Neural Networks, Perceptrons, SVM

STAT261: Introduction to Machine Learning

May 25, 2016

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Outline

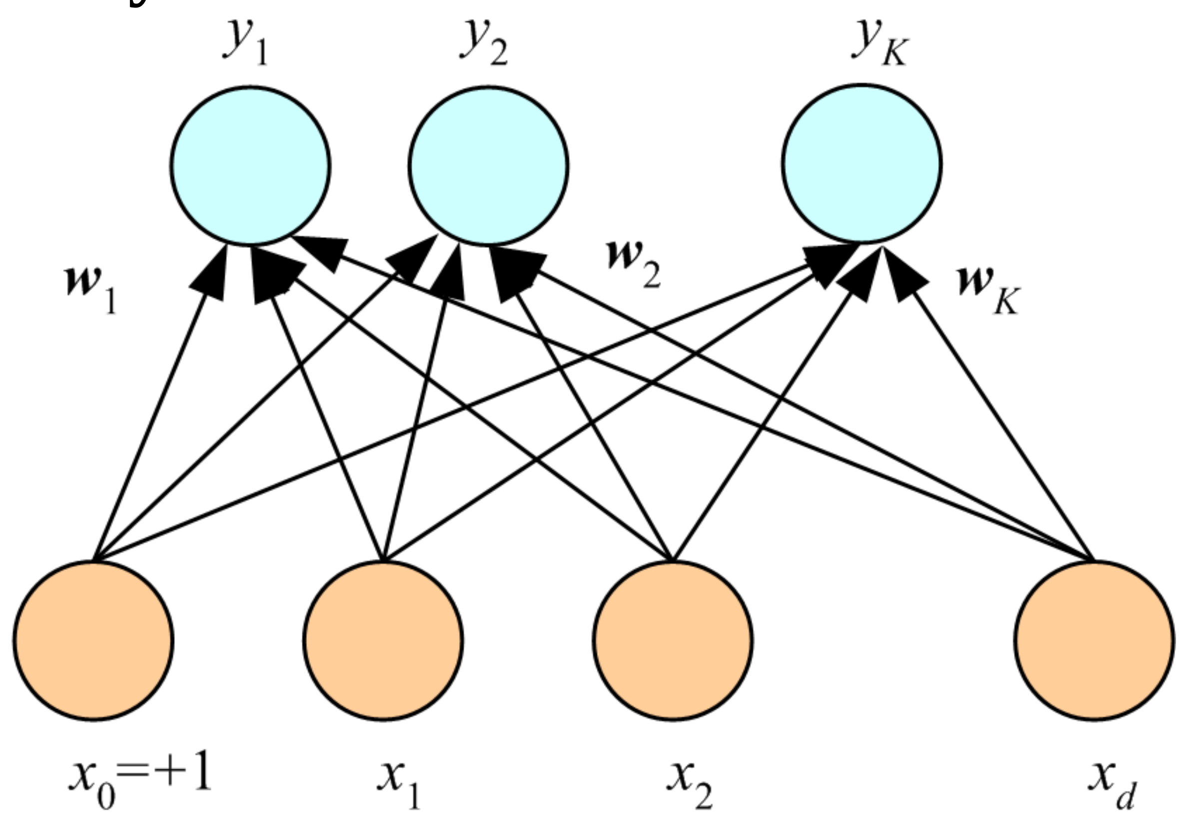
- Multilayer Perceptron

K Outputs

Regression:

$$y_i = \sum_{j=1}^{d} w_{ij} x_j + w_{i0} = \mathbf{w}_i^T \mathbf{x}$$

$$\mathbf{y} = \mathbf{W}\mathbf{x}$$



Classification:

$$o_i = \mathbf{w}_i^T \mathbf{x}$$

$$y_i = \frac{\exp o_i}{\sum_k \exp o_k}$$

choose C_i

if $y_i = \max_k y_k$

Training

- Online (instances seen one by one) vs batch (whole sample) learning:
  - No need to store the whole sample
  - Problem may change in time
  - Wear and degradation in system components
- Stochastic gradient-descent: Update after a single pattern
- Generic update rule (LMS rule):

$$\Delta w_{ij}^t = \eta\left(r_i^t - y_i^t\right)x_j^t$$

$$\text{Update} = \text{LearningFactor} \cdot \left(\text{DesiredOutput} - \text{ActualOutput}\right) \cdot \text{Input}$$

Training a Perceptron: Regression

- Regression (Linear output):

$$E^t\left(\mathbf{w} \mid \mathbf{x}^t, r^t\right) = \frac{1}{2}\left(r^t - y^t\right)^2 = \frac{1}{2}\left[r^t - \left(\mathbf{w}^T\mathbf{x}^t\right)\right]^2$$

$$\Delta w_j^t = \eta\left(r^t - y^t\right)x_j^t$$

Classification

- Single sigmoid output

$$y^t = \text{sigmoid}\left(\mathbf{w}^T \mathbf{x}^t\right)$$

$$E^t\left(\mathbf{w} \mid \mathbf{x}^t, \mathbf{r}^t\right) = -r^t \log y^t - \left(1 - r^t\right) \log\left(1 - y^t\right)$$

$$\Delta w_j^t = \eta\left(r^t - y^t\right) x_j^t$$

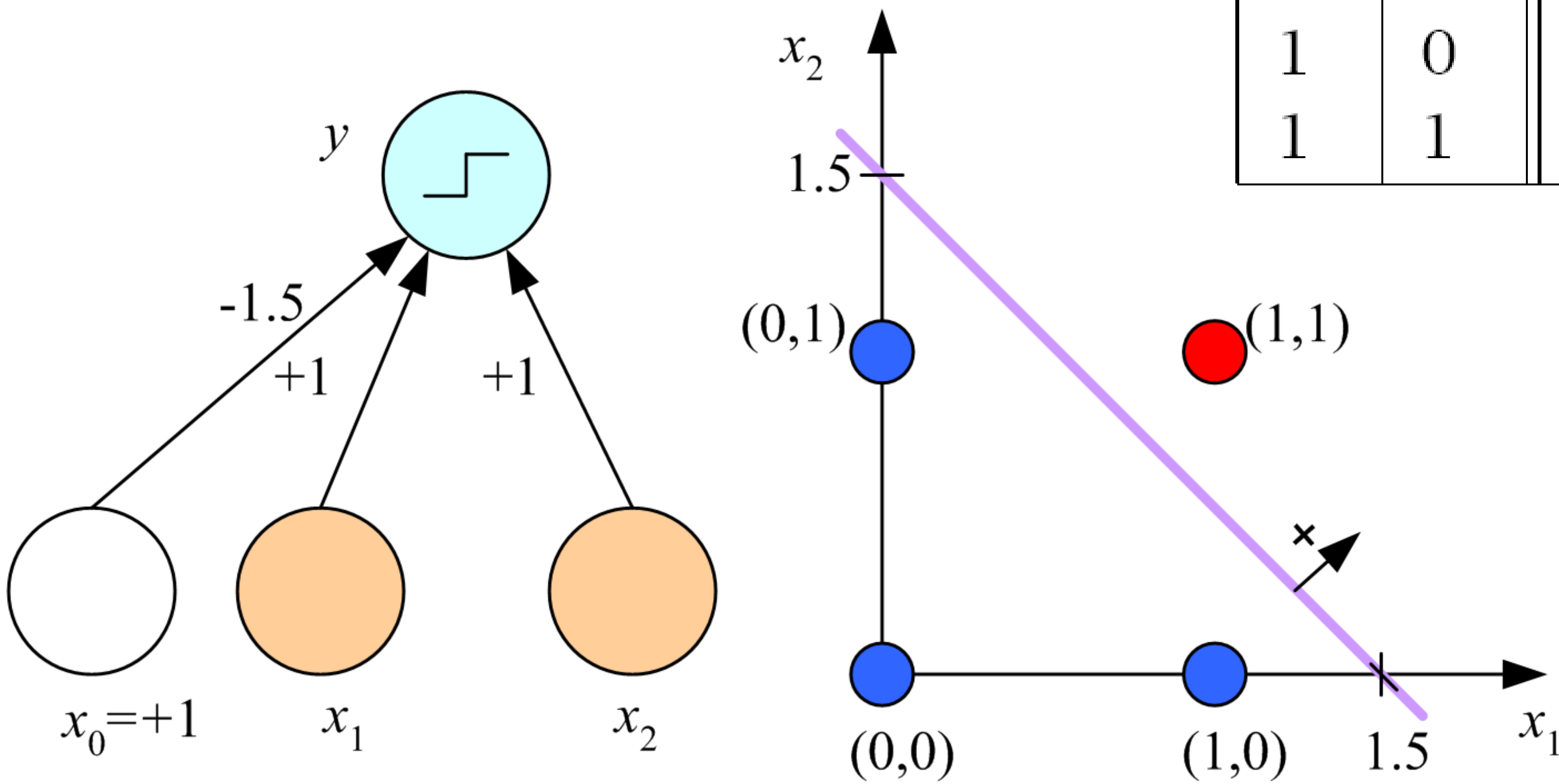
- K>2 softmax outputs

$$y^t = \frac{\exp \mathbf{w}_i^T \mathbf{x}^t}{\sum_k \exp \mathbf{w}_k^T \mathbf{x}^t} \qquad E^t\left(\{\mathbf{w}_i\}_i \mid \mathbf{x}^t, \mathbf{r}^t\right) = -\sum_i r_i^t \log y_i^t$$

