	1.257E+1
		1.0	-	2	-	-	9	-	-	-	-	-	-	9.160E+0	1.061E+1	7.003E+0
		2.0	-	2	-	-	9	-	-	-	-	-	-	1.619E+1	1.206E+1	5.403E+0
		5.0	-	2	-	-	9	-	-	-	-	-	-	4.922E+1	1.888E+1	4.822E+0
	2.0	0.1	-	-	-	-	11	-	-	1	-	-	-	3.506E+1	1.471E+1	2.398E+2
		0.5	-	1	-	-	10	-	-	-	-	1	-	2.594E+1	1.341E+1	1.400E+1
		1.0	-	2	-	-	9	-	-	-	-	-	-	1.968E+1	1.337E+1	5.723E+0
		2.0	-	2	-	-	9	-	-	-	-	-	-	3.232E+1	1.503E+1	3.344E+0
		5.0	-	4	-	-	6	-	-	-	-	-	-	6.075E+1	2.453E+1	2.458E+0
	5.0	0.1	-	-	-	-	1	-	-	1	-	20	-	1.434E+3	6.503E+1	5.503E+2
		0.5	-	-	-	-	3	-	-	2	-	14	-	3.452E+2	3.440E+1	2.697E+1
		1.0	-	-	-	-	4	-	-	3	-	10	-	2.193E+2	3.033E+1	8.802E+0
		2.0	-	-	-	-	5	-	-	5	-	4	-	1.581E+2	2.973E+1	3.628E+0
		5.0	-	-	-	-	5	-	-	7	-	-	-	2.465E+2	3.842E+1	1.811E+0

D-OPTIMUM DESIGNS IN $\mathcal{C}_{4,2}(120)$

			Atom										
ρ_1	ρ_2	ρ_3	1	2	3	4	5	6	7	8	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
0.1	0.1	0.1	15	-	-	-	-	-	-	-	0.000E+0	1.112E-1	7.819E+0
		0.5	15	-	-	-	-	-	-	-	0.000E+0	1.683E-1	6.301E+0
		1.0	15	-	-	-	-	-	-	-	0.000E+0	3.040E-1	6.211E+0
		2.0	15	-	-	-	-	-	-	-	0.000E+0	7.898E-1	6.174E+0
		5.0	15	-	-	-	-	-	-	-	1.000E-4	3.961E+0	6.155E+0
	0.5	0.1	15	-	-	-	-	-	-	-	0.000E+0	2.140E-1	9.337E+0
		0.5	15	-	-	-	-	-	-	-	0.000E+0	2.940E-1	4.180E+0
		1.0	15	-	-	-	-	-	-	-	0.000E+0	4.583E-1	3.933E+0
		2.0	15	-	-	-	-	-	-	-	1.000E-4	1.001E+0	3.843E+0
		5.0	15	-	-	-	-	-	-	-	3.000E-4	4.344E+0	3.800E+0
	1.0	0.1	15	-	-	-	-	-	-	-	0.000E+0	4.337E-1	1.717E+1
		0.5	15	-	-	-	-	-	-	-	0.000E+0	5.423E-1	4.479E+0
		1.0	15	-	-	-	-	-	-	-	1.000E-4	7.423E-1	3.943E+0
		2.0	15	-	-	-	-	-	-	-	2.000E-4	1.357E+0	3.763E+0
		5.0	15	-	-	-	-	-	-	-	8.000E-4	4.914E+0	3.683E+0
	2.0	0.1	15	-	-	-	-	-	-	-	1.000E-4	1.177E+0	4.340E+1
		0.5	15	-	-	-	-	-	-	-	2.000E-4	1.342E+0	5.706E+0
		1.0	15	-	-	-	-	-	-	-	4.000E-4	1.614E+0	4.281E+0
		2.0	15	-	-	-	-	-	-	-	8.000E-4	2.371E+0	3.843E+0
		5.0	-	-	-	-	-	-	-	24	2.900E-3	4.691E+0	4.399E+0
	5.0	0.1	15	-	-	-	-	-	-	-	3.200E-3	5.834E+0	2.051E+2
		0.5	15	-	-	-	-	-	-	-	4.200E-3	6.171E+0	1.283E+1
		1.0	15	-	-	-	-	-	-	-	5.700E-3	6.657E+0	6.256E+0
		2.0	-	-	-	-	-	-	-	24	9.200E-3	6.308E+0	5.067E+0
		5.0	-	-	-	-	-	-	-	24	2.180E-2	1.003E+1	4.481E+0
0.5	0.1	0.1	15	-	-	-	-	-	-	-	0.000E+0	2.079E-1	1.029E+1
		0.5	15	-	-	-	-	-	-	-	0.000E+0	2.764E-1	7.214E+0
		1.0	15	-	-	-	-	-	-	-	0.000E+0	4.264E-1	7.053E+0
		2.0	15	-	-	-	-	-	-	-	1.000E-4	9.407E-1	6.992E+0
		5.0	15	-	-	-	-	-	-	-	4.000E-4	4.198E+0	6.961E+0
	0.5	0.1	15	-	-	-	-	-	-	-	0.000E+0	3.431E-1	9.410E+0
		0.5	15	-	-	-	-	-	-	-	0.000E+0	4.345E-1	1.638E+0

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ρ_1	ρ_2	ρ_3	1	2	3	4	5	6	7	8	Det(**V**)	Tr(**V**)	Tr($\mathbf{V}_s$)
		1.0	15	-	-	-	-	-	-	-	1.000E-4	6.131E-1	1.288E+0
		2.0	15	-	-	-	-	-	-	-	3.000E-4	1.185E+0	1.165E+0
		5.0	15	-	-	-	-	-	-	-	1.300E-3	4.613E+0	1.108E+0
	1.0	0.1	15	-	-	-	-	-	-	-	1.000E-4	6.032E-1	1.847E+1
		0.5	15	-	-	-	-	-	-	-	1.000E-4	7.232E-1	1.843E+0
		1.0	15	-	-	-	-	-	-	-	3.000E-4	9.375E-1	1.163E+0
		2.0	15	-	-	-	-	-	-	-	7.000E-4	1.580E+0	9.388E-1
		5.0	15	-	-	-	-	-	-	-	3.100E-3	5.223E+0	8.419E-1
	2.0	0.1	15	-	-	-	-	-	-	-	5.000E-4	1.427E+0	4.741E+1
		0.5	15	-	-	-	-	-	-	-	8.000E-4	1.604E+0	3.129E+0
		1.0	15	-	-	-	-	-	-	-	1.300E-3	1.890E+0	1.477E+0
		2.0	15	-	-	-	-	-	-	-	2.800E-3	2.676E+0	9.751E-1
		5.0	-	-	14	-	-	-	6	-	1.020E-2	5.407E+0	7.833E-1
	5.0	0.1	15	-	-	-	-	-	-	-	1.040E-2	6.327E+0	2.174E+2
		0.5	15	-	-	-	-	-	-	-	1.350E-2	6.676E+0	1.056E+1
		1.0	15	-	-	-	-	-	-	-	1.800E-2	7.176E+0	3.513E+0
		2.0	1	16	-	-	-	-	-	-	2.880E-2	7.594E+0	1.477E+0
		5.0	-	-	-	-	-	-	-	24	6.930E-2	1.073E+1	8.406E-1
1.0	0.1	0.1	15	-	-	-	-	-	-	-	0.000E+0	3.890E-1	1.992E+1
		0.5	15	-	-	-	-	-	-	-	1.000E-4	4.718E-1	1.416E+1
		1.0	15	-	-	-	-	-	-	-	1.000E-4	6.397E-1	1.389E+1
		2.0	15	-	-	-	-	-	-	-	4.000E-4	1.190E+0	1.379E+1
		5.0	15	-	-	-	-	-	-	-	2.000E-3	4.554E+0	1.374E+1
	0.5	0.1	15	-	-	-	-	-	-	-	1.000E-4	5.647E-1	1.389E+1
		0.5	15	-	-	-	-	-	-	-	2.000E-4	6.704E-1	2.107E+0
		1.0	15	-	-	-	-	-	-	-	4.000E-4	8.668E-1	1.604E+0
		2.0	15	-	-	-	-	-	-	-	1.000E-3	1.474E+0	1.434E+0
		5.0	6	-	12	-	-	-	-	-	4.700E-3	4.355E+0	1.301E+0
	1.0	0.1	15	-	-	-	-	-	-	-	3.000E-4	8.754E-1	2.443E+1
		0.5	15	-	-	-	-	-	-	-	6.000E-4	1.010E+0	2.126E+0
		1.0	15	-	-	-	-	-	-	-	1.000E-3	1.242E+0	1.242E+0
		2.0	3	-	16	-	-	-	-	-	2.400E-3	1.702E+0	8.843E-1
		5.0	-	-	20	-	-	-	-	-	9.600E-3	4.489E+0	7.598E-1
	2.0	0.1	12	-	-	4	-	-	-	-	1.600E-3	1.751E+0	5.463E+1

