# Elements of Nonlinear Statistics and Neural Networks


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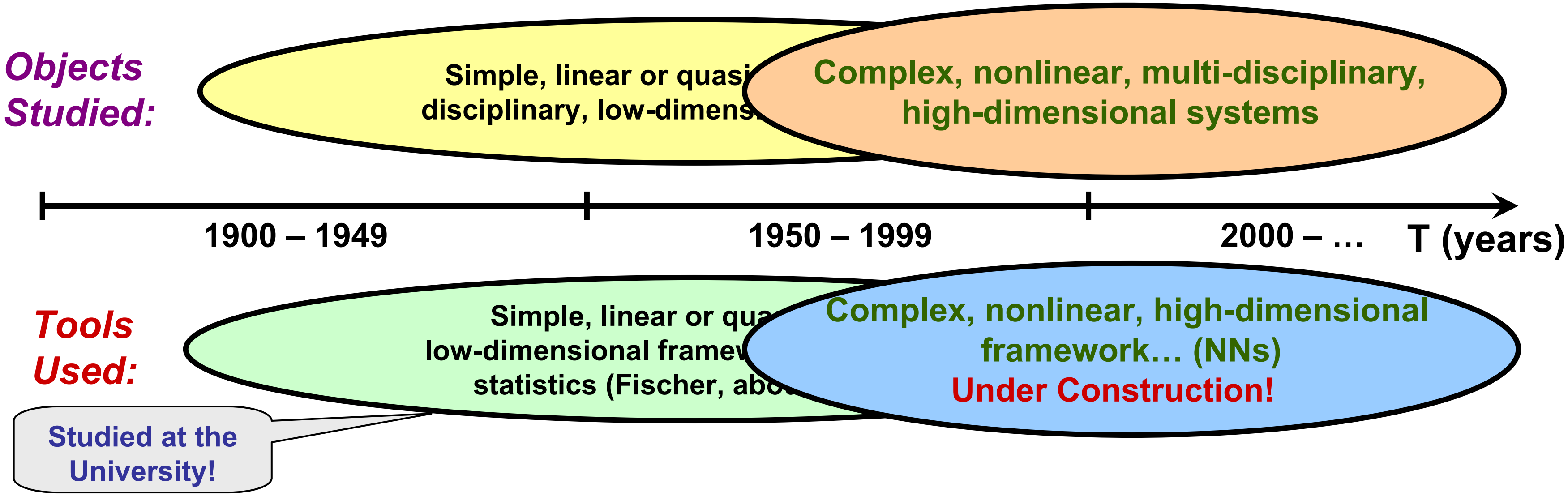
# Outline

- Introduction: Motivation
- Classical Statistic Framework: Regression Analysis
- Regression Models (Linear & Nonlinear)
- NN Tutorial
- Some Atmospheric & Oceanic Applications
  – Accelerating Calculations of Model Physics in Numerical Models
- How to Apply NNs
- Conclusions

# Motivations for This Seminar




- **Problems for Classical Paradigm:**
  - **Nonlinearity & Complexity**
  - **High Dimensionality - *Curse of Dimensionality***
- **New Paradigm under Construction:**
  - **Is still quite fragmentary**
  - **Has many different names and gurus**
  - **NNs are one of the tools developed inside this paradigm**

***Materials presented here reflect personal opinions and experience of the author!***

# Statistical Inference:
## *A Generic Problem*

**Problem:**

Information exists in the form of sets of values of several *related variables* (sample or training set) – a part of the population:

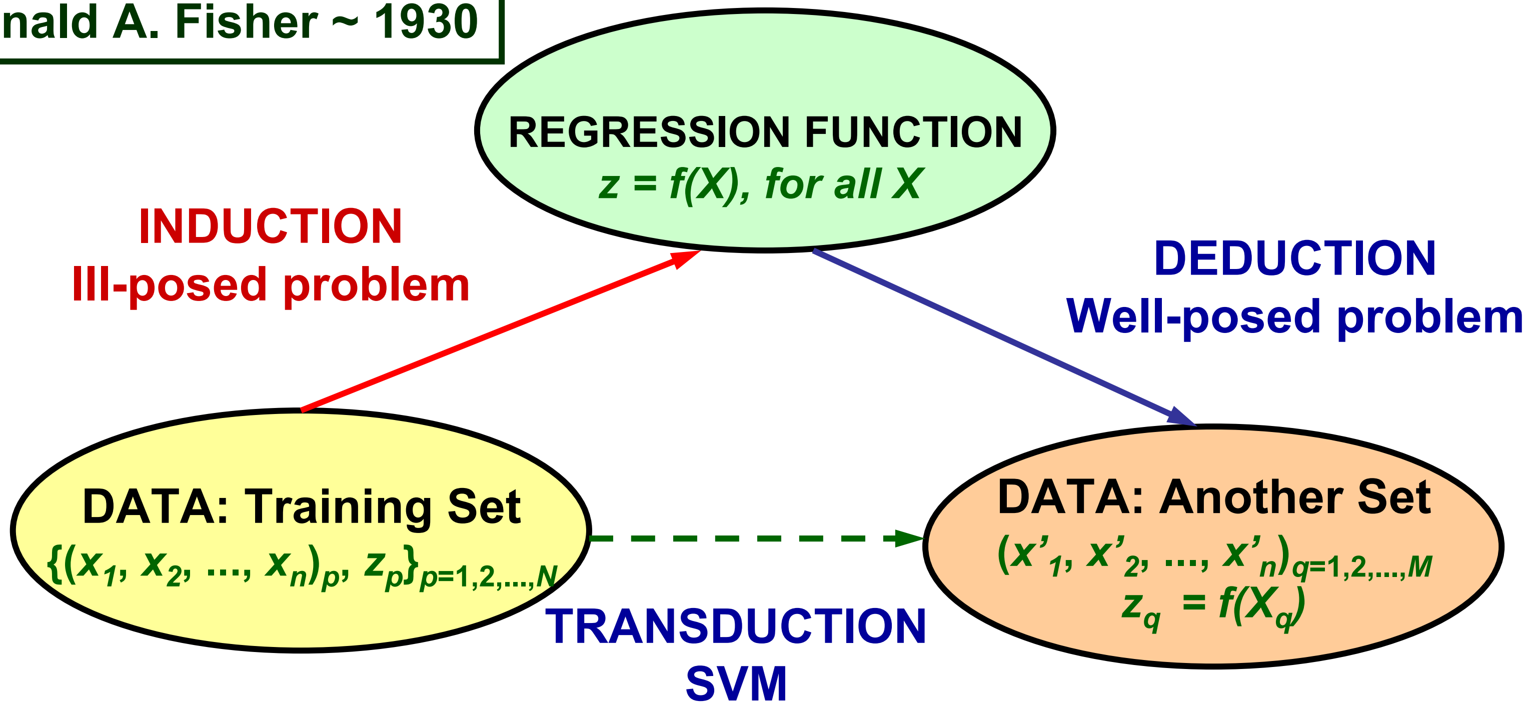
$$\{(x_1, x_2, \ldots, x_n)_p, z_p\}_{p=1,2,\ldots,N}$$

– $x_1, x_2, \ldots, x_n$ - independent variables (accurate),
– $z$ - response variable (may contain observation errors $\varepsilon$)

We want to find responses $z'_q$ for another set of independent variables $\{(x'_1, x'_2, \ldots, x'_n)_q\}_{q=1,\ldots,M}$

# Regression Analysis (1):
## *General Solution and Its Limitations*

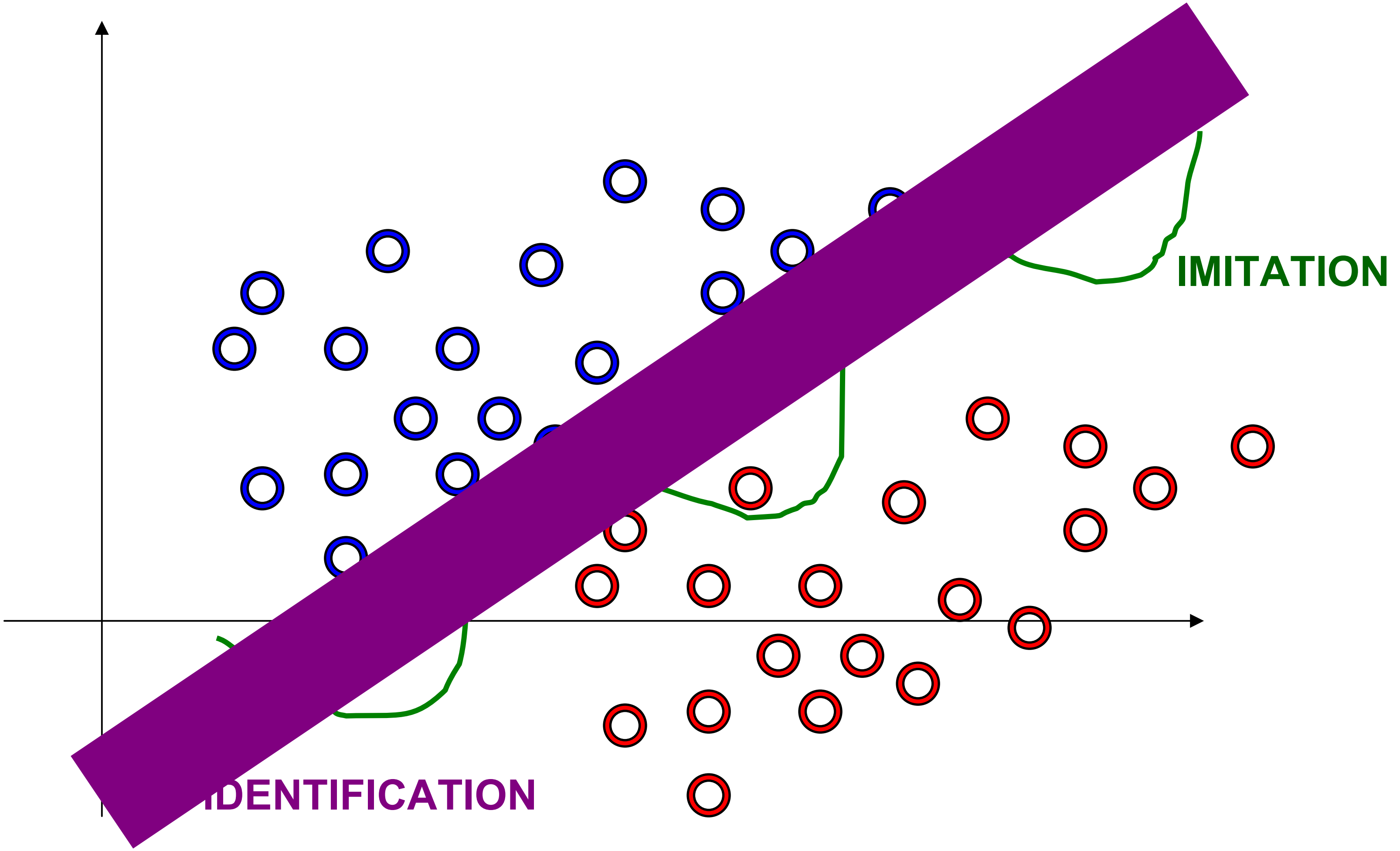
**Sir Ronald A. Fisher ~ 1930**




**Find mathematical function *f* which describes this relationship:**

1. **Identify the unknown function *f***
2. **Imitate or emulate the unknown function *f***

# Regression Analysis (2):
## Identification vs. Imitation



# Regression Analysis (2):
## *A Generic Solution*

- The effect of ***independent variables*** on the ***response*** is expressed mathematically be the ***regression or response function f:***

$$y = f(x_1, x_2, \ldots, x_n; a_1, a_2, \ldots, a_q)$$

- $y$ - dependent variable
- $a_1, a_2, \ldots, a_q$ - regression parameters (unknown!)
- $f$ - the form is usually assumed to be known
- Regression model for observed response variable:

$$z = y + \varepsilon = f(x_1, x_2, \ldots, x_n; a_1, a_2, \ldots, a_q) + \varepsilon$$

- $\varepsilon$ - error in observed value z

# Regression Models (1):
## Maximum Likelihood

- **Fischer suggested to determine unknown regression parameters $\{a_i\}_{i=1,..,q}$ maximizing the functional:**

$$L(a) = \sum_{i=1}^{N} \ln\left[\rho(y_i - f(x_i, a))\right]$$

Not always!!!

