

Levenberg-Marquardt learning

- Multi-layer neural networks
- MLP (Multilayer Perceptrons)
- RBF (Radial Basis Functions)

Taylor expansion

$$E(\theta + \Delta\theta)$$

$$\approx E(\theta) + E'(\theta) \Delta\theta$$

$$E(\theta + \Delta\theta)$$

$$= E(\theta) + E'(\theta) \Delta\theta +$$

$$\frac{1}{2} \Delta\theta^T E''(\theta) \Delta\theta$$

Function Approximation

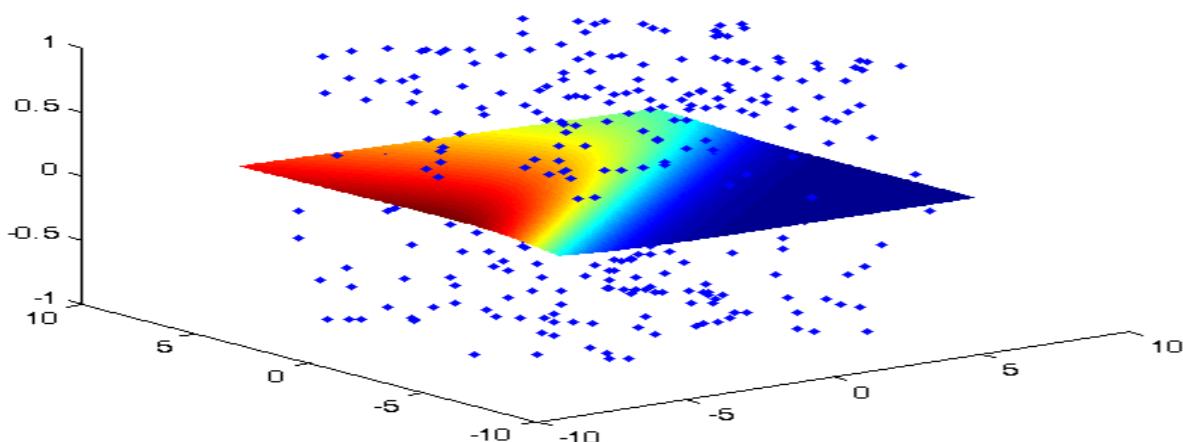
- High-dimensional nonlinear function approximation
- Linear combination of basis functions
 - Projective basis function
 - Radial basis function

Function approximation

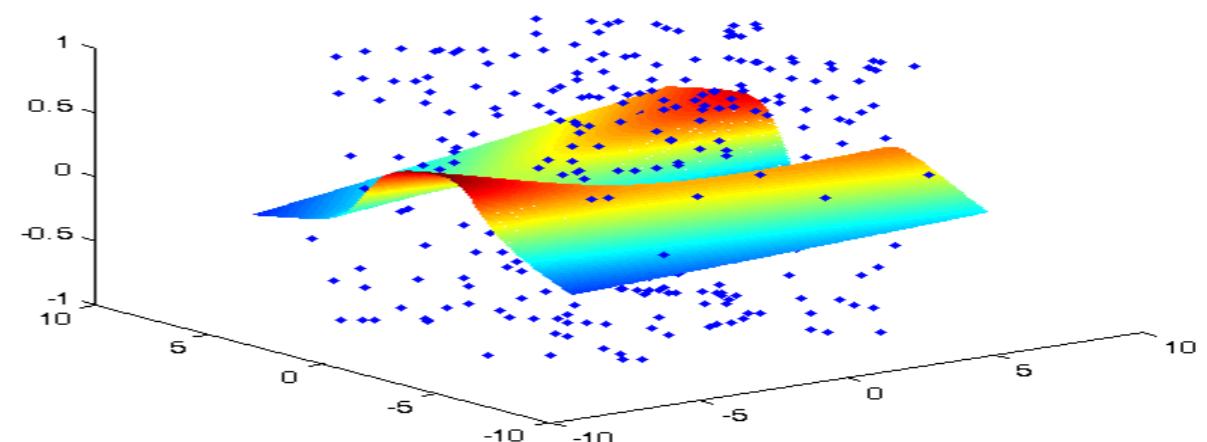
- Data oriented function approximation
- Paired data sampled from an unknown target function : $\mathbb{R}^d \rightarrow \mathbb{R}$
 $(\mathbf{x}[t], y[t]), t=1, \dots, N$

Desired target (output)
Predictor (input)

