Artificial Neural Networks

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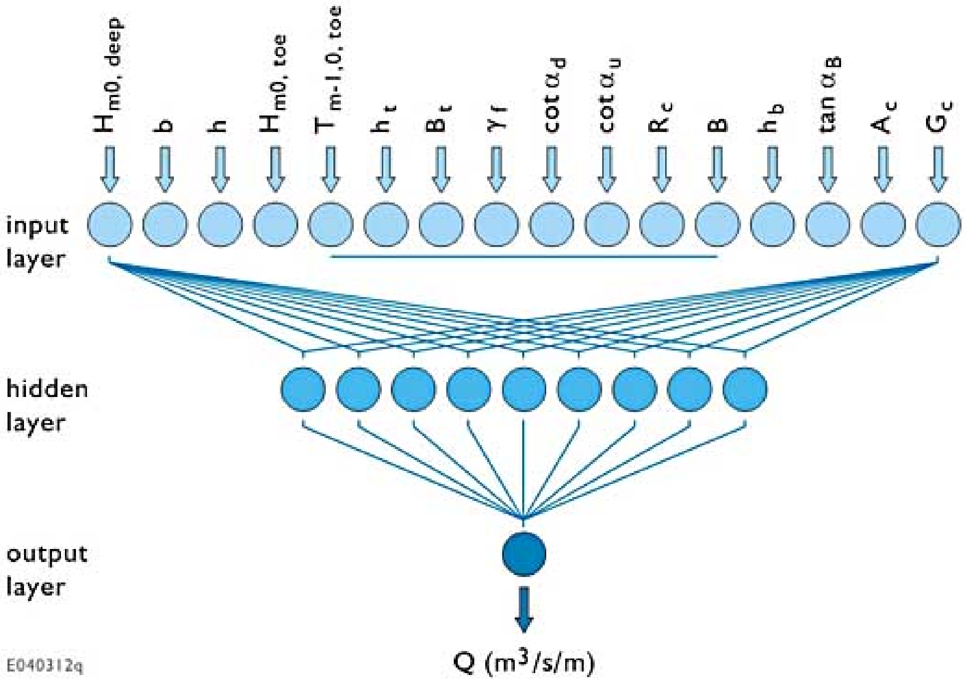


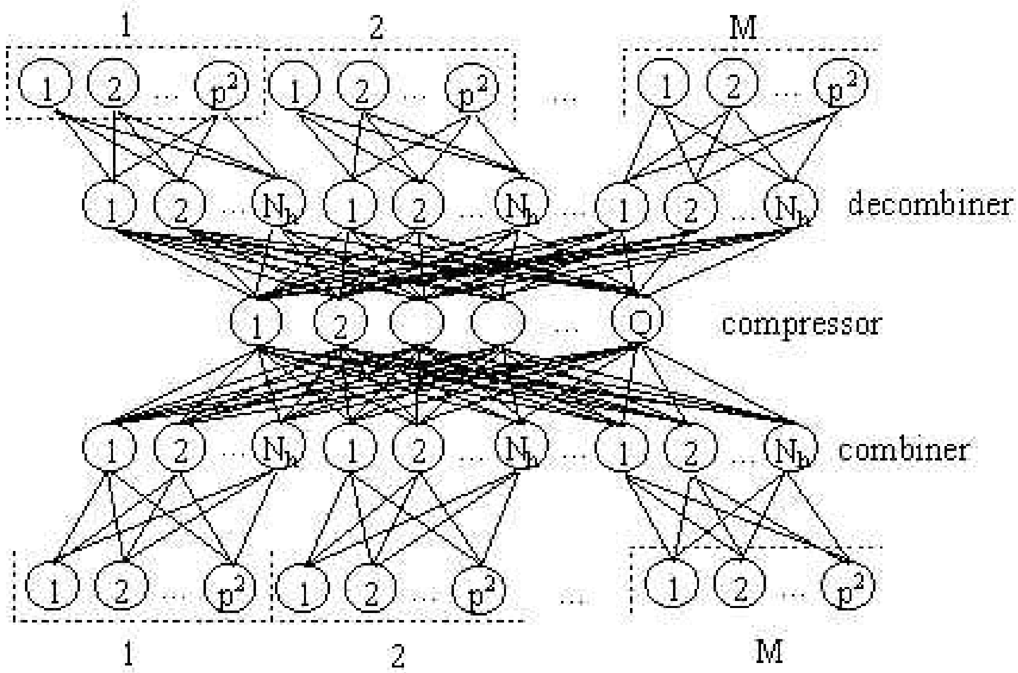
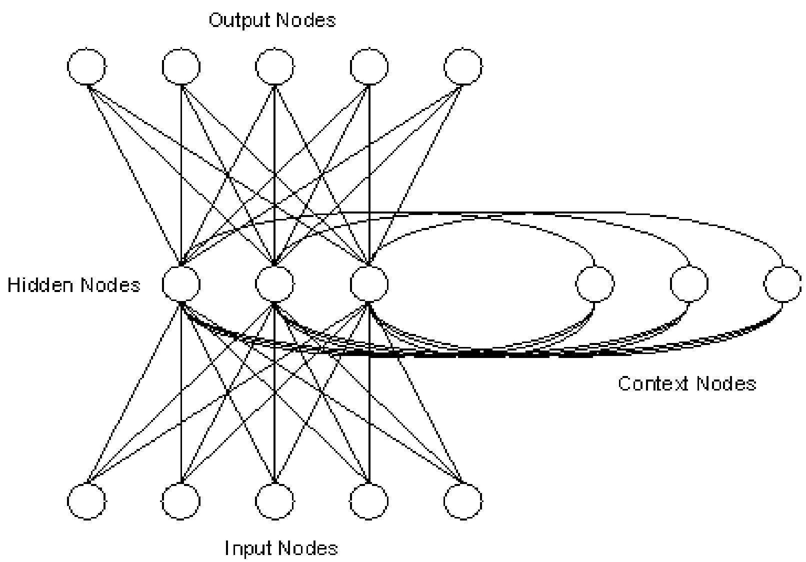
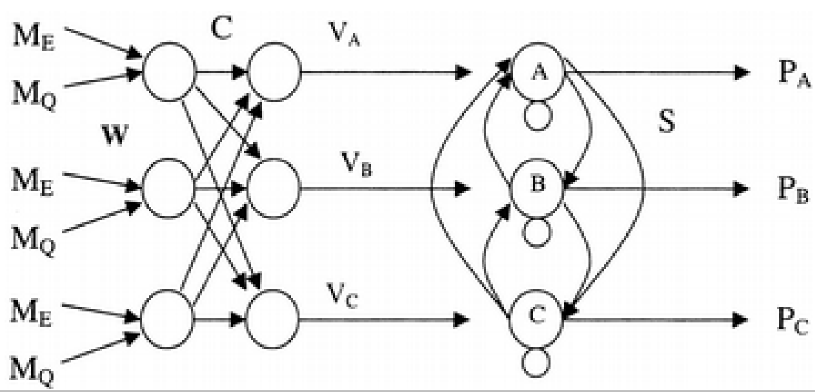
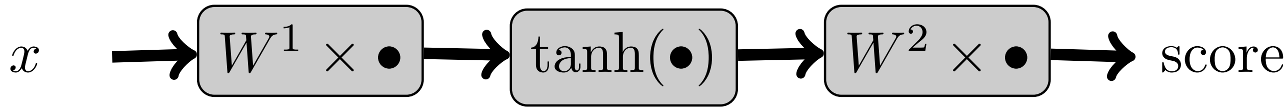