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ρ_1	ρ_2	ρ_3	1	2	3	4	5	6	7	8	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
		0.5	9	-	-	8	-	-	-	-	2.500E-3	1.877E+0	3.224E+0
		1.0	-	12	-	6	-	-	-	-	4.000E-3	2.078E+0	1.373E+0
		2.0	-	-	20	-	-	-	-	-	7.900E-3	2.627E+0	8.192E-1
		5.0	-	-	20	-	-	-	-	-	2.700E-2	5.820E+0	6.220E-1
	5.0	0.1	-	-	-	20	-	-	-	-	2.590E-2	5.586E+0	1.846E+2
		0.5	-	-	-	20	-	-	-	-	3.320E-2	5.860E+0	8.835E+0
		1.0	-	-	-	20	-	-	-	-	4.350E-2	6.248E+0	2.877E+0
		2.0	-	-	-	20	-	-	-	-	6.830E-2	7.184E+0	1.232E+0
		5.0	-	-	-	19	-	-	1	-	1.764E-1	1.131E+1	6.742E-1
2.0	0.1	0.1	15	-	-	-	-	-	-	-	3.000E-4	9.521E-1	4.951E+1
		0.5	14	-	-	-	-	2	-	-	7.000E-4	1.046E+0	3.518E+1
		1.0	14	-	-	-	-	2	-	-	1.300E-3	1.243E+0	3.463E+1
		2.0	-	-	20	-	-	-	-	-	3.300E-3	1.634E+0	3.158E+1
		5.0	-	-	20	-	-	-	-	-	1.440E-2	4.336E+0	3.150E+1
	0.5	0.1	14	-	-	-	-	2	-	-	8.000E-4	1.188E+0	2.531E+1
		0.5	13	-	-	-	-	4	-	-	1.500E-3	1.292E+0	3.504E+0
		1.0	-	-	20	-	-	-	-	-	2.800E-3	1.412E+0	2.450E+0
		2.0	-	-	20	-	-	-	-	-	6.300E-3	1.938E+0	2.195E+0
		5.0	-	-	20	-	-	-	-	-	2.520E-2	4.780E+0	2.090E+0
	1.0	0.1	13	-	-	-	-	4	-	-	2.000E-3	1.554E+0	3.705E+1
		0.5	12	-	-	-	-	6	-	-	3.500E-3	1.669E+0	2.854E+0
		1.0	-	-	20	-	-	-	-	-	5.800E-3	1.804E+0	1.504E+0
		2.0	-	-	20	-	-	-	-	-	1.200E-2	2.389E+0	1.129E+0
		5.0	-	-	20	-	-	-	-	-	4.420E-2	5.407E+0	9.805E-1
	2.0	0.1	-	-	-	20	-	-	-	-	7.800E-3	2.394E+0	6.509E+1
		0.5	-	-	-	20	-	-	-	-	1.170E-2	2.564E+0	3.740E+0
		1.0	-	-	-	20	-	-	-	-	1.750E-2	2.824E+0	1.551E+0
		2.0	-	-	-	20	-	-	-	-	3.270E-2	3.502E+0	9.131E-1
		5.0	-	-	20	-	-	-	-	-	1.057E-1	6.895E+0	6.669E-1
	5.0	0.1	-	-	-	20	-	-	-	-	9.120E-2	6.914E+0	2.203E+2
		0.5	-	-	-	20	-	-	-	-	1.145E-1	7.211E+0	1.031E+1
		1.0	-	-	-	20	-	-	-	-	1.473E-1	7.629E+0	3.237E+0
		2.0	-	-	-	20	-	-	-	-	2.254E-1	8.623E+0	1.299E+0
		5.0	-	-	-	20	-	-	-	-	5.587E-1	1.287E+1	6.481E-1

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													continued from previous page
ρ_1	ρ_2	ρ_3	1	2	3	4	5	6	7	8	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
5.0	0.1	0.1	10	-	-	-	-	10	-	-	2.290E-2	3.703E+0	1.888E+2
		0.5	-	-	20	-	-	-	-	-	3.610E-2	3.839E+0	1.350E+2
		1.0	-	-	20	-	-	-	-	-	5.530E-2	4.087E+0	1.332E+2
		2.0	-	-	20	-	-	-	-	-	1.058E-1	4.742E+0	1.326E+2
		5.0	-	-	20	-	-	-	-	-	3.550E-1	7.970E+0	1.324E+2
	0.5	0.1	10	-	-	-	-	10	-	-	3.780E-2	4.124E+0	7.276E+1
		0.5	-	-	18	-	-	3	-	-	5.660E-2	4.130E+0	9.553E+0
		1.0	-	-	18	-	-	3	-	-	8.370E-2	4.392E+0	7.313E+0
		2.0	-	-	18	-	-	3	-	-	1.534E-1	5.067E+0	6.661E+0
		5.0	-	-	20	-	-	-	-	-	4.881E-1	8.603E+0	6.630E+0
	1.0	0.1	10	-	-	-	-	10	-	-	6.540E-2	4.727E+0	8.901E+1
		0.5	-	-	18	-	-	3	-	-	9.330E-2	4.705E+0	6.236E+0
		1.0	-	-	18	-	-	3	-	-	1.327E-1	4.995E+0	3.346E+0
		2.0	-	-	18	-	-	3	-	-	2.322E-1	5.726E+0	2.517E+0
		5.0	-	-	15	-	6	-	-	-	6.963E-1	9.119E+0	2.233E+0
	2.0	0.1	-	-	-	18	-	3	-	-	1.593E-1	5.966E+0	1.351E+2
		0.5	-	-	-	15	6	-	-	-	2.109E-1	6.181E+0	7.157E+0
		1.0	-	-	-	15	6	-	-	-	2.851E-1	6.515E+0	2.761E+0
		2.0	-	-	-	10	12	-	-	-	4.664E-1	7.055E+0	1.477E+0
		5.0	-	-	10	-	12	-	-	-	1.271E+0	1.055E+1	1.040E+0
	5.0	0.1	-	-	-	18	-	3	-	-	9.857E-1	1.179E+1	3.340E+2
		0.5	-	-	-	18	-	3	-	-	1.185E+0	1.214E+1	1.515E+1
		1.0	-	-	-	15	6	-	-	-	1.458E+0	1.259E+1	4.574E+0
		2.0	-	-	-	15	6	-	-	-	2.088E+0	1.372E+1	1.717E+0
		5.0	-	-	-	10	12	-	-	-	4.650E+0	1.757E+1	7.626E-1