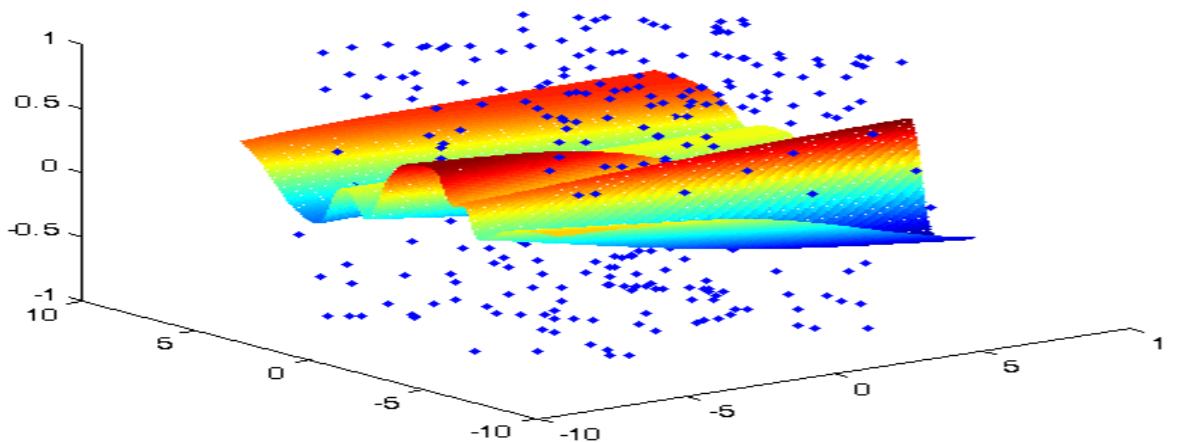
NRBF(3) by annealed FE



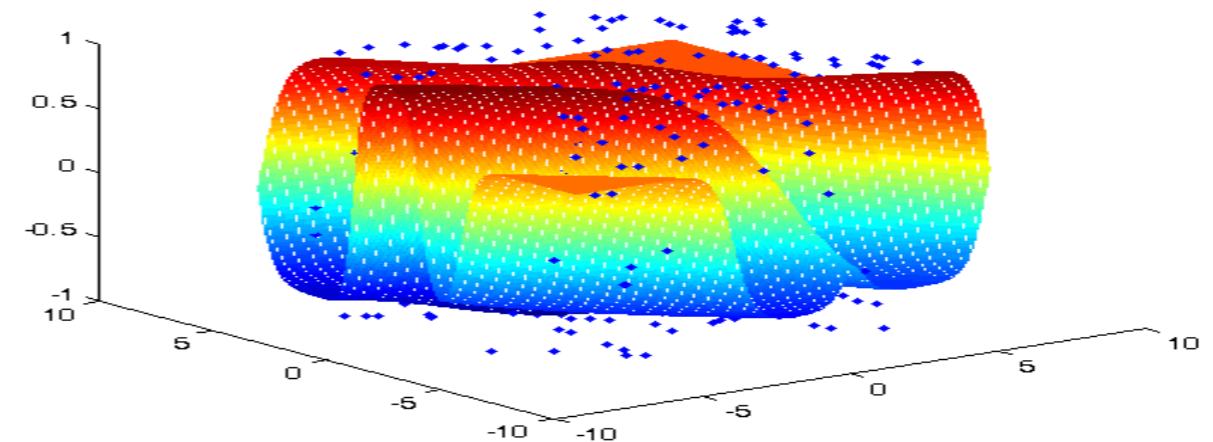
NRBF(6) by annealed FE



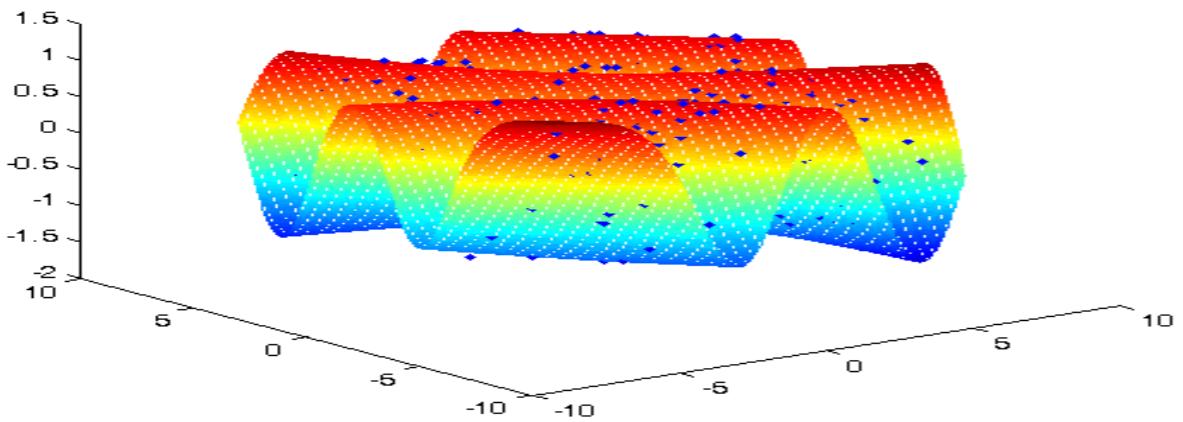
NRBF(9) by annealed FE



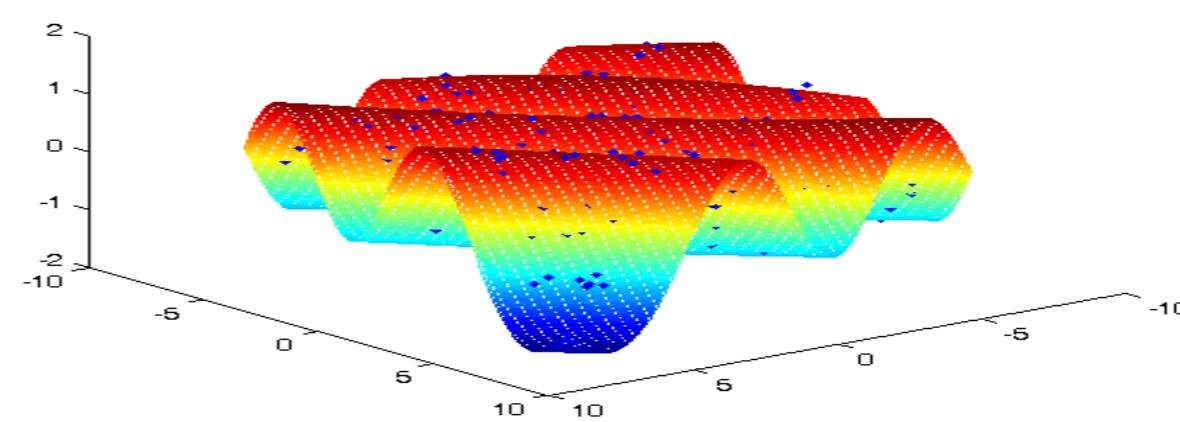
NRBF(12) by annealed FE



NRBF(15) by annealed FE



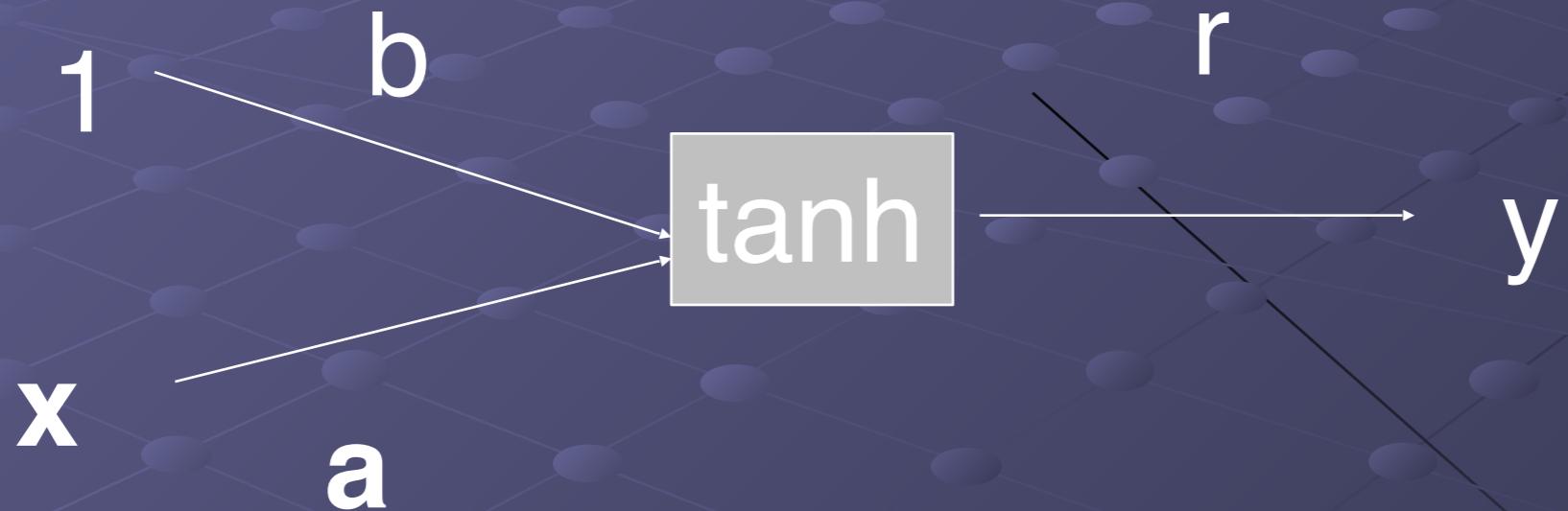
NRBF(18) by annealed FE



Perceptron

Projective basis function

$$y = r \tanh(\mathbf{a}^T \mathbf{x} + b)$$



Post-tanh projection

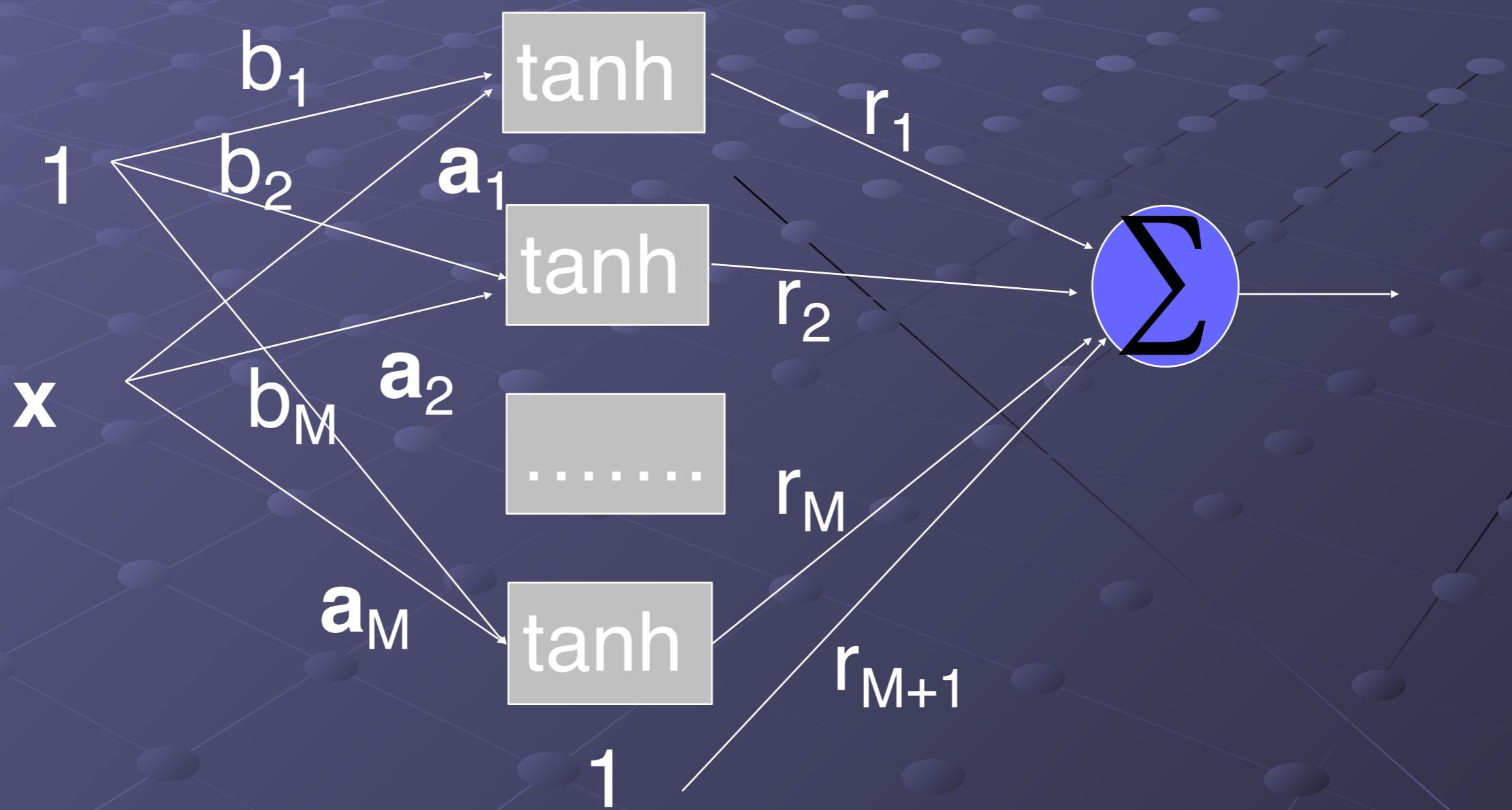
Posterior Weight

$$y = r \tanh(\mathbf{a}^T \mathbf{x} + b)$$

Linear projection

Post-nonlinear function

Multiple (Multi-layer) perceptrons



MLP (multilayer perceptrons)

Weight sum of post-tanh projections

$$F(\mathbf{x}; \theta) = \sum_{m=1}^M r_m \tanh(\mathbf{a}_m^T \mathbf{x} + b_m) + r_0$$

$$\theta = \{\mathbf{a}_m\} \cup \{b_m\} \cup \{r_m\}$$

Why Projection?

• Why projection?