**here $\rho(\varepsilon)$ is the probability density function of errors $\varepsilon_i$**

- ***In a case*** **when $\rho(\varepsilon)$ is a** ***normal distribution*** **the maximum likelihood => least squares**

# Regression Models (2):
## *Method of Least Squares*

- To find ***unknown regression parameters*** $\{a_i\}_{i=1,2,\ldots,q}$ , the ***method of least squares*** can be applied:

$$E(a_1,a_2,\ldots,a_q)=\sum_{p=1}^{N}(z_p-y_p)^2=\sum_{p=1}^{N}[z_p-f((x_1,\ldots,x_n)_p;a_1,a_2,\ldots,a_q)]^2$$

- ***E(a$_1$,…,a$_q$)*** - **error function** = the sum of squared deviations.
- To estimate $\{a_i\}_{i=1,2,\ldots,q}$ => **minimize** ***E*** => solve the system of equations:

$$\frac{\partial E}{\partial a_i}=0;\quad i=1,2,\ldots,q$$

- **Linear** and **nonlinear** cases.

# Regression Models (3):
## *Examples of Linear Regressions*

- **Simple Linear Regression:**

  $$z = a_0 + a_1 x_1 + \varepsilon$$

- **Multiple Linear Regression:**

  $$z = a_0 + a_1 x_1 + a_2 x_2 + \dots + \varepsilon = a_0 + \sum_{i=1}^{n} a_i x_i + \varepsilon$$

- **Generalized Linear Regression:**

  $$z = a_0 + a_1 f_1(x_1) + a_2 f_2(x_2) + \dots + \varepsilon = a_0 + \sum_{i=1}^{n} a_i f_i(x_i) + \varepsilon$$

  No free parameters

  – **Polynomial regression,** $f_i(x) = x^i$,

  $$z = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \dots + \varepsilon$$

  – **Trigonometric regression,** $f_i(x) = \cos(ix)$

  $$z = a_0 + a_1 \cos(x) + a_1 \cos(2x) + \dots + \varepsilon$$

# Regression Models (4):
## *Examples of Nonlinear Regressions*

- **Response Transformation Regression:**

  $G(z) = a_0 + a_1 x_1 + \varepsilon$

- **Example:**

  $z = \exp(a_0 + a_1 x_1)$

  $G(z) = \ln(z) = a_0 + a_1 x_1$

- **Projection-Pursuit Regression:**

$$y = a_0 + \sum_{j=1}^{k} a_j f\left(\sum_{i=1}^{n} \Omega_{ji} x_i\right)$$

- **Example:**

$$z = a_0 + \sum_{j=1}^{k} a_j \tanh\left(b_j + \sum_{i=1}^{n} \Omega_{ji} x_i\right) + \varepsilon$$

# NN Tutorial:
## *Introduction to Artificial NNs*

- **NNs as Continuous Input/Output Mappings**
  - **Continuous Mappings: definition and some examples**
  - **NN Building Blocks: neurons, activation functions, layers**
  - **Some Important Theorems**
- **NN Training**
- **Major Advantages of NNs**
- **Some Problems of Nonlinear Approaches**

# Mapping

## Generalization of Function

- **Mapping: A** *rule of correspondence established between vectors* **in vector spaces and that associates each vector** *X* **of a vector space $\Re^n$ with a vector** *Y* **in another vector space $\Re^m$.**

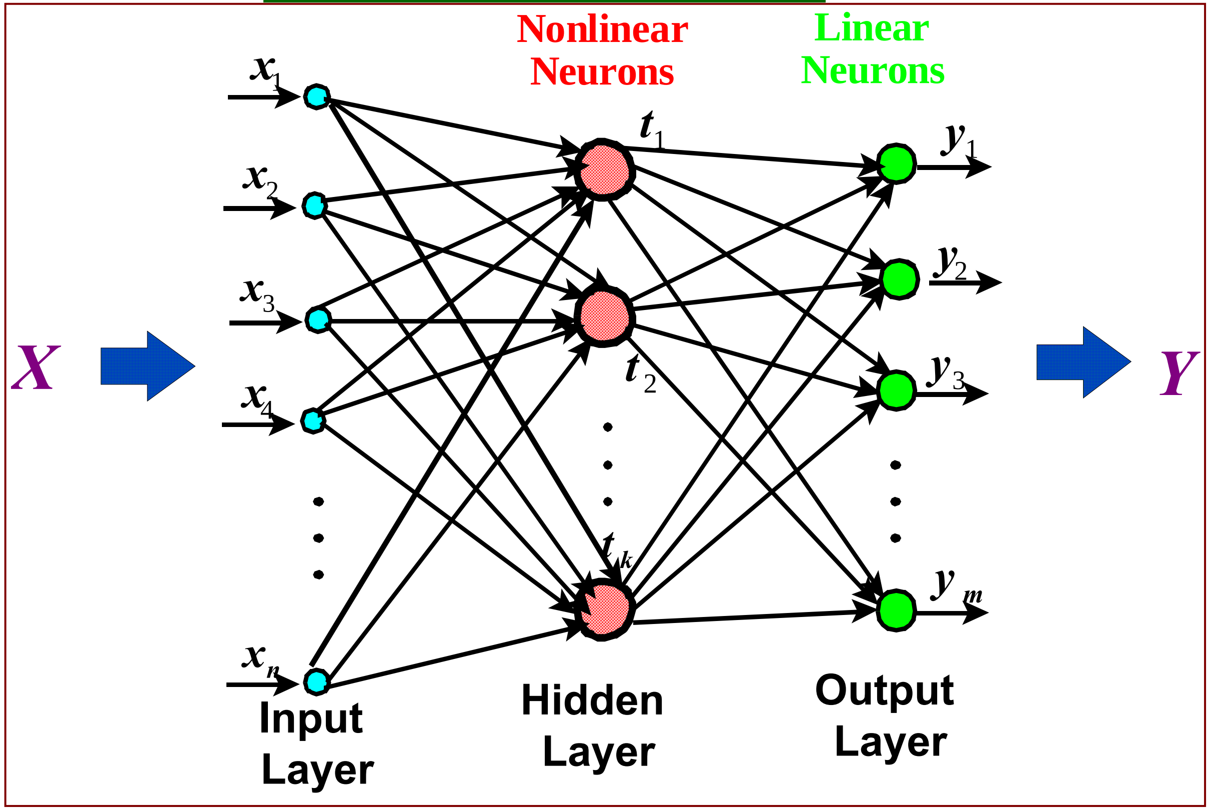
$$
\left.
\begin{aligned}
&Y = F(X) \\
&X = \{x_1, x_2, \ldots, x_n\}, \in \Re^n \\
&Y = \{y_1, y_2, \ldots, y_m\}, \in \Re^m
\end{aligned}
\right\}
\Rightarrow
\begin{bmatrix}
y_1 = f_1(x_1, x_2, \ldots, x_n) \\
y_2 = f_2(x_1, x_2, \ldots, x_n) \\
\vdots \\
y_m = f_m(x_1, x_2, \ldots, x_n)
\end{bmatrix}
$$

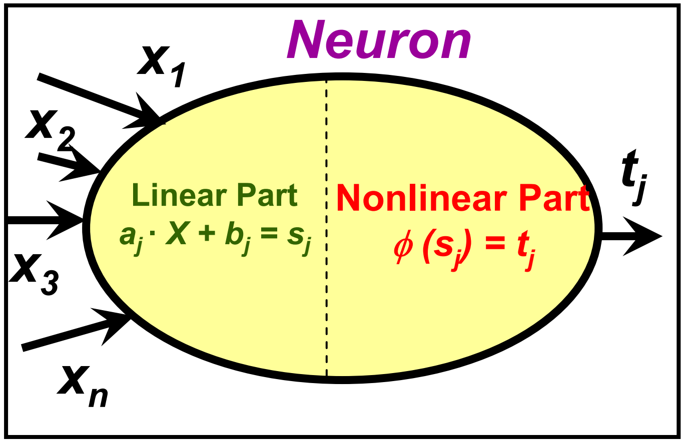
# Mapping $Y = F(X)$: examples

- **Time series prediction:**
  - $X = \{x_t, x_{t-1}, x_{t-2}, ..., x_{t-n}\}$, - Lag vector
  - $Y = \{x_{t+1}, x_{t+2}, ..., x_{t+m}\}$ - Prediction vector
  - (Weigend & Gershenfeld, “Time series prediction”, 1994)
- **Calculation of precipitation climatology:**
  - $X$ = {*Cloud parameters, Atmospheric parameters*}
  - $Y$ = {*Precipitation climatology*}
  - (Kondragunta & Gruber, 1998)
- **Retrieving surface wind speed over the ocean from satellite data (SSM/I):**
  - $X$ = {*SSM/I brightness temperatures*}
  - $Y = \{W, V, L, SST\}$
  - (Krasnopolsky, et al., 1999; operational since 1998)
- **Calculation of long wave atmospheric radiation:**
  - $X$ = {*Temperature, moisture, $O_3$, $CO_2$, cloud parameters profiles, surface fluxes, etc.*}
  - $Y$ = {*Heating rates profile, radiation fluxes*}
  - (Krasnopolsky et al., 2005)

# NN - Continuous Input to Output Mapping

## *Multilayer Perceptron:* Feed Forward, Fully Connected




$$t_j = \phi(b_{j0} + \sum_{i=1}^{n} b_{ji} \cdot x_i) =$$

$$= \tanh(b_{j0} + \sum_{i=1}^{n} b_{ji} \cdot x_i)$$

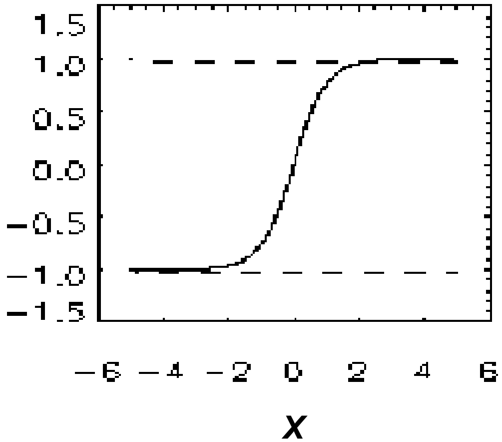
**$Y = F_{NN}(X)$**

**Jacobian !**

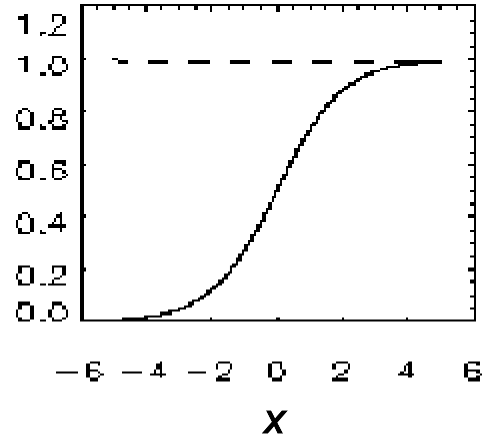
$$\begin{cases} y_q = a_{q0} + \sum_{j=1}^{k} a_{qj} \cdot t_j = a_{q0} + \sum_{j=1}^{k} a_{qj} \cdot \phi(b_{j0} + \sum_{i=1}^{n} b_{ji} \cdot x_i) = \\ = a_{q0} + \sum_{j=1}^{k} a_{qj} \cdot \tanh(b_{j0} + \sum_{i=1}^{n} b_{ji} \cdot x_i); \quad q = 1,2,\ldots,m \end{cases}$$