$$\Delta w_{ij}^t = \eta\left(r_i^t - y_i^t\right) x_j^t$$

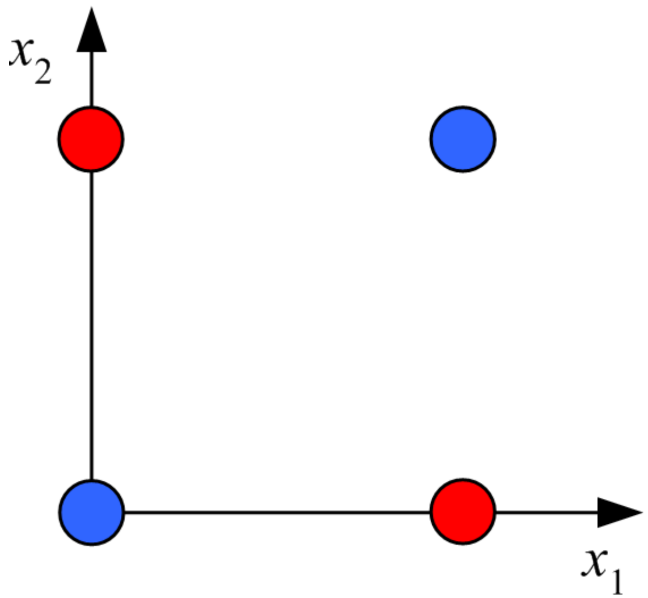
Learning Boolean AND

x_1	x_2	r
0	0	0
0	1	0
1	0	0
1	1	1



XOR

x_1	x_2	r
0	0	0
0	1	1
1	0	1
1	1	0

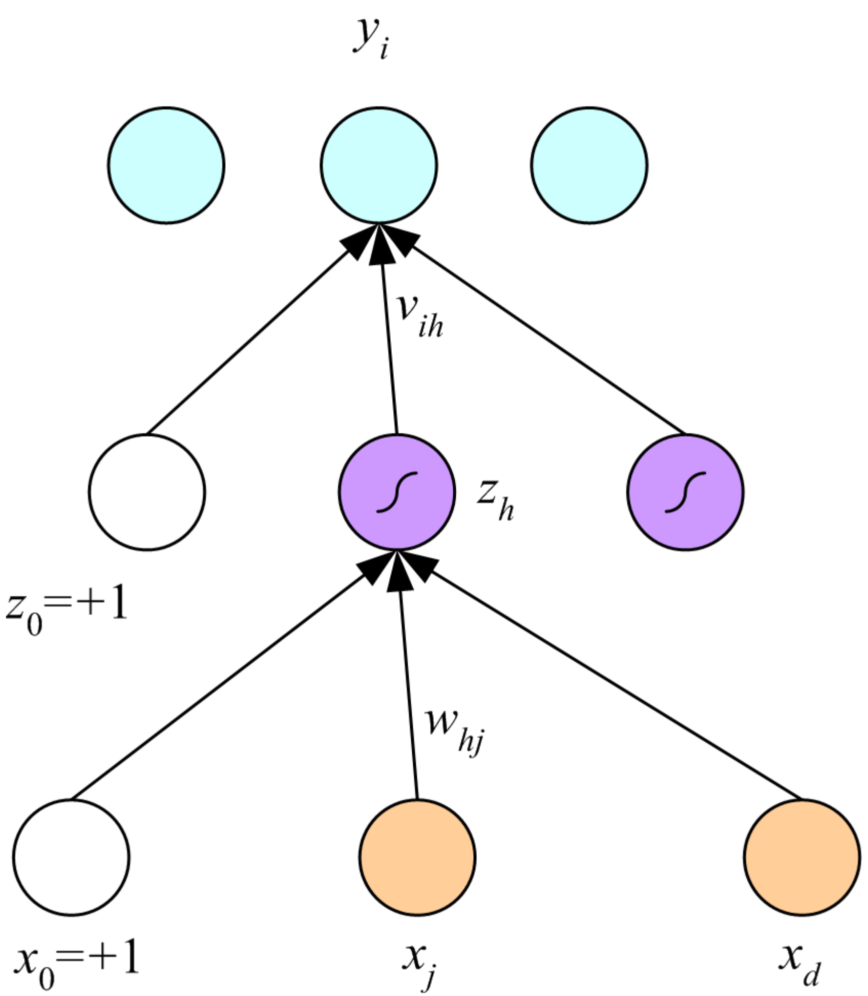


- No w_0, w_1, w_2 satisfy:

$$\begin{aligned} w_0 &\le 0 \\ w_2 + w_0 &> 0 \\ w_1 + w_0 &> 0 \\ w_1 + w_2 + w_0 &\le 0 \end{aligned}$$

(Minsky and Papert, 1969)

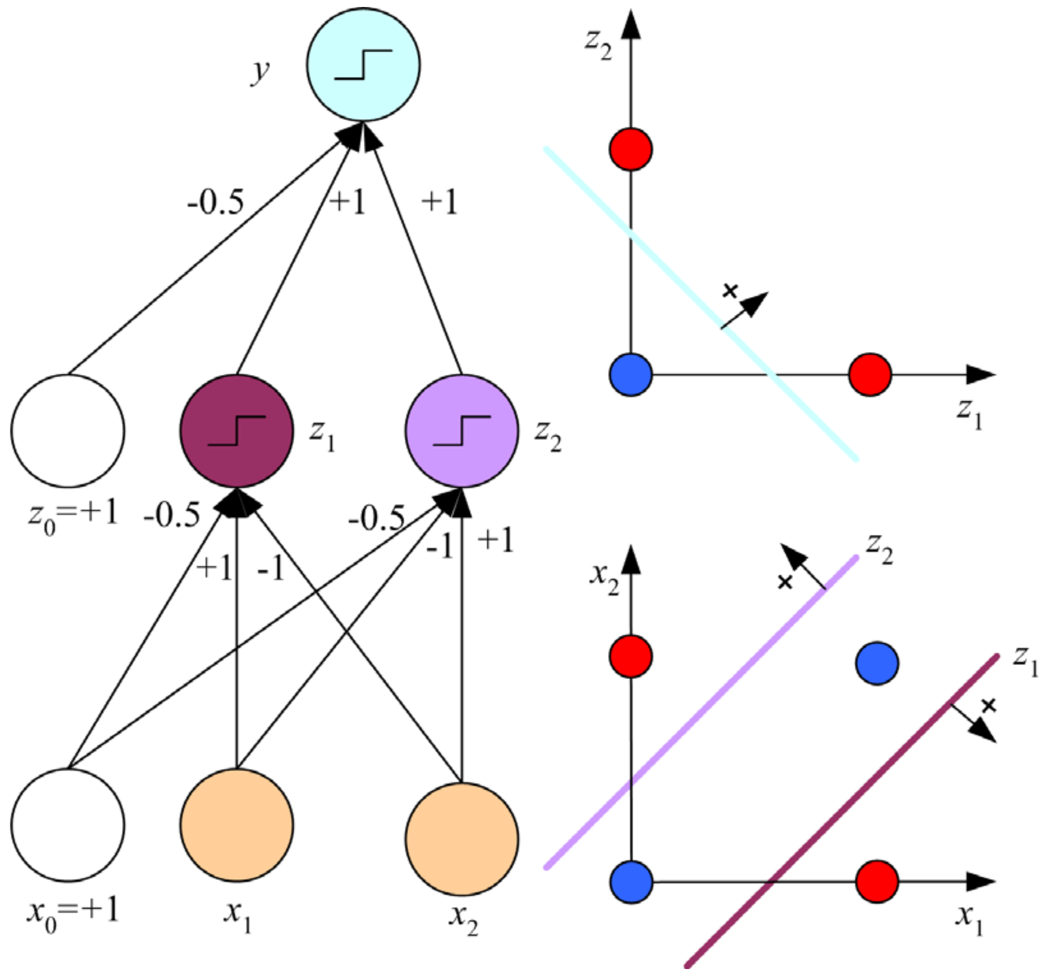
Multilayer Perceptrons



$$y_i = \mathbf{v}_i^T \mathbf{z} = \sum_{h=1}^{H} v_{ih} z_h + v_{i0}$$

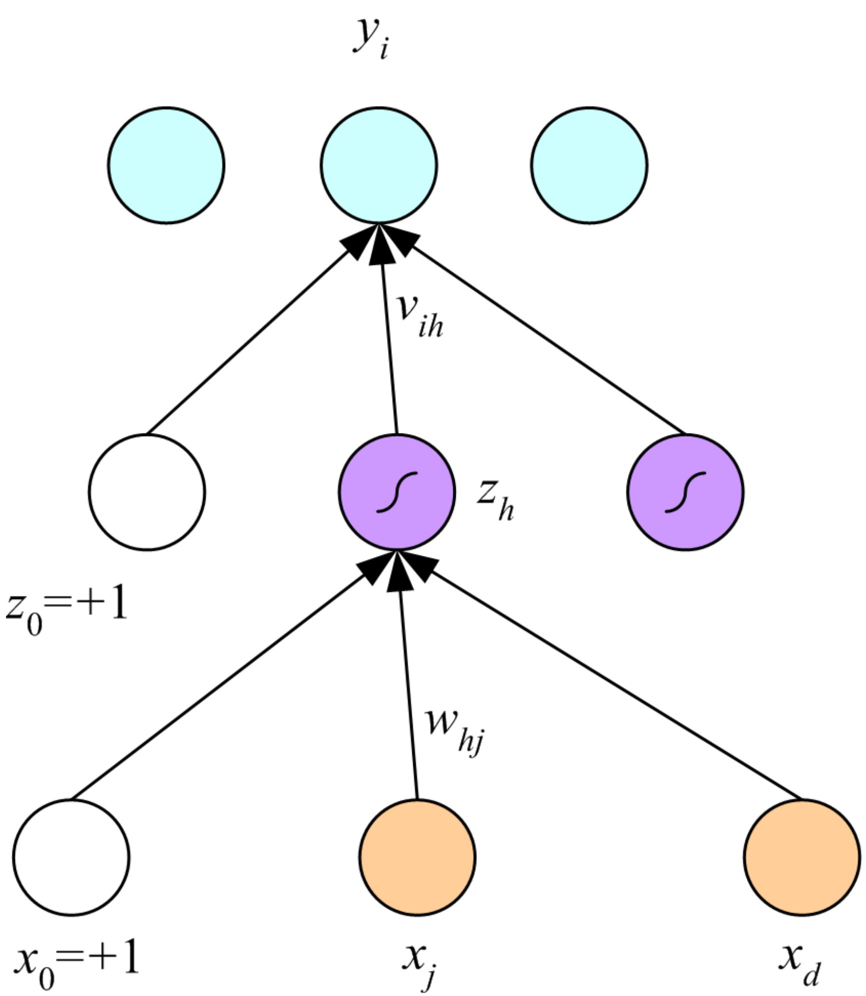
$$z_h = \text{sigmoid}\left(\mathbf{w}_h^T \mathbf{x}\right)$$
$$= \frac{1}{1 + \exp\left[-\left(\sum_{j=1}^{d} w_{hj} x_j + w_{h0}\right)\right]}$$

(Rumelhart et al., 1986)



x_1 XOR x_2 = (x_1 AND ~x_2) OR (~x_1 AND x_2)

Backpropagation



$$y_i = \mathbf{v}_i^T \mathbf{z} = \sum_{h=1}^{H} v_{ih} z_h + v_{i0}$$

$$z_h = \text{sigmoid}\left(\mathbf{w}_h^T \mathbf{x}\right)$$

$$= \frac{1}{1+\exp\left[-\left(\sum_{j=1}^{d} w_{hj} x_j + w_{h0}\right)\right]}$$

$$\boxed{\frac{\partial E}{\partial w_{hj}} = \frac{\partial E}{\partial y_i} \frac{\partial y_i}{\partial z_h} \frac{\partial z_h}{\partial w_{hj}}}$$