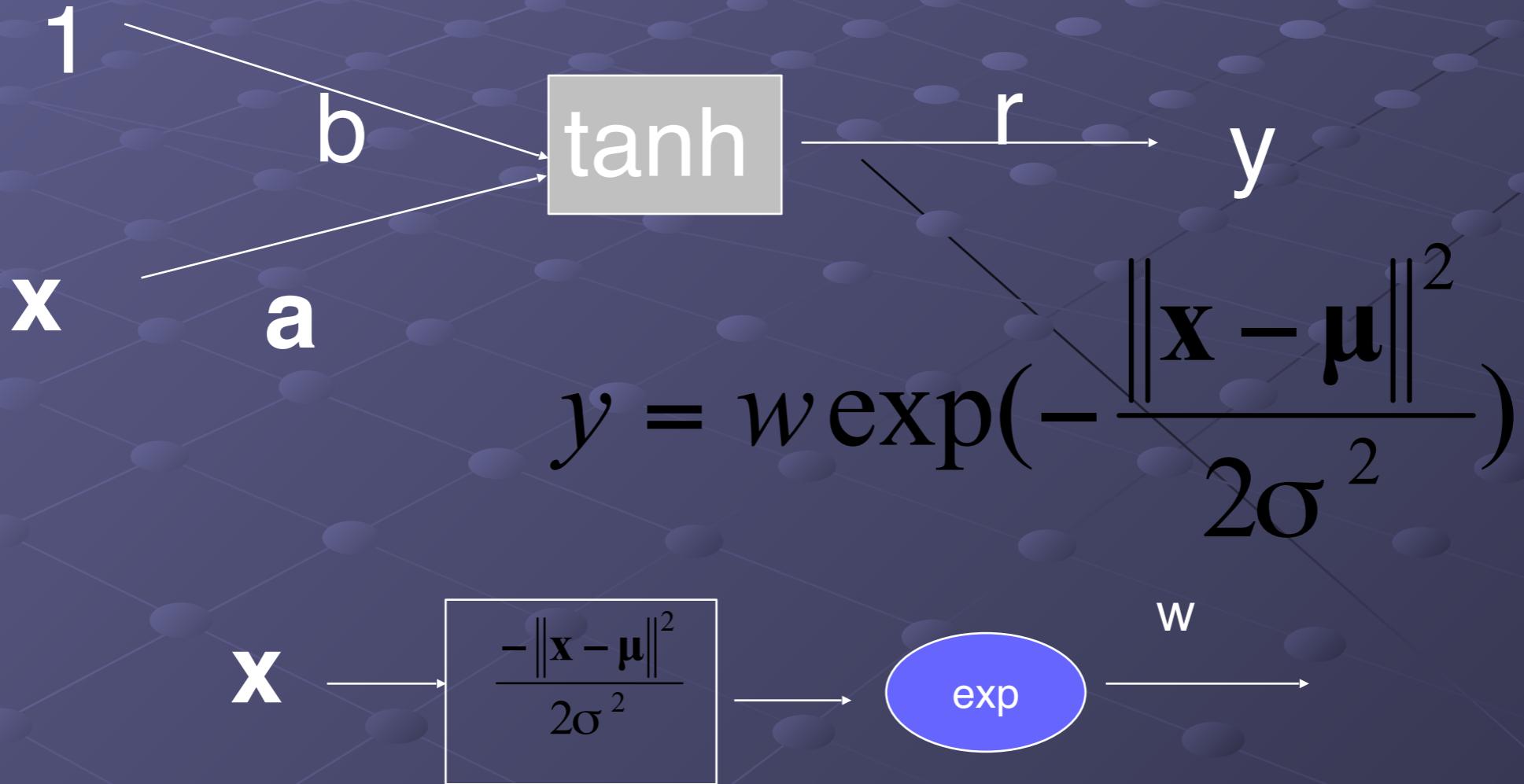
- Linear projection versus Radial basis function

• Why hyper-tangent

- Hyper-tangent function versus exponential function

Radial basis function

$$y = r \tanh(\mathbf{a}^T \mathbf{x} + b)$$



RBF Network function

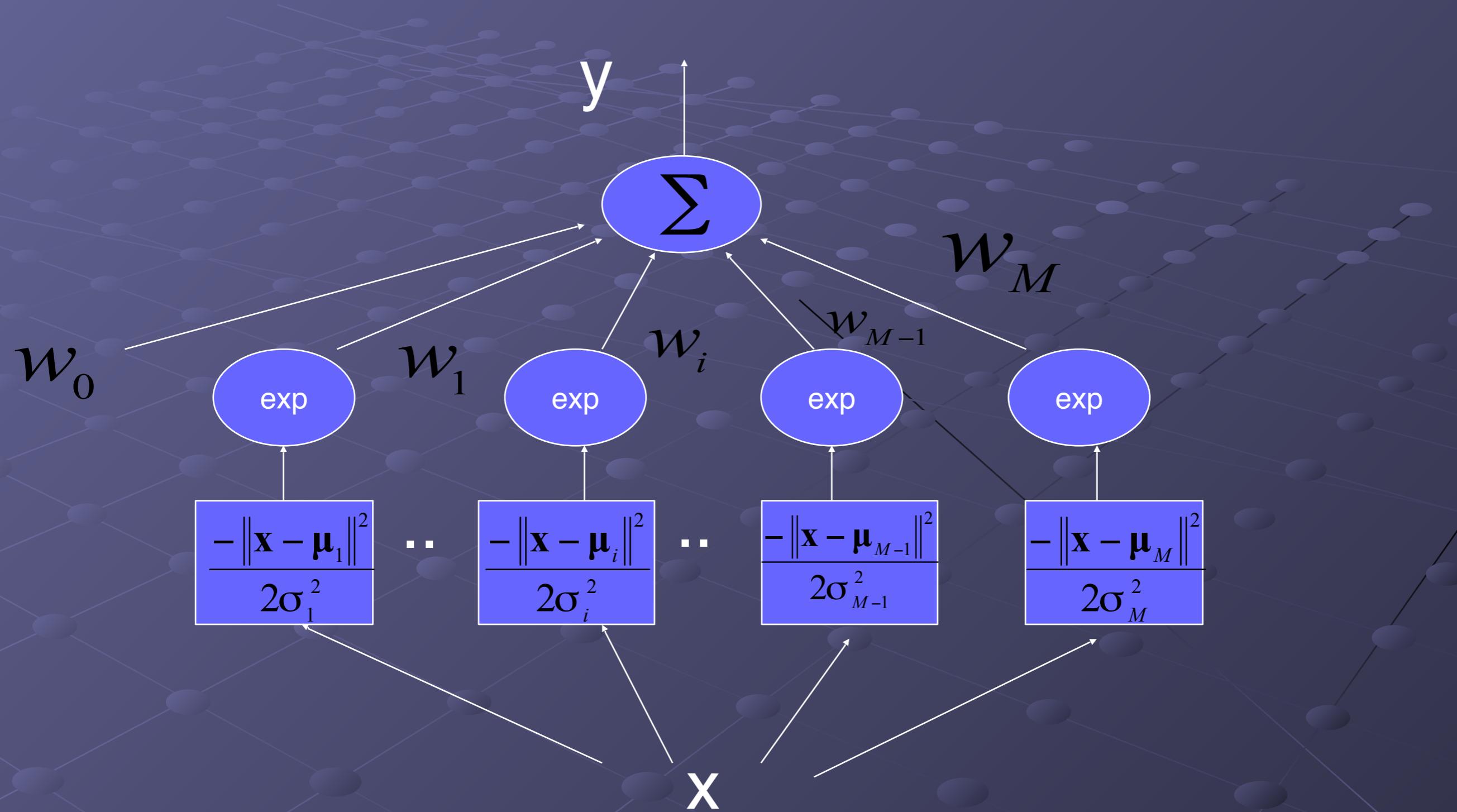
$$y(t | \theta) = G(\mathbf{x}[t] | \theta)$$

$$= w_0 + \sum_{m=1}^M w_m \exp\left(-\frac{\|\mathbf{x}[t] - \boldsymbol{\mu}_m\|^2}{2\sigma_m^2}\right)$$

Network parameter

$$\theta = \{w_i\}_i \cup \{\boldsymbol{\mu}_i\}_i \cup \{\sigma_i\}_i$$

RBF Network



Posterior weights

- Two stages
- Calculation of radial basis functions
- A linear combination

Stage I

Radial basis functions

$$f_m(x | \mu_m, \beta_m)$$

$$\equiv \exp\left(-\frac{\|x - \mu_m\|^2}{2\beta_m^2}\right)$$

$$\mathbf{o}[t] = (o_1[t], \dots, o_M[t])^\top$$

$$o_m[t] = f_m(x[t])$$

Stage II Posterior weighting

$$y[t] = \gamma_o[t]^T + \gamma_o$$

$$x[t] \rightarrow o[t] \rightarrow y[t]$$

Given $\{u_m\}$, $\{\delta_m\}$
optimiser

$$\mathbf{O} = \begin{bmatrix} \mathbf{o}[1]^T \\ \mathbf{o}[2]^T \\ \vdots \\ \mathbf{o}[N]^T \end{bmatrix}^T, \quad N \times d$$

$$\mathbf{O} = [\mathbf{o} \ \text{ones}(N, 1)]$$

$$O\gamma = y$$

$$Or = y$$

$$O^T Or = O^T y$$

$$C(r) = Y^T O^T Or - O^T y$$

$C(r)$

$$= \gamma^T \Omega r - \gamma^T y + \lambda \gamma^T r$$

Regularization

$$\frac{dc}{dr}$$

$$= D^T \sigma r - D^T y + \lambda r = \emptyset$$
$$(D^T D + \lambda I) r = D^T y$$

$$Y = \text{pinv}(O + \lambda I) Y$$

optimization of

Y for given

$\{\mu_m\}$ and $\{\sigma_m\}$

Ratsch Algorithm

Algorithm RBF-Net(K, λ, O)

Input:

Sequence of labeled training patterns $\mathbf{Z} = \langle (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_l, y_l) \rangle$

Number of RBF centers K

Regularization constant λ

Number of iterations O

Initialize:

Run K -means clustering to find initial values for μ_k and determine $\sigma_k, k = 1, \dots, K$, as the distance between μ_k and the closest μ_i ($i \neq k$).