# Some Popular Activation Functions

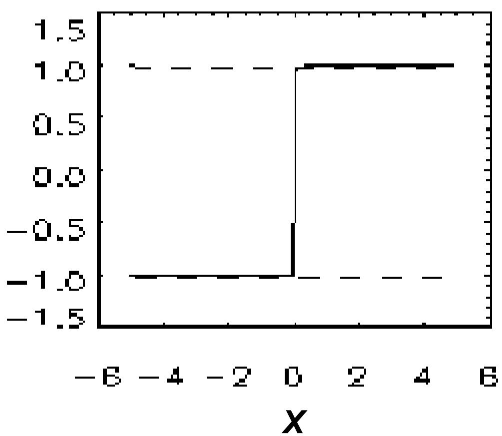
*tanh(x)*



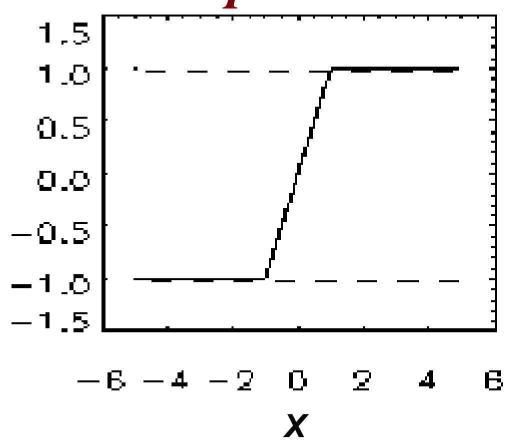

*Sigmoid, $(1 + exp(-x))^{-1}$*




*Hard Limiter*




*Ramp Function*



# NN as a Universal Tool for Approximation of Continuous & Almost Continuous Mappings

## Some Basic Theorems:

- **Any function or mapping *Z = F (X)*, continuous on a compact subset, *can be approximately represented by* a p (p ≥ 3) layer *NN in the sense of uniform convergence* (e.g., Chen & Chen, 1995; Blum and Li, 1991, Hornik, 1991; Funahashi, 1989, etc.)**

- **The error bounds for the uniform approximation on compact sets (Attali & Pagès, 1997):**

$$||Z - Y|| = ||F(X) - F_{NN}(X)|| \sim C/k$$

***k*** **-number of neurons in the hidden layer**
***C*** **– does not depend on *n* (avoiding *Curse of Dimensionality!*)**

# NN training (1)

- For the mapping $Z = F(X)$ create a ***training set*** - set of matchups $\{X_i, Z_i\}_{i=1,\dots,N}$, where $X_i$ is ***input vector*** and $Z_i$ - ***desired output vector***
- Introduce ***an error or cost function E***:

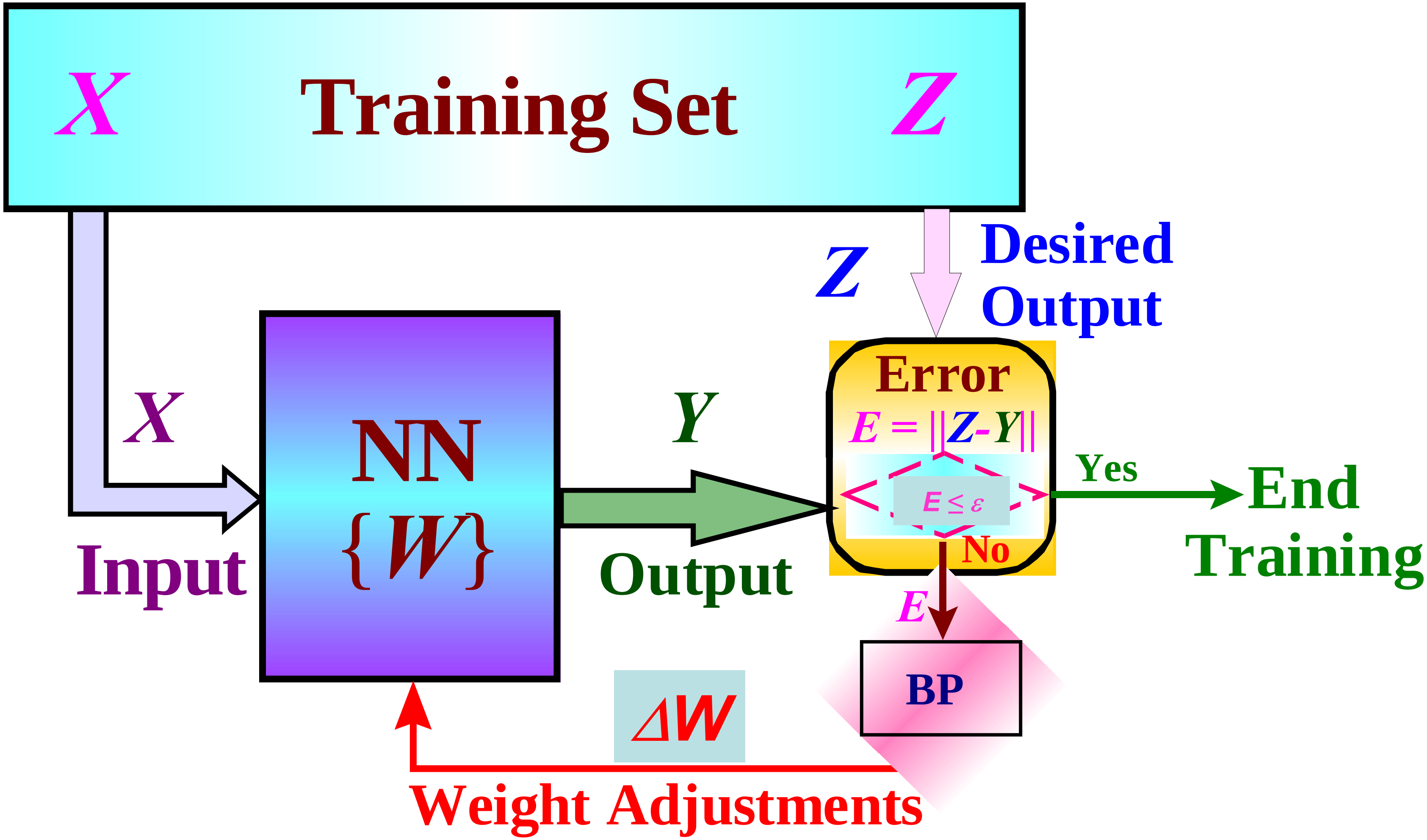
$$E(a,b) = ||Z - Y|| = \sum_{i=1}^{N} \left| Z_i - F_{NN}(X_i) \right|^2 ,$$

where $Y = F_{NN}(X)$ is neural network

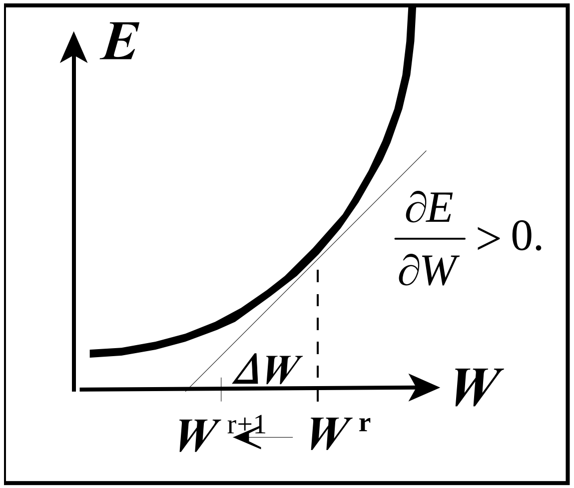
- Minimize the cost function: $min\{E(a,b)\}$ and find optimal weights $(a_0, b_0)$
- Notation: $W = \{a, b\}$ - all weights.

# NN Training (2)

## One Training Iteration



# Backpropagation (BP) Training Algorithm




- **BP is a simplified steepest descent:**

$$\Delta W = -\eta \frac{\partial E}{\partial W}$$

**where *W* - any weight, *E* - error function,**

**$\eta$ - learning rate, and $\Delta W$ - weight increment**

- **Derivative can be calculated analytically:**

$$\frac{\partial E}{\partial W} = -2\sum_{i=1}^{N}[Z_i - F_{NN}(X_i)] \cdot \frac{\partial F_{NN}(X_i)}{\partial W}$$

- **Weight adjustment after r-th iteration:**

$$W^{r+1} = W^{r} + \Delta W$$

- **BP training algorithm is robust but slow**

# Generic Neural Network

## FORTRAN Code:

```
DATA W1/.../, W2/.../, B1/.../, B2/.../, A/.../, B/.../ !  Task specific part
!===================================================================
DO K = 1,OUT
!
    DO I = 1, HID
        X1(I) = tanh(sum(X * W1(:,I) + B1(I))
    ENDDO !  I
!
    X2(K) = tanh(sum(W2(:,K)*X1) + B2(K))
    Y(K) = A(K) * X2(K) + B(K)
! ---
    XY = A(K) * (1. -X2(K) * X2(K))
    DO J = 1, IN
        DUM = sum((1. -X1 * X1) * W1(J,:) * W2(:,K))
        DYDX(K,J) = DUM * XY
    ENDDO !  J
!
ENDDO !  K
```