Regression

$$E(\mathbf{W},\mathbf{v}\,|\,\mathcal{X})=\frac{1}{2}\sum_t \left(r^t-y^t\right)^2$$

$$\boxed{\Delta v_h=\sum_t \left(r^t-y^t\right)z_h^t}$$

Backward

$$\boxed{\begin{aligned}\Delta w_{hj}&=-\eta\frac{\partial E}{\partial w_{hj}}\\&=-\eta\sum_t \frac{\partial E}{\partial y^t}\frac{\partial y^t}{\partial z_h^t}\frac{\partial z_h^t}{\partial w_{hj}}\\&=-\eta\sum_t -\left(r^t-y^t\right)v_h\boxed{z_h^t\left(1-z_h^t\right)}x_j^t\\&=\eta\sum_t \left(r^t-y^t\right)v_h z_h^t\left(1-z_h^t\right)x_j^t\end{aligned}}$$

$$y^t=\sum_{h=1}^{H} v_h z_h^t+v_0$$

Forward

$$z_h=\boxed{\text{sigmoid}}\left(\mathbf{w}_h^T\mathbf{x}\right)$$

$$\boldsymbol{x}$$

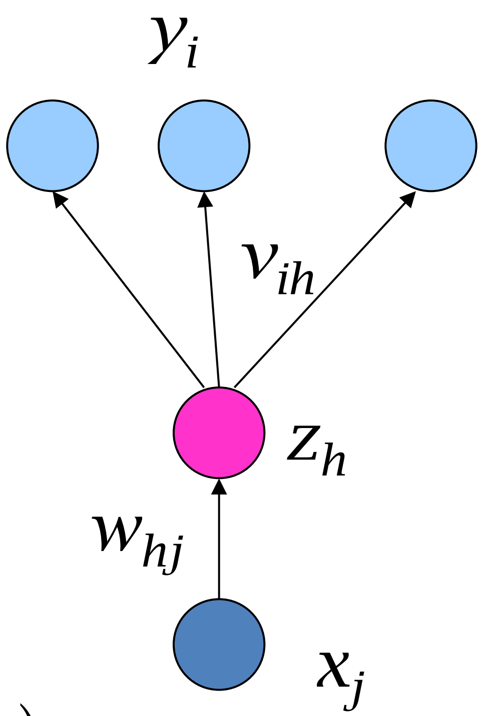
Regression with Multiple Outputs

$$E(\mathbf{W},\mathbf{V}\mid\mathcal{X})=\frac{1}{2}\sum_t\sum_i\left(r_i^t-y_i^t\right)^2$$

$$y_i^t=\sum_{h=1}^{H}v_{ih}z_h^t+v_{i0}$$

$$\Delta v_{ih}=\eta\sum_t\left(r_i^t-y_i^t\right)z_h^t$$

$$\Delta w_{hj}=\eta\sum_t\left[\sum_i\left(r_i^t-y_i^t\right)v_{ih}\right]z_h^t\left(1-z_h^t\right)x_j^t$$



Initialize all v_{ih} and w_{hj} to rand$(-0.01, 0.01)$

Repeat

    For all $(\boldsymbol{x}^t, r^t) \in \mathcal{X}$ in random order

        For $h = 1, \ldots, H$

            $z_h \leftarrow \mathrm{sigmoid}(\boldsymbol{w}_h^T \boldsymbol{x}^t)$

        For $i = 1, \ldots, K$

            $y_i = \boldsymbol{v}_i^T \boldsymbol{z}$

        For $i = 1, \ldots, K$

            $\Delta \boldsymbol{v}_i = \eta(r_i^t - y_i^t)\boldsymbol{z}$

        For $h = 1, \ldots, H$

            $\Delta \boldsymbol{w}_h = \eta(\sum_i (r_i^t - y_i^t) v_{ih}) z_h (1 - z_h) \boldsymbol{x}^t$