Do for $o = 1 : O$,

1. Compute optimal output weights $\mathbf{w} = (G^\top G + 2\frac{\lambda}{l}\mathbf{I})^{-1} G^\top \mathbf{y}$
- 2a. Compute gradients $\frac{\partial}{\partial \mu_k} E$ and $\frac{\partial}{\partial \sigma_k} E$ as in (28) and (27) with optimal \mathbf{w} and form a gradient vector \mathbf{v}
- 2b. Estimate the conjugate direction $\bar{\mathbf{v}}$ with Fletcher-Reeves-Polak-Ribiere CG-Method (Press et al., 1992)
- 3a. Perform a line search to find the minimizing step size δ in direction $\bar{\mathbf{v}}$; in each evaluation of E recompute the optimal output weights \mathbf{w} as in line 1
- 3b. Update μ_k and σ_k with $\bar{\mathbf{v}}$ and δ

Output: Optimized RBF net

K Means

- Given $\{x[t]\}$, find centers and variances
- Matlab kmeans.m

[http://134.208.26.59/MathProgramming2010/Lecture10/
Lecture10II.pdf](http://134.208.26.59/MathProgramming2010/Lecture10/Lecture10II.pdf)

$\{x[t]\}, \{y[t]\}$
 M, λ

$u = kmeans(x, M)$
 $\delta = kvar(x, u)$

$O = g(x | M, \delta)$
 $R = \text{inv}(O^T O + \lambda I) O^T g$
 $V = \left[-\frac{\partial E}{\partial u} \quad -\frac{\partial E}{\partial \delta} \right]$

$P = V$
 $S_{\text{new}} = V^T V$

$k = 0$
 $n = \text{size}([M \delta])$

not HC

EXIT

$\delta = \text{linmin}(u, \delta, r, x)$
 $[u, \delta] = [u, \delta] + \delta \nabla P$

$O = g(x | M, \delta)$
 $R = \text{inv}(O^T O + \lambda I) O^T g$
 $V = \left[-\frac{\partial E}{\partial u} \quad -\frac{\partial E}{\partial \delta} \right]$

$S_{\text{old}} = S_{\text{new}}$
 $S_{\text{new}} = V^T V$
 $\beta = S_{\text{new}} / S_{\text{old}}$
 $P = V + \beta P$
 $K = K + 1$

if $K = n \mid V^T P \leq 0$
 $P = V$
 $K = 0$

Relation between RBF and MLP

- Why Euclidean distance?
- Why exponential function?
- Why hyper-tangent function?

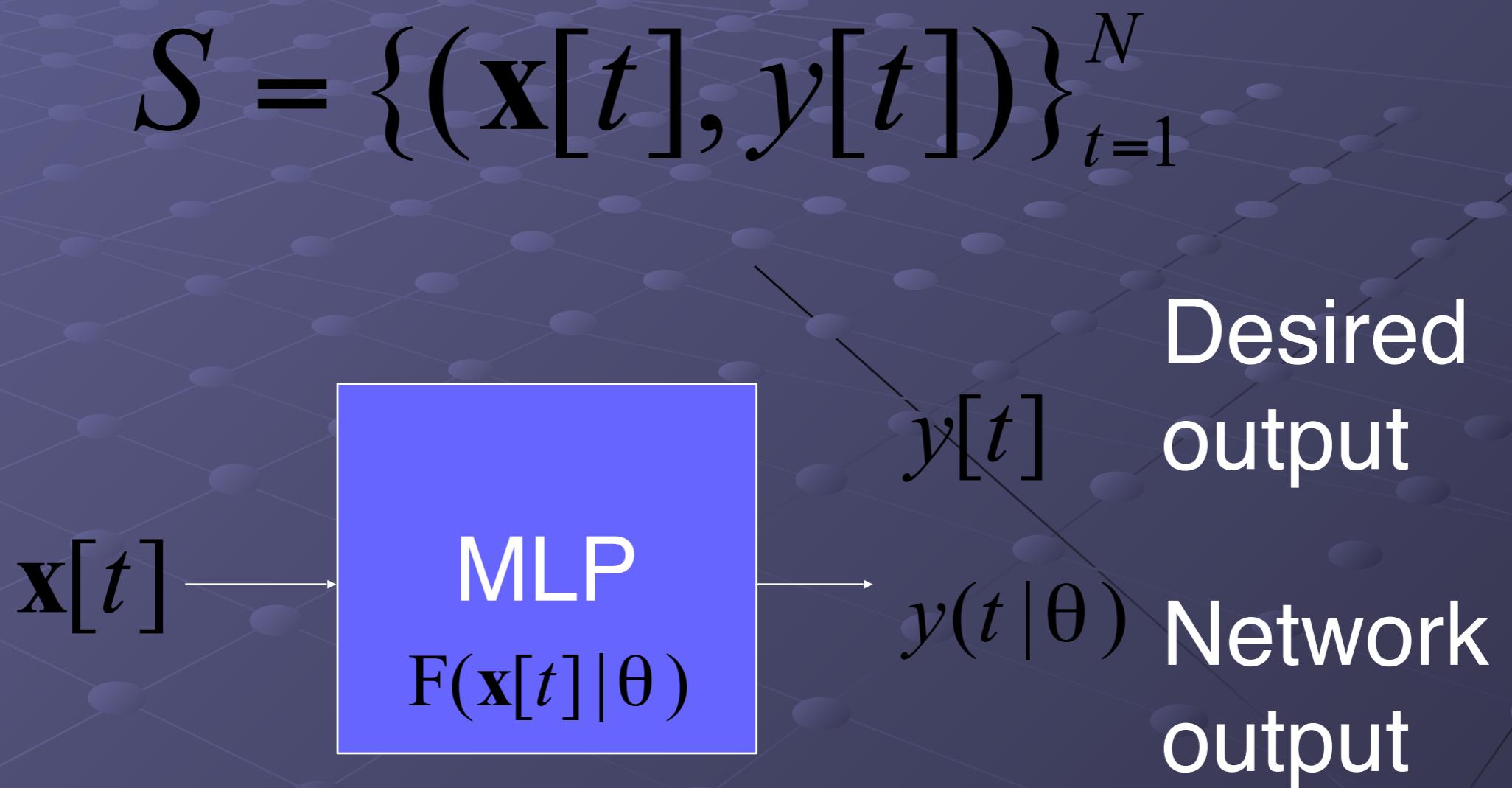
Network parameter

$$\theta = [\mathbf{u}_1^T \mathbf{u}_2^T \cdots \mathbf{u}_M^T \sigma_1 \sigma_2 \cdots \sigma_M w_0 w_1 w_2 \cdots w_M]^T$$
$$= [\theta_1, \dots, \theta_{M*d+2M+1}]$$