NN Output

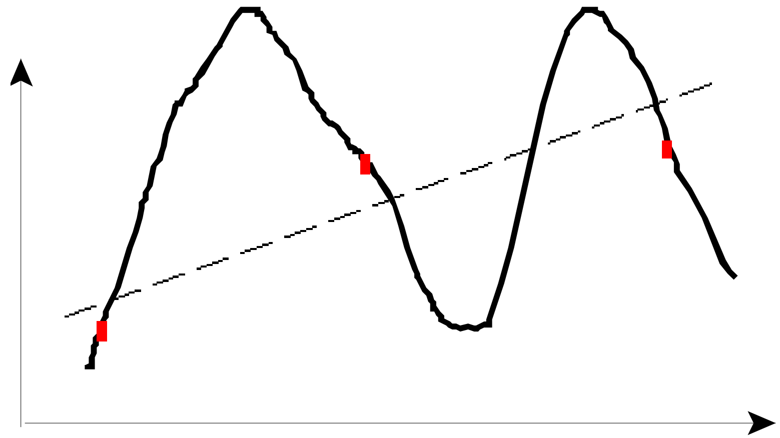
Jacobian

# Major Advantages of NNs :

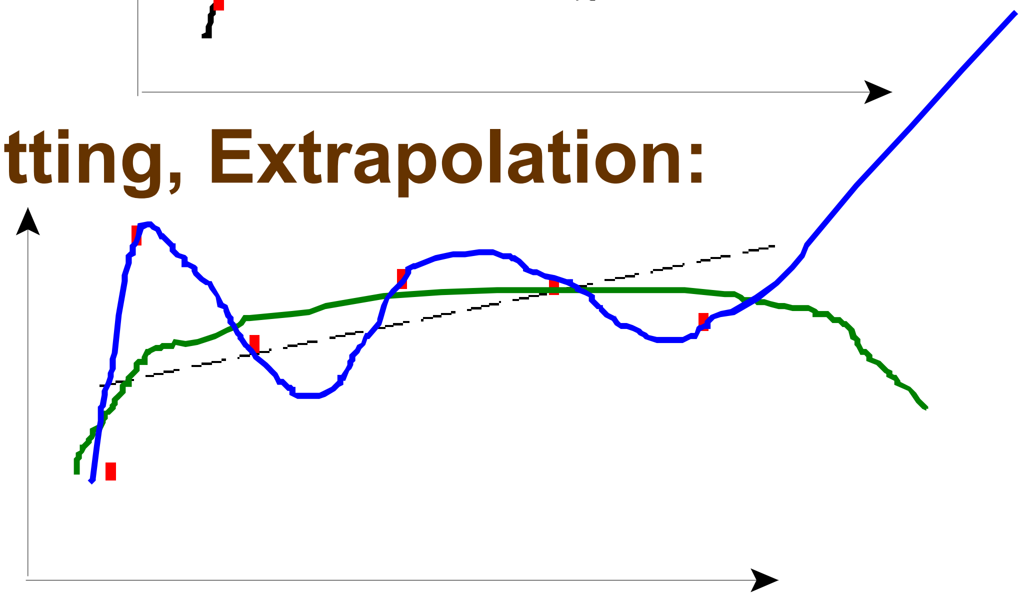
- **NNs are very *generic, accurate and convenient* mathematical (statistical) models which are able to emulate numerical model components, which are complicated nonlinear input/output relationships (continuous or almost continuous mappings ).**
- **NNs avoid *Curse of Dimensionality***
- **NNs are** *robust* **with respect to random noise and fault-tolerant.**
- **NNs are *analytically differentiable* (training, error and sensitivity analyses): almost free Jacobian!**
- **NNs emulations are** accurate and fast but NO FREE LUNCH!
- **Training is complicated and time consuming nonlinear optimization task; *however, training should be done only once for a particular application!***
- **Possibility of online adjustment**
- **NNs are well-suited for parallel and vector processing**

# NNs & Nonlinear Regressions: Limitations (1)

- **Flexibility and Interpolation:**



- **Overfitting, Extrapolation:**

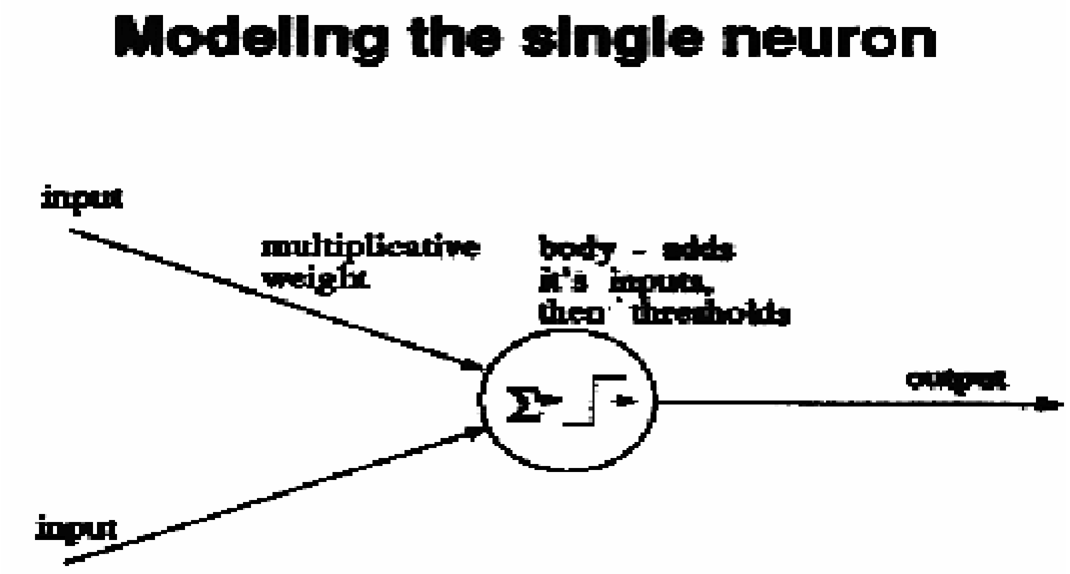


# NNs & Nonlinear Regressions: Limitations (2)

- **Consistency** of estimators: $\alpha$ is a **consistent estimator** of parameter $A$, if $\alpha \rightarrow A$ as the size of the **sample** $n \rightarrow N$, where $N$ is the size of the **population**.
- For **NNs** and **Nonlinear Regressions** **consistency** can be usually "proven" only **numerically**.
- Additional **independent** data sets are required for test (demonstrating **consistency** of estimates).

# ARTIFICIAL NEURAL NETWORKS:
## BRIEF HISTORY

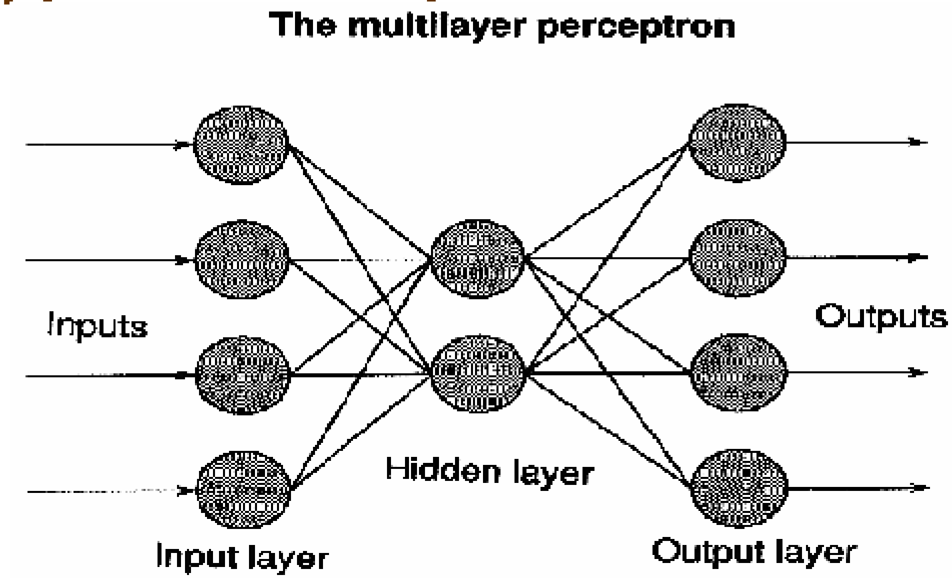
- **1943 - McCulloch and Pitts introduced a model of the neuron**




- **1962 - Rosenblat introduced the one layer "perceptrons", the model neurons, connected up in a simple fashion.**
- **1969 - Minsky and Papert published the book which practically "closed the field"**

# ARTIFICIAL NEURAL NETWORKS:
## BRIEF HISTORY

- **1986 - Rumelhart and McClelland proposed the "multilayer perceptron" (MLP) and showed that it is a perfect application for parallel distributed processing.**




- **From the end of the 80's there has been explosive growth in applying NNs to various problems in different fields of science and technology**

# Atmospheric and Oceanic NN Applications

- **Satellite Meteorology and Oceanography**
  - Classification Algorithms
  - Pattern Recognition, Feature Extraction Algorithms
  - Change Detection & Feature Tracking Algorithms
  - Fast Forward Models for Direct Assimilation
  - Accurate Transfer Functions (Retrieval Algorithms)
- **Predictions**
  - Geophysical time series
  - Regional climate
  - Time dependent processes
- **Accelerating and Inverting Blocks in Numerical Models**
- **Data Fusion & Data Mining**
- **Interpolation, Extrapolation & Downscaling**
- **Nonlinear Multivariate Statistical Analysis**
- **Hydrological Applications**

# Developing Fast NN Emulations for Parameterizations of Model Physics

**Atmospheric Long & Short Wave Radiations**

# General Circulation Model

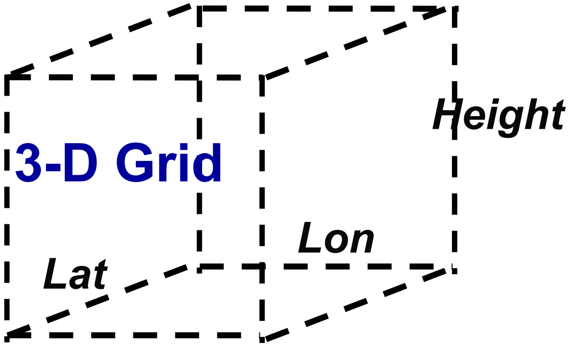
***The set of conservation laws (mass, energy, momentum, water vapor, ozone, etc.)***

- ***First Priciples/Prediction 3-D Equations on the Sphere:***

$$\frac{\partial \psi}{\partial t} + D(\psi, x) = P(\psi, x)$$

  - **$\psi$ - a 3-D prognostic/dependent variable, e.g., temperature**
  - ***x* - a 3-D independent variable: *x, y, z* & *t***
  - ***D* - dynamics (spectral or gridpoint)**
  - ***P* - physics or parameterization of physical processes (1-D vertical r.h.s. forcing)**

- ***Continuity Equation***
- ***Thermodynamic Equation***
- ***Momentum Equations***