$\mathbf{A}_s$-OPTIMUM DESIGNS IN $\mathcal{C}_{4,2}(120)$

			Atom													
ρ_1	ρ_2	ρ_3	1	3	4	5	6	7	8	11	13	15	18	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
0.1	0.1	0.1	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	1.112E-1	7.819E+0
		0.5	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	1.683E-1	6.301E+0
		1.0	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	3.040E-1	6.211E+0
		2.0	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	7.898E-1	6.174E+0
		5.0	15	-	-	-	-	-	-	-	-	-	-	1.000E-4	3.961E+0	6.155E+0
	0.5	0.1	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	2.140E-1	9.337E+0
		0.5	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	2.940E-1	4.180E+0
		1.0	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	4.583E-1	3.933E+0
		2.0	15	-	-	-	-	-	-	-	-	-	-	1.000E-4	1.001E+0	3.843E+0
		5.0	15	-	-	-	-	-	-	-	-	-	-	3.000E-4	4.344E+0	3.800E+0
	1.0	0.1	11	-	-	-	-	-	-	-	-	16	-	0.000E+0	4.288E-1	1.676E+1
		0.5	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	5.423E-1	4.479E+0
		1.0	15	-	-	-	-	-	-	-	-	-	-	1.000E-4	7.423E-1	3.943E+0
		2.0	15	-	-	-	-	-	-	-	-	-	-	2.000E-4	1.357E+0	3.763E+0
		5.0	15	-	-	-	-	-	-	-	-	-	-	8.000E-4	4.914E+0	3.683E+0
	2.0	0.1	6	-	-	-	-	-	-	-	-	36	-	3.000E-4	9.429E-1	3.414E+1
		0.5	15	-	-	-	-	-	-	-	-	-	-	2.000E-4	1.342E+0	5.706E+0
		1.0	15	-	-	-	-	-	-	-	-	-	-	4.000E-4	1.614E+0	4.281E+0
		2.0	15	-	-	-	-	-	-	-	-	-	-	8.000E-4	2.371E+0	3.843E+0
		5.0	15	-	-	-	-	-	-	-	-	-	-	3.000E-3	6.357E+0	3.668E+0
	5.0	0.1	-	-	-	-	-	4	-	-	-	48	-	2.100E-2	2.941E+0	1.056E+2
		0.5	10	-	-	-	-	-	-	-	-	20	-	5.500E-3	4.807E+0	1.214E+1
		1.0	15	-	-	-	-	-	-	-	-	-	-	5.700E-3	6.657E+0	6.256E+0
		2.0	15	-	-	-	-	-	-	-	-	-	-	9.300E-3	7.842E+0	4.423E+0
		5.0	15	-	-	-	-	-	-	-	-	-	-	2.500E-2	1.311E+1	3.789E+0
0.5	0.1	0.1	14	-	-	-	2	-	-	-	-	-	-	0.000E+0	2.125E-1	1.028E+1
		0.5	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	2.764E-1	7.214E+0
		1.0	15	-	-	-	-	-	-	-	-	-	-	0.000E+0	4.264E-1	7.053E+0
		2.0	15	-	-	-	-	-	-	-	-	-	-	1.000E-4	9.407E-1	6.992E+0
		5.0	15	-	-	-	-	-	-	-	-	-	-	4.000E-4	4.198E+0	6.961E+0
	0.5	0.1	4	-	-	-	22	-	-	-	-	-	-	0.000E+0	4.898E-1	8.110E+0
		0.5	10	-	-	-	10	-	-	-	-	-	-	1.000E-4	4.366E-1	1.596E+0

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ρ_1	ρ_2	ρ_3	1	3	4	5	6	7	8	11	13	15	18	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
		1.0	12	-	-	-	6	-	-	-	-	-	-	1.000E-4	5.927E-1	1.277E+0
		2.0	13	-	-	-	4	-	-	-	-	-	-	3.000E-4	1.130E+0	1.161E+0
		5.0	14	-	-	-	2	-	-	-	-	-	-	1.300E-3	4.459E+0	1.106E+0
	1.0	0.1	-	-	-	-	17	-	-	13	-	-	-	2.000E-4	7.813E-1	1.375E+1
		0.5	8	-	-	-	14	-	-	-	-	-	-	2.000E-4	6.810E-1	1.718E+0
		1.0	-	20	-	-	-	-	-	-	-	-	-	3.000E-4	8.597E-1	1.135E+0
		2.0	3	16	-	-	-	-	-	-	-	-	-	8.000E-4	1.401E+0	9.289E-1
		5.0	9	8	-	-	-	-	-	-	-	-	-	3.200E-3	4.766E+0	8.381E-1
	2.0	0.1	-	-	-	-	3	-	-	8	-	38	-	4.800E-3	1.775E+0	2.724E+1
		0.5	-	-	6	-	7	-	-	14	-	-	-	1.200E-3	1.284E+0	2.580E+0
		1.0	-	17	-	-	2	-	-	-	-	5	-	1.600E-3	1.568E+0	1.378E+0
		2.0	-	20	-	-	-	-	-	-	-	-	-	2.900E-3	2.259E+0	9.459E-1
		5.0	6	12	-	-	-	-	-	-	-	-	-	1.040E-2	5.916E+0	7.693E-1
	5.0	0.1	-	1	-	-	-	-	-	1	-	55	-	4.487E-1	5.441E+0	8.597E+1
		0.5	-	6	-	-	-	-	-	-	-	42	-	5.160E-2	3.686E+0	6.164E+0
		1.0	-	10	-	-	-	-	-	-	-	30	-	3.510E-2	4.249E+0	2.614E+0
		2.0	-	16	-	-	-	-	-	-	-	12	-	3.470E-2	5.977E+0	1.387E+0
		5.0	-	-	-	-	-	-	24	-	-	-	-	6.930E-2	1.073E+1	8.406E-1
1.0	0.1	0.1	2	-	-	-	26	-	-	-	-	-	-	1.000E-4	7.710E-1	1.737E+1
		0.5	3	-	-	-	24	-	-	-	-	-	-	2.000E-4	6.618E-1	1.266E+1
		1.0	3	-	-	-	24	-	-	-	-	-	-	4.000E-4	7.658E-1	1.244E+1
		2.0	3	-	-	-	24	-	-	-	-	-	-	1.000E-3	1.098E+0	1.237E+1
		5.0	3	-	-	-	24	-	-	-	-	-	-	4.800E-3	3.084E+0	1.234E+1
	0.5	0.1	2	-	-	-	26	-	-	-	-	-	-	3.000E-4	8.873E-1	1.060E+1
		0.5	5	-	-	-	20	-	-	-	-	-	-	3.000E-4	6.853E-1	1.816E+0
		1.0	-	12	-	-	12	-	-	-	-	-	-	5.000E-4	7.996E-1	1.420E+0
		2.0	-	12	-	-	12	-	-	-	-	-	-	1.300E-3	1.203E+0	1.284E+0
		5.0	-	12	-	-	12	-	-	-	-	-	-	5.900E-3	3.495E+0	1.225E+0
	1.0	0.1	-	-	-	-	24	-	-	6	-	-	-	1.200E-3	1.299E+0	1.687E+1
		0.5	-	-	10	-	15	-	-	-	-	-	-	8.000E-4	9.352E-1	1.729E+0
		1.0	-	12	-	-	12	-	-	-	-	-	-	1.300E-3	1.068E+0	1.068E+0
		2.0	-	14	-	-	9	-	-	-	-	-	-	2.800E-3	1.543E+0	8.452E-1
		5.0	-	16	-	-	6	-	-	-	-	-	-	1.040E-2	4.211E+0	7.501E-1
	2.0	0.1	-	-	-	-	4	-	-	4	-	44	-	3.020E-2	3.073E+0	3.205E+1