Figure 2 *Hierarchical neural network structure*



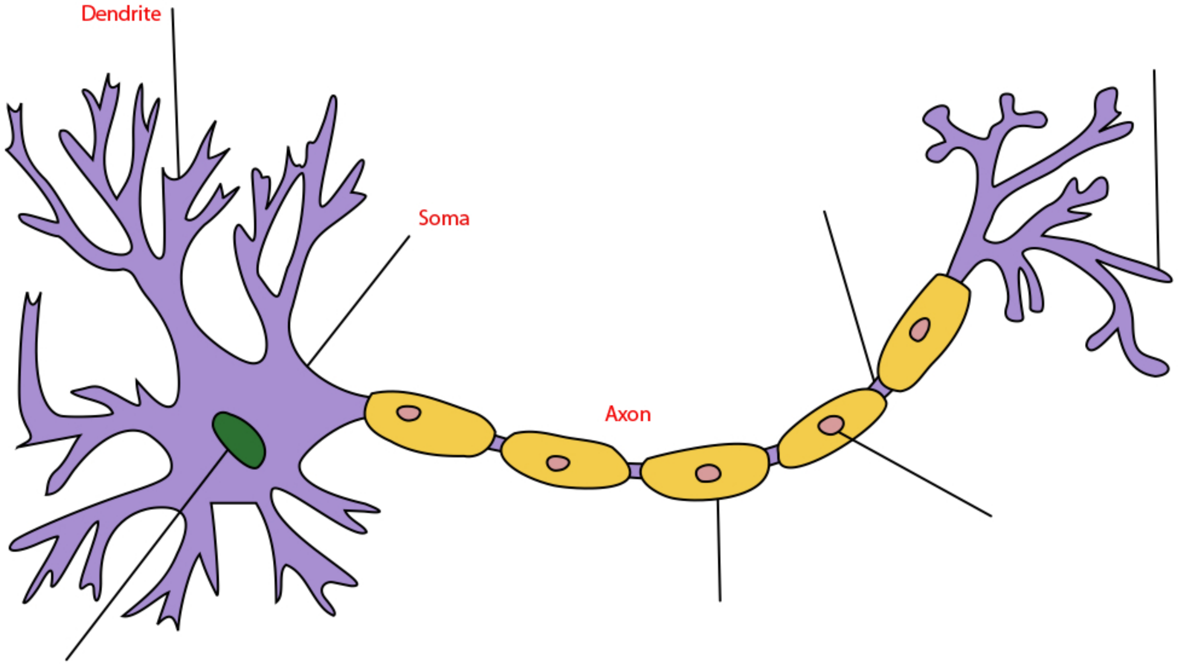


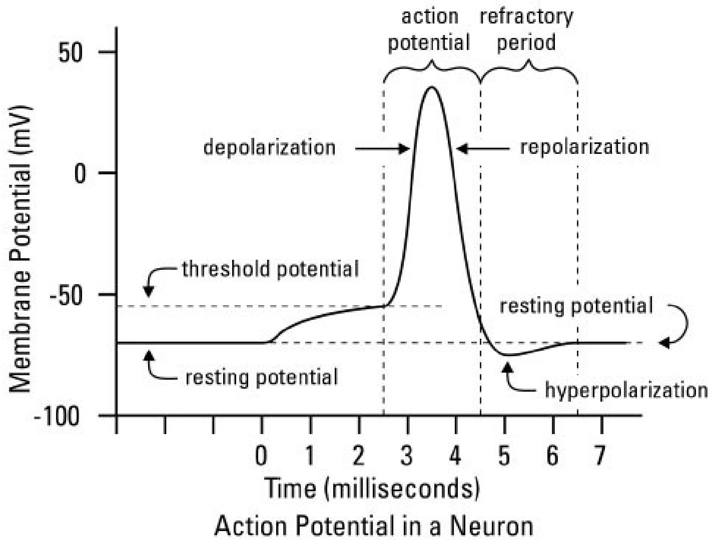
Introduction: Neural Networks in 2011



- Stack matrix-vector multiplications interleaved with non-linearity

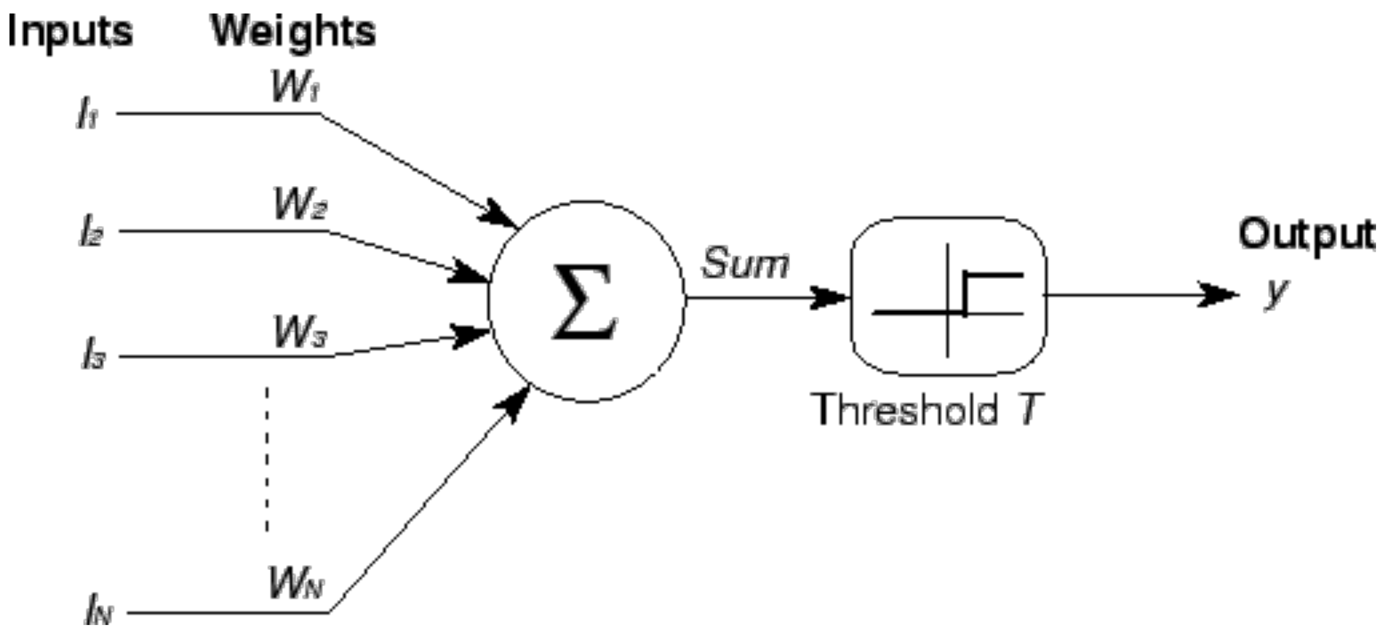
- Where does this come from?
- How to train them?
- Why does it generalize?
- What about real-life inputs (other than vectors x)?
- Any applications?





- Dendrites connected to other neurons through synapses
- Excitatory and inhibitory signals are integrated
- If stimulus reaches a threshold, the neuron fires along the axon

- Neuron as linear threshold units

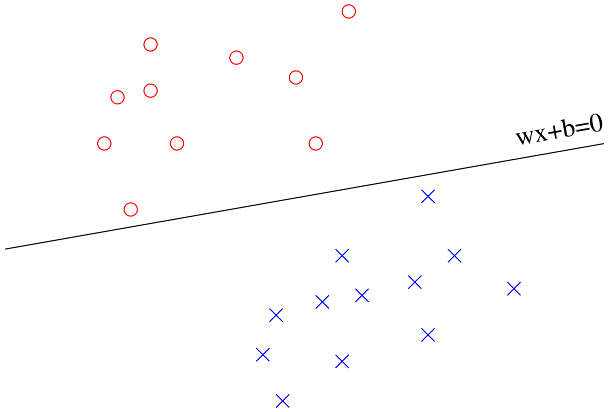


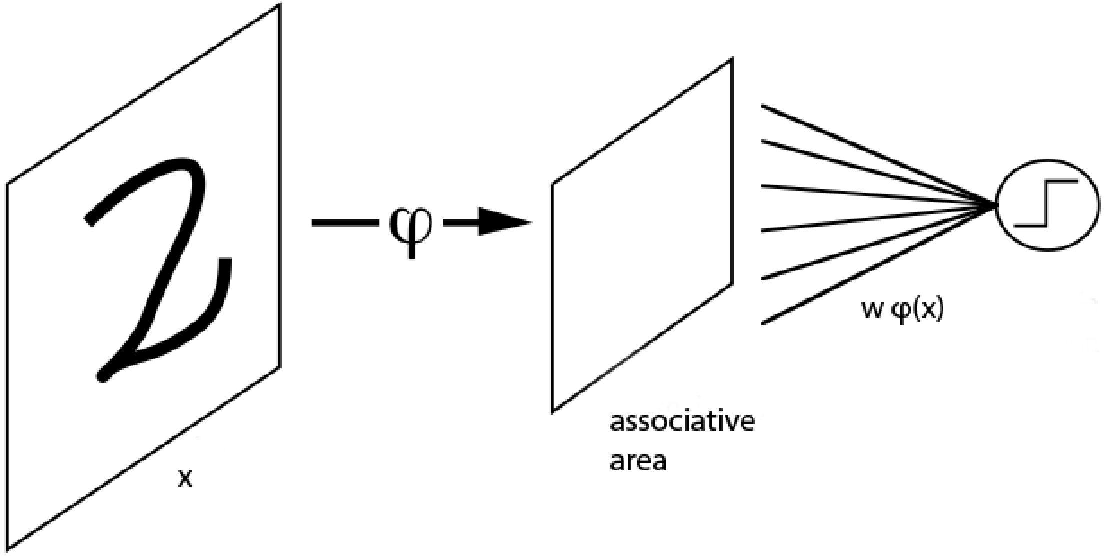
- Binary inputs $x \in \{0, 1\}^d$, binary output, vector of weights $w \in \mathbb{R}^d$

$$f(x) = \begin{cases} 1 & \text{if } w \cdot x > T \\ 0 & \text{otherwise} \end{cases}$$

- A unit can perform OR and AND operations
- Combine these units to represent any boolean function

- How to train them?