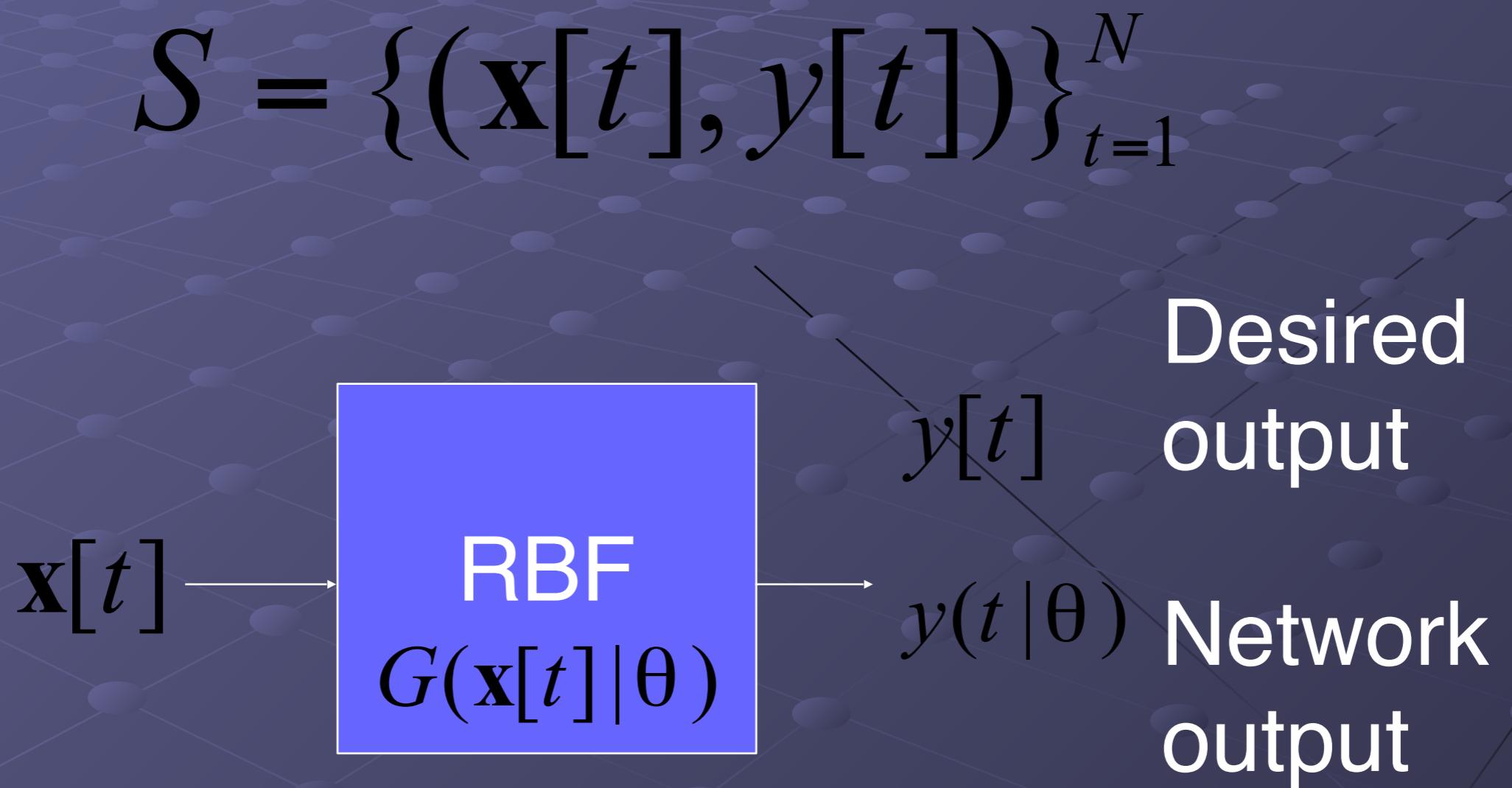
a vector of d elements

scalar

Training set



Training set



Mean square errors

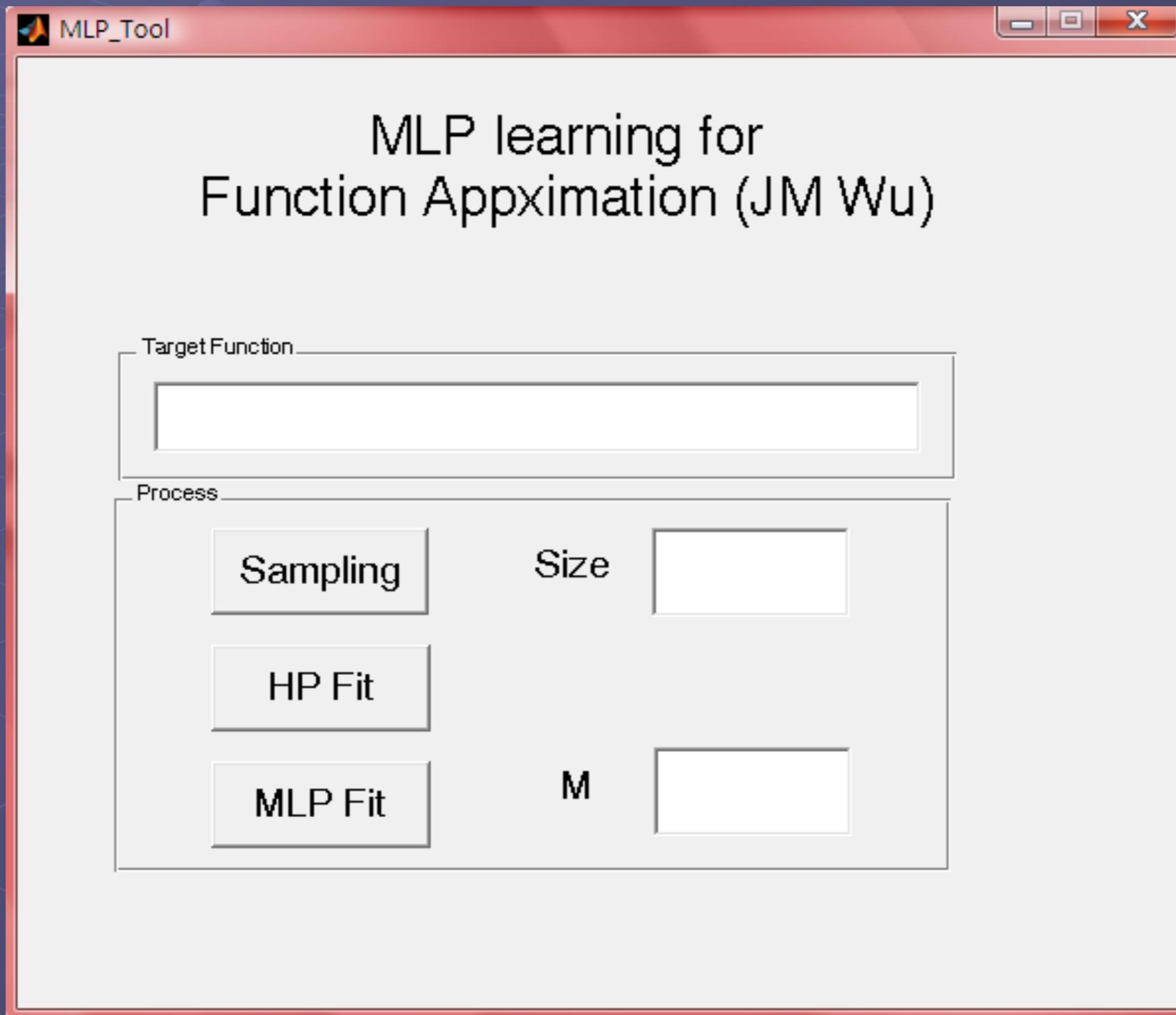
$$E_S(\theta) = \frac{1}{2N} \sum_{t=1}^N (y[t] - y(t | \theta))^2$$

Unconstrained optimization

$$\hat{\theta} = \arg \min_{\{\theta\}} E_S(\theta)$$

Find θ to minimize $E_S(\theta)$

Revisit hyper-plane Fitting



Sampling

Blue : training data
Red : testing data

MLP learning for
Function Approximation (JM Wu)