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ρ_1	ρ_2	ρ_3	1	3	4	5	6	7	8	11	13	15	18	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
		0.5	-	-	-	-	12	-	-	16	-	4	-	4.700E-3	1.644E+0	2.443E+0
		1.0	-	-	-	12	5	-	-	10	-	-	-	5.400E-3	1.770E+0	1.204E+0
		2.0	-	5	-	18	-	-	-	-	-	-	-	8.800E-3	2.377E+0	7.913E-1
		5.0	-	16	-	-	6	-	-	-	-	-	-	2.880E-2	5.436E+0	6.163E-1
	5.0	0.1	-	-	-	-	1	-	-	2	-	54	-	1.600E+0	8.488E+0	9.363E+1
		0.5	-	-	-	-	3	-	-	9	-	36	-	1.607E-1	4.566E+0	5.783E+0
		1.0	-	-	-	-	6	-	-	16	-	16	-	8.440E-2	4.610E+0	2.235E+0
		2.0	-	-	-	-	7	-	-	23	-	-	-	8.610E-2	5.482E+0	1.104E+0
		5.0	-	3	-	18	-	-	-	-	3	-	-	1.859E-1	9.865E+0	6.563E-1
2.0	0.1	0.1	-	2	-	-	27	-	-	-	-	-	-	1.600E-3	1.629E+0	3.609E+1
		0.5	-	2	-	-	27	-	-	-	-	-	-	3.300E-3	1.693E+0	2.652E+1
		1.0	-	2	-	-	27	-	-	-	-	-	-	6.300E-3	1.805E+0	2.613E+1
		2.0	-	2	-	-	27	-	-	-	-	-	-	1.520E-2	2.137E+0	2.601E+1
		5.0	-	2	-	-	27	-	-	-	-	-	-	6.540E-2	4.005E+0	2.595E+1
	0.5	0.1	1	-	-	-	28	-	-	-	-	-	-	3.700E-3	1.784E+0	1.767E+1
		0.5	-	6	-	-	21	-	-	-	-	-	-	2.800E-3	1.247E+0	2.770E+0
		1.0	-	6	-	-	21	-	-	-	-	-	-	4.900E-3	1.386E+0	2.152E+0
		2.0	-	8	-	-	18	-	-	-	-	-	-	9.200E-3	1.753E+0	1.956E+0
		5.0	-	8	-	-	18	-	-	-	-	-	-	3.670E-2	3.996E+0	1.873E+0
	1.0	0.1	1	-	-	-	28	-	-	-	-	-	-	8.800E-3	2.025E+0	2.516E+1
		0.5	-	-	-	12	15	-	-	-	-	-	-	6.000E-3	1.534E+0	2.260E+0
		1.0	-	8	-	-	18	-	-	-	-	-	-	8.300E-3	1.647E+0	1.328E+0
		2.0	-	10	-	-	15	-	-	-	-	-	-	1.510E-2	2.125E+0	1.032E+0
		5.0	-	10	-	-	15	-	-	-	-	-	-	5.570E-2	4.603E+0	9.113E-1
	2.0	0.1	-	-	-	-	18	-	-	3	-	18	-	6.270E-2	3.304E+0	4.635E+1
		0.5	-	-	-	-	20	-	-	10	-	-	-	2.440E-2	2.383E+0	2.991E+0
		1.0	-	-	-	4	14	-	-	11	-	-	-	2.760E-2	2.526E+0	1.344E+0
		2.0	-	-	-	20	5	-	-	-	-	-	-	3.930E-2	3.023E+0	8.307E-1
		5.0	-	-	-	24	-	-	-	-	-	-	-	1.156E-1	5.856E+0	6.292E-1
	5.0	0.1	-	-	-	-	1	-	-	1	-	56	-	1.544E+1	1.903E+1	1.178E+2
		0.5	-	-	-	-	4	-	-	6	-	40	-	8.441E-1	6.822E+0	6.535E+0
		1.0	-	-	-	-	6	-	-	11	-	26	-	4.288E-1	6.135E+0	2.341E+0
		2.0	-	-	-	-	8	-	-	19	-	6	-	3.196E-1	6.718E+0	1.067E+0
		5.0	-	-	-	4	5	-	-	20	-	-	-	6.393E-1	9.977E+0	5.931E-1