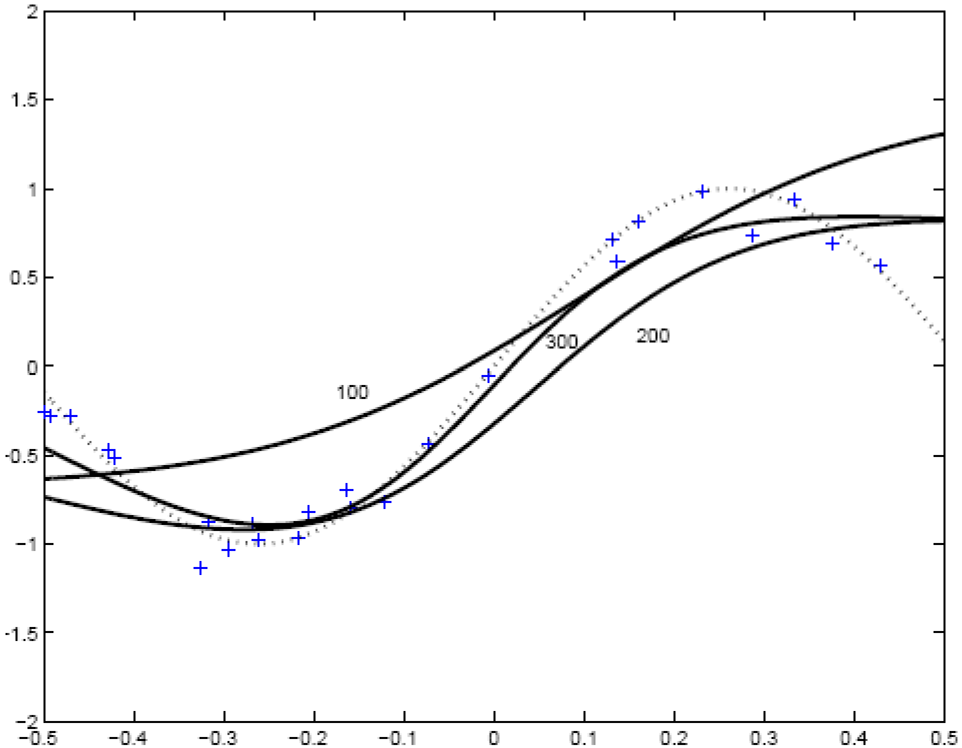
        For $i = 1, \ldots, K$

            $\boldsymbol{v}_i \leftarrow \boldsymbol{v}_i + \Delta \boldsymbol{v}_i$

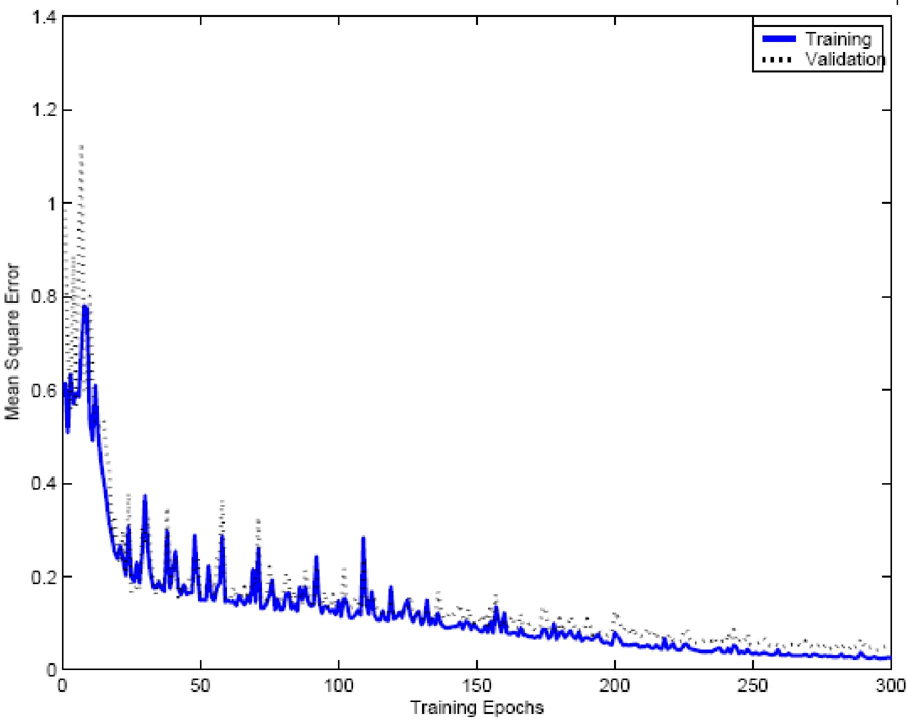
        For $h = 1, \ldots, H$

            $\boldsymbol{w}_h \leftarrow \boldsymbol{w}_h + \Delta \boldsymbol{w}_h$

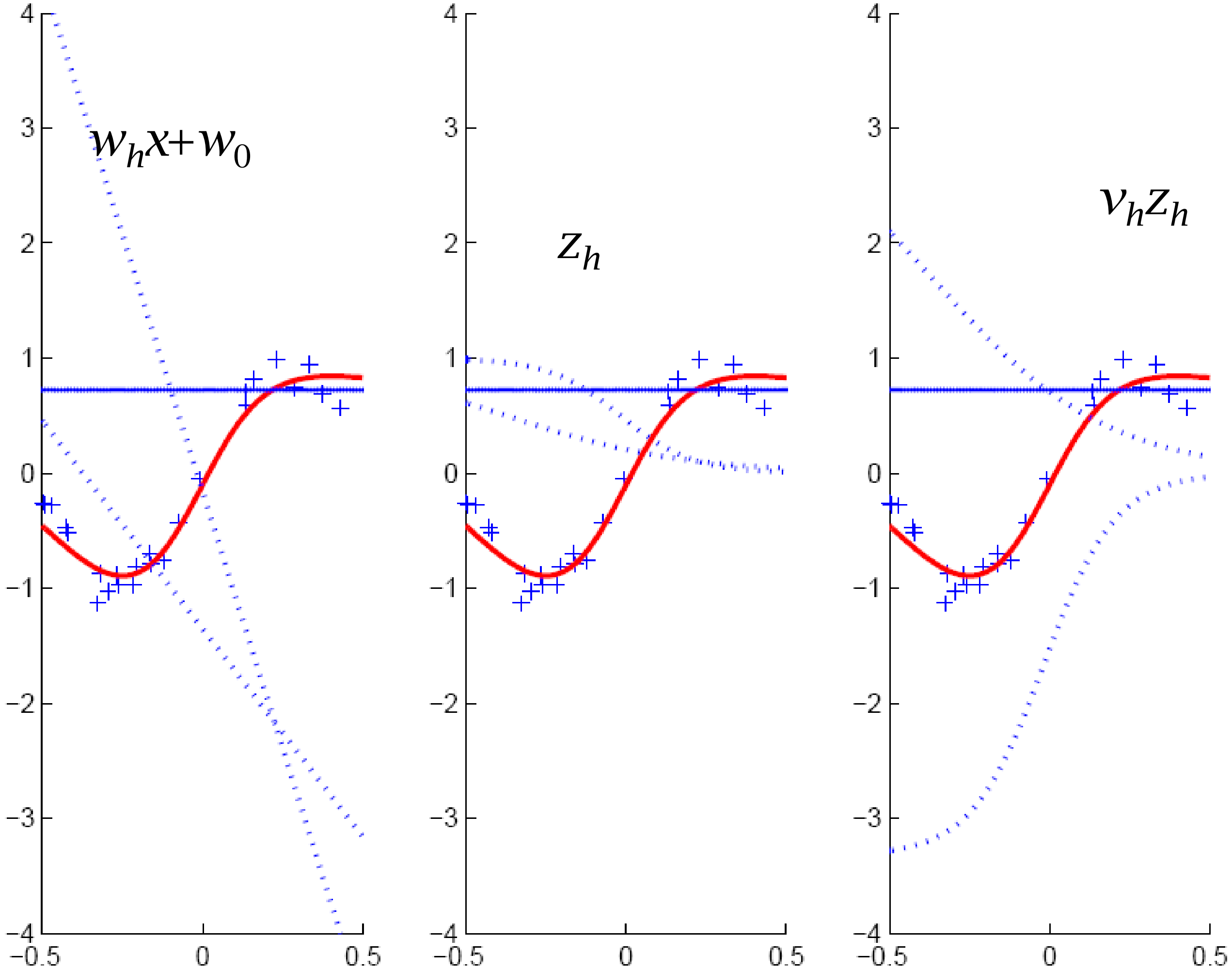
Until convergence



100
300
200



Training
Validation
Mean Square Error
Training Epochs


$w_h x + w_0$
z_h
$v_h z_h$
4
3
2
1
0
−1
−2
−3
−4
−0.5
0
0.5

Two-Class Discrimination

- One sigmoid output y^t for $P(C_1|x^t)$ and $P(C_2|x^t) \equiv 1-y^t$

$$y^t = \text{sigmoid}\left(\sum_{h=1}^{H} v_h z_h^t + v_0\right)$$

$$E(\mathbf{W},\mathbf{v}|\mathcal{X}) = -\sum_t r^t \log y^t + \left(1-r^t\right)\log\left(1-y^t\right)$$

$$\Delta v_h = \eta \sum_t \left(r^t - y^t\right) z_h^t$$

$$\Delta w_{hj} = \eta \sum_t \left(r^t - y^t\right) v_h z_h^t \left(1 - z_h^t\right) x_j^t$$

$K > 2$ Classes

$$o_i^t = \sum_{h=1}^{H} v_{ih} z_h^t + v_{i0} \qquad y_i^t = \frac{\exp o_i^t}{\sum_k \exp o_k^t} \equiv P(C_i \mid \mathbf{x}^t)$$

$$E(\mathbf{W}, \mathbf{v} \mid \mathcal{X}) = -\sum_t \sum_i r_i^t \log y_i^t$$

$$\Delta v_{ih} = \eta \sum_t \left(r_i^t - y_i^t\right) z_h^t$$

$$\Delta w_{hj} = \eta \sum_t \left[\sum_i \left(r_i^t - y_i^t\right) v_{ih} \right] z_h^t \left(1 - z_h^t\right) x_j^t$$

Multiple Hidden Layers

- MLP with one hidden layer is a universal approximator (Hornik et al., 1989), but using multiple layers may lead to simpler networks

$$z_{1h} = \text{sigmoid}\left(\mathbf{w}_{1h}^T \mathbf{x}\right) = \text{sigmoid}\left(\sum_{j=1}^{d} w_{1hj} x_j + w_{1h0}\right), h = 1, \ldots, H_1$$

$$z_{2l} = \text{sigmoid}\left(\mathbf{w}_{2l}^T \mathbf{z}_1\right) = \text{sigmoid}\left(\sum_{h=1}^{H_1} w_{2lh} z_{1h} + w_{2l0}\right), l = 1, \ldots, H_2$$

$$y = \mathbf{v}^T \mathbf{z}_2 = \sum_{l=1}^{H_2} v_l z_{2l} + v_0$$

Improving Convergence

- Momentum

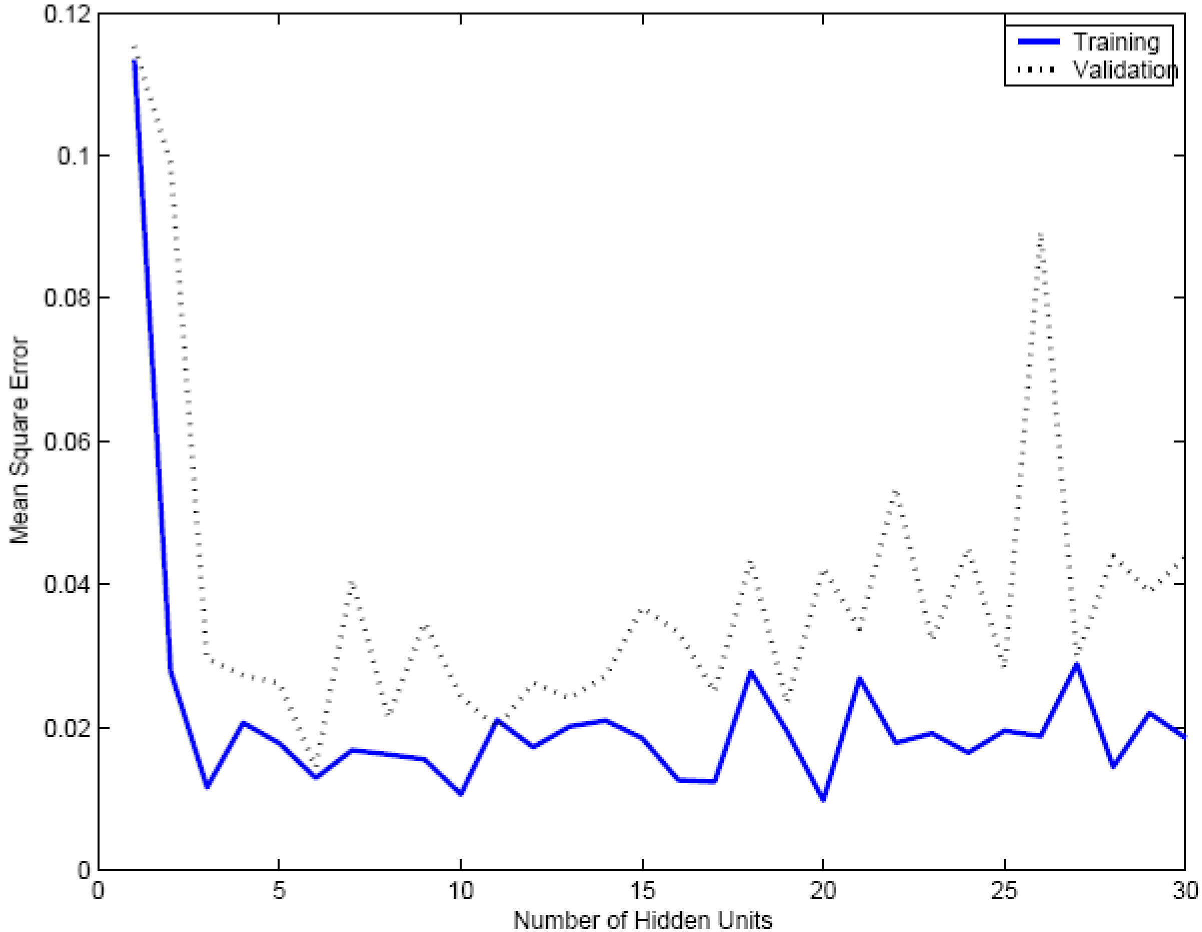
$$\Delta w_i^t = -\eta \frac{\partial E^t}{\partial w_i} + \alpha \Delta w_i^{t-1}$$

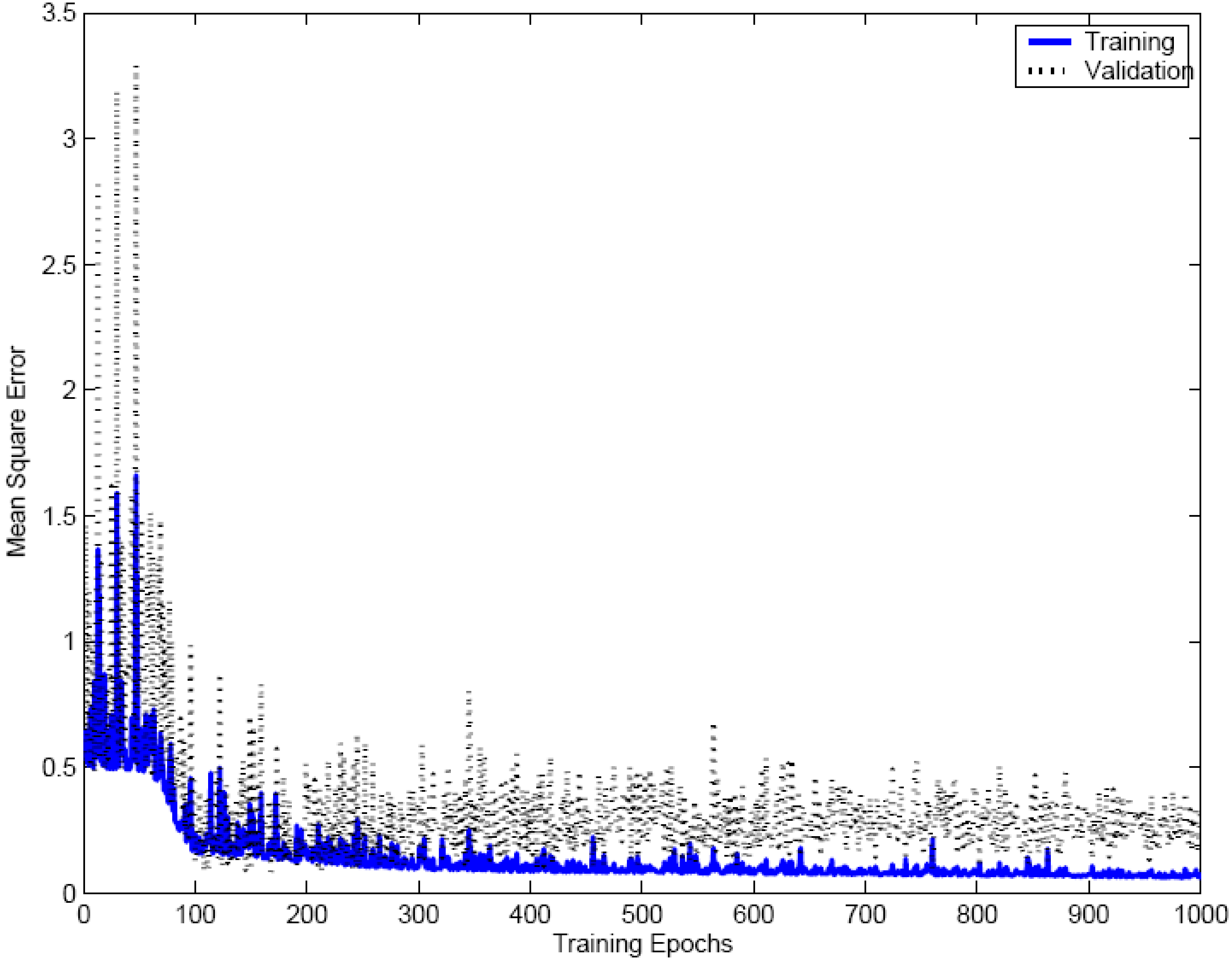
- Adaptive learning rate

$$\Delta \eta = \begin{cases} +a & \text{if } E^{t+\tau} < E^t \\ -b\eta & \text{otherwise} \end{cases}$$