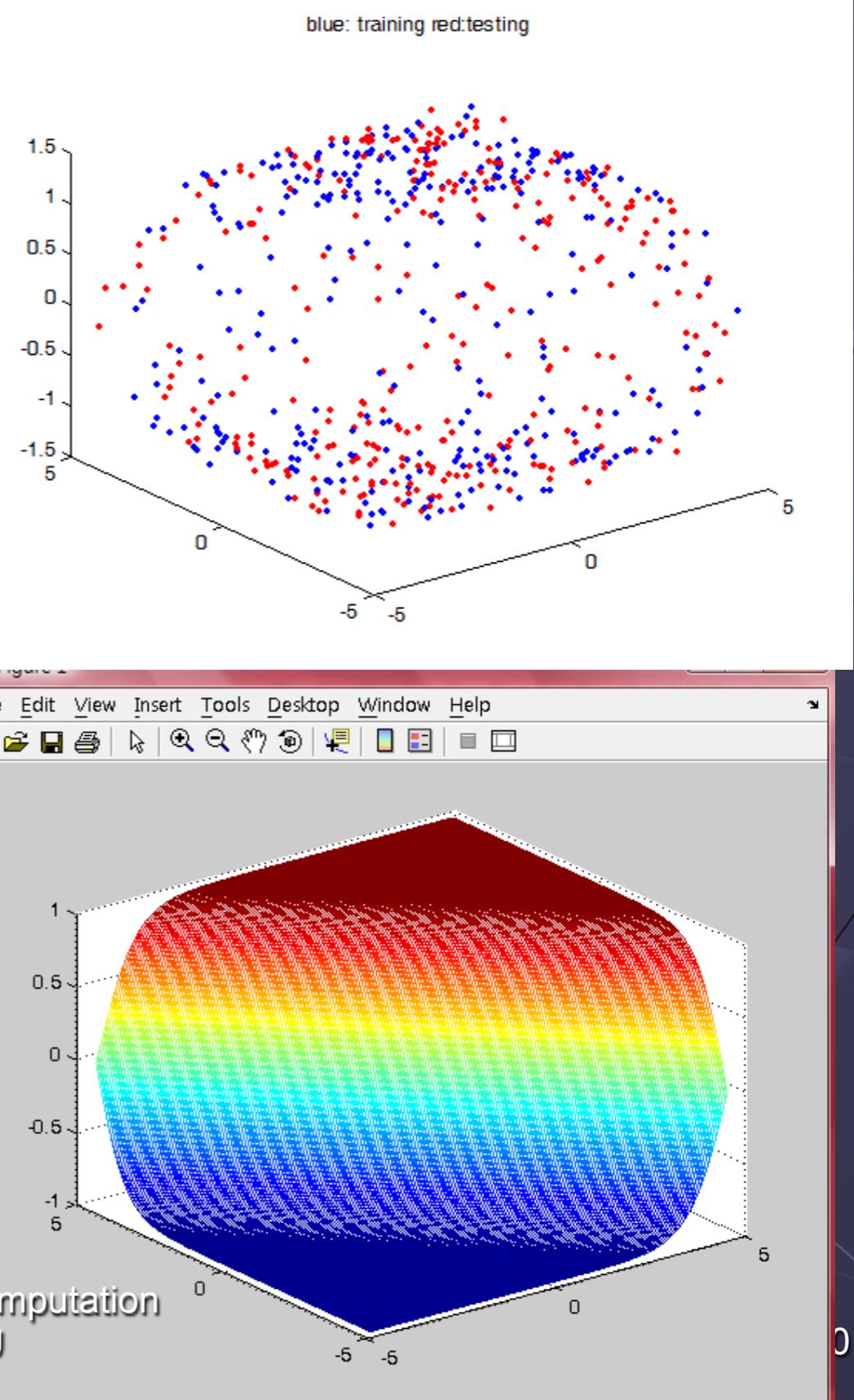
Target Function

Process

Sampling Size 300

HP Fit

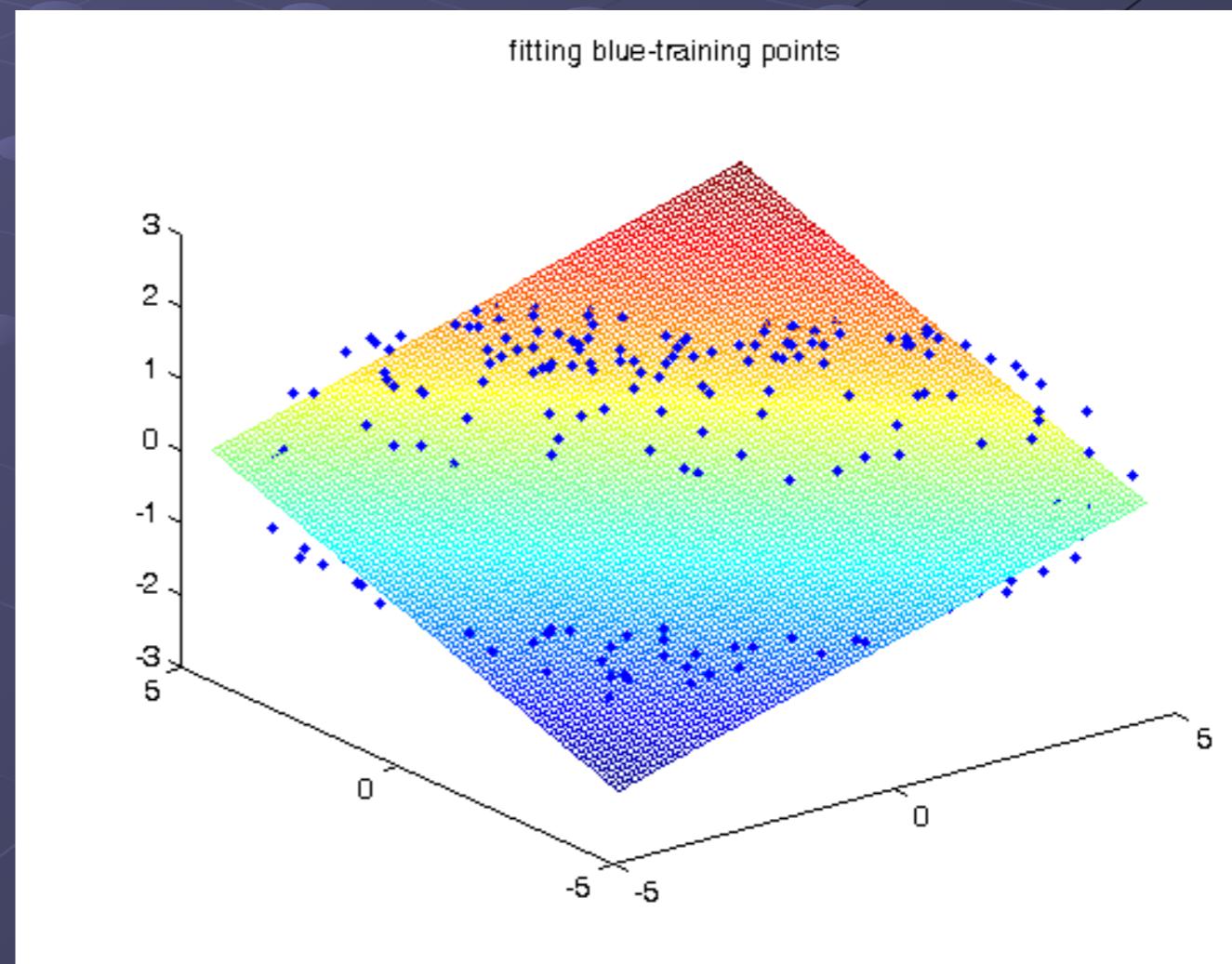
MLP Fit M



Fitting

1. Fitting blue training data
2. The performance is reflected by the mean square testing error

mean square training error 0.159647
mean square testing error 0.160200



Verification of Generalization

Training phase

- Given a training set, find θ to minimize $E_s(\theta)$

Testing phase

- Verify $F(x; \theta_{\text{opt}})$ by a testing set, which is assumed unknown during training phase

Both training and testing sets are assumed oriented from the same generating process

Performance evaluation

Mean square error of training

- Substitute each predictor in a training set to a network function
- Determine the mean square error of approximating the desired target by the network output

Mean square error of testing indicates generalization capability of a network function

Mean square training error

$$E_S(\theta) = \frac{1}{2N} \sum_{t=1}^N (y[t] - F(\mathbf{x}[t]; \theta))^2$$

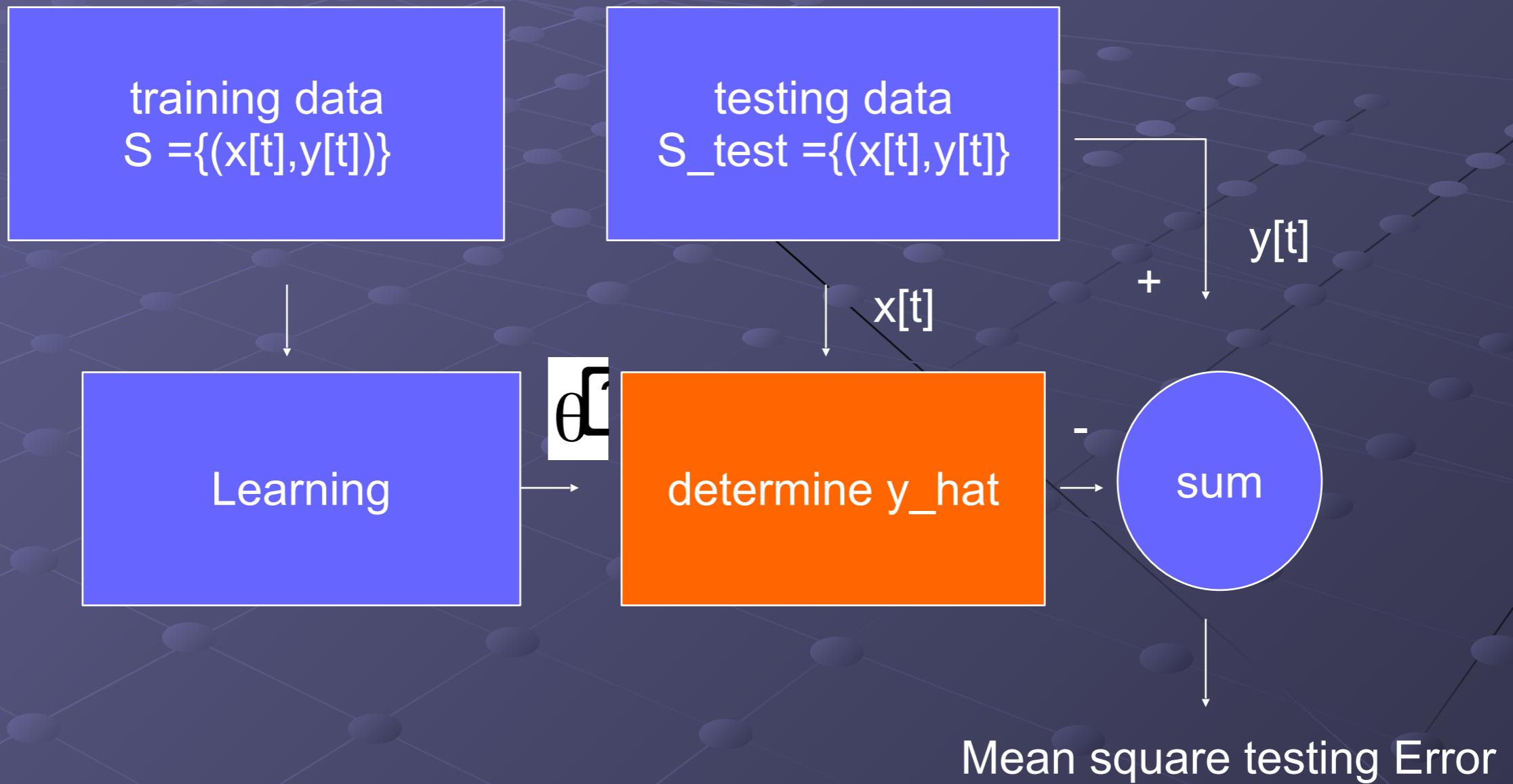
$S = \{(\mathbf{x}[t], y[t])\}_t$: training set

Mean square testing error

$$E_{S_{\text{Test}}}(\theta) = \frac{1}{2N} \sum_{t=1}^N (y[t] - F(x[t]; \theta))^2$$

$S_{\text{Test}} = \{(x[t], y[t])\}_t$: testing set

Prediction



Over-fitting

- ➊ Extremely low training error but high testing error
- ➋ Over-fitting implies false generalization