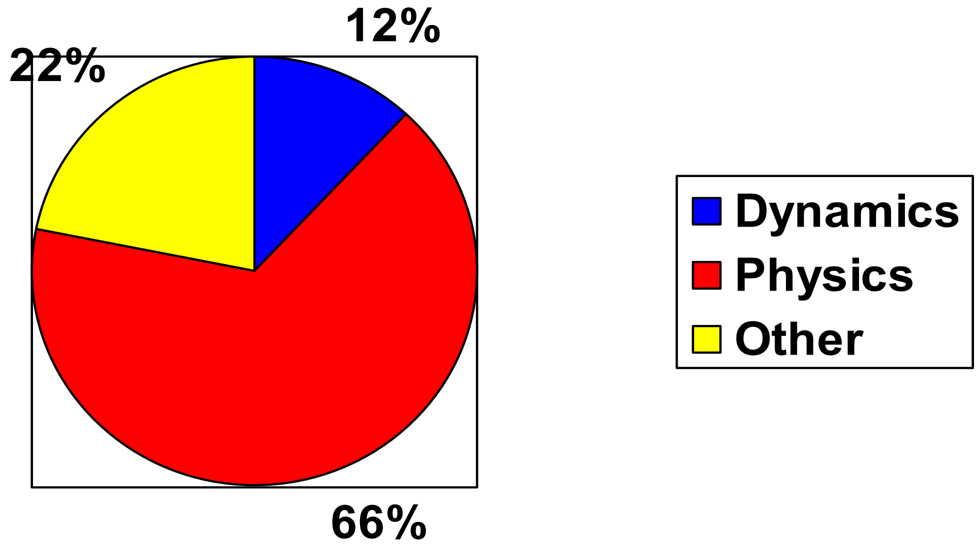
# General Circulation Model

***Physics – P, represented by 1-D (vertical) parameterizations***

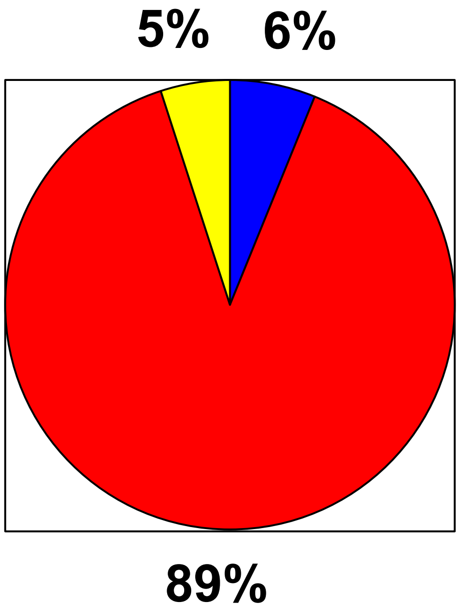
- **Major components of *P* = {*R, W, C, T, S*}:**
  - ***R* - radiation (long & short wave processes)**
  - ***W* – convection, and large scale precipitation processes**
  - **C - clouds**
  - ***T* – turbulence**
  - ***S* – surface model (land, ocean, ice – air interaction)**
- **Each component of *P* is a 1-D parameterization of complicated set of multi-scale theoretical and empirical physical process models *simplified for computational reasons***
- **P is the *most time consuming* part of GCMs*!***

# Distribution of Total Climate Model Calculation Time

Current NCAR Climate Model (T42 x L26): ~ 3° x 3.5°

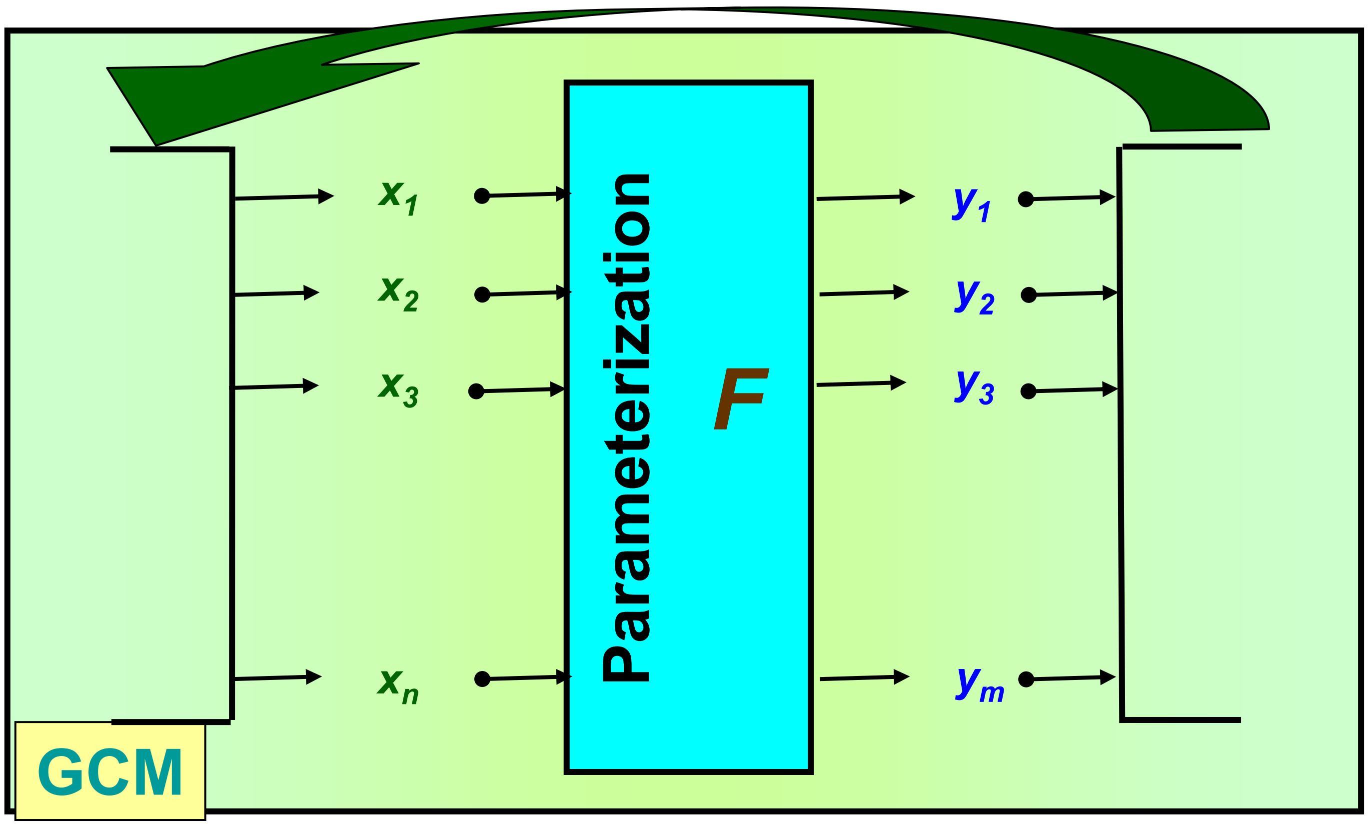



Near-Term Upcoming Climate Models (estimated) : ~ 1° x 1°



# Generic Problem in Numerical Models

## Parameterizations of Physics are Mappings

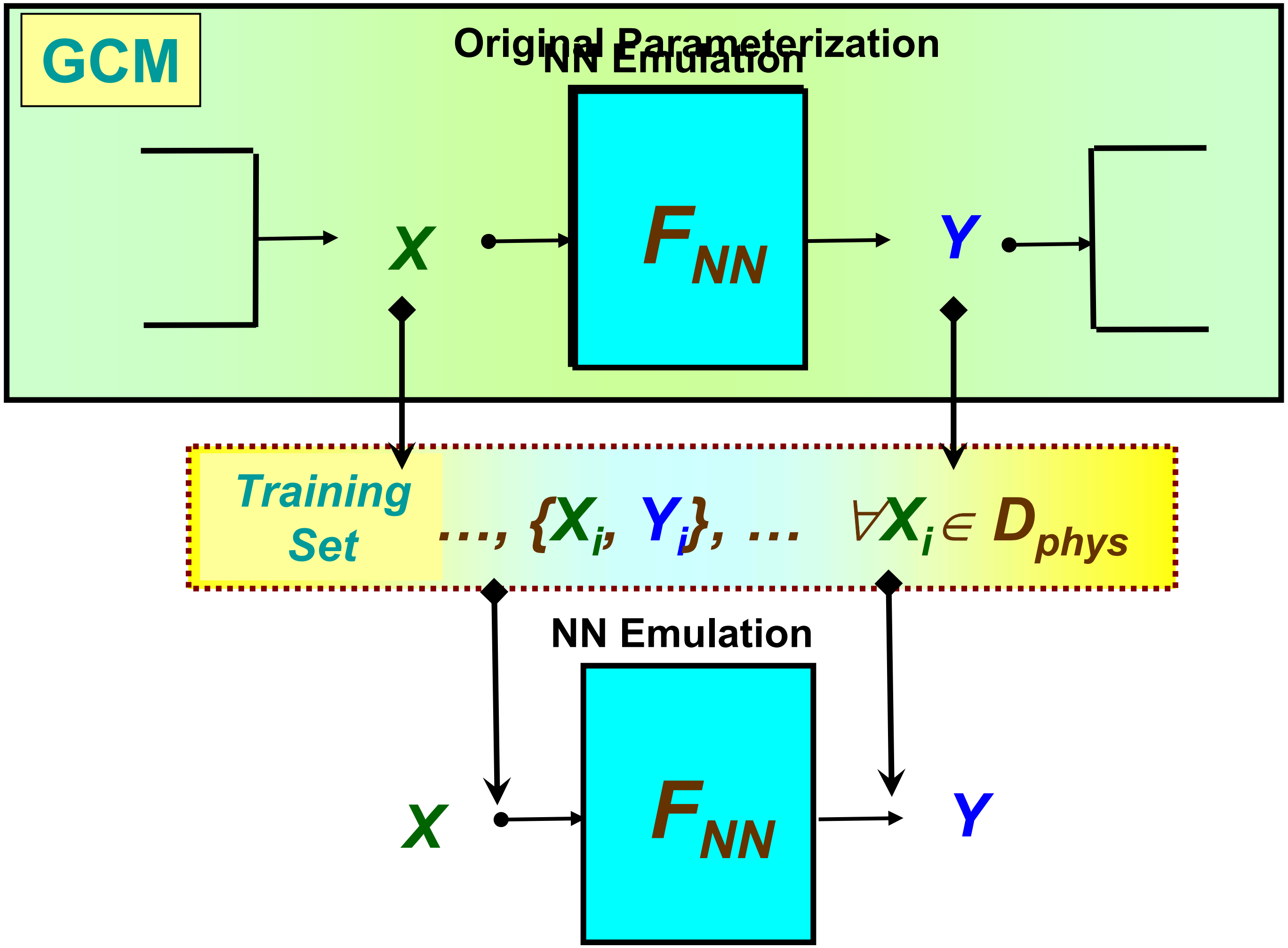



$$Y=F(X)$$

# Generic Solution – “NeuroPhysics”

## Accurate and Fast NN Emulation for Physics Parameterizations

*Learning from Data*



# NN for NCAR CAM Physics

## *CAM Long Wave Radiation*

- **Long Wave Radiative Transfer:**

$$F^{\downarrow}(p) = B(p_t)\cdot\varepsilon(p_t, p) + \int_{p_t}^{p} \alpha(p_t, p)\cdot dB(p')$$

$$F^{\uparrow}(p) = B(p_s) - \int_{p}^{p_s} \alpha(p, p')\cdot dB(p')$$

$$B(p) = \sigma\cdot T^4(p) \quad - \textit{the Stefan} - \textit{Boltzman relation}$$

- **Absorptivity & Emissivity (optical properties):**

$$\alpha(p, p') = \frac{\int_0^\infty \{dB_\nu(p')/dT(p')\}\cdot(1-\tau_\nu(p, p'))\cdot d\nu}{dB(p)/dT(p)}$$

$$\varepsilon(p_t, p) = \frac{\int_0^\infty B_\nu(p_t)\cdot(1-\tau_\nu(p_t, p))\cdot d\nu}{B(p_t)}$$

$$B_\nu(p) \quad - \textit{the Plank function}$$

# Magic of NN performance


$Y = F(X)$


$Y_{NN} = F_{NN}(X)$

- OP Numerical Performance is Determined by:
  - Numerical complexity (NC) of OP
    - Complexity of OP Mathematics
      - Complexity of Physical Processes

- NN Emulation Numerical Performance is Determined by:
  - NC of NN emulation
    - Functional Complexity (FC) of OP, i.e. Complexity of I/O Relationship: $Y = F(X)$

- <u>Explanation of Magic of NN Performance:</u>
  - Usually, FC of OP << NC of OP