Overfitting/Overtraining

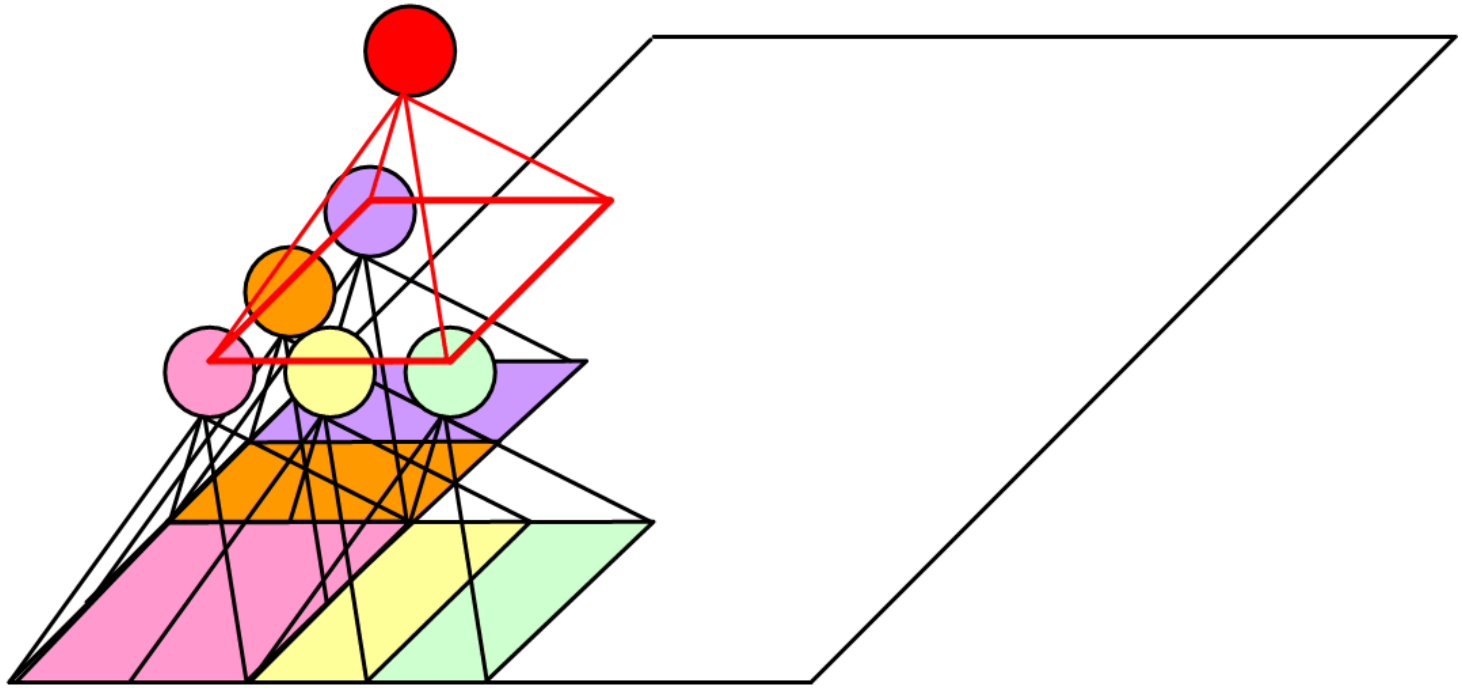
Number of weights: $H\ (d+1)+(H+1)K$





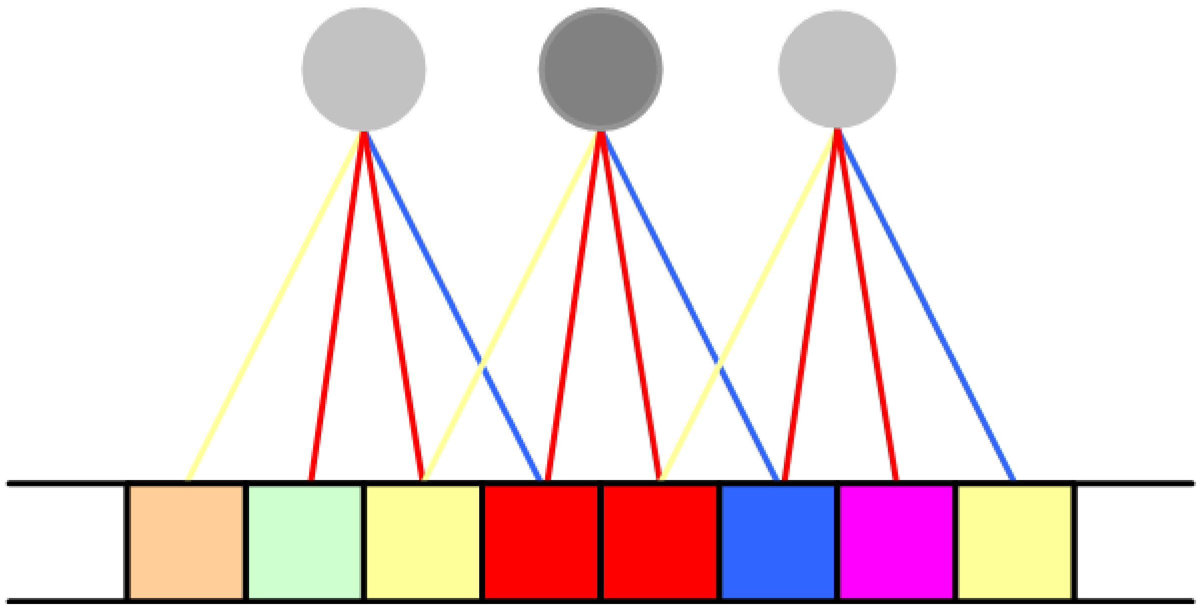
Training
Validation
Mean Square Error
Training Epochs
0
0.5
1
1.5
2
2.5
3
3.5
0
100
200
300
400
500
600
700
800
900
1000

Structured MLP



(Le Cun et al, 1989)

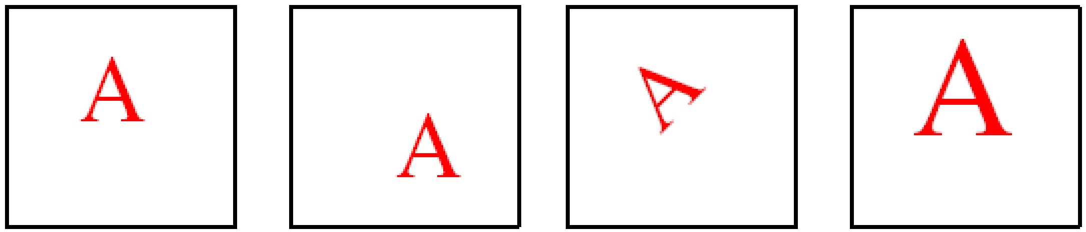
Weight Sharing



Hints

(Abu-Mostafa, 1995)

- Invariance to translation, rotation, size



- Virtual examples
- Augmented error: $E' = E + \lambda_h E_h$

If $\boldsymbol{x'}$ and $\boldsymbol{x}$ are the “same”: $E_h = [g(x|\theta) - g(x'|\theta)]^2$

Approximation hint:

$$E_h = \begin{cases} 0 & \text{if } g(x|\theta) \in [a_x, b_x] \\ (g(x|\theta) - a_x)^2 & \text{if } g(x|\theta) < a_x \\ (g(x|\theta) - b_x)^2 & \text{if } g(x|\theta) > b_x \end{cases}$$

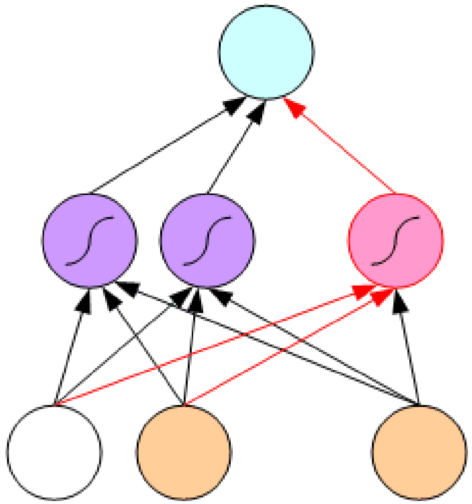
Tuning the Network Size

- Destructive
- Weight decay:

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i} - \lambda w_i$$

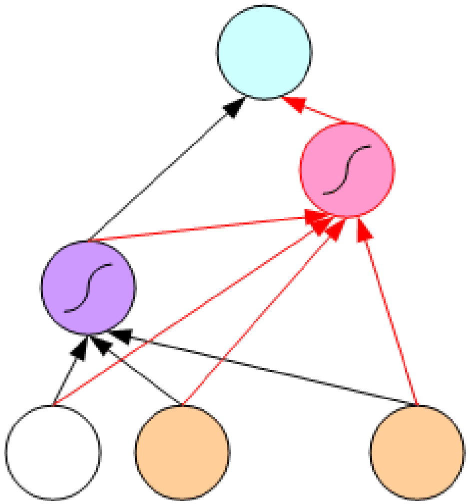
$$E' = E + \frac{\lambda}{2} \sum_i w_i^2$$

- Constructive
- Growing networks



Dynamic Node Creation

(Ash, 1989)



Cascade Correlation

(Fahlman and Lebiere, 1989)

Bayesian Learning

- Consider weights w_i as random vars, prior $p(w_i)$

$$p(\mathbf{w}|\mathcal{X}) = \frac{p(\mathcal{X}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{X})} \quad \hat{\mathbf{w}}_{MAP} = \arg\max_{\mathbf{w}} \log p(\mathbf{w}|\mathcal{X})$$

$$\log p(\mathbf{w}|\mathcal{X}) = \log p(\mathcal{X}|\mathbf{w}) + \log p(\mathbf{w}) + C$$

$$p(\mathbf{w}) = \prod_i p(w_i) \text{ where } p(w_i) = c \cdot \exp\left[-\frac{w_i^2}{2(1/2\lambda)}\right]$$