Table lookup

- Over-fitting
- S: training set

$$f(x) = y[t^*]$$
$$t^* = \arg \min_t \| \mathbf{x} - \mathbf{x}[t] \|^2$$

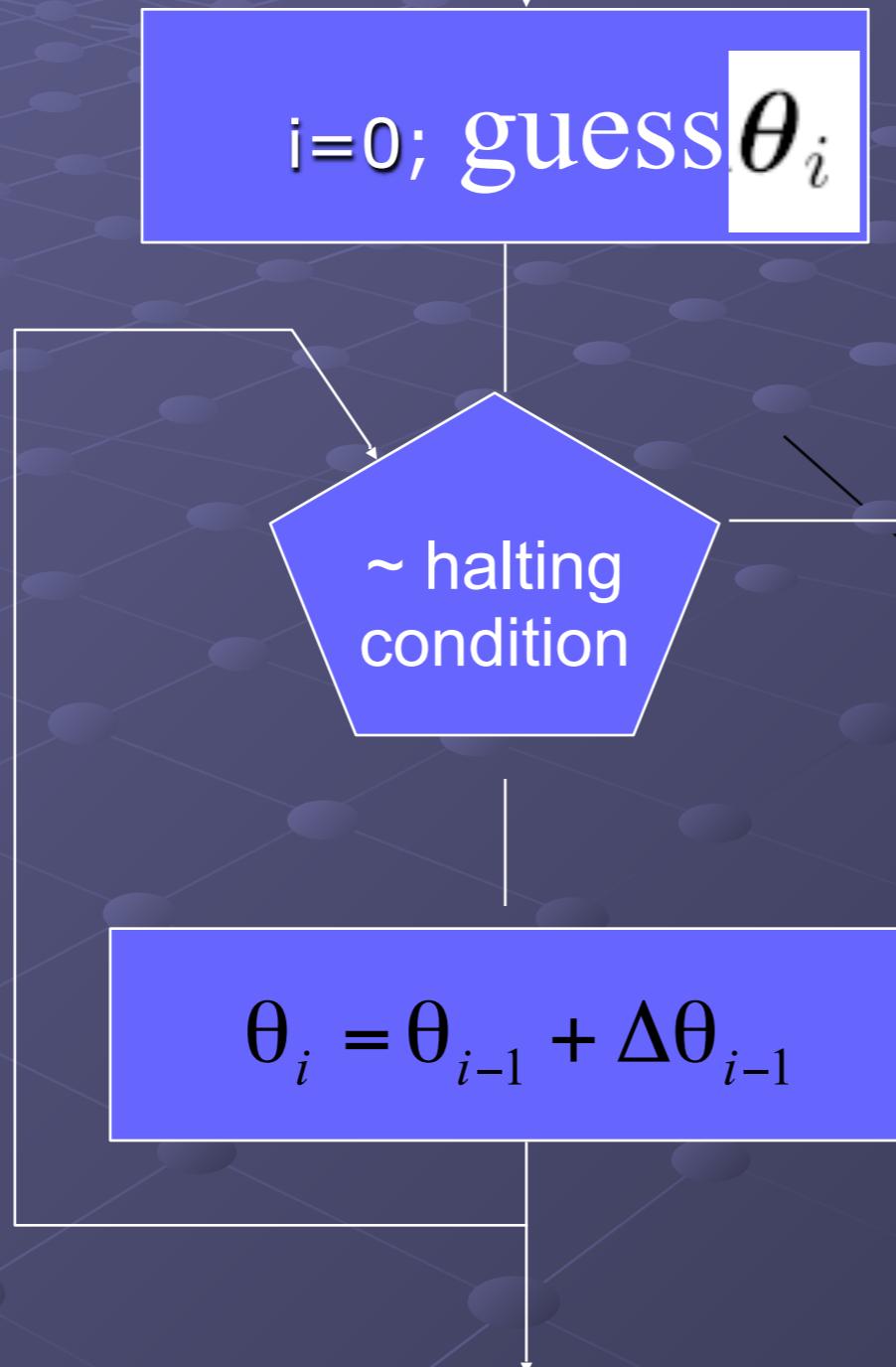
Iterative approaches

- Gradient method
- Newton-Gauss method
- Levenberg-Marquardt method

Iterative approach

1. Initialize θ_i with $i=0$
2. Determine $\Delta\theta_i$
3. Update network parameters
$$\theta_{i+1} = \theta_i + \Delta\theta_i$$
4. If halting condition holds, exit
otherwise $i=i+1$, go to step 2

Flow Chart



Objective function

$$E_S(\theta) = \frac{1}{2N} \sum_{t=1}^N \varepsilon^2(t, \theta)$$

$$\varepsilon(t, \theta) = y[t] - y(t|\theta)$$

Error of
the ith paired data

Desired
output

Network
output

Gradient method

$$\Delta\theta_i \propto -\frac{dE_S(\theta)}{d\theta} |_{\theta=\theta_i}$$

- Derive the derivative of E_S with respect to θ
- Substitute θ to $\frac{dE_S(\theta)}{d\theta}$

Gradient

$$E_S(\theta) = \frac{1}{2N} \sum_{t=1}^N (y[t] - y(t|\theta))^2$$

$$\frac{dE_S(\theta)}{d\theta} = \frac{-1}{N} \sum_{t=1}^N (y[t] - y(t|\theta)) \frac{dy(t|\theta)}{d\theta}$$

Derivation

$$y(t | \theta)$$

$$= F(x[t]; \theta) = \sum_{m=1}^M r_m \tanh(a_m^T x[t] + b_m) + r_0$$

$$\begin{aligned}\theta &= [a_1^T \ a_2^T \ \cdots \ a_M^T \ b_1 \ b_2 \ \cdots \ b_M \ r_0 \ r_1 \ r_2 \ \cdots \ r_M]^T \\ &= [\theta_1, \dots, \theta_{M^*d+2M+1}]\end{aligned}$$

$$\begin{aligned}
& \frac{dy(t | \theta)}{d\theta} \\
&= \left(\frac{dy(t | \theta)}{d\theta_1}, \frac{dy(t | \theta)}{d\theta_2}, \dots, \dots, \frac{dy(t | \theta)}{d\theta_{Md+2M+1}} \right)^T \\
&\theta = [\mathbf{a}_1^T \ \mathbf{a}_2^T \ \dots \ \mathbf{a}_M^T \ b_1 \ b_2 \ \dots \ b_M \ r_0 \ r_1 \ r_2 \ \dots \ r_M]^T \\
&= [\theta_1, \dots, \theta_{Md+2M+1}]
\end{aligned}$$

$$\frac{dy(t | \theta)}{d\theta}$$

$$= \left(\frac{dy(t | \theta)}{da_1^T} \quad \frac{dy(t | \theta)}{da_2^T} \quad \dots \frac{dy(t | \theta)}{db_1^T} \quad \dots \frac{dy(t | \theta)}{dr_1^T} \dots \frac{dy(t | \theta)}{dr_M^T} \right)^T$$

$$\theta = [a_1^T \ a_2^T \ \dots \ a_M^T \ b_1 \ b_2 \ \dots \ b_M \ r_0 \ r_1 \ r_2 \ \dots \ r_M]^T$$

$$= [\theta_1, \dots, \theta_{M*d+2M+1}]$$

$$y(t | \theta)$$

$$= F(\mathbf{x}[t]; \theta) = \sum_{m=1}^M r_m \tanh(\mathbf{a}_m^T \mathbf{x}[t] + b_m) + r_0$$

$$\frac{dy(t | \theta)}{d\mathbf{a}_k}$$

$$= \frac{d}{d\mathbf{a}_k} \sum_{m=1}^M r_m \tanh(\mathbf{a}_m^T \mathbf{x}[t] + b_m) + r_0$$

$$= r_k (1 - \tanh(\mathbf{a}_k^T \mathbf{x}[t] + b_k)^2) \mathbf{x}[t]$$

$$\begin{aligned}\frac{dy(t | \theta)}{db_k} &= \frac{d}{db_k} \sum_{m=1}^M r_m \tanh(\mathbf{a}_m^T \mathbf{x}[t] + b_m) + r_0 \\ &= r_k (1 - \tanh(\mathbf{a}_k^T \mathbf{x}[t] + b_k)^2)\end{aligned}$$

$$\frac{dy(t | \theta)}{dr_k}$$

$$= \frac{d}{dr_k} \sum_{m=1}^M r_m \tanh(\mathbf{a}_m^T \mathbf{x}[t] + b_m) + r_0$$

$$= \tanh(\mathbf{a}_k^T \mathbf{x}[t] + b_k)$$

Error

derivative

$$\varepsilon(t, \theta) = y[t] - y(t|\theta)$$

$$\psi(t, \theta) = \frac{dy(t|\theta)}{d\theta}$$

$$\frac{dE_S(\theta)}{d\theta} \Big|_{\theta=\theta_i} = \nabla(\theta_i) = \frac{-1}{N} \sum_{t=1}^N \varepsilon(t, \theta_i) \psi(t, \theta_i)$$

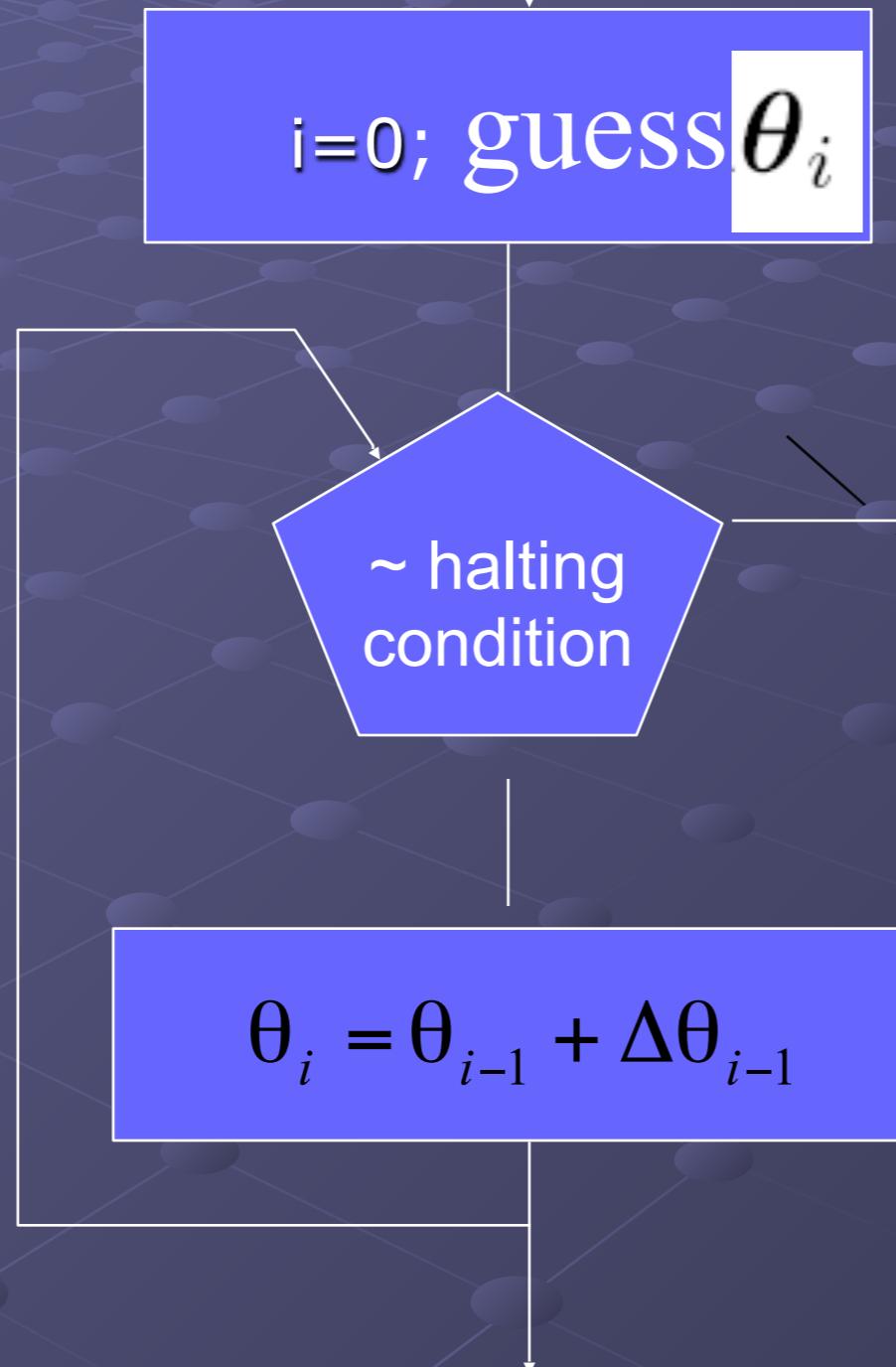
$$\Delta\theta_i \propto -\frac{dE_S(\theta)}{d\theta} |_{\theta=\theta_i}$$

$$= -\nabla(\theta_i)$$

Exercise

- Gradient descent method for learning
MLP networks
- Gradient descent method for learning
RBF networks