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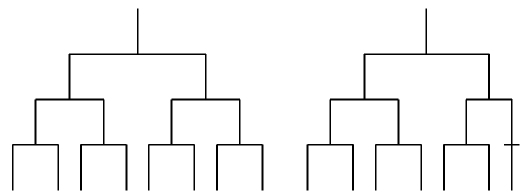
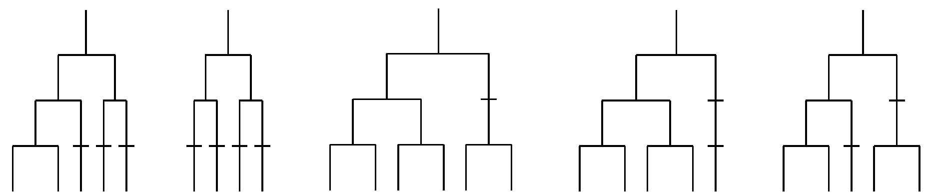
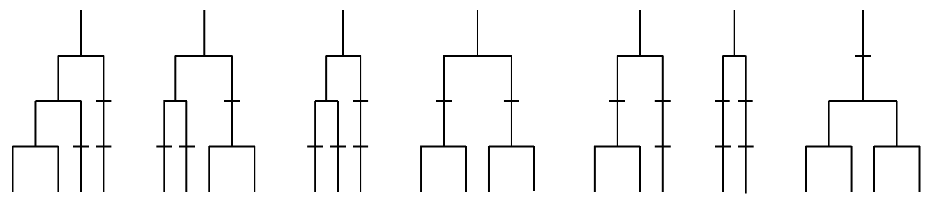
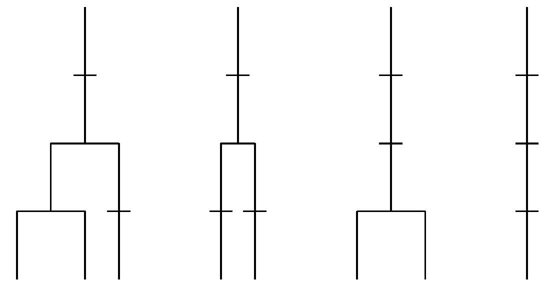
ρ_1	ρ_2	ρ_3	1	3	4	5	6	7	8	11	13	15	18	Det($\mathbf{V}$)	Tr($\mathbf{V}$)	Tr($\mathbf{V}_s$)
5.0	0.1	0.1	-	2	-	-	27	-	-	-	-	-	-	8.260E-2	3.561E+0	1.345E+2
		0.5	-	1	-	-	28	-	-	-	-	-	1	2.445E-1	4.635E+0	9.986E+1
		1.0	-	1	-	-	28	-	-	-	-	-	1	3.764E-1	4.798E+0	9.861E+1
		2.0	-	1	-	-	28	-	-	-	-	-	1	7.257E-1	5.228E+0	9.824E+1
		5.0	-	1	-	-	28	-	-	-	-	-	1	2.457E+0	7.358E+0	9.810E+1
	0.5	0.1	-	1	-	-	28	-	-	-	-	1	-	2.580E-1	4.834E+0	5.135E+1
		0.5	-	2	-	-	27	-	-	-	-	-	-	1.960E-1	3.961E+0	7.524E+0
		1.0	-	4	-	-	24	-	-	-	-	-	-	1.664E-1	3.778E+0	5.909E+0
		2.0	-	4	-	-	24	-	-	-	-	-	-	3.082E-1	4.275E+0	5.431E+0
		5.0	-	4	-	-	24	-	-	-	-	-	-	9.933E-1	6.677E+0	5.255E+0
	1.0	0.1	-	1	-	-	28	-	-	-	-	1	-	4.323E-1	5.222E+0	6.151E+1
		0.5	-	4	-	-	24	-	-	-	-	-	-	1.814E-1	4.016E+0	4.865E+0
		1.0	-	4	-	-	24	-	-	-	-	-	-	2.602E-1	4.227E+0	2.762E+0
		2.0	-	6	-	-	21	-	-	-	-	-	-	3.482E-1	4.780E+0	2.146E+0
		5.0	-	6	-	-	21	-	-	-	-	-	-	1.057E+0	7.423E+0	1.917E+0
	2.0	0.1	-	-	-	-	29	-	-	1	-	-	-	1.967E+0	8.131E+0	9.236E+1
		0.5	-	-	-	6	22	-	-	-	-	1	-	5.173E-1	5.163E+0	5.419E+0
		1.0	-	-	-	8	20	-	-	-	-	-	-	5.474E-1	5.285E+0	2.239E+0
		2.0	-	6	-	-	21	-	-	-	-	-	-	6.963E-1	5.975E+0	1.304E+0
		5.0	-	8	-	-	18	-	-	-	-	-	-	1.622E+0	9.163E+0	9.637E-1
	5.0	0.1	-	-	-	-	2	-	-	1	-	54	-	1.282E+2	3.784E+1	2.142E+2
		0.5	-	-	-	-	8	-	-	4	-	36	-	1.043E+1	1.383E+1	1.060E+1
		1.0	-	-	-	-	11	-	-	8	-	22	-	4.746E+0	1.168E+1	3.453E+0
		2.0	-	-	-	-	15	-	-	13	-	4	-	3.361E+0	1.142E+1	1.418E+0
		5.0	-	-	-	4	11	-	-	14	-	-	-	5.803E+0	1.510E+1	7.107E-1

Stage	Atom 1	Atom 2	Atom 3	Atom 4
1				
2				
3				
4				
b_i	2	2	2	2
c_{ij}	2,2	2,2	2,2	2,2
n_{ijk}	2,2,2,2	2,2,2,1	2,2,1,1	2,1,2,1

Stage	5	6	7	8	9
1					
2					
3					
4					
b_i	2	2	2	2	2
c_{ij}	2,2	2,2	2,1	2,1	2,1
n_{ijk}	2,1,1,1	1,1,1,1	2,2,2	2,2,1	2,1,2

Stage	10	11	12	13	14	15	16
1							
2							
3							
4							
b_i	2	2	2	2	2	2	1
c_{ij}	2,1	2,1	2,1	1,1	1,1	1,1	2
n_{ijk}	2,1,1	1,1,2	1,1,1	2,2	2,1	1,1	2,2

	Atom			
Stage	17	18	19	20
1				
2				
3				
4				
b_i	1	1	1	1
c_{ij}	2	2	1	1
n_{ijk}	2,1	1,1	2	1

SMALL SAMPLE RESULTS (*continued*)

- With few exceptions the D-optimal designs found are constructed using either atom A_1 or A_4 when $\rho_1 \leq 1$, this regardless of the values of the other parameters.
- For larger values of ρ_1 the designs make use of atoms 3, 4 and 5. These are some of the staggered structures originally proposed by Anderson (1960) and Bainbridge (1963).
- A-optimality is quite sensitive to the prior parameter configuration. A slight change in the prior parameter values can lead to very different design configurations.

$\boxed{\textbf{LARGE SAMPLE DESIGNS}}$

- A complete search is not practical when the sample size is large. So, for experiments with a large sample size, we look for Optimal Design Measures in the class $\mathcal{C}^*_{4,s}$.
- We let N and k be arbitrary, but use $s = 2$. The number of atoms for this case is 20.
- Let $w_\alpha = r_\alpha/N$, for $\alpha = 1, 2, \ldots, 20$ be the proportion of experimental resources allocated to atom $\mathrm{A}_\alpha \in \mathcal{A}_{4,2}$.

LARGE SAMPLE DESIGNS (*continued*)

- Define $\mathbf{w}$, $\mathbf{n}$, $\mathbf{c}$ and $\mathbf{b}$ as 20×1 vectors whose elements are w_α, $n_{\alpha**}$, $c_{\alpha*}$ and b_α for atom α. In terms of these vectors, (since the total number of observations equals N) we have

$$\mathbf{n}'\mathbf{w} = 1.$$

The total number of first, second and third stage classes are, respectively

$$a = N\,\mathbf{1}'\,\mathbf{w},$$

$$b_* = N\,\mathbf{b}'\,\mathbf{w},$$

and

$$c_{**} = N\,\mathbf{c}'\,\mathbf{w},$$

where $\mathbf{1}$ is a 20×1 vector of 1's.