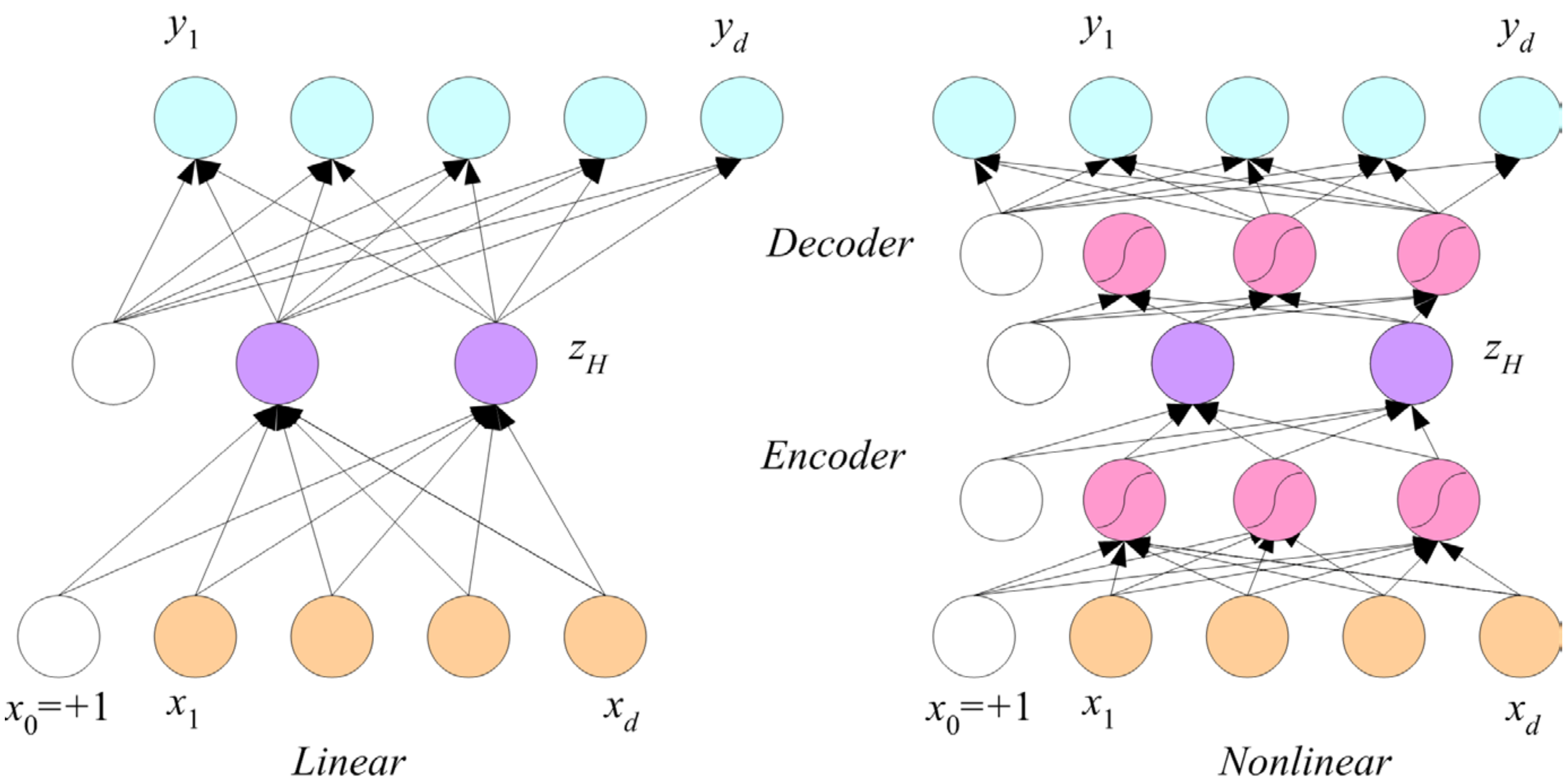
$$E' = E + \lambda\|\mathbf{w}\|^2$$

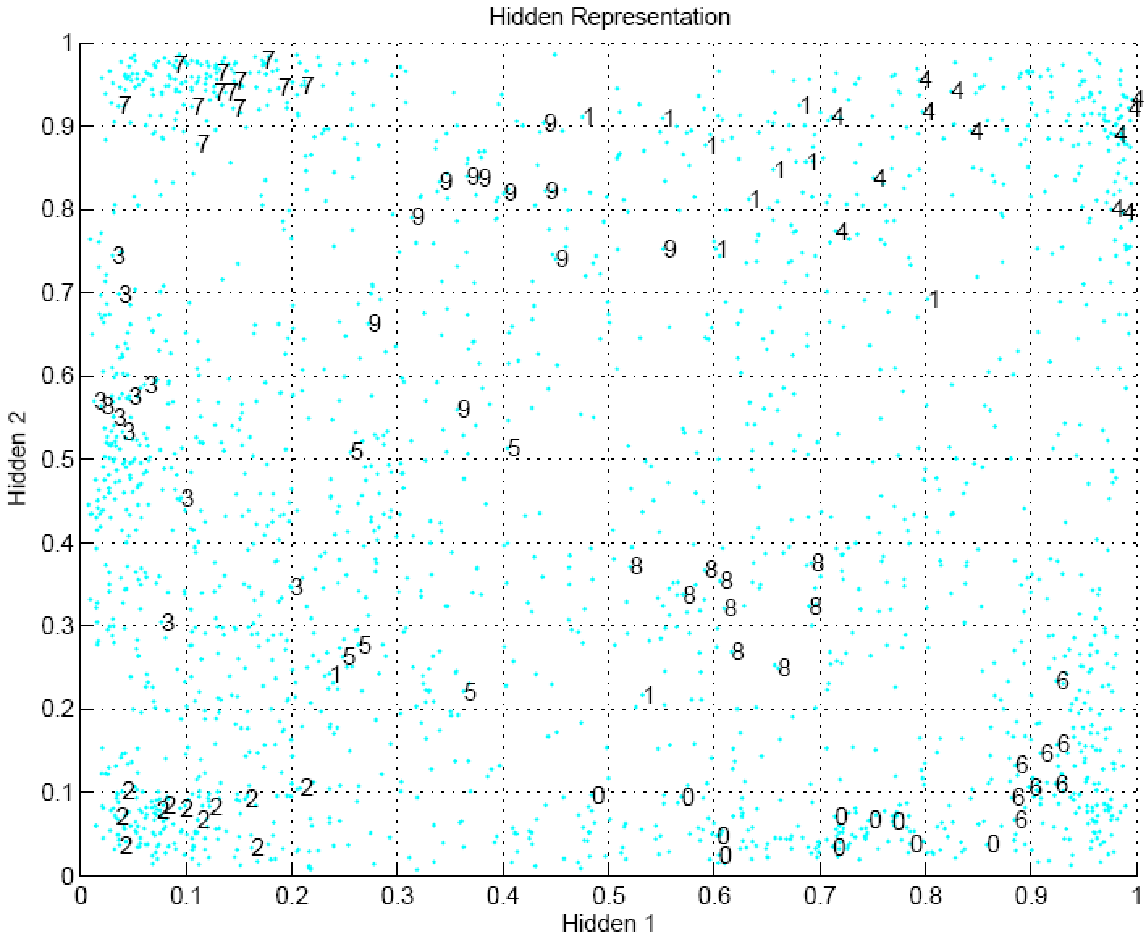
- Weight decay, ridge regression, regularization

  cost=data-misfit + λ complexity

  More about Bayesian methods in chapter 14

Dimensionality Reduction

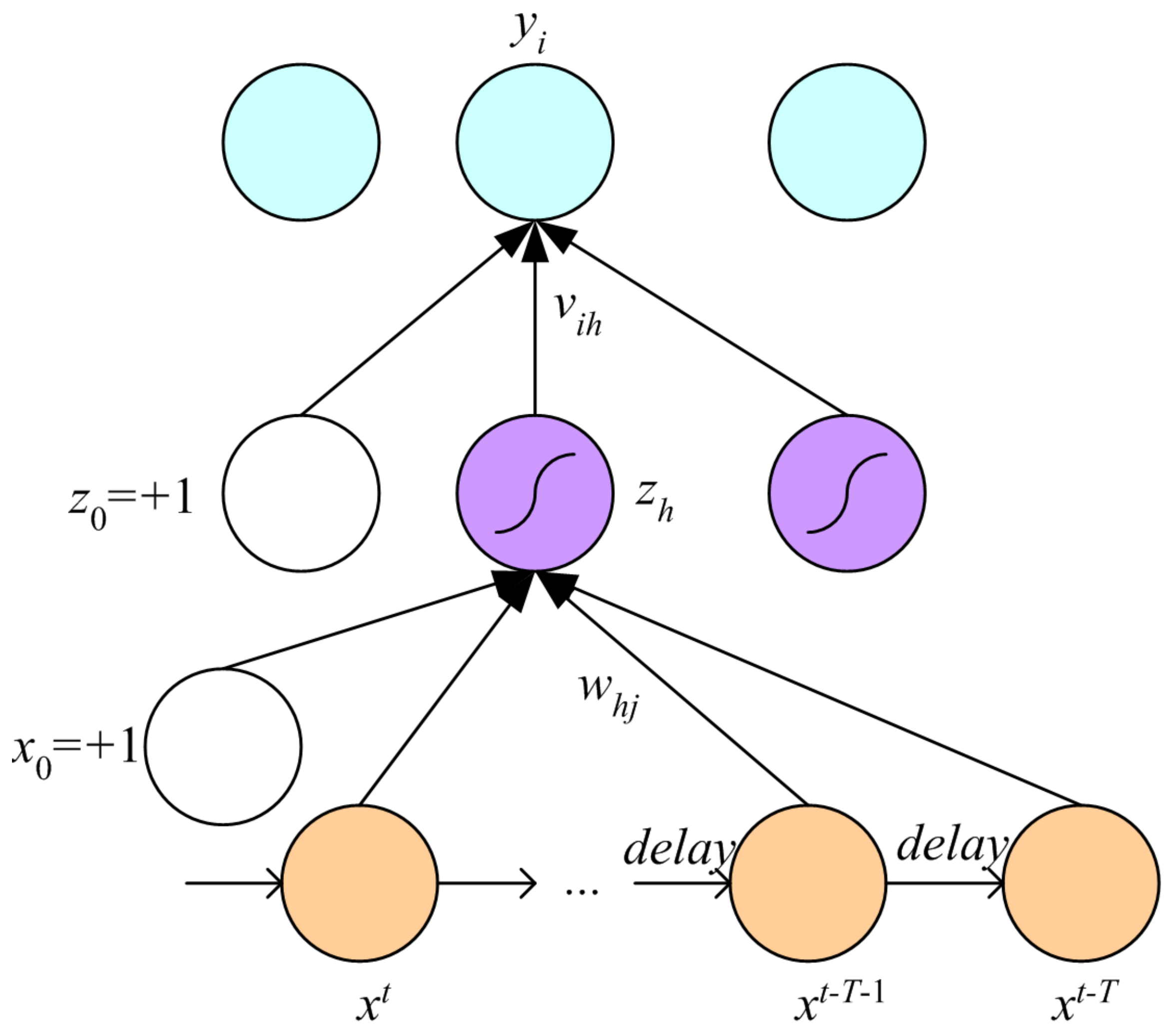



Hidden Representation
Hidden 2
Hidden 1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