    AS A RESULT
  - NC of NN Emulation ~ FC of OP

    and

    NC of NN Emulation << NC of OP

# Neural Network for NCAR LW Radiation

## NN characteristics

- **220 Inputs:**
  - ***10 Profiles:*** temperature; humidity; ozone, methane, cfc11, cfc12, & $N_2O$ mixing ratios, pressure, cloudiness, emissivity
  - ***Relevant surface characteristics*:** surface pressure, upward LW flux on a surface - *flwupcgs*
- **33 Outputs:**
  - Profile of heating rates (26)
  - 7 LW radiation fluxes: *flns, flnt, flut, flnsc, flntc, flutc, flwds*
- **Hidden Layer: One layer with 50 to 300 neurons**
- **Training: *nonlinear optimization in the space with dimensionality of 15,000 to 100,000***
  - Training Data Set: Subset of about 200,000 instantaneous profiles simulated by CAM for the 1-st year
  - Training time: about 2 to 40 days (SGI workstation)
  - Training iterations: 1,500 to 8,000
- **Validation on Independent Data:**
  - Validation Data Set (independent data): about 200,000 instantaneous profiles simulated by CAM for the 2-nd year

# Neural Network for NCAR SW Radiation

## NN characteristics

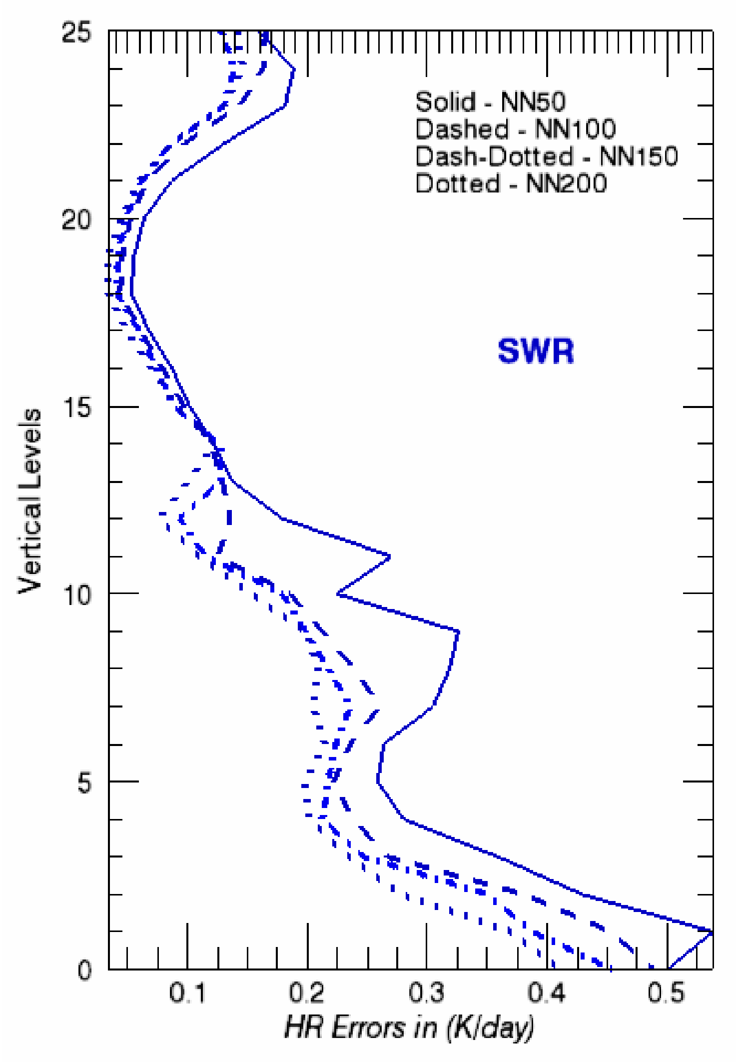
- **451 Inputs:**
  - ***21 Profiles:*** specific humidity, ozone concentration, pressure, cloudiness, aerosol mass mixing ratios, etc
  - ***7 Relevant surface characteristics***
- **33 Outputs:**
  - Profile of heating rates (26)
  - 7 LW radiation fluxes: *fsns, fsnt, fsdc, sols, soll, solsd, solld*
- **Hidden Layer: One layer with 50 to 200 neurons**
- **Training: *nonlinear optimization in the space with dimensionality of 25,000 to 130,000***
  - Training Data Set: Subset of about 100,000 instantaneous profiles simulated by CAM for the 1-st year
  - Training time: about 2 to 40 days (SGI workstation)
  - Training iterations: 1,500 to 8,000
- **Validation on Independent Data:**
  - Validation Data Set (independent data): about 100,000 instantaneous profiles simulated by CAM for the 2-nd year

# NN Approximation Accuracy and Performance vs. Original Parameterization

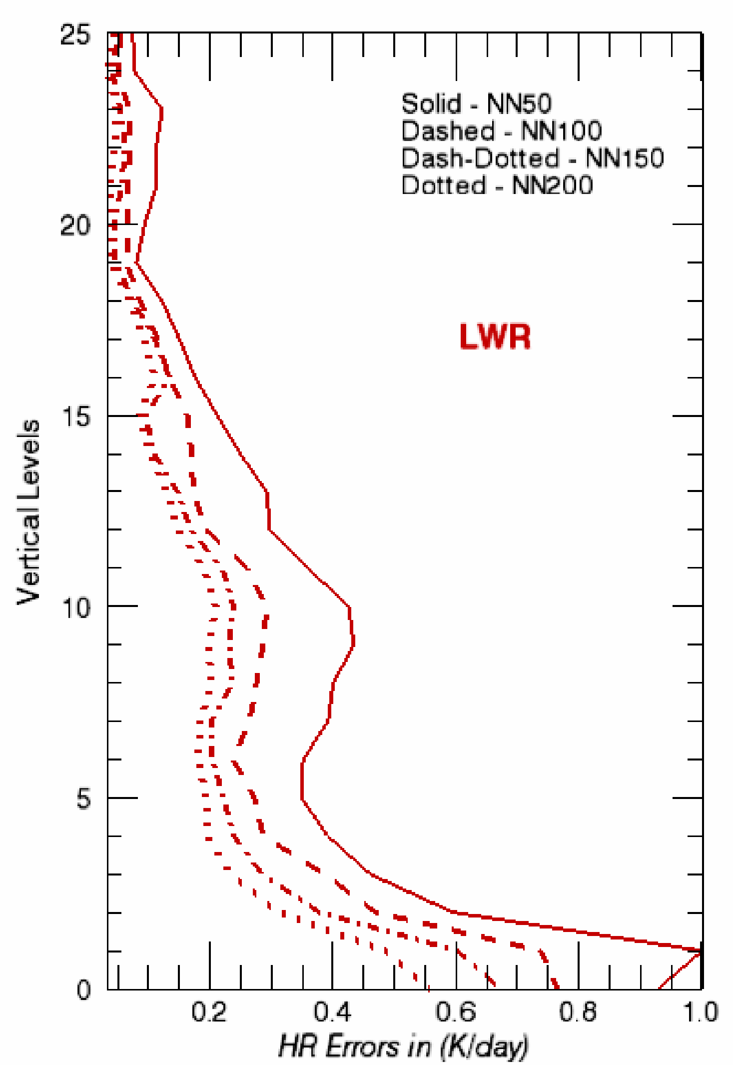
| Parameter | Model | Bias | RMSE | Mean | $\sigma$ | Performance |
|---|---|---|---|---|---|---|
| **LWR** (°*K/day*) **NN150** | NASA | $1.\ 10^{-4}$ | 0.32 | 1.52 | 1.46 | |
| | NCAR | $3.\ 10^{-5}$ | 0.28 | -1.40 | 1.98 | ~ 150 times faster |
| **SWR** (°*K/day*) **NN150** | NCAR | $6.\ 10^{-4}$ | 0.19 | 1.47 | 1.89 | ~ 20 times faster |