$\boxed{\textbf{VALUES OF DESIGN CONSTANTS } k_m}$

The values for the k_m, for $m = 1, 2, \ldots, 25$, are given by

$$k_1 = \frac{1}{N}\sum_{\alpha} w_\alpha n^2_{\alpha**}, \qquad k_2 = \frac{1}{N}\sum_{\alpha} w_\alpha \sum_{j} n^2_{\alpha j*},$$

$$k_3 = \frac{1}{N}\sum_{\alpha} w_\alpha \sum_{j}\sum_{k} n^2_{\alpha jk}, \qquad k_4 = N\sum_{\alpha} w_\alpha \frac{\sum_j n^2_{\alpha j*}}{n_{\alpha**}},$$

$$k_5 = N\sum_{\alpha} w_\alpha \frac{\sum_j \sum_k n^2_{\alpha jk}}{n_{\alpha**}}, \qquad k_6 = N\sum_{\alpha} w_\alpha \frac{\sum_j \sum_k n^2_{\alpha jk}}{n_{\alpha j*}},$$

$$k_7 = N\sum_{\alpha} w_\alpha n^3_{\alpha**}, \qquad k_8 = N\sum_{\alpha} w_\alpha \sum_{j} n^3_{\alpha j*},$$

$$k_9 = N\sum_{\alpha} w_\alpha \sum_{j}\sum_{k} n^3_{\alpha jk}, \qquad k_{10} = N\sum_{\alpha} w_\alpha \frac{\sum_j \sum_k n^3_{\alpha jk}}{n_{\alpha**}},$$

$$k_{11} = N\sum_{\alpha} w_\alpha \sum_{j} \frac{\sum_k n^3_{\alpha jk}}{n_{\alpha j*}}, \qquad k_{12} = N\sum_{\alpha} w_\alpha \frac{\sum_j n^3_{\alpha j*}}{n_{\alpha**}},$$

VALUES OF DESIGN CONSTANTS k_m (*continued*)

$$k_{13} = N \sum_{\alpha} w_{\alpha} \frac{\left(\sum_j n^2_{\alpha j *}\right)^2}{n_{\alpha **}}, \qquad k_{14} = N \sum_{\alpha} w_{\alpha} \frac{\left(\sum_j \sum_k n^2_{\alpha j k}\right)^2}{n_{\alpha **}},$$

$$k_{15} = N \sum_{\alpha} w_{\alpha} \sum_j \frac{\left(\sum_k n^2_{\alpha j k}\right)^2}{n_{\alpha j *}}, \qquad k_{16} = N \sum_{\alpha} w_{\alpha} \frac{\sum_j n_{\alpha j *} \left(\sum_k n^2_{\alpha j k}\right)}{n_{\alpha **}},$$

$$k_{17} = N \sum_{\alpha} w_{\alpha} \frac{\left(\sum_j n^2_{\alpha j *}\right)\left(\sum_j \sum_k n^2_{\alpha j k}\right)}{n_{\alpha **}}, \qquad k_{18} = N \sum_{\alpha} w_{\alpha} \frac{\sum_j \left(\sum_k n^2_{\alpha j k}\right)^2 / n_{\alpha j *}}{n_{\alpha **}},$$

$$k_{19} = N \sum_{\alpha} w_{\alpha} \sum_j \frac{\left(\sum_k n^2_{\alpha j k}\right)^2}{n^2_{\alpha j *}}, \qquad k_{20} = N \sum_{\alpha} w_{\alpha} \frac{\left(\sum_j n^2_{i j *}\right)\left(\sum_j \sum_k n^2_{\alpha j k}\right)}{n^2_{\alpha **}},$$

$$k_{21} = N \sum_{\alpha} w_{\alpha} \frac{\left(\sum_j \sum_k n^2_{\alpha j k}\right)^2}{n^2_{\alpha **}}, \qquad k_{22} = N \sum_{\alpha} w_{\alpha} \frac{\left(\sum_j n^2_{\alpha j *}\right)^2}{n^2_{\alpha **}},$$

$$k_{23} = N \sum_{\alpha} w_{\alpha} n_{\alpha **} \left(\sum_j n^2_{\alpha j *} \right), \qquad k_{24} = N \sum_{\alpha} w_{\alpha} n_{\alpha **} \left(\sum_j \sum_k n^2_{\alpha , j k} \right)$$

$$k_{25} = N \sum_{\alpha} w_{\alpha} \sum_j n_{\alpha j *} \left(\sum_k n^2_{i j k} \right)$$

$\boxed{\textbf{VARIANCE OF } \hat{\boldsymbol{\sigma}}^2}$

- We express $\text{Var}(\hat{\boldsymbol{\sigma}}^2)$ as a function of w_α and the parameter configuration.
- As $N \to \infty$, we find that $\text{Var}(\hat{\boldsymbol{\sigma}}^2)$ is proportional to

$$\mathbf{H}^{-1}\mathbf{G}\boldsymbol{\mathcal{V}}(\mathbf{H}^{-1}\mathbf{G})'$$

  where this matrix depends only on w_α, the quantities (ρ_1, ρ_2, ρ_3) and the specific structure of the atoms in $\mathcal{A}_{4,2}$.
- The constant of proportionality is $2\sigma_\epsilon^4/N$.
- In this expression the matrix $\mathbf{G}$ and the matrix $\mathbf{H}$ are

$$\mathbf{G} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{bmatrix}; \qquad \mathbf{H} = \begin{bmatrix} 1 - c_{**} & 0 & 0 & 0 \\ c_{**} - b_* & 1 - k_6 & 0 & 0 \\ b_* - a & k_6 - k_5 & 1 - k_4 & 0 \\ a & k_5 & k_4 & 1 \end{bmatrix},$$

$\boxed{\textbf{VARIANCE OF } \hat{\boldsymbol{\sigma}}^2}$

The individual elements of the symmetric matrix $\boldsymbol{\mathcal{V}}$ are

$$
\begin{aligned}
\mathcal{V}_{5,q} &= 0, \quad \text{for } q = 1, 2, \ldots, 5, \\
\mathcal{V}_{4,4} &= K_1\,\rho_3^2 + K_{22}\,\rho_2^2 + K_{21}\,\rho_1^2 + a + 2K_2\,\rho_3\,\rho_2 + 2K_3\,\rho_3\,\rho_1 \\
&\quad +2\,\rho_3 + 2K_{20}\,\rho_2\,\rho_1 + 2K_4\,\rho_2 + 2K_5\,\rho_1, \\
\mathcal{V}_{4,3} &= \mathcal{V}_{4,4} + (K_{12} - K_{22})\,\rho_2^2 + (K_{18} - K_{21})\,\rho_1^2 + 2(K_{16} - K_{20})\,\rho_2\,\rho_1, \\
\mathcal{V}_{4,2} &= \mathcal{V}_{4,3} + (K_{10} - K_{18})\,\rho_1^2 \\
\mathcal{V}_{4,1} &= K_1\,\rho_3^2 + K_{12}\,\rho_2^2 + K_{10}\,\rho_1^2 + a + 2K_2\,\rho_3\,\rho_2 + 2K_3\,\rho_3\,\rho_1 \\
&\quad +2\,\rho_3 + 2K_{16}\,\rho_2\,\rho_1 + 2K_4\,\rho_2 + 2K_5\,\rho_1), \\
\mathcal{V}_{3,3} &= \mathcal{V}_{4,4} + (K_2 - K_{22})\,\rho_2^2 + (K_{19} - K_{21})\,\rho_1^2 + (b_* - a) \\
&\quad +2(K_3 - K_{20})\,\rho_2\,\rho_1 + 2(1 - K_4)\,\rho_2 + 2(K_6 - K_5)\,\rho_1, \\
\mathcal{V}_{3,2} &= \mathcal{V}_{3,3} + (K_{11} - K_{19})\,\rho_1^2 \\
\mathcal{V}_{3,1} &= K_1\,\rho_3^2 + K_2\,\rho_2^2 + K_{11}\,\rho_1^2 + b_* + 2K_2\,\rho_3\,\rho_2 + 2K_3\,\rho_3\,\rho_1 \\
&\quad +2\,\rho_3 + 2K_3\,\rho_2\,\rho_1 + 2\,\rho_2 + 2K_6\,\rho_1),
\end{aligned}
$$