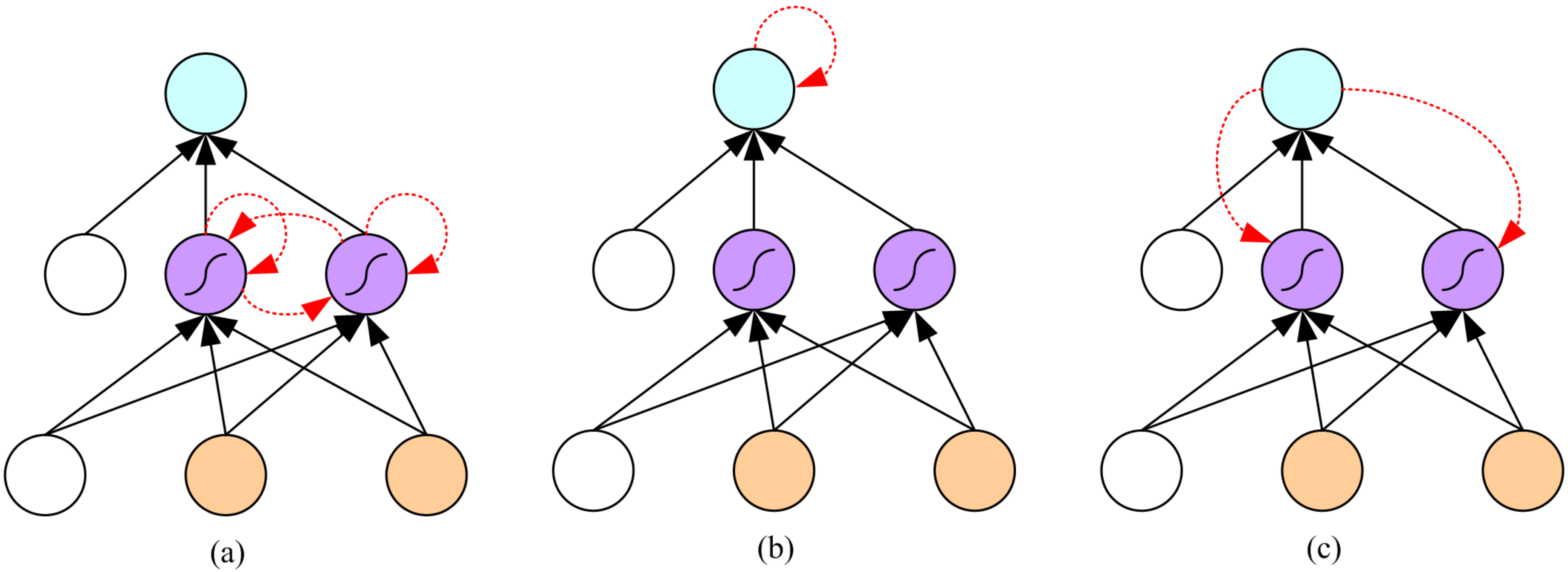
Learning Time

- Applications:
  - Sequence recognition: Speech recognition
  - Sequence reproduction: Time-series prediction
  - Sequence association
- Network architectures
  - Time-delay networks (Waibel et al., 1989)
  - Recurrent networks (Rumelhart et al., 1986)

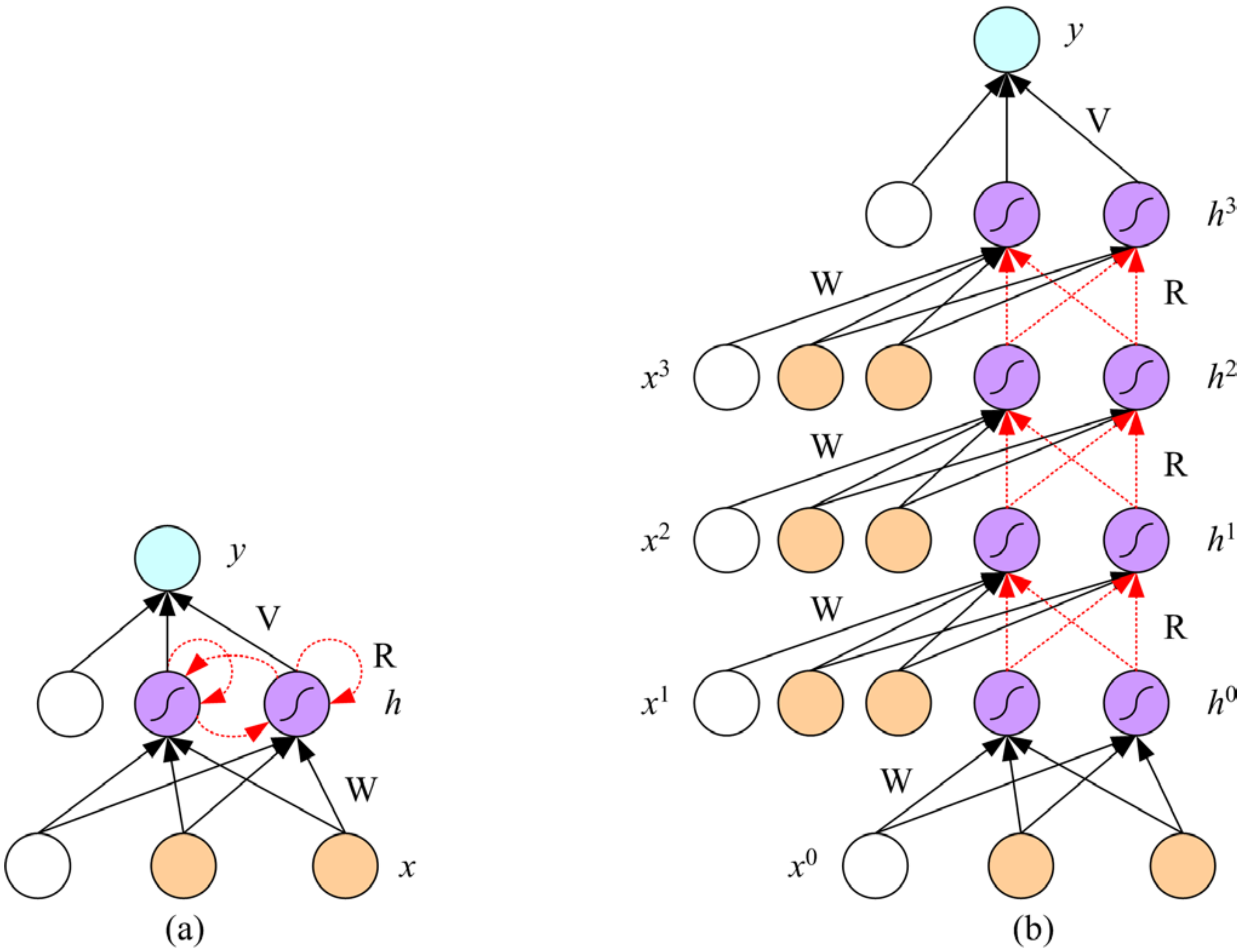
Time-Delay Neural Networks



Recurrent Networks



Unfolding in Time



Kernel Machines

- Discriminant-based: No need to estimate densities first
- Define the discriminant in terms of support vectors
- The use of kernel functions, application-specific measures of similarity
- No need to represent instances as vectors
- Convex optimization problems with a unique solution

Optimal Separating Hyperplane

$$\mathcal{X} = \{\mathbf{x}^t, r^t\}_t \text{ where } r^t = \begin{cases} +1 & \text{if } \mathbf{x}^t \in C_1 \\ -1 & \text{if } \mathbf{x}^t \in C_2 \end{cases}$$

find $\mathbf{w}$ and w_0 such that

$$\mathbf{w}^T\mathbf{x}^t + w_0 \geq +1 \text{ for } r^t = +1$$

$$\mathbf{w}^T\mathbf{x}^t + w_0 \leq +1 \text{ for } r^t = -1$$

which can be rewritten as

$$r^t\left(\mathbf{w}^T\mathbf{x}^t + w_0\right) \geq +1$$

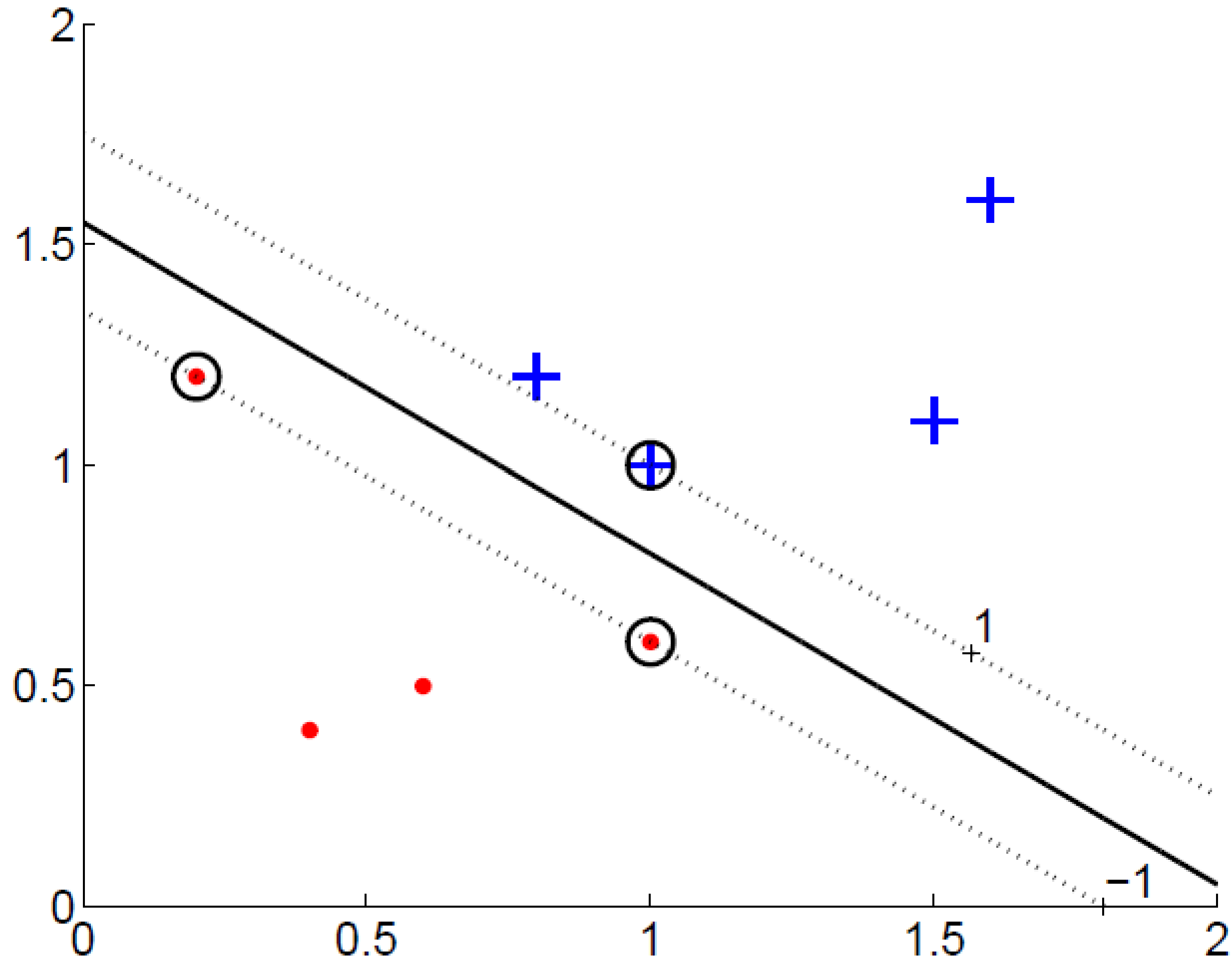
(Cortes and Vapnik, 1995; Vapnik, 1995)