# Error Vertical Variability Profiles

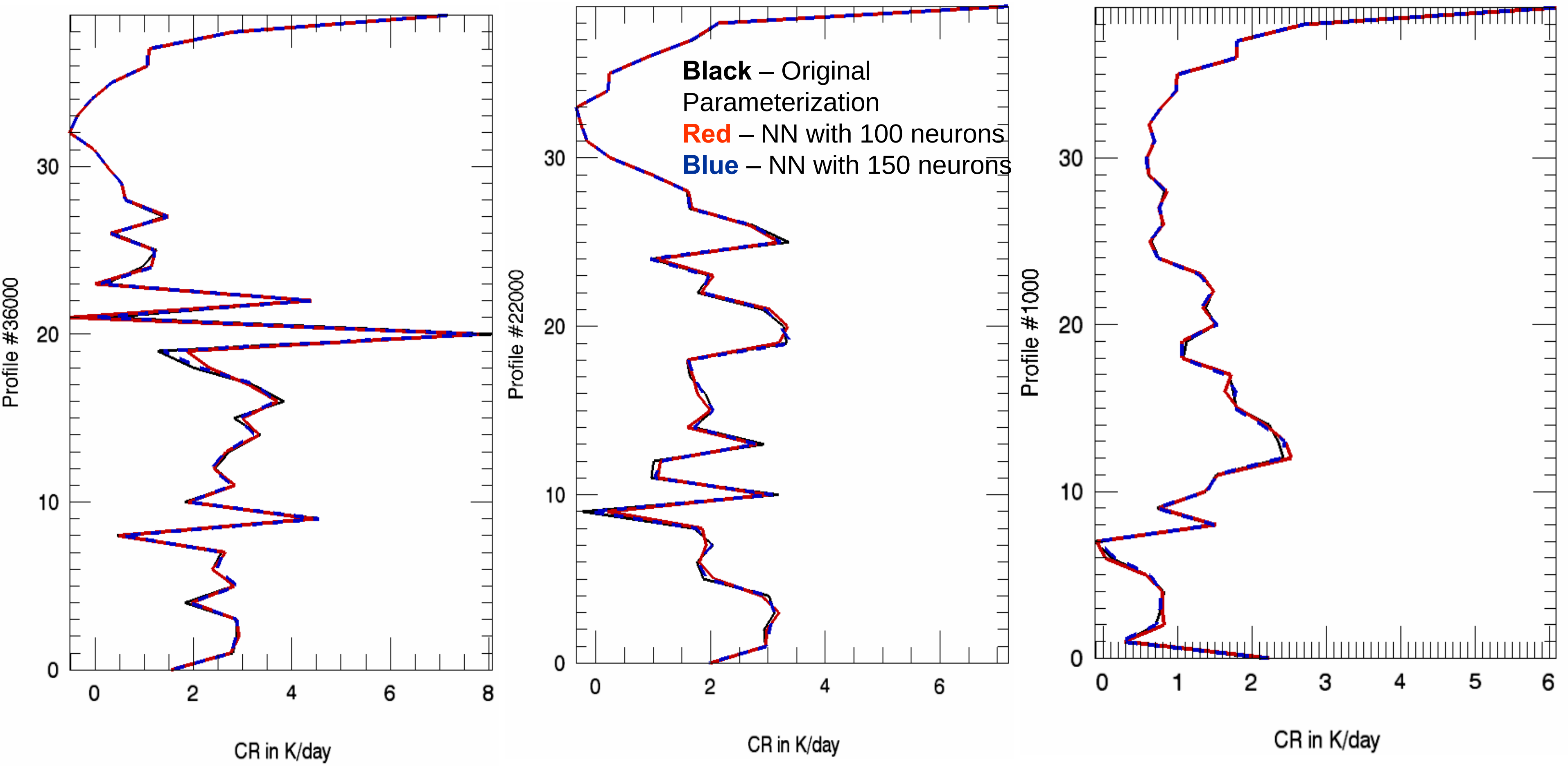
## RMSE profiles in K/day




## RMSE Profiles in K/day



# Individual Profiles



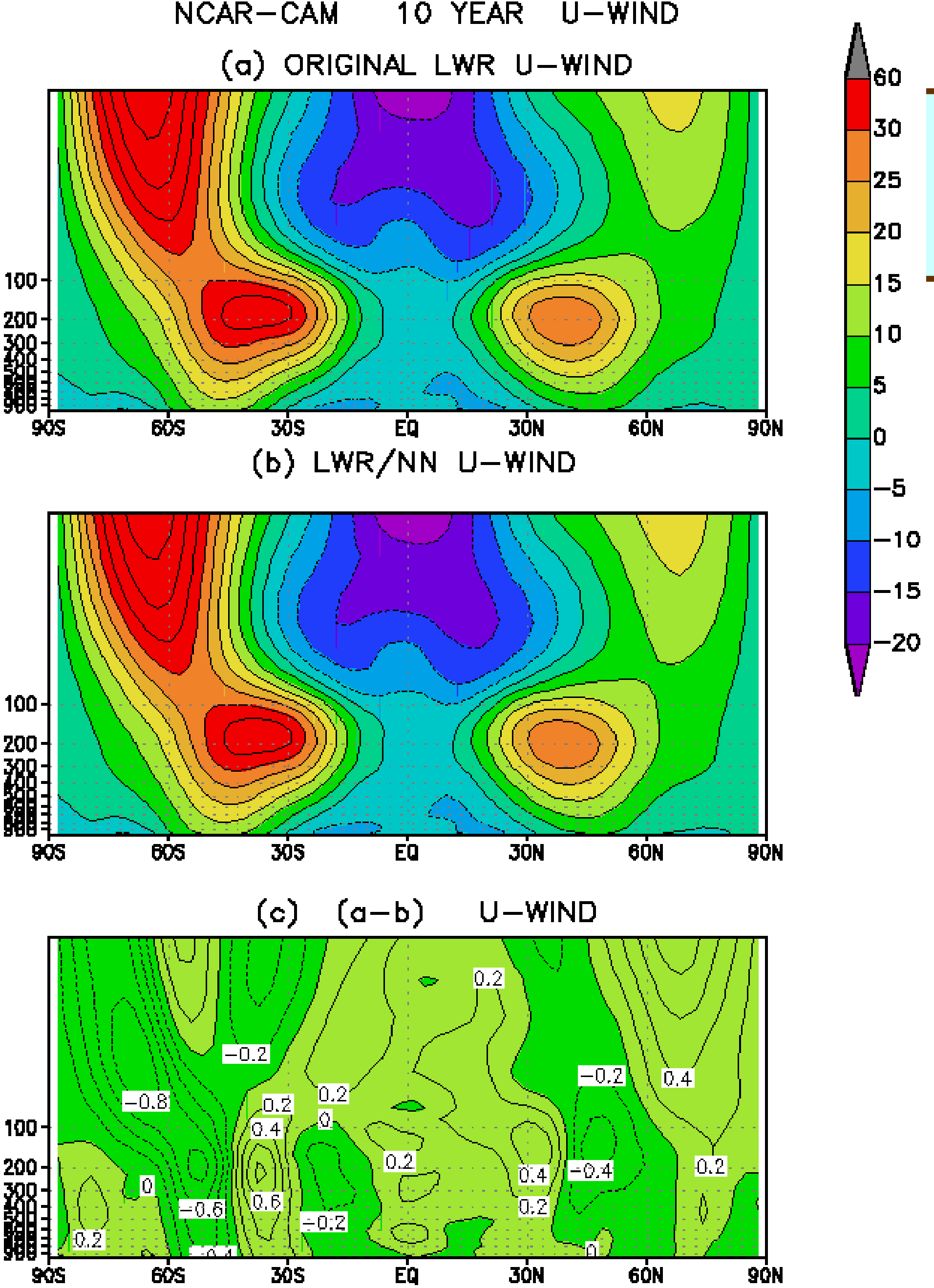

**PRMSE = 0.18 & 0.10 K/day** **PRMSE = 0.11 & 0.06 K/day** **PRMSE = 0.05 & 0.04 K/day**

# NCAR CAM-2: 10 YEAR EXPERIMENTS

- **CONTROL: the standard NCAR CAM version (available from the CCSM web site) with the original Long-Wave Radiation (LWR) (e.g. Collins, JAS, v. 58, pp. 3224-3242, 2001)**
- **LWR/NN: the hybrid version of NCAR CAM with NN emulation of the LWR (Krasnopolsky, Fox-Rabinovitz, and Chalikov, 2005, *Monthly Weather Review*, *133*, 1370-1383)**

# PRESERVATION of *Global Annual Means*

| Parameter | Original LWR Parameterization | NN Approximation | Difference in % |
|---|---|---|---|
| Mean Sea Level Pressure (*hPa*) | 1011.480 | 1011.481 | 0.0001 |
| Surface Temperature (*°K*) | 289.003 | 289.001 | 0.0007 |
| Total Precipitation (*mm/day*) | 2.275 | 2.273 | 0.09 |
| Total Cloudiness (*fractions 0.1 to 1.*) | 0.607 | 0.609 | 0.3 |
| LWR Heating Rates (*°K/day*) | -1.698 | -1.700 | 0.1 |
| Outgoing LWR – OLR (*W/m²*) | 234.4 | 234.6 | 0.08 |
| Latent Heat Flux (*W/m²*) | 82.84 | 82.82 | 0.03 |