$\boxed{\textbf{VARIANCE OF } \hat{\boldsymbol{\sigma}}^2 \ (\textit{continued})}$

$$
\begin{aligned}
\mathcal{V}_{2,2} &= \mathcal{V}_{3,3} + (K_3 - K_{19})\,\rho_1^2 + (c_{**} - b_*) + 2(1 - K_6)\,\rho_1, \\
\mathcal{V}_{2,1} &= K_1\,\rho_3^2 + K_2\,\rho_2^2 + K_3\,\rho_1^2 + c_{**} + 2K_2\,\rho_3\,\rho_2 + 2K_3\,\rho_3\,\rho_1 \\
&\quad +2\,\rho_3 + 2K_3\,\rho_2\,\rho_1 + 2\,\rho_2 + 2\,\rho_1), \\
\mathcal{V}_{1,1} &= K_1\,\rho_3^2 + K_2\,\rho_2^2 + K_3\,\rho_1^2 + 1 + 2K_2\,\rho_3\,\rho_2 + 2K_3\,\rho_3\,\rho_1 \\
&\quad +2\,\rho_3 + 2K_3\,\rho_2\,\rho_1 + 2\,\rho_2 + 2\,\rho_1),
\end{aligned}
$$

K_m are the same as k_m but the coefficients N or $1/N$ is omitted.

VARIANCE OF $\hat{\boldsymbol{\sigma}}^2$ (*continued*)

- To assure that the parameters of the model are estimable, the following restrictions must be incorporated into the problem:

$$\mathbf{n}'\,\mathbf{w} = 1, \qquad \mathbf{c}'\,\mathbf{w} \le 1,$$

$$K_6 \le 1, \qquad K_4 \le 1,$$

  where again the coefficient N of k_4 and k_6 are dropped to obtain K_4 and K_6.

- For a given variance component configuration (ρ_1, ρ_2, ρ_3), the design criteria are functions only of w_α. Hence the determinant, the trace or the scaled trace may be numerically optimized to obtain the large sample D-optimal, A-optimal or A$_s$-optimal designs.

- The following Table shows the results of minimization of the A$_s$ criterion for a selected set of prior values of the variance component configuration.

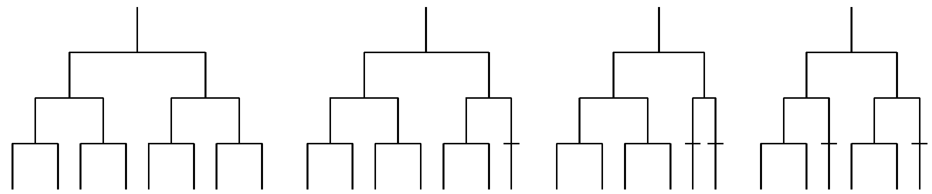
EXAMPLE: LARGE SAMPLE A_s-OPTIMAL DESIGNS

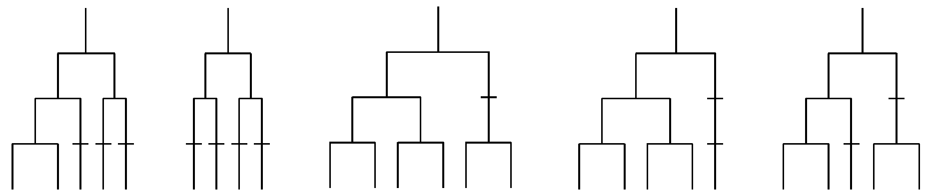
			Atom																	
ρ_1	ρ_2	ρ_3	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	$\mathrm{Tr}(\mathbf{V}_s)$	$\mathrm{Det}(\mathbf{V})$	$\mathrm{Tr}(\mathbf{V})$
0.5	1.0	0.1	-	-	-	-	-	0.143	-	-	-	-	0.107	-	-	-	-	8.110E2	2.804E3	4.695E1
		0.5	0.070	-	-	-	-	0.109	-	-	-	-	-	-	-	-	-	1.012E2	2.399E3	4.036E1
		1.0	0.094	-	-	-	0.001	0.061	-	-	-	-	-	-	-	-	-	6.696E1	3.979E3	5.149E1
		2.0	0.106	-	-	-	-	0.038	-	-	-	-	-	-	-	-	-	5.508E1	9.265E3	8.600E1
		5.0	0.118	-	0.003	-	-	0.011	-	-	-	-	-	-	-	-	-	4.974E1	3.871E4	2.879E2
	2.0	0.1	-	-	-	-	-	0.027	-	-	-	-	0.063	-	-	-	0.320	1.618E3	6.402E4	1.078E2
		0.5	-	-	-	0.062	-	0.056	-	-	-	-	0.102	-	-	-	-	1.522E2	1.492E4	7.665E1
		1.0	0.008	0.059	-	0.051	-	0.053	-	-	-	-	-	-	-	-	-	8.112E1	1.897E4	9.454E1
		2.0	0.004	-	0.161	-	-	-	-	-	-	-	-	-	-	-	-	5.583E1	3.610E4	1.327E2
		5.0	0.093	-	0.040	-	-	0.003	-	-	-	-	-	-	-	-	-	4.559E1	1.265E5	3.634E2
	5.0	0.1	-	-	0.001	-	0.010	-	0.004	-	-	-	-	0.001	-	0.002	0.458	5.131E3	5.938E6	3.300E2
		0.5	-	-	-	-	0.015	0.079	-	-	-	-	-	-	-	0.110	0.138	3.745E2	4.434E5	2.221E2
		1.0	-	-	0.045	-	-	0.061	0.003	-	-	-	0.031	-	0.037	0.001	0.098	1.562E2	3.416E5	2.610E2
		2.0	-	0.041	0.001	0.059	0.001	0.060	0.008	-	0.005	-	-	-	0.009	-	-	8.257E1	3.928E5	3.717E2
		5.0	0.073	-	0.037	0.019	-	0.021	-	-	-	-	-	-	-	-	-	5.078E1	9.587E5	7.086E2
1.0	0.1	0.1	0.018	-	-	-	-	0.214	-	-	-	-	-	-	-	-	-	1.036E3	1.004E3	4.434E1
		0.5	0.022	-	-	-	-	0.206	-	-	-	-	-	-	-	-	-	7.583E2	2.263E3	4.228E1
		1.0	0.022	-	-	-	-	0.206	-	-	-	-	-	-	-	-	-	7.460E2	4.988E3	4.795E1
		2.0	0.022	-	-	-	-	0.206	-	-	-	-	-	-	-	-	-	7.417E2	1.370E4	6.681E1
		5.0	0.022	-	-	-	-	0.205	-	-	-	-	-	-	-	-	-	7.397E2	6.563E4	1.802E2
	0.5	0.1	0.016	-	-	-	-	0.217	-	-	-	-	-	-	-	-	-	6.254E2	3.608E3	5.377E1
		0.5	0.042	-	-	-	-	0.167	-	-	-	-	-	-	-	-	-	1.078E2	3.831E3	4.082E1
		1.0	-	-	0.097	-	-	0.105	-	-	-	-	-	-	-	-	-	8.454E1	6.880E3	4.746E1
		2.0	-	-	0.104	-	-	0.093	-	-	-	-	-	-	-	-	-	7.660E1	1.636E4	7.059E1
		5.0	-	-	0.109	-	-	0.086	-	-	-	-	-	-	-	-	-	7.311E1	7.029E4	2.055E2
	1.0	0.1	0.001	-	-	-	-	0.205	-	-	-	-	0.042	-	-	-	-	9.946E2	1.585E4	7.978E1
		0.5	-	-	-	0.009	0.137	0.065	-	-	-	-	-	-	-	-	-	1.020E2	1.074E4	5.594E1
		1.0	-	-	0.101	-	-	0.098	-	-	-	-	-	-	-	-	-	6.323E1	1.632E4	6.323E1
		2.0	-	-	0.119	-	-	0.071	-	-	-	-	-	-	-	-	-	5.017E1	3.378E4	9.066E1
		5.0	-	-	0.131	-	-	0.054	-	-	-	-	-	-	-	-	-	4.463E1	1.296E5	2.420E2
	2.0	0.1	-	-	-	-	-	0.029	-	-	-	-	0.033	-	-	-	0.375	1.905E3	4.140E5	1.909E2
		0.5	-	-	-	-	-	0.105	-	-	-	-	0.140	-	-	-	0.009	1.443E2	5.488E4	9.694E1
		1.0	0.036	-	-	-	-	0.178	-	-	-	-	-	-	-	-	-	2.099E1	4.612E2	2.834E1
		2.0	-	-	0.042	-	0.149	-	-	-	-	-	-	-	-	-	-	4.674E1	1.088E5	1.398E2
		5.0	-	-	0.075	-	0.110	-	-	-	-	-	-	-	-	-	-	3.665E1	3.577E5	3.077E2