Margin

- Distance from the discriminant to the closest instances on either side
- Distance of x to the hyperplane is $\frac{\left|\mathbf{w}^T\mathbf{x}^t + w_0\right|}{\|\mathbf{w}\|}$
- We require $\frac{r^t\left(\mathbf{w}^T\mathbf{x}^t + w_0\right)}{\|\mathbf{w}\|} \geq \rho, \forall t$
- For a unique sol'n, fix $\rho\|w\|=1$, and to max margin

$$\min \frac{1}{2}\|\mathbf{w}\|^2 \text{ subject to } r^t\left(\mathbf{w}^T\mathbf{x}^t + w_0\right) \geq +1, \forall t$$

Margin



$$\min \frac{1}{2}\|\mathbf{w}\|^2 \text{ subject to } r^t\left(\mathbf{w}^T\mathbf{x}^t + w_0\right) \geq +1, \forall t$$

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{t=1}^{N} \alpha^t \left[r^t\left(\mathbf{w}^T\mathbf{x}^t + w_0\right) - 1 \right]$$

$$= \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{t=1}^{N} \alpha^t r^t \left(\mathbf{w}^T\mathbf{x}^t + w_0\right) + \sum_{t=1}^{N} \alpha^t$$

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_{t=1}^{N} \alpha^t r^t \mathbf{x}^t$$

$$\frac{\partial L_p}{\partial w_0} = 0 \Rightarrow \sum_{t=1}^{N} \alpha^t r^t = 0$$

$$L_d = \frac{1}{2}\left(\mathbf{w}^T\mathbf{w}\right) - \mathbf{w}^T\sum_t \alpha^t r^t \mathbf{x}^t - w_0 \sum_t \alpha^t r^t + \sum_t \alpha^t$$

$$= -\frac{1}{2}\left(\mathbf{w}^T\mathbf{w}\right) + \sum_t \alpha^t$$

$$= -\frac{1}{2}\sum_t\sum_s \alpha^t \alpha^s r^t r^s \left(\mathbf{x}^t\right)^T \mathbf{x}^s + \sum_t \alpha^t$$

subject to $\sum_{\mathrm{t}} \alpha^t r^t = 0$ and $\alpha^t \geq 0, \forall t$

Most α^t are 0 and only a small number have $\alpha^t > 0$; they are the support vectors

Soft Margin Hyperplane

- Not linearly separable

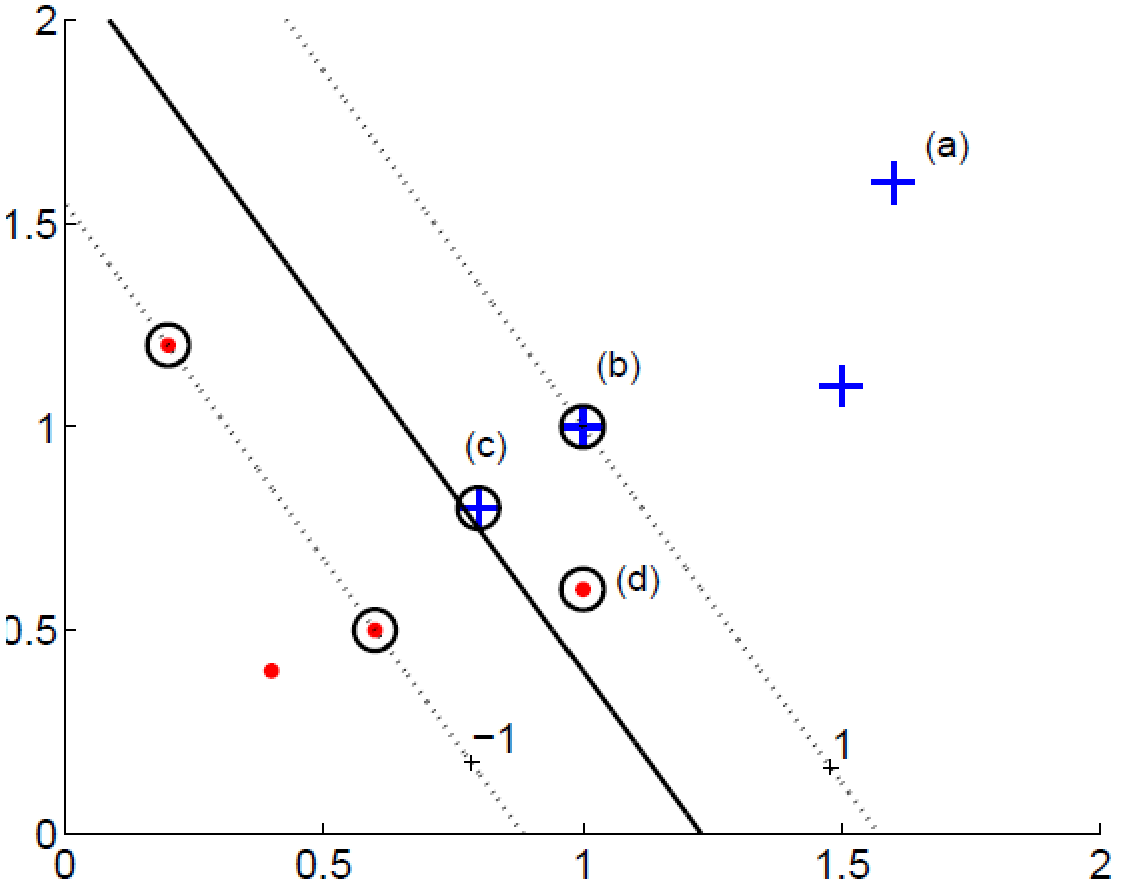
$$r^t\left(\mathbf{w}^T x^t + w_0\right) \geq 1 - \xi^t$$

- Soft error

$$\sum_t \xi^t$$

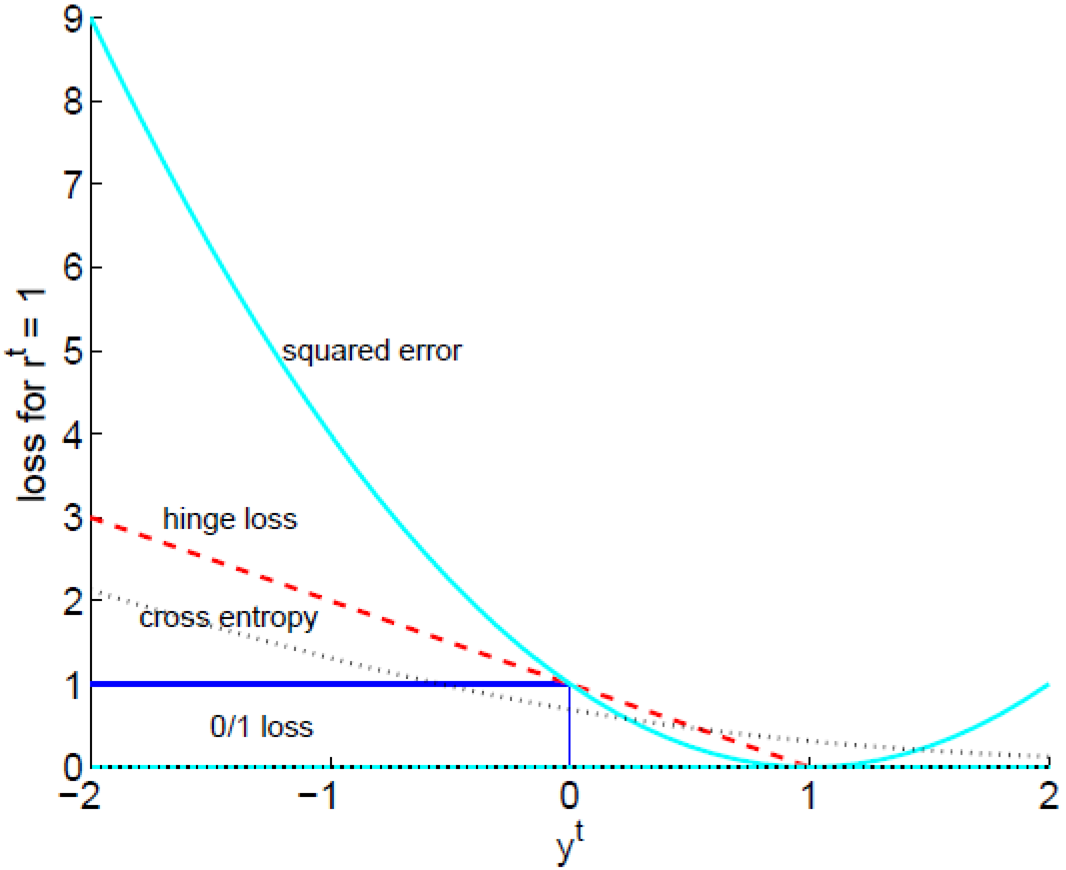
- New primal is

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_t \xi^t - \sum_t \alpha^t\left[r^t\left(\mathbf{w}^T x^t + w_0\right) - 1 + \xi^t\right] - \sum_t \mu^t \xi^t$$


(a)
(b)
(c)
(d)
−1
1
0
0.5
1
1.5
2

Hinge Loss

$$L_{hinge}(y^t, r^t) = \begin{cases} 0 & \text{if } y^t r^t \geq 1 \\ 1 - y^t r^t & \text{otherwise} \end{cases}$$



ν-SVM

$$\min \frac{1}{2}\|\mathbf{w}\|^2 - \nu\rho + \frac{1}{N}\sum_t \xi^t$$

subject to

$$r^t\left(\mathbf{w}^T\mathbf{x}^t + w_0\right) \geq \rho - \xi^t, \xi^t \geq 0, \rho \geq 0$$

$$L_d = -\frac{1}{2}\sum_{t=1}^{N}\sum_s \alpha^t\alpha^s r^t r^s \left(x^t\right)^T x^s$$

subject to

$$\sum_{\mathrm{t}} \alpha^t r^t = 0, 0 \leq \alpha^t \leq \frac{1}{N}, \sum_t \alpha^t \leq \nu$$

ν controls the fraction of support vectors