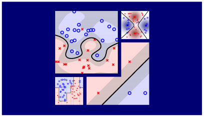
Machine Learning Techniques
(機器學習技法)



Lecture 12: Neural Network

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Roadmap

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models

Lecture 11: Gradient Boosted Decision Tree

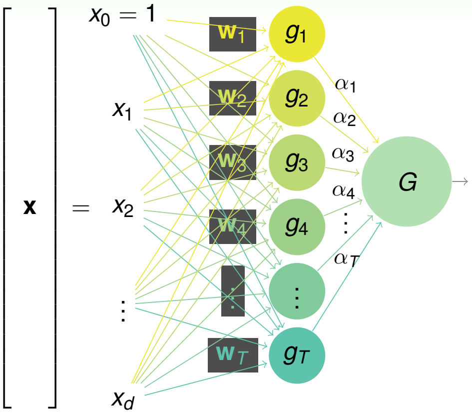
aggregating trees from **functional gradient** and **steepest descent** subject to **any error measure**

3. Distilling Implicit Features: Extraction Models

Lecture 12: Neural Network

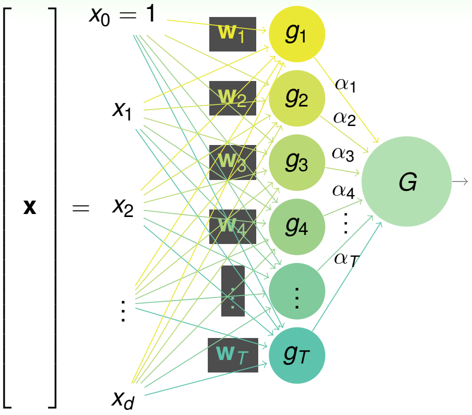
- Motivation
- Neural Network Hypothesis
- Neural Network Learning
- Optimization and Regularization

Linear Aggregation of Perceptrons: Pictorial View



$$G(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t \underbrace{\text{sign}\left(\mathbf{w}_t^T \mathbf{x}\right)}_{g_t(\mathbf{x})}\right)$$

Linear Aggregation of Perceptrons: Pictorial View



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- two layers of weights: $\mathbf{w}_t$ and $\boldsymbol{\alpha}$

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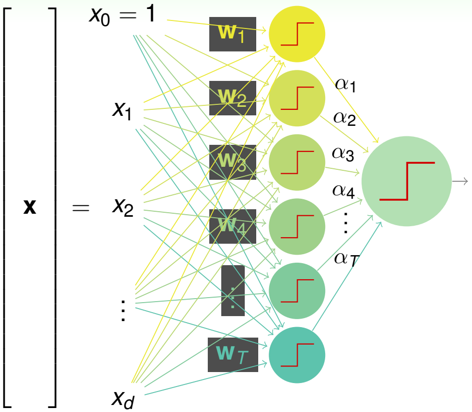

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- two layers of sign functions: in g_t and in G

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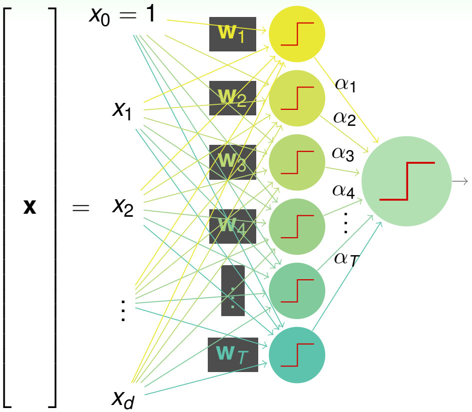

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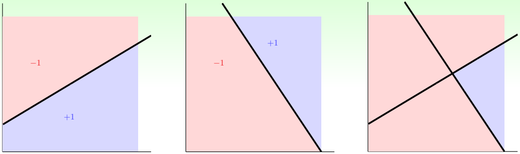
- two layers of sign functions: in g_t and in G

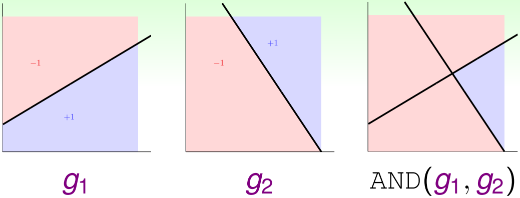
what boundary can G **implement**?