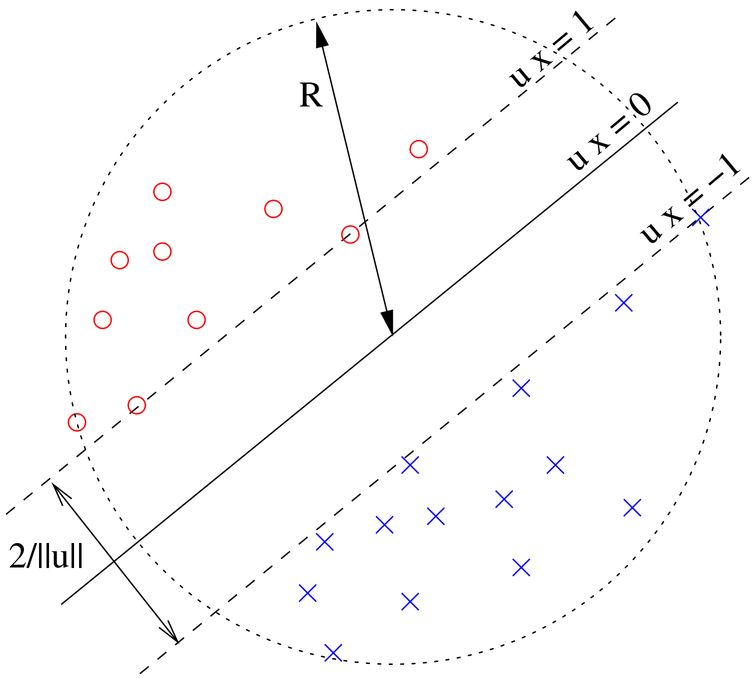
- Input: retina $x \in \mathbb{R}^n$
- Associative area: any kind of (fixed) function $\varphi(x) \in \mathbb{R}^d$
- Decision function:

$$f(x) = \begin{cases} 1 & \text{if } w \cdot \varphi(x) > 0 \\ -1 & \text{otherwise} \end{cases}$$

- Training: minimize $\sum_t \max(0, -y^t\, w^t \cdot \varphi(x^t))$, given $(x^t, y^t) \in \mathbb{R}^d \times \{-1, 1\}$

$$w^{t+1} = w^t + \begin{cases} y^t\, \varphi(x^t) & \text{if } y^t\, w \cdot \varphi(x^t) \leq 0 \\ 0 & \text{otherwise} \end{cases}$$

Assuming classes are separable



- Cauchy-Schwarz ($\rho_{max} \triangleq 2/||u||$)...

$$u \cdot w^t \leq ||u|| \, ||w^t|| \leq \frac{2}{\rho_{max}} ||w^t||$$

- u defines maximum margin separating hyperplane...

$$u \cdot w^t = u \cdot w^{t-1} + y^t \, u \cdot x^t \geq u \cdot w^{t-1} + 1 \geq t$$

- When we do a "mistake" ...

$$||w^t||^2 = ||w^{t-1}||^2 + 2y^t \, w^{t-1} \cdot x^t + ||x^t||^2 \leq ||w^{t-1}||^2 + R^2 \leq t \, R^2$$

- We get:

$$t \leq \frac{4 \, R^2}{\rho_{max}^2}$$

Adaline: Widrow & Hoff (1960)

- Problems of the Perceptron:
  - ⋆ Separable case:
    does not find a hyperplane equidistant from the two classes
  - ⋆ Non-separable case: does not converge
- Adaline (Widrow & Hoff, 1960) minimizes

$$\frac{1}{2}\sum_t (y^t - w^t \cdot \varphi(x^t))^2$$

- Delta rule:

$$w^{t+1} = w^t + \lambda(y^t - w^t \cdot x^t)\, x^t$$

Perceptron: Margin

See (Duda & Hart, 1973), (Krauth & Mézard, 1987), (Collobert, 2004)

- Poor generalization capabilities in practice
- No control on the margin:

$$\rho = \frac{2}{||w^T||} \geq \frac{\rho_{max}}{R^2}$$

- Margin Perceptron: minimize $\sum_t \max(0, 1 - y^t\, w^t \cdot \varphi(x^t))$

$$w^{t+1} = w^t + \lambda \begin{cases} y^t\, \varphi(x^t) & \text{if } y^t\, w \cdot \varphi(x^t) \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

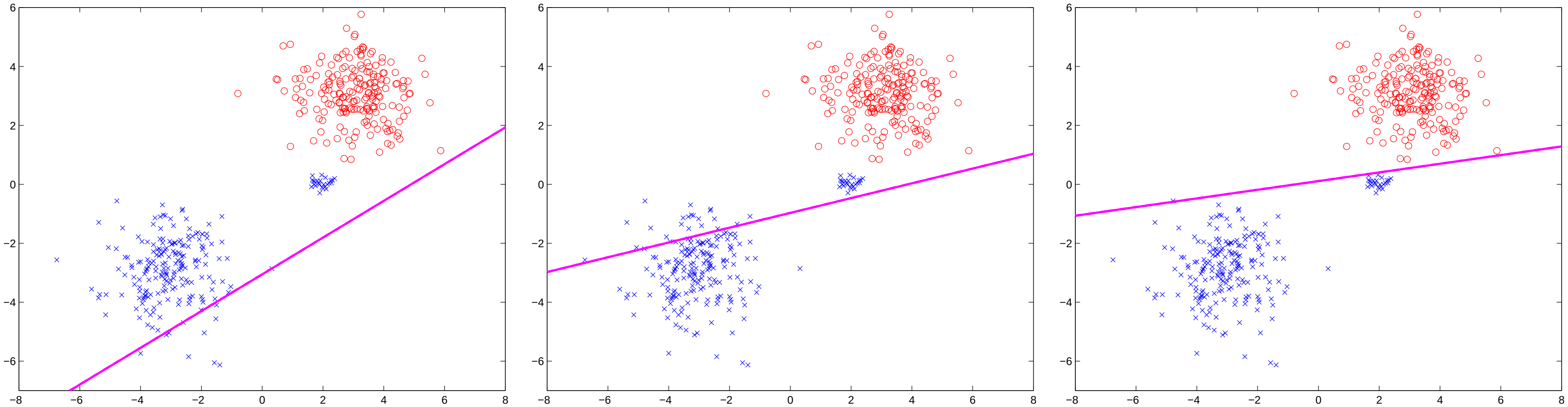
- Finite number of updates:

$$t \leq \frac{4}{\rho_{max}^2}(\frac{2}{\lambda} + R^2)$$

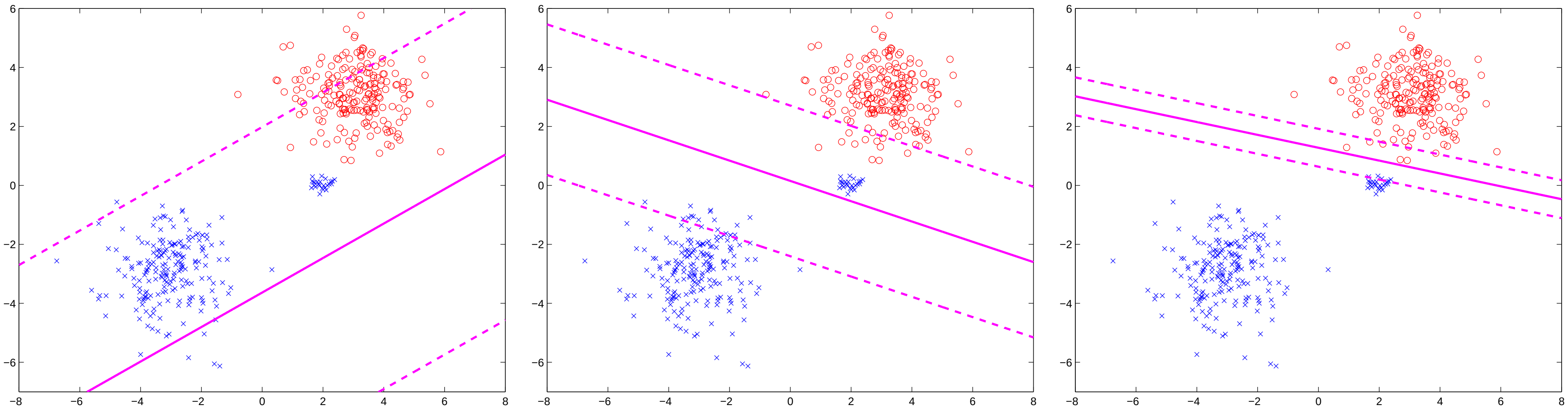
- Control on the margin:

$$\rho \geq \rho_{max} \frac{1}{2 + R^2\, \lambda}$$

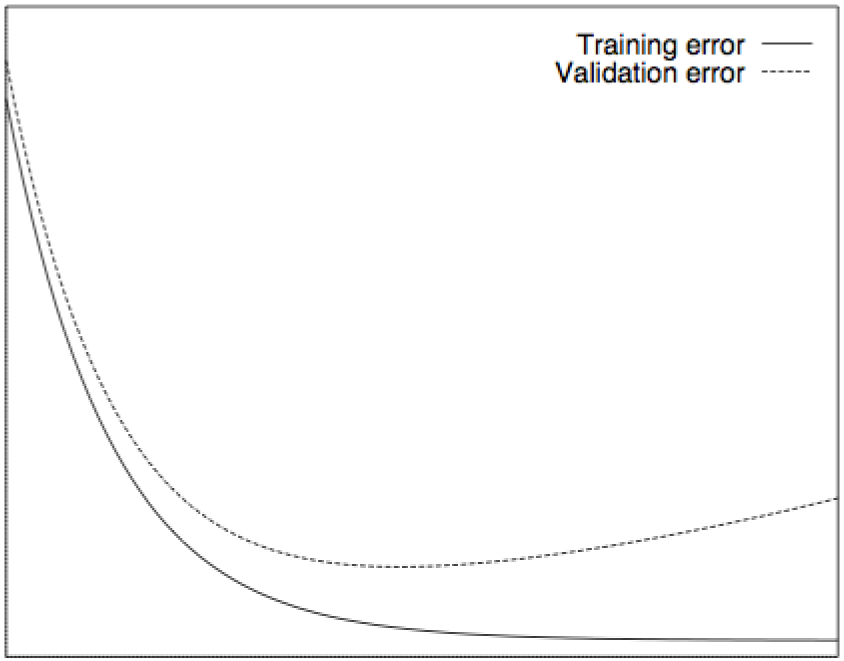
Original Perceptron (10/40/60 iter)