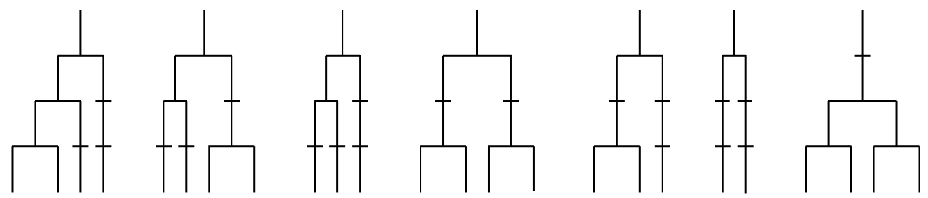
$\boxed{\textbf{EXAMPLE}}$

- Suppose $\rho_1 = 1.0$, $\rho_2 = 0.1$ and $\rho_3 = 0.1$ and that a sample size $N = 120$ is desired.
- Our results indicate that (see Table) an A$_s$-optimal design should be constructed using atoms A_1 and A_6. The values of $w_1 = 0.018$ and $w_6 = 0.214$ imply that $r_1 = 2.16$ and $r_6 = 25.68$. Tr$(\mathbf{V}_s)$ is equal to $17.267\sigma_\epsilon^4$. Since only integer replicates of atoms A_1 and A_6 are possible, we could take 2 replicates of atom 1 and 26 of atom 6. This design should not depart much from the large sample optimal design with noninteger values of r_α.
- In this example the design is, in fact, A$_s$-optimal when complete search of $\mathcal{C}_{4,2,3}(120)$ is done.
- An important finding is that in some cases the number of atoms for which $r_\alpha \neq 0$ is more than 3. However, typically only two or three of the w_α are non-negligible.

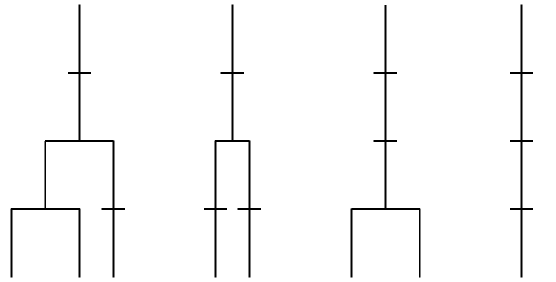
ATOMS IN $\mathcal{A}_{4,2}$

Stage	Atom 1	2	3	4
1 2 3 4				
b_i	2	2	2	2
c_{ij}	2,2	2,2	2,2	2,2
n_{ijk}	2,2,2,2	2,2,2,1	2,2,1,1	2,1,2,1

	5	6	7	8	9
1 2 3 4					
b_i	2	2	2	2	2
c_{ij}	2,2	2,2	2,1	2,1	2,1
n_{ijk}	2,1,1,1	1,1,1,1	2,2,2	2,2,1	2,1,2

	10	11	12	13	14	15	16
1 2 3 4							
b_i	2	2	2	2	2	2	1
c_{ij}	2,1	2,1	2,1	1,1	1,1	1,1	2
n_{ijk}	2,1,1	1,1,2	1,1,1	2,2	2,1	1,1	2,2

ATOMS IN $\mathcal{A}_{4,2}$ (*continued*)

	Atom			
Stage	17	18	19	20
1				
2				
3				
4				
b_i	1	1	1	1
c_{ij}	2	2	1	1
n_{ijk}	2,1	1,1	2	1

$\boxed{\textbf{SUMMARY}}$

- We considered the optimum design problem for estimating variance components in the 4-stage nested model.
- We used ANOVA estimators for the variance components.
- Three functions of the variance–covariance matrix of the estimators were considered: the trace, the determinant and the scaled trace. The scaled trace criterion uses the trace of the generalized squared coefficients of variation matrix rather than the trace of the variance–covariance matrix.
- In all cases, sampling cost was assumed to be proportional to N. Other cost structures are easily accommodated.
- Classes of designs were considered that allow the estimation of all the model parameters. For the most part, the proposed classes of designs include designs proposed by earlier authors.

SUMMARY

- For the l–stage model, the class $\mathcal{C}_{l,s,k}(N)$ consisting of all N–observation designs in which the number of sublevels at each level is at most s and the number of distinct atoms in the design is at most k.
- Delgado & Iyer (1999) studied the three–stage nested model with the design classes restricted to $s = 2$ and $s = 3$. Here we have extended the study to four–stage nested models with $s = 2$.
- Computer programs are available to find locally optimal designs. Search for small sample optimal designs in the four–stage model was restricted to $\mathcal{C}_{4,2,3}(N)$. Staggered designs of Anderson (1960) and Bainbridge (1963) to make the degrees of freedom more or less equal are elements of this class.
- Large sample design measures were studied for the four-stage model for the case $s = 2$.
- It was found that, even when the number of atoms, k, was not restricted (large sample designs), the best designs attempted to concentrate all the resources on three or less atoms.
- A computer program is available for large sample optimum designs in the class $\mathcal{C}^*_{4,2}$, for given prior parameter configuration.

$\boxed{\textbf{LIST OF THINGS TO DO}}$

- Modify our algorithm for small sample optimum designs to accommodate specified cost structures.
- Examine large sample optimum designs for 4-stage nested models for the case $s = 3$ (feasibility is an issue)
- Compare our results with optimum designs based on ML or REML estimation.
- Define classes of designs to extend our work to cross classified random effects models.
- Investigate Bayesian approaches in which the expected risk relative to an assumed prior distribution for (ρ_1, ρ_2, ρ_3) is minimized.

$\boxed{\textbf{THANK YOU}}$