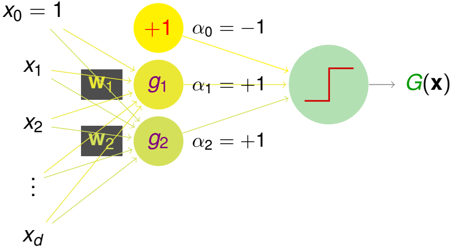
Logic Operations with Aggregation



g_1 g_2 $\texttt{AND}(g_1, g_2)$

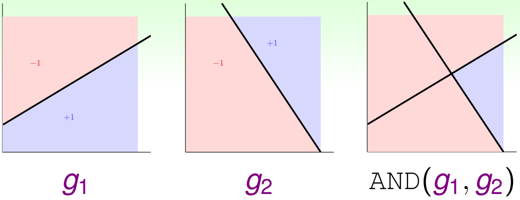
Logic Operations with Aggregation

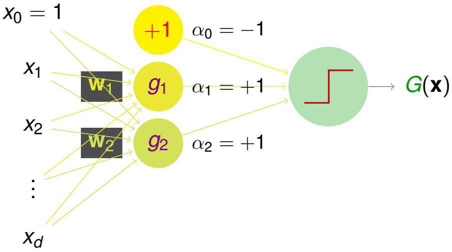




$$G(\mathbf{x}) = \text{sign}\left(-1 + g_1(\mathbf{x}) + g_2(\mathbf{x})\right)$$

Logic Operations with Aggregation

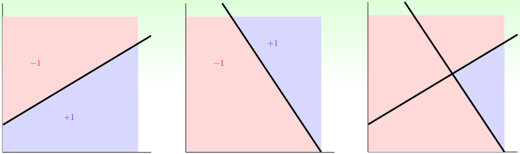




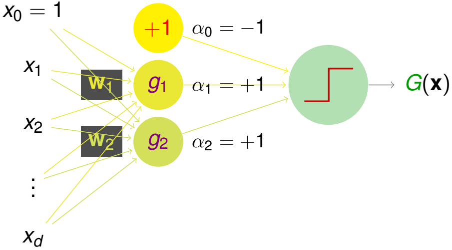
$G(\mathbf{x}) = \mathrm{sign}\left(-1 + g_1(\mathbf{x}) + g_2(\mathbf{x})\right)$

- $g_1(\mathbf{x}) = g_2(\mathbf{x}) = +1$ (TRUE):
  $G(\mathbf{x}) = \quad (\quad)$
- otherwise:
  $G(\mathbf{x}) = \quad (\quad)$

Logic Operations with Aggregation



g_1 g_2 $\mathrm{AND}(g_1, g_2)$



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- $g_1(\mathbf{x}) = g_2(\mathbf{x}) = +1$ (TRUE): $G(\mathbf{x}) = +1$ (TRUE)
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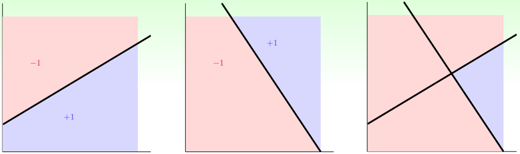
Logic Operations with Aggregation



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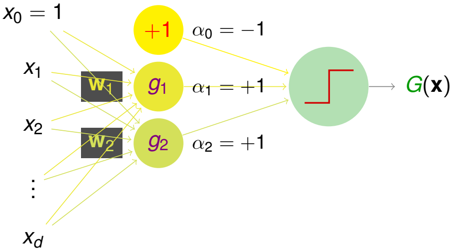

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- $g_1(\mathbf{x}) = g_2(\mathbf{x}) = +1$ (TRUE): $G(\mathbf{x}) = +1$ (TRUE)
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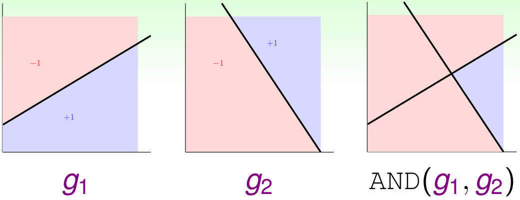
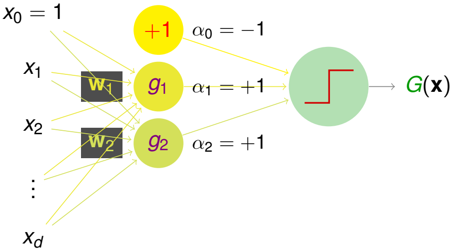
- $G \equiv \text{AND}(g_1, g_2)$

Logic Operations with Aggregation





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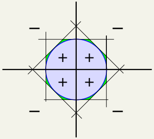
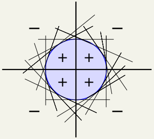
- otherwise: $G(\mathbf{x}) = -1$ (FALSE)
- $G \equiv$ AND(g_1, g_2)

OR, NOT can be **similarly implemented**

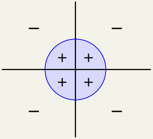
Powerfulness and Limitation



8 perceptrons

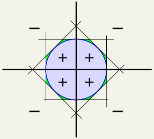


16 perceptrons



target boundary

Powerfulness and Limitation



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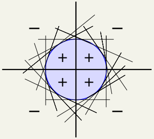

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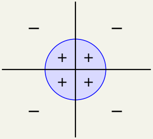