Flow Chart



Calculate the change

$$\Delta\theta_i \propto -\frac{dE_S(\boldsymbol{\theta})}{d\theta} |_{\theta=\theta_i}$$

$$= \frac{-1}{N} \sum_{t=1}^N \varepsilon(t, \theta_i) \psi(t, \theta_i)$$

- Prepare a, b, r from given theta
 - Substitute a, b, r to
 - Substitute a, b, r to
- $$\varphi(t, \theta) = \frac{dy(t|\theta)}{d\theta}$$
- $$\varepsilon(t, \theta) = y[t] - y(t|\theta)$$
- for all t

Substitute a, b, r to

$$\varphi(t, \theta) = \frac{dy(t|\theta)}{d\theta}$$

Substitute current a, b, r to

$$\frac{dy(t | \theta)}{d\theta} = \left(\frac{dy(t | \theta)}{da_1^T} \frac{dy(t | \theta)}{da_2^T} \dots \frac{dy(t | \theta)}{db_1^T} \dots \frac{dy(t | \theta)}{dr_1^T} \dots \frac{dy(t | \theta)}{dr_M^T} \right)^T$$

Substitute a,b,r to

$$\frac{dy(t | \theta)}{da_k} = r_k (1 - \tanh(a_k^T x[t] + b_k)^2) x[t]$$

$$\frac{dy(t | \theta)}{db_k} = r_k (1 - \tanh(a_k^T x[t] + b_k)^2)$$

$$\frac{dy(t | \theta)}{dr_k} = \tanh(a_k^T x[t] + b_k)$$

for all k

Newton-Gauss Method

Second order expansion

Linear expansion of errors

Error : nonlinear function of θ

$$\varepsilon(t, \boldsymbol{\theta}) = y[t] - y(t|\boldsymbol{\theta})$$

Linear expansion at $\theta = \theta_i$

$$\begin{aligned}\tilde{\varepsilon}_i(t, \boldsymbol{\theta}) &= \varepsilon(t, \boldsymbol{\theta}_i) + (\boldsymbol{\theta} - \boldsymbol{\theta}_i)^T \frac{d\varepsilon(t, \boldsymbol{\theta})}{d\boldsymbol{\theta}}|_{\boldsymbol{\theta}=\boldsymbol{\theta}_i} \\ &= \varepsilon(t, \boldsymbol{\theta}_i) - (\boldsymbol{\theta} - \boldsymbol{\theta}_i)^T \frac{dy(t|\boldsymbol{\theta})}{d\boldsymbol{\theta}}|_{\boldsymbol{\theta}=\boldsymbol{\theta}_i}\end{aligned}$$

Linear expansion of error

Let

$$\psi(t, \theta) = \frac{dy(t|\theta)}{d\theta}$$

$$\tilde{\varepsilon}_i(t, \theta) = \varepsilon(t, \theta_i) - (\theta - \theta_i)^T \psi(t, \theta_i)$$

is a linear function of θ

Criteria for Newton-Gauss

Mean square
error

$$E_S(\theta) = \frac{1}{2N} \sum_{t=1}^N \varepsilon^2(t, \theta)$$

Quadratic form

$$L_i(\theta) = \frac{1}{2N} \sum_{t=1}^N \tilde{\varepsilon}_i^2(t, \theta)$$

Quadratic form

Expansion at $\theta = \theta_i$

$$L_i(\boldsymbol{\theta}) = L_i(\boldsymbol{\theta}_i) + \nabla(\boldsymbol{\theta}_i)^T(\boldsymbol{\theta} - \boldsymbol{\theta}_i) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_i)^T R(\boldsymbol{\theta}_i)(\boldsymbol{\theta} - \boldsymbol{\theta}_i),$$

gradient $\nabla(\boldsymbol{\theta}_i) = \frac{-1}{N} \sum_{t=1}^N \varepsilon(t, \boldsymbol{\theta}_i) \psi(t, \boldsymbol{\theta}_i)$

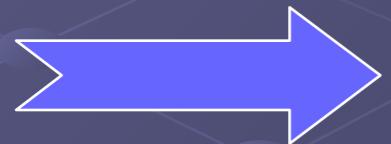
Gauss-Newton Hessian

$$R(\boldsymbol{\theta}_i) = \frac{1}{N} \sum_{t=1}^N \psi(t, \boldsymbol{\theta}_i) \psi^T(t, \boldsymbol{\theta}_i)$$

Newton-Gauss method

$$\frac{dL_i(\theta)}{d\theta} = \nabla(\theta_i) + R(\theta_i)(\theta - \theta_i) = 0$$

$$\Delta\theta_i = \theta - \theta_i$$



$$R(\theta_i)\Delta\theta_i = -\nabla(\theta_i)$$

$$R(\theta_i) \Delta\theta_i = -\nabla(\theta_i)$$

$$\Delta\theta_i = -(R(\theta_i))^{-1} \nabla(\theta_i)$$

Levenberg-Marquardt method

$\Delta\theta_i$ is determined by

$$(R(\theta_i) + \lambda I)\Delta\theta_i = -\nabla(\theta_i)$$

$$\lambda = 0$$

$$(R(\theta_i) + \lambda \mathbf{I}) \Delta \theta_i = -\nabla(\theta_i)$$



$$R(\theta_i) \Delta \theta_i = -\nabla(\theta_i)$$

Newton-Gauss method

Sufficiently large λ

$$(R(\theta_i) + \lambda \mathbf{I}) \Delta \theta_i = -\nabla(\theta_i)$$



$$\Delta \theta_i \propto -\nabla(\theta_i)$$

Gradient method

Control λ

Current parameter

Next parameter

$$\alpha_i = \frac{E_S(\boldsymbol{\theta}_i) - E_S(\boldsymbol{\theta}_i + \Delta\boldsymbol{\theta}_i)}{E_S(\boldsymbol{\theta}_i) - L_i(\boldsymbol{\theta}_i + \Delta\boldsymbol{\theta}_i)}$$

Actual cost reduction

Predicted cost reduction

High α_i

Reduce λ

improve efficiency

Force to
Newton-Gauss
method

Low

α_i

Increase

λ

Improve reliability

Force to
gradient
method

Heuristic adaption

- (a) If $\alpha_i > 0.75$, $\lambda \leftarrow 0.5\lambda$.
- (b) If $\alpha_i < 0.25$, $\lambda \leftarrow 2\lambda$.

LM method

1. Initialize $\theta_i, i=0$ and set λ
2. Calculate $\nabla(\theta_i)$ and $R(\theta_i)$ and $\Delta\theta_i$
3. Update network parameters
$$\theta_{i+1} = \theta_i + \Delta\theta_i$$
4. Calculate α_i
5. Update λ
 - (a) If $\alpha_i > 0.75$, $\lambda \leftarrow 0.5\lambda$.
 - (b) If $\alpha_i < 0.25$, $\lambda \leftarrow 2\lambda$.
6. If halting condition hold, exit otherwise go to step 2

Initialize θ , set λ

exit

~ halting cond

Calculate
 $R(\theta)$ and $\nabla(\theta)$

Calculate
 $\Delta(\theta)$
 $\theta = \theta + \Delta(\theta)$

calculate α_i

α_i

> 0.75

$\lambda=0.5 * \lambda$

< 0.25

$\lambda=2 * \lambda$

Project

Learning RBF by the LM method

1. (30 pt) Derivation

$$\frac{dy(t | \theta)}{d\theta} = ?$$

2. (140 pt) Matlab codes
3. (50 pt) Testing

Derivative

$$\begin{aligned}\theta &= [\mathbf{u}_1^T \ \mathbf{u}_2^T \cdots \mathbf{u}_M^T \ \boldsymbol{\sigma}_1 \ \boldsymbol{\sigma}_2 \cdots \boldsymbol{\sigma}_M \ \mathbf{w}_0 \ \mathbf{w}_1 \ \mathbf{w}_2 \cdots \mathbf{w}_M]^T \\ &= [\theta_1, \dots, \theta_{M^*d+2M+1}]\end{aligned}$$

$$\frac{dy(t|\theta)}{d\theta} = \left[\frac{dy(t|\theta)}{d\theta_1}, \dots, \frac{dy(t|\theta)}{d\theta_{M^*d+2M+1}} \right]^T$$

Derivative

$$\frac{dy(t|\theta)}{d\mathbf{u}_m} = ?$$
$$\frac{dy(t|\theta)}{d\sigma_m} = ?$$
$$\frac{dy(t|\theta)}{dw_m} = ?$$

Matlab coding

- (30 pt) Main program
- Matlab Functions
 - a. (10 pt) Calculate $E_S(\theta_i)$
 - b. (10 pt) Calculate $L_i(\theta_i)$

Matlab coding

- Matlab functions

- (10 pt) Calculate

$$\frac{dy(t | \theta)}{d\mathbf{u}_m} \Big|_{\theta = \theta_i}$$

- (10 pt) Calculate

$$\frac{dy(t | \theta)}{d\sigma_m} \Big|_{\theta = \theta_i}$$

- (10 pt) Calculate

$$\frac{dy(t | \theta)}{dw_m} \Big|_{\theta = \theta_i}$$

Matlab coding

- Matlab functions
- (20 pt) Calculate $\nabla(\theta_i)$
- (20 pt) Calculate $R(\theta_i)$
- (20 pt) Calculate $G(x|\theta)$

Test

- Give two examples to test your matlab codes for learning RBF networks by Levenberg-Marquardt method