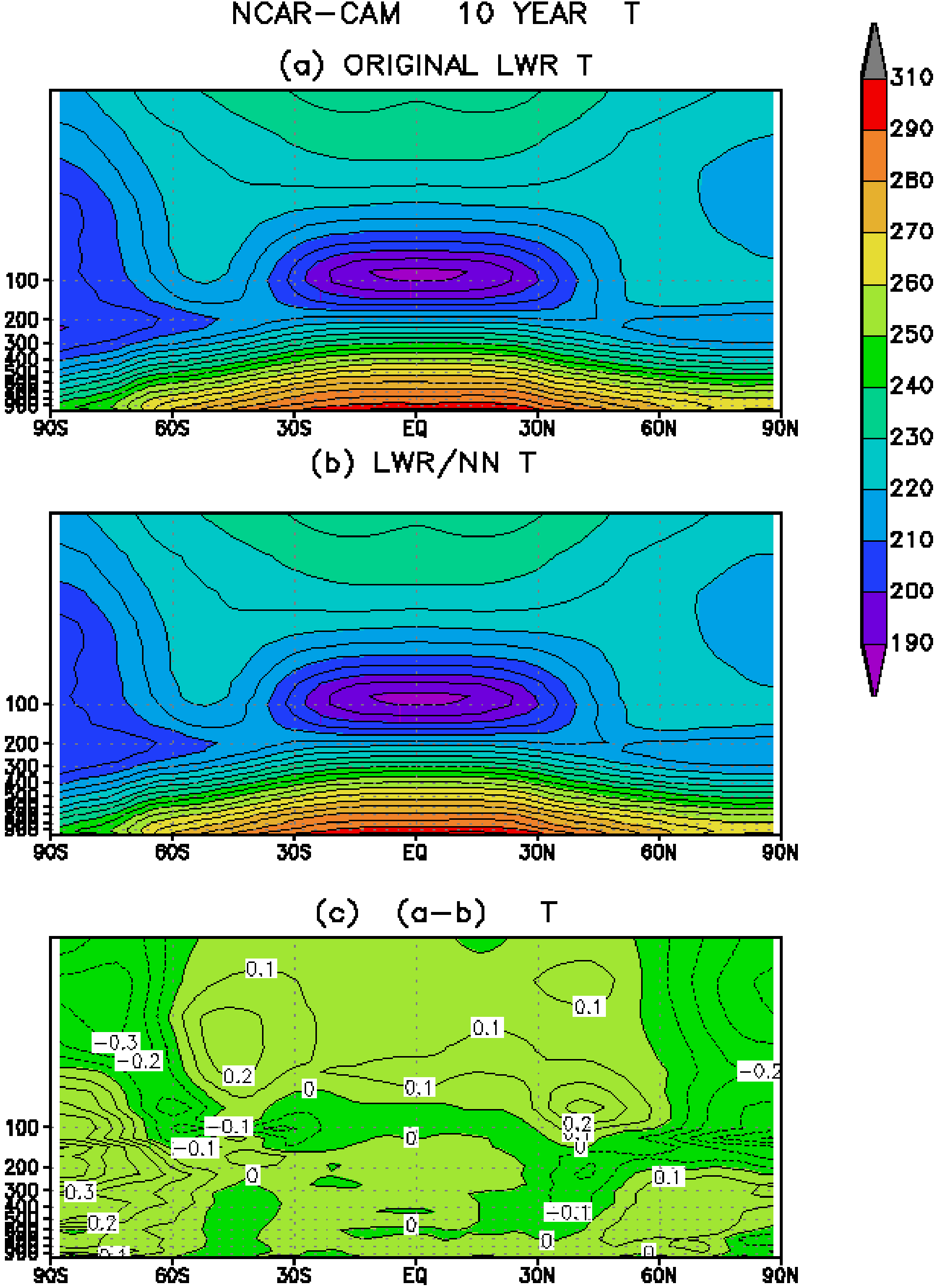

# NCAR CAM-2 Zonal Mean U 10 Year Average

(a)– Original LWR Parameterization

(b)- NN Approximation

(c)- Difference (a) – (b), contour 0.2 *m/sec*

all in *m/sec*



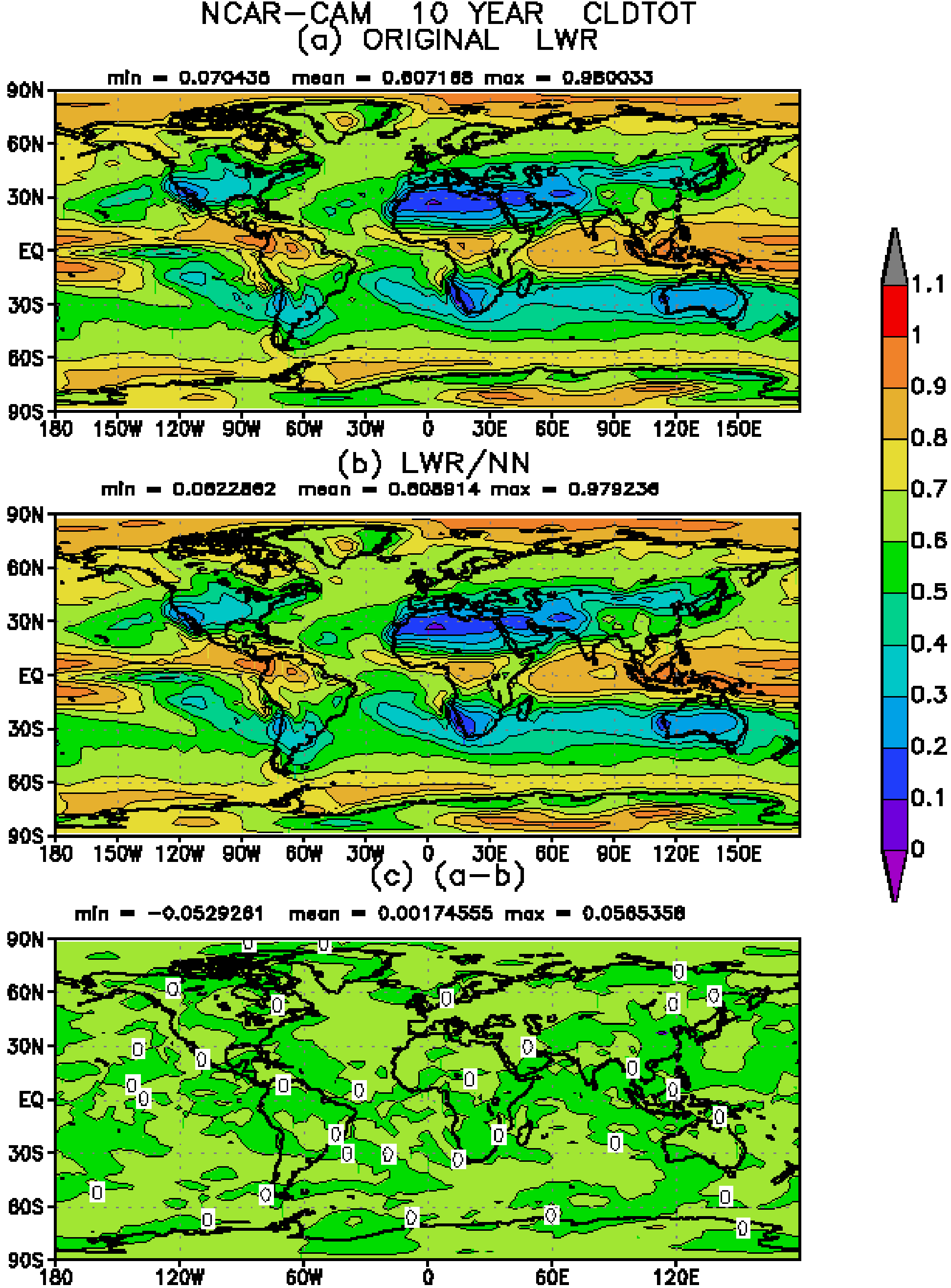

# NCAR CAM-2 Zonal Mean Temperature 10 Year Average

(a)– Original LWR Parameterization

(b)- NN Approximation

(c)- Difference (a) – (b), contour 0.1 °K

all in °K




# NCAR CAM-2 Total Cloudiness 10 Year Average

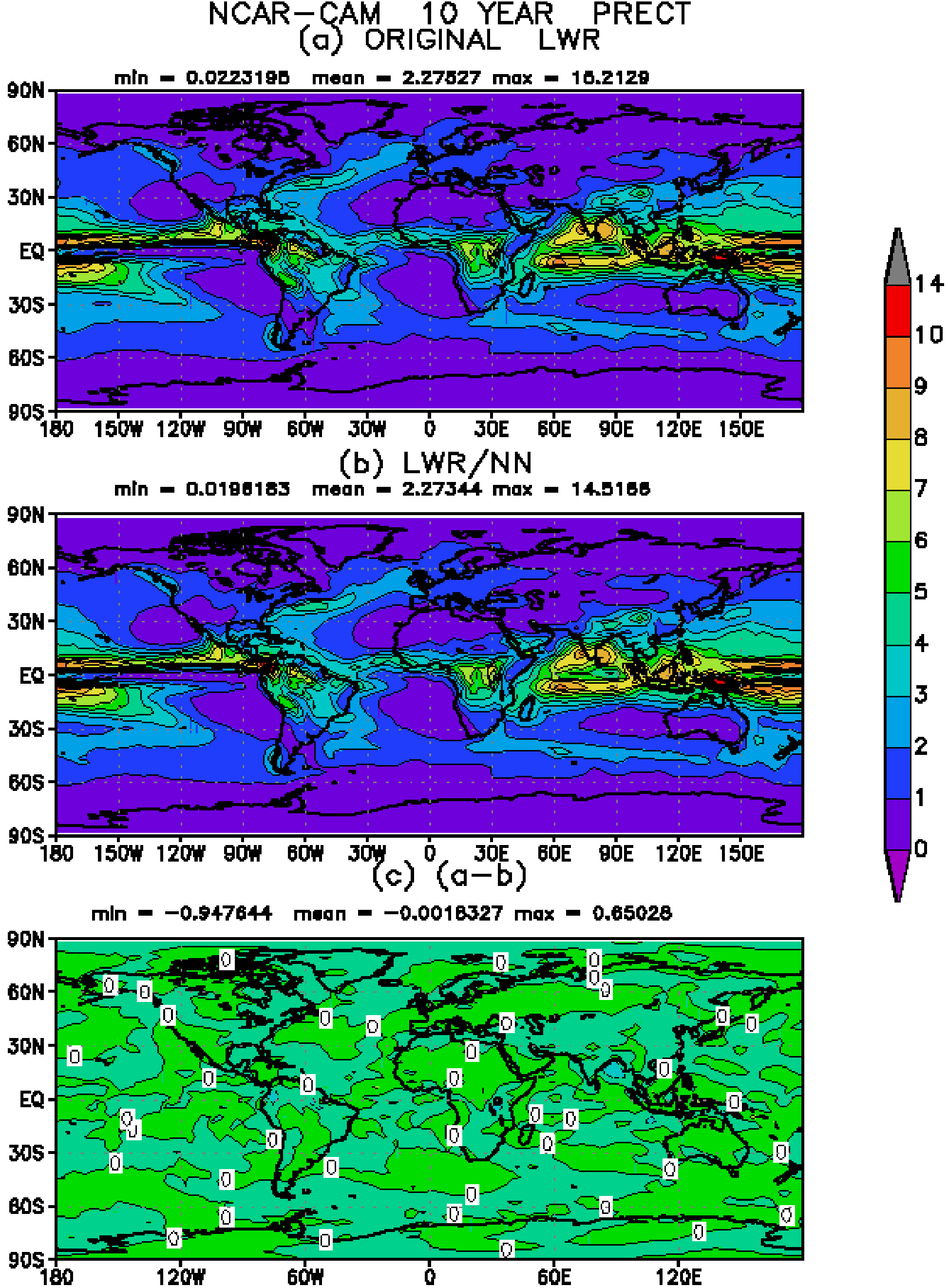
(a)– Original LWR Parameterization

(b)- NN Approximation

(c)- Difference (a) – (b),

all *in fractions*

| | Mean | Min | Max |
|---|---|---|---|
| (a) | 0.607 | 0.07 | 0.98 |
| (b) | 0.608 | 0.06 | 0.98 |
| (c) | 0.002 | -0.05 | 0.05 |




# NCAR CAM-2 Total Precipitation 10 Year Average

(a)– Original LWR Parameterization

(b)- NN Approximation

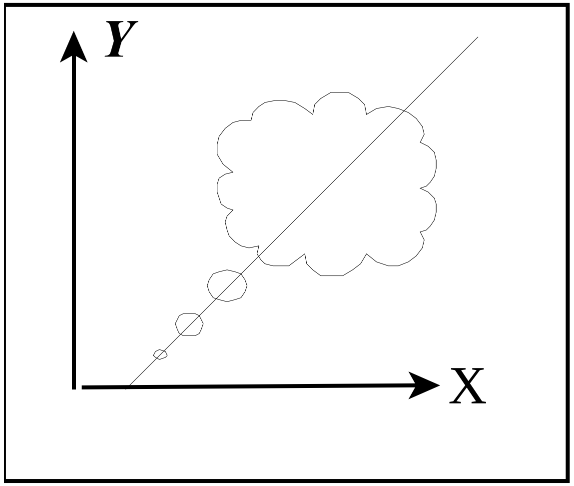
(c)- Difference (a) – (b), all in *mm/day*

| | Mean | Min | Max |
|---|---|---|---|
| (a) | 2.275 | 0.02 | 15.21 |
| (b) | 2.273 | 0.02 | 14.52 |
| (c) | 0.002 | 0.94 | 0.65 |

# How to Develop NNs:
## An Outline of the Approach (1)

- **Problem Analysis:**
  - Are traditional approaches unable to solve your problem?
    - At all
    - With desired accuracy
    - With desired speed, etc.
  - Are NNs well-suited for solving your problem?
    - Nonlinear mapping
    - Classification
    - Clusterization, etc.
  - Do you have a first guess for NN architecture?
    - Number of inputs and outputs
    - Number of hidden neurons

# How to Develop NNs:
## An Outline of the Approach (2)




- **Data Analysis**
  - **How noisy are your data?**
    - **May change architecture or even technique**
  - **Do you have enough data?**
  - **For selected architecture:**
    - **1) Statistics => $N^1_A > n_W$**
    - **2) Geometry => $N^2_A > 2^n$**
    - **$N^1_A < N_A < N^2_A$**
    - **To represent all possible patterns => $N_R$**
      **$N_{TR} = \max(N_A, N_R)$**
  - **Add for test set: $N = N_{TR} \times (1 + \tau)$; $\tau > 0.5$**
  - **Add for validation: $N = N_{TR} \times (1 + \tau + \nu)$; $\nu > 0.5$**

# How to Develop NNs:
## An Outline of the Approach (3)

- **Training**
  - **Try different initializations**
  - **If results are not satisfactory, then goto Data Analysis or Problem Analysis**
- **Validation (must for any nonlinear tool!)**
  - **Apply trained NN to independent validation data**
  - **If statistics are not consistent with those for training and test sets, go back to Training or Data Analysis**

# Conclusions

- **There is an obvious trend in scientific studies:**
  - **From simple, linear, single-disciplinary, low dimensional systems**
  - **To complex, nonlinear, multi-disciplinary, high dimensional systems**
- **There is a corresponding trend in math & statistical tools:**
  - **From simple, linear, single-disciplinary, low dimensional tools and models**
  - **To complex, nonlinear, multi-disciplinary, high dimensional tools and models**
- **Complex, nonlinear tools have advantages & limitations: learn how to use advantages & avoid limitations!**
- **Check your toolbox and follow the trend, otherwise you may miss the train!**

# Recommended Reading

- **Regression Models:**
  - **B. Ostle and L.C. Malone, "Statistics in Research", 1988**
- **NNs, Introduction:**
  - **R. Beale and T. Jackson, "Neural Computing: An Introduction", 240 pp., Adam Hilger, Bristol, Philadelphia and New York., 1990**
- **NNs, Advanced:**
  - **Bishop, C.M. (1995), *Neural Networks for Pattern Recognition*, 482 pp., Oxford University Press, Oxford, U.K.**
  - **Haykin, S. (1994), *Neural Networks: A Comprehensive Foundation*, 696 pp., Macmillan College Publishing Company, New York, U.S.A.**
  - **Ripley, B.D. (1996), *Pattern Recognition and Neural Networks*, 403 pp., Cambridge University Press, Cambridge, U.K.**
  - **Vapnik, V.N., and S. Kotz (2006), *Estimation of Dependences Based on Empirical Data (Information Science and Statistics)*, 495 pp., Springer, New York.**
- **NNs and Statistics:**
  - **B. Cheng and D.M. Titterington, "Neural Networks: A Review from a Statistical Perspective", 1994**

# Share with your Colleagues!