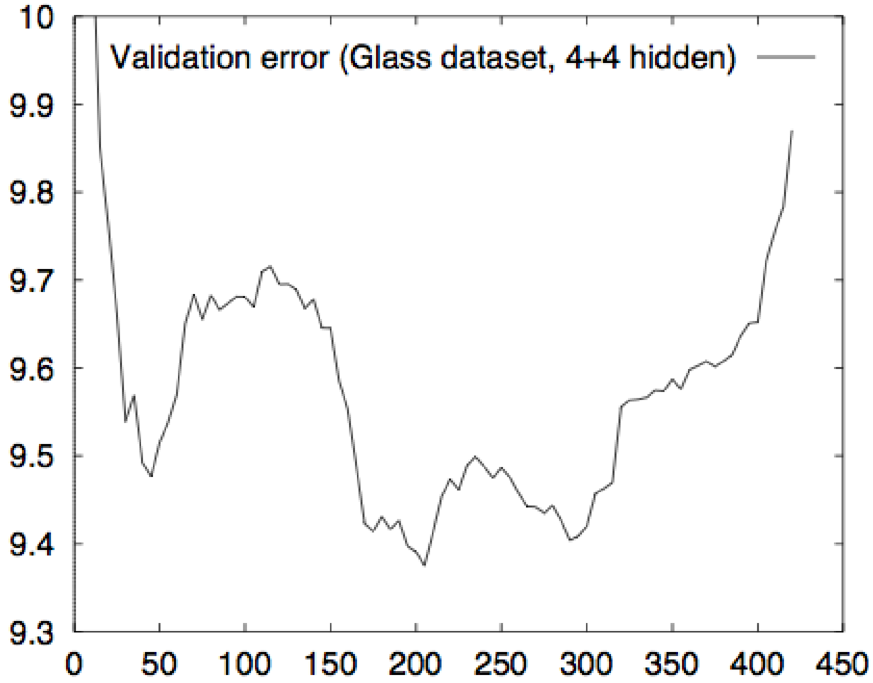


Margin Perceptron (10/120/2000 iter)



- In many machine-learning algorithms (including SVMs!) early stopping (on a validation set) is a good idea





From (Prechelt, 1997)

- Weight decay

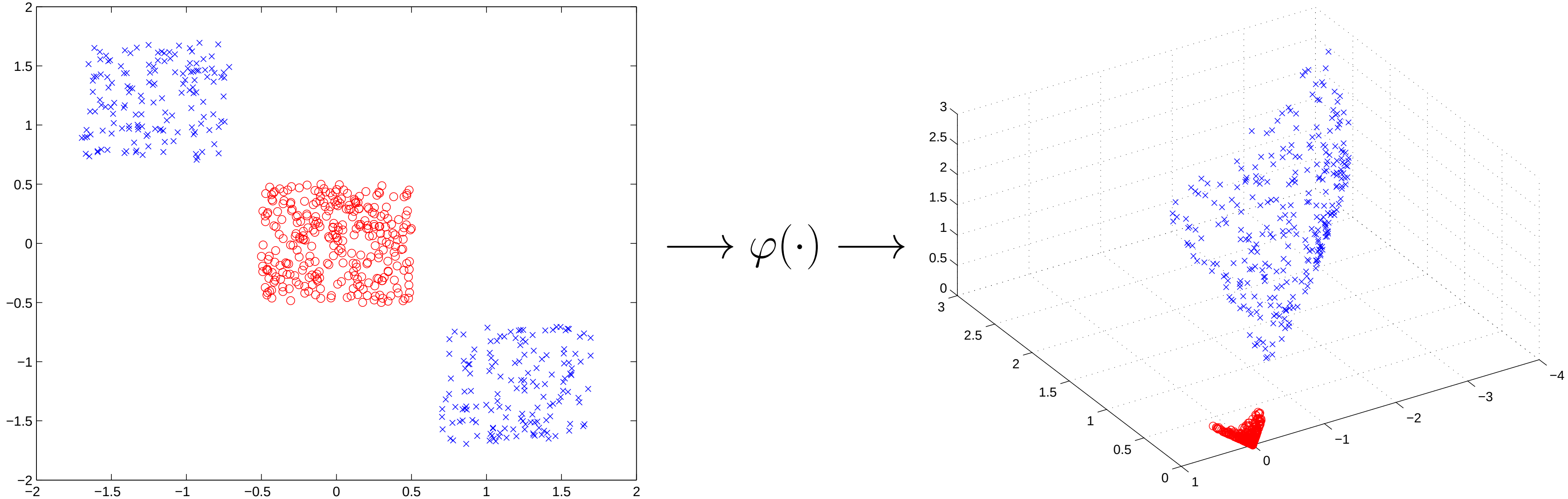
$$\mu||w||^2 + \max(0, 1 - y^t\, w^t \cdot \varphi(x^t))$$

This is the SVM cost!

- Consider the decision function

$$f(x) = \begin{cases} 1 & \text{if } w \cdot \varphi(x) > 0 \\ -1 & \text{otherwise} \end{cases}$$

- Non-linearity achieved by hand-crafting a non-linear $\varphi(\cdot)$



- Here $\varphi(x) = \varphi(x_1, x_2) = (x_1^2,\ \sqrt{2}\, x_1\, x_2,\ x_2^2)$
- Problem: the dot product is slow to compute in high dimensions

- See (Aizerman, Braverman and Rozonoer, 1964)
- Consider now the update

$$w^{t+1} = w^t + \begin{cases} y^t \varphi(x^t) & \text{if } y^t w \cdot \varphi(x^t) \leq 0 \\ 0 & \text{otherwise} \end{cases}$$

- Decision function at the t^{th} example can be written as:

$$f^t(x) = \sum_{t \in \text{“updated”}} y^t \varphi(x^t) \cdot \varphi(x)$$

- Can use a kernel instead

$$K(x, x^t) = \varphi(x^t) \cdot \varphi(x)$$

- E.g., for $\varphi(x) = \varphi(x_1, x_2) = (x_1^2, \sqrt{2}\, x_1 x_2, x_2^2)$ a possible kernel is

$$K(x, x^t) = (x \cdot x^t)^2$$

- $K(\cdot, \cdot)$ is a kernel if $\forall g$

such that $\int g(x)^2 dx < \infty$ then $\int K(x, y)\, g(x)\, g(y)\, dx\, dy \geq 0$

Link with SVMs

- Support Vector Machines unify nicely all the previous concepts

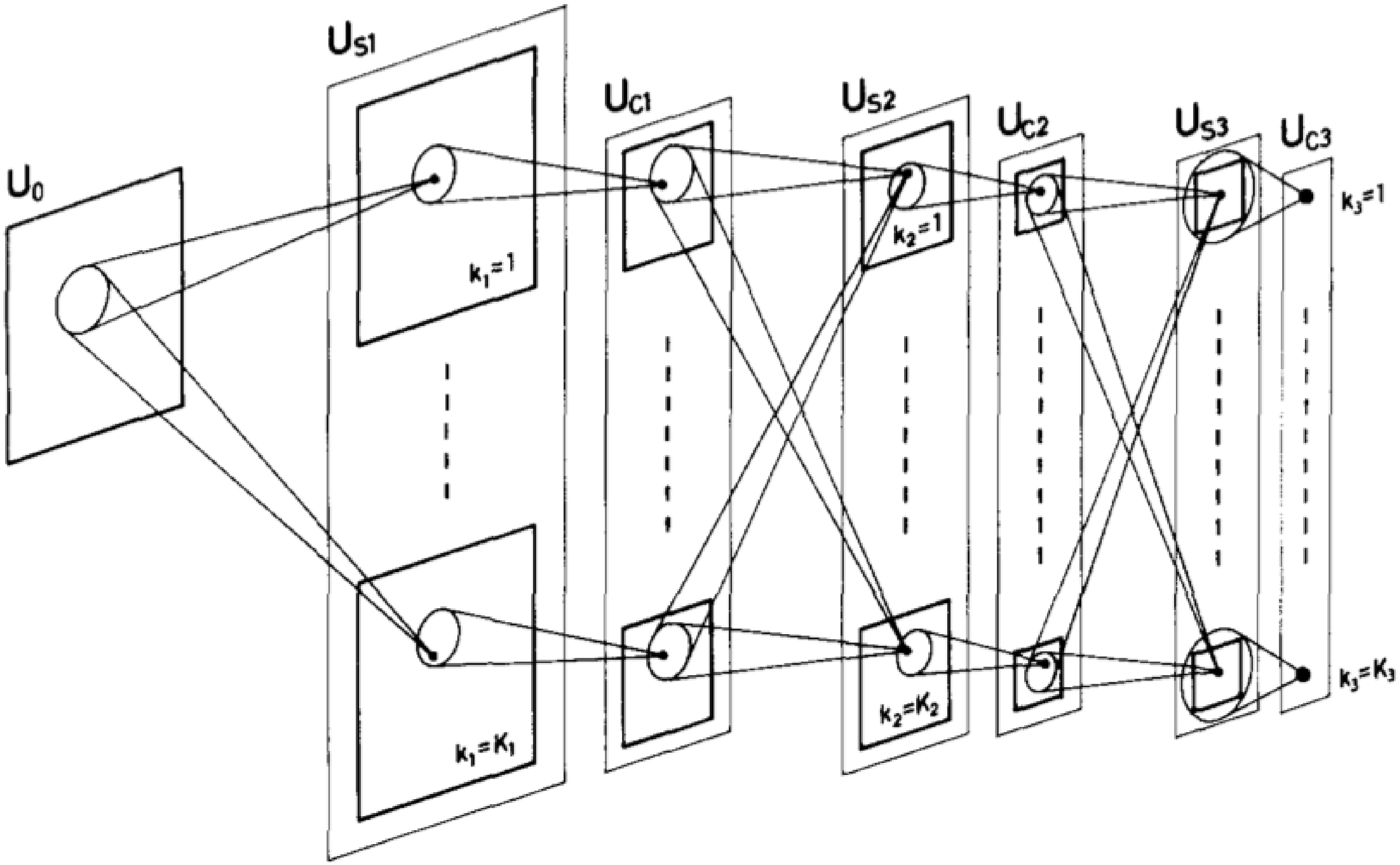
  ⋆ Early versions: (Vapnik & Lerner, 1963), (Vapnik, 1979)

  ⋆ Perceptron + Margin + Regularization
  = soft-margin Support Vector Machines
  (Cortes & Vapnik, 1995)

  ⋆ Perceptron + Margin + Regularization + Kernel
  = non-linear Support Vector Machines
  (Hard-margin SVMs: Boser, Guyon & Vapnik, 1992)

- For linear SVM, primal optimization is ok
- For non-linear kernels, sparsity issues with gradient descent in the primal
  $\longrightarrow$ efficient algorithms exist in the dual, or consider a budget
- see SVM course

- How to train a "good" $\varphi(\cdot)$?
- Neocognitron: (Fukushima, 1980)



- Madaline: (Winter & Widrow, 1988)

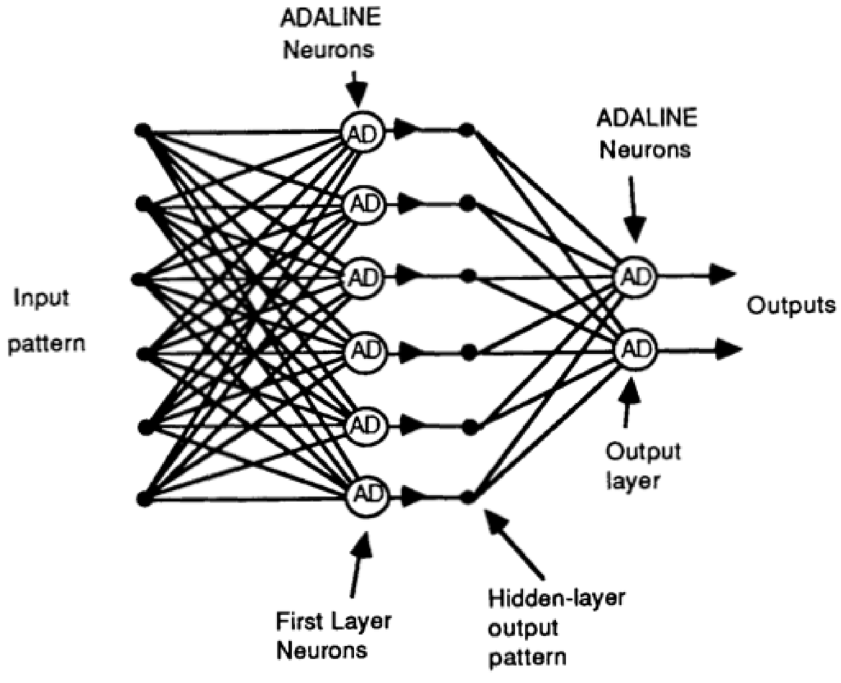
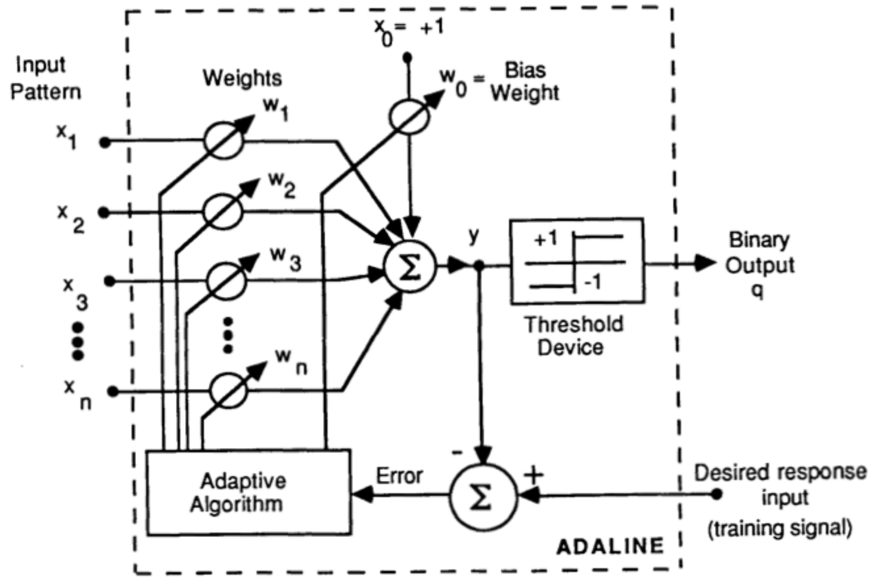


Figure 1: Layered feed-forward ADALINE network.



- Multi-Layer Perceptron

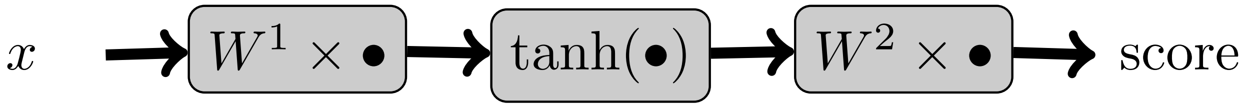
$$x \rightarrow \boxed{W^1 \times \bullet} \rightarrow \boxed{\tanh(\bullet)} \rightarrow \boxed{W^2 \times \bullet} \rightarrow \text{score}$$

- Training solution: gradient descent

- Any function

$$g : \mathbb{R}^d \longrightarrow \mathbb{R}$$

can be approximated (on a compact) by a two-layer neural network



- Cybenko used
  - ⋆ The Hahn Banach theorem
  - ⋆ The Riesz representation theorem

- Given a set of examples $(x^t, y^t) \in \mathbb{R}^d \times \mathbb{N}$, $t = 1 \dots T$, we want to minimize

$$C(\theta) = \sum_{t=1}^{T} c(f_\theta(x^t),\, y^t)$$

- Batch gradient descent

$$\theta \longleftarrow \theta - \lambda \frac{\partial C(\theta)}{\partial \theta}$$

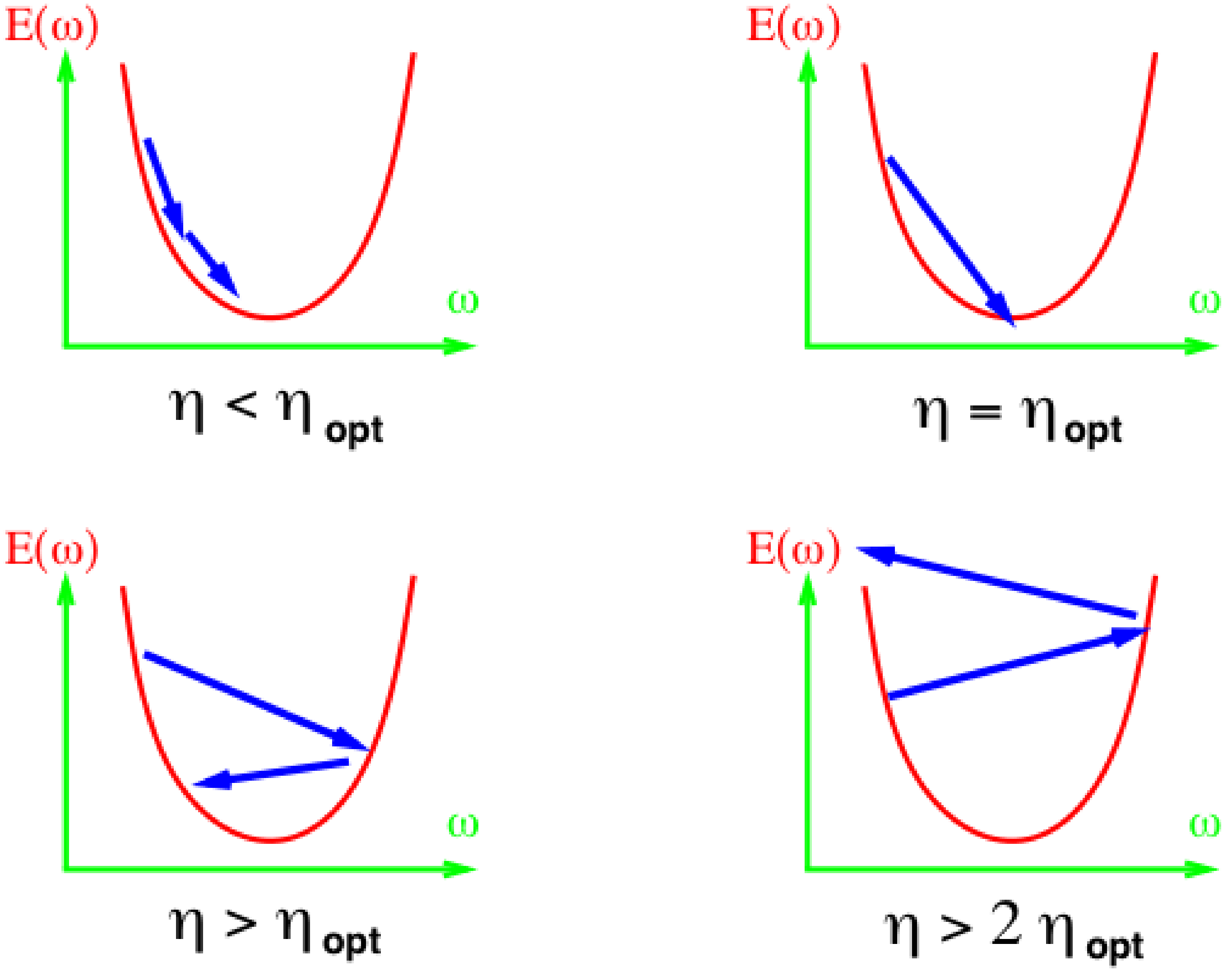
  - ⋆ Update after seeing all examples
  - ⋆ Variants: see your optimization book (Conjugate gradient, BFGS...)
  - ⋆ Slow in practice

- Take advantage of redundancy: stochastic gradient descent
  Pick a random example t

$$\theta \longleftarrow \theta - \lambda \frac{\partial c(f_\theta(x^t),\, y^t)}{\partial \theta}$$

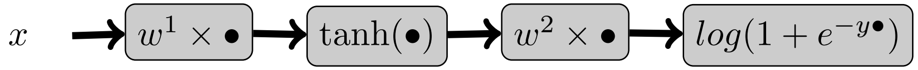
  - ⋆ Update after seeing one example

- The learning rate must be chosen carefully
- Good idea to use a validation set

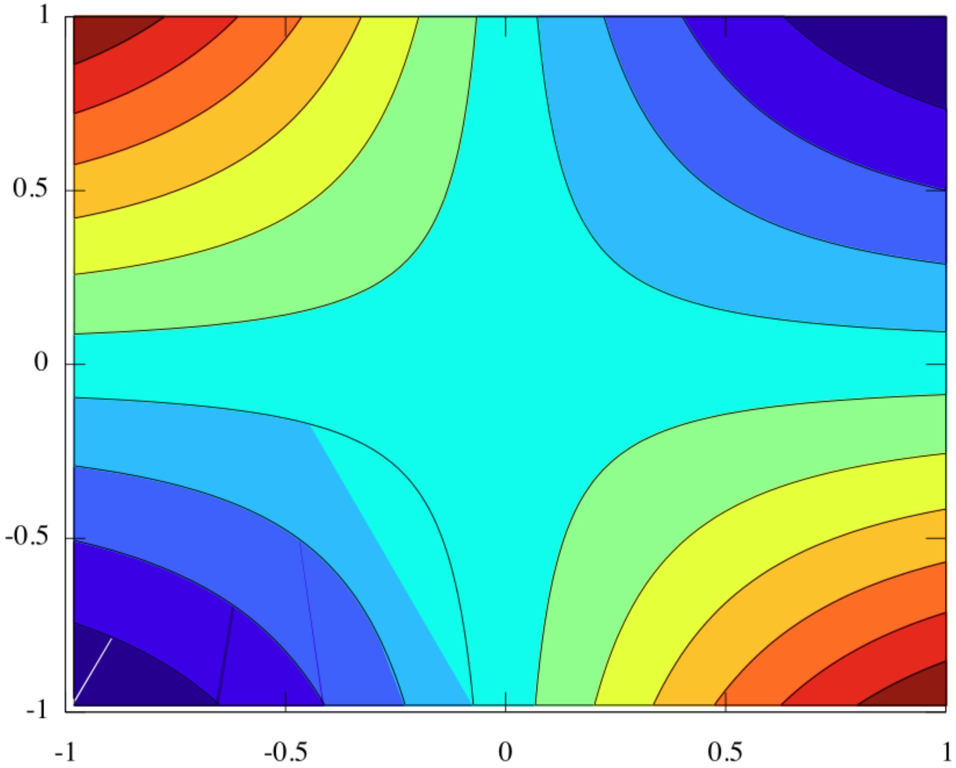


From (LeCun, 2006)

- Consider the network



With one example $(x = 1, y = 1)$ and one hidden unit!



- No progress in some directions
- Saddle points, plateaux..

- Initialize properly the weights
  - ⋆ Not too big: $tanh(\bullet)$ saturates
  - ⋆ Not too small: all units would do the same!
- Normalize properly your data (mean/variance)
  - ⋆ Again, you want to be in the right part of the $tanh(\bullet)$
- Use a second order approach (H is the Hessian)

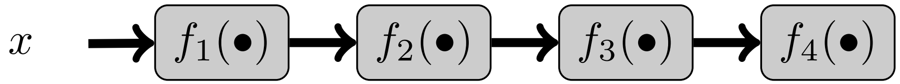
$$C(\theta+\epsilon) \approx C(\theta) + \frac{\partial C(\theta)}{\partial \theta}\epsilon + \epsilon^{\mathrm{T}} H(\theta)\epsilon$$

  - ⋆ Costly with full Hessian, consider only the diagonal
  - ⋆ Estimated on a training subset
  - ⋆ Be sure it is positive definite!
  - ⋆ Can be "backpropagated" as the gradient
  - ⋆ Update with

$$\lambda = \frac{\gamma}{\frac{\partial^2 C}{\partial \theta_k^2} + \mu} \quad \forall k$$

- In the neural network field: (Rumelhart, Hinton, Williams, 1986)
- However, previous possible references exist, including (Leibniz, 1675) and (Newton, 1687)

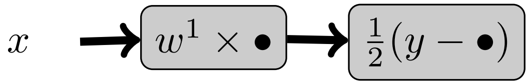
- View the network+loss as a "stack" of layers



- Minimize the score by gradient descent

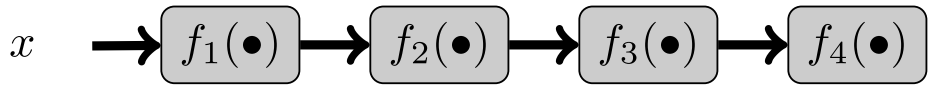
$$f(x) = f_L(f_{L-1}(\dots f_1(x)) \quad \longrightarrow \quad \text{How to compute } \frac{\partial f}{\partial w^l} \quad \forall l \quad ??$$

- For e.g., in the Adaline $L = 2$



  - ⋆ $f_1(x) = w_1 \cdot x$
  - ⋆ $f_2(f_1) = \frac{1}{2}(y - f_1)^2$

$$\frac{\partial f}{\partial w_1} = \underbrace{\frac{\partial f_2}{\partial f_1}}_{=y-f_1} \underbrace{\frac{\partial f_1}{\partial w^1}}_{=x} \qquad \text{chain rule}$$



- Brutal way:

$$\frac{\partial f}{\partial w^l} = \frac{\partial f_L}{\partial f_{L-1}} \frac{\partial f_{L-1}}{\partial f_{L-2}} \cdots \frac{\partial f_{l+1}}{\partial f_l} \frac{\partial f_l}{\partial w^l}$$

- In the backprop way, each module $f_l()$
  - ⋆ Receive the gradient w.r.t. its own outputs f_l
  - ⋆ Computes the gradient w.r.t. its own input f_{l-1} (backward)
  - ⋆ Computes the gradient w.r.t. its own parameters w^l (if any)

$$\frac{\partial f}{\partial f_{l-1}} = \frac{\partial f}{\partial f_l} \frac{\partial f_l}{\partial f_{l-1}}$$
$$\frac{\partial f}{\partial w^l} = \frac{\partial f}{\partial f_l} \frac{\partial f_l}{\partial w^l}$$

- Often, gradients are efficiently computed using outputs of the module

Do a forward before each backward

Examples Of Modules

- For simplicity, we denote
  - ⋆ x the input of a module
  - ⋆ z target of a loss module
  - ⋆ y the output of a module $f_l(x)$
  - ⋆ $\tilde{y}$ the gradient w.r.t. the output of each module

Module	**Forward**	**Backward**	**Gradient**
Linear	$y = W\,x$	$W^{\mathrm{T}}\,\tilde{y}$	$\tilde{y}\,x^{\mathrm{T}}$
MSE Loss	$y = \frac{1}{2}(x - z)^2$	$x - z$	
Tanh	$y = \tanh(x)$	$\tilde{y}\,(1 - y^2)$	
Sigmoid	$y = 1/(1 + e^{-x})$	$\tilde{y}\,(1 - y)\,y$	
Perceptron Loss	$y = max(0, -z\,x)$	$-\mathbf{1}_{z\cdot x \leq 0}$	

See Lush, Torch5, Theano...

- Given a set of examples $(x^t, y^t) \in \mathbb{R}^d \times \mathbb{N}$, $t = 1 \dots T$ we want to maximize the (log-)likelihood

$$\log \prod_{t=1}^{T} p(y^t|x^t) = \sum_{t=1}^{T} \log p(y^t|x^t)$$

- The network outputs a score $f_y(x)$ per class y
- Interpret scores as conditional probabilities using a softmax:

$$p(y|x) = \frac{e^{f_y(x)}}{\sum_i e^{f_i(x)}}$$

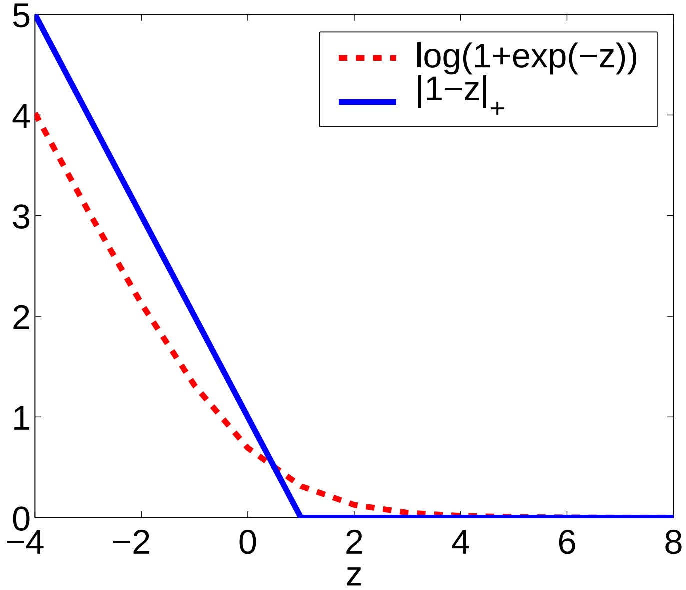
- In practice we prefer log-probabilites:

$$\log p(y|x) = f_y(x) - \log \left[\sum_i e^{f_i(x)} \right]$$

- Assume only two class problems, $y \in \{-1, +1\}$

$$\log p(y = 1|x) = \log \frac{e^{f_1(x)}}{e^{f_1(x)} + e^{f_{-1}(x)}} = -\log(1 + e^{-y\,(f_1(x) - f_{-1}(x))})$$
$$\log p(y = -1|x) = \log \frac{e^{f_{-1}(x)}}{e^{f_1(x)} + e^{f_{-1}(x)}} = -\log(1 + e^{-y\,(f_1(x) - f_{-1}(x))})$$

- Note: only one network output needed
- Taking $z = y\,(f_1(x) - f_{-1}(x))$,
  $z \mapsto log(1 + e^{-z})$ is a smooth version of SVM cost



Likelihood For Regression

- The target variables $y \in \mathbb{R}$ are now continuous
- We often consider

$$y|x \quad \sim \quad \mathcal{N}(f(x), \sigma^2)$$

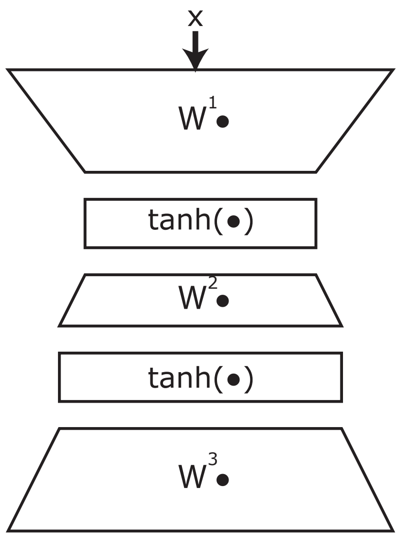
- In this case,

$$\log p(y|x) = -\frac{1}{2\sigma^2}||y - f(x)||^2 \; + \; \text{cste}$$

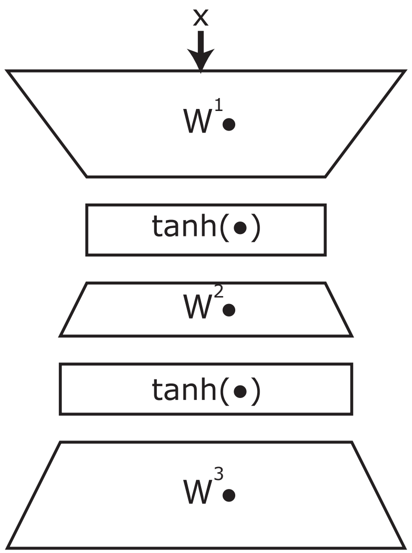
- Equivalent to Mean Squared Error (MSE) criterion...
- Not great to classification

- How to leverage unlabeled data (when there is no y)?
- Deep architectures are hard to train: how to pretrain each layer?

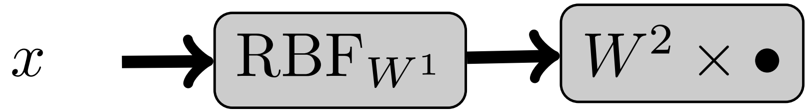
- "Auto-encoder/bottleneck" network: try to reconstruct the input



- Caveats:
  - ⋆ PCA if no W^2 layer (Bourlard & Kamp, 1988)
  - ⋆ It is a *bottleneck* mapping...

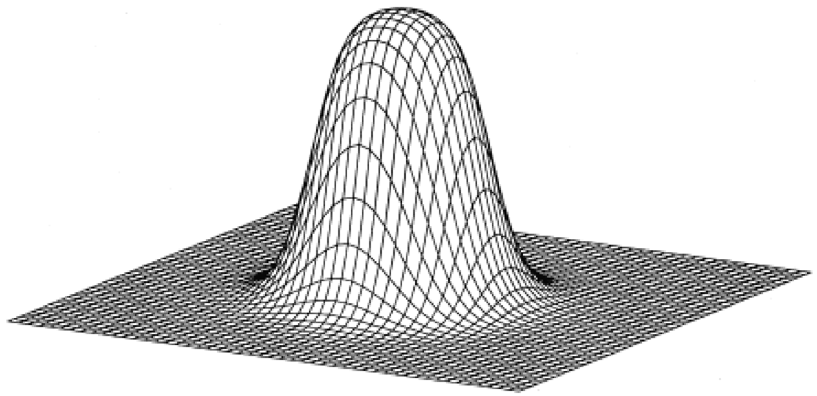


- Possible improvements:
  - ⋆ No W^2 layer, $W^3 = \left[W^1\right]^{\mathrm{T}}$ (Bengio et al., 2006)
  - ⋆ Inject noise in x, try to reconstruct the true x (Bengio et al., 2008)
  - ⋆ Impose sparsity constraints
    on the projection (Kavukcuoglu et al., 2008)



- A Radial Basis Function (RBF) layer is defined by:

$$f_{1,i}(x) = e^{-\frac{||x - W^1_{\bullet,i}||^2}{2\sigma^2}}$$

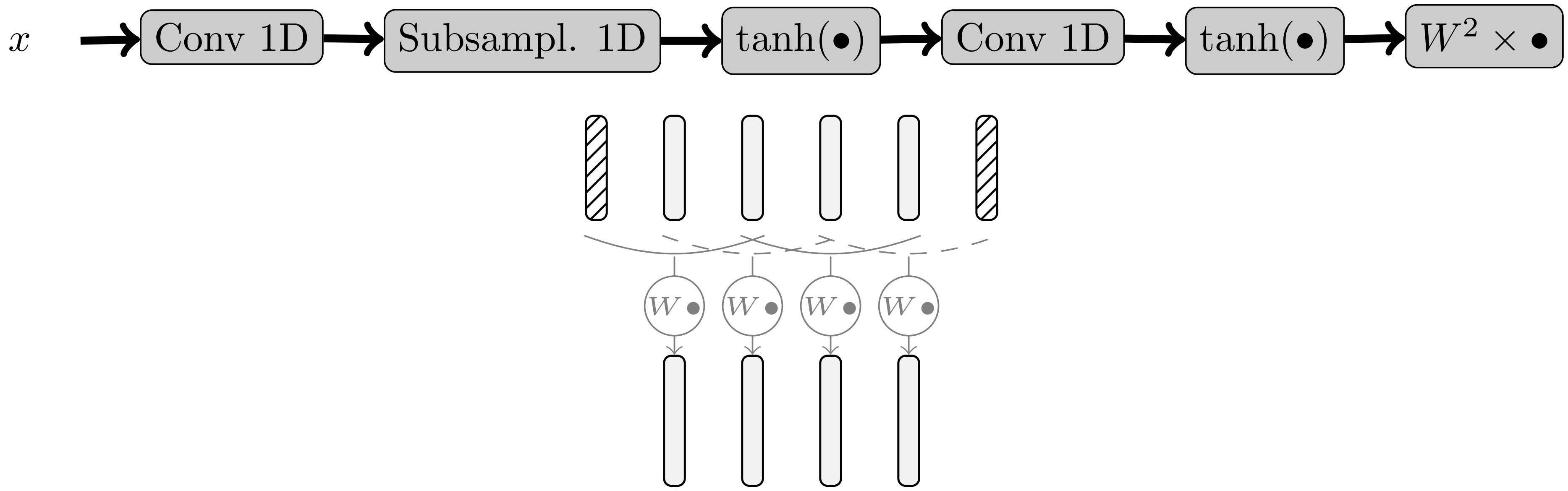


- Better to find parametrization of σ such that it is strictly positive:

$$\sigma = \tilde{\sigma} + \theta$$

- Gradient is zero if W^1 colums are far from training examples

$\longrightarrow$ Initialize with K-Means

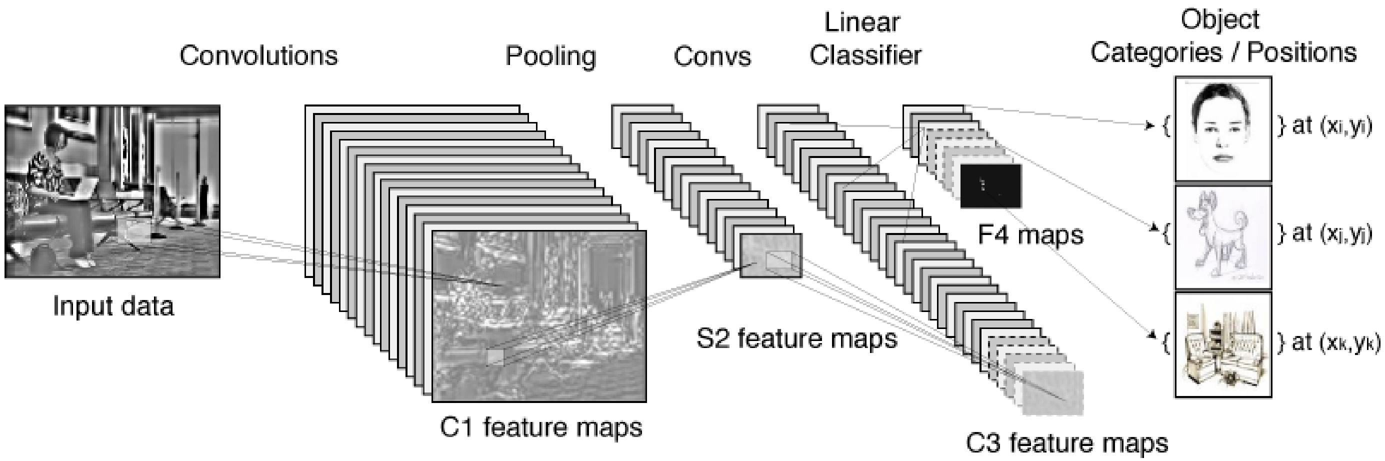


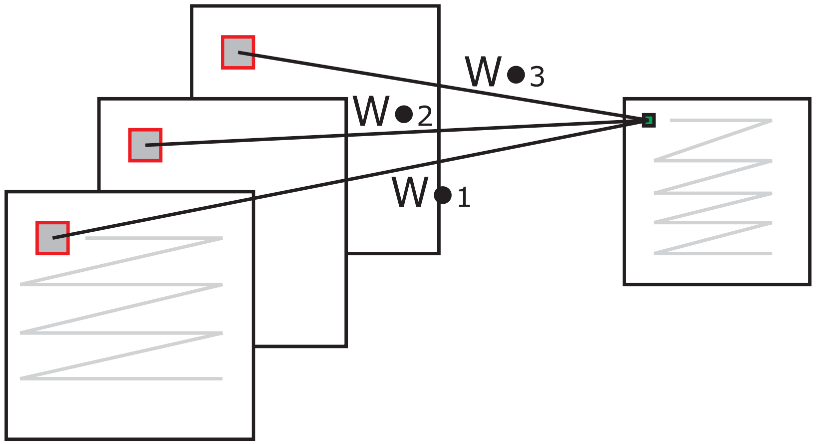
- Weights are "shared" through time

$$X = (X_{\bullet 1}, X_{\bullet 2} \cdots)$$ input (matrix)

$$W \times \begin{pmatrix} X_{\bullet 1} & X_{\bullet 2} & \\ X_{\bullet 2} & X_{\bullet 3} & \cdots \\ X_{\bullet 3} & X_{\bullet 4} & \end{pmatrix}$$ convolution (local embedding for each input column)

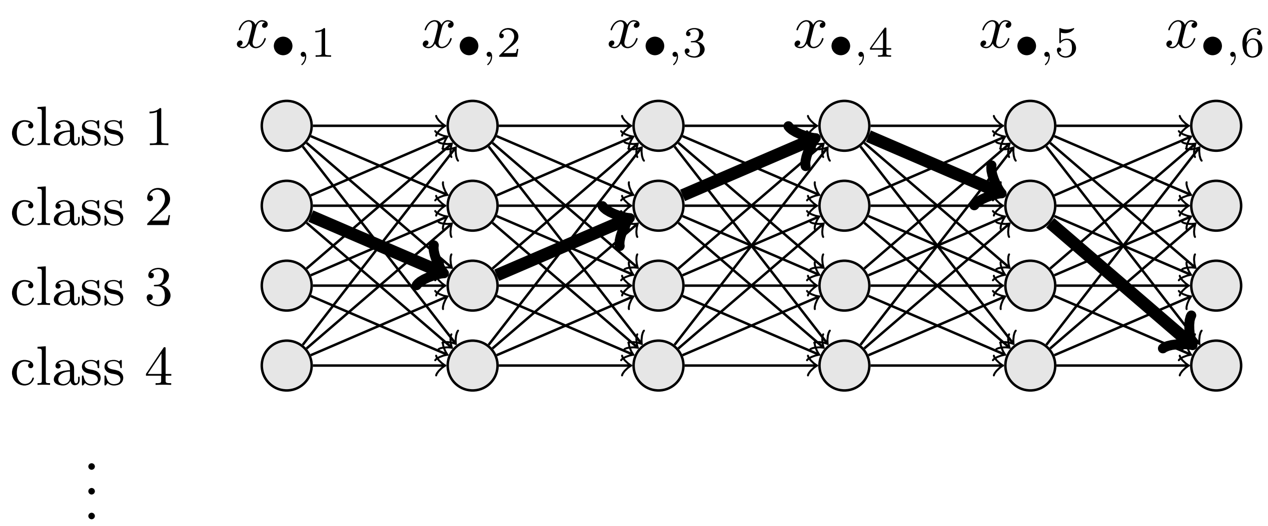
- Robustness to time shifts:
  Apply sub-sampling (as convolution, but $W_{\bullet,i}$ contains single value)
- Also called Time Delay Neural Networks (TDNNs)





- Same story than in 1D but... in 2D

- Sequence of T frames $[\boldsymbol{x}]_1^T$
- The network score for class k at the t^{th} frame is $f([\boldsymbol{x}]_1^T,\, k,\, t,\, \boldsymbol{\theta})$
- A_{kl} transition score to jump from class k to class l



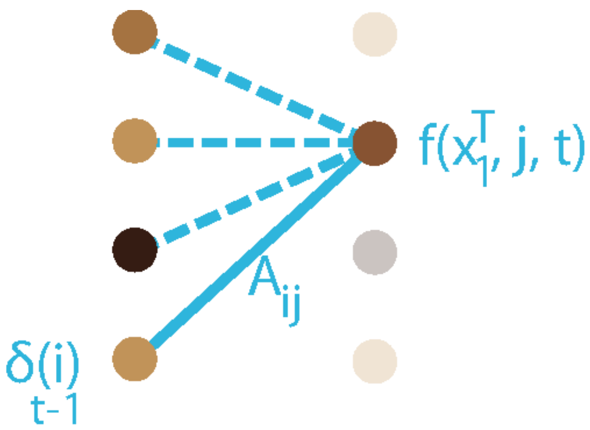
- Sentence score for a class label path $[i]_1^T$

$$s([\boldsymbol{x}]_1^T,\, [i]_1^T,\, \tilde{\boldsymbol{\theta}}) = \sum_{t=1}^{T} \left(A_{[i]_{t-1}[i]_t} + f([\boldsymbol{x}]_1^T,\, [i]_t,\, t,\, \boldsymbol{\theta}) \right)$$

- Conditional likelihood by normalizing w.r.t all possible paths:

$$\log p([y]_1^T \,|\, [\boldsymbol{x}]_1^T,\, \tilde{\boldsymbol{\theta}}) = s([\boldsymbol{x}]_1^T,\, [y]_1^T,\, \tilde{\boldsymbol{\theta}}) - \operatorname*{logadd}_{\forall [j]_1^T} s([\boldsymbol{x}]_1^T,\, [j]_1^T,\, \tilde{\boldsymbol{\theta}})$$

- Normalization computed with recursive Forward algorithm:



$$\delta_t(j) = \text{logAdd}_i \left[\delta_{t-1}(i) + A_{i,j} + f_\theta(j, x_1^T, t)\right]$$

Termination:

$$\underset{\forall [j]_1^T}{\text{logadd}}\, s([\boldsymbol{x}]_1^T,\ [j]_1^T,\ \tilde{\boldsymbol{\theta}}) = \text{logAdd}_i\, \delta_T(i)$$

- Simply backpropagate through this recursion with chain rule

- Non-linear CRFs: Graph Transformer Networks (Bottou et al., 1997)
- Compared to CRFs, we train features (network parameters $\boldsymbol{\theta}$ and transitions scores A_{kl})

- Inference: Viterbi algorithm (replace logAdd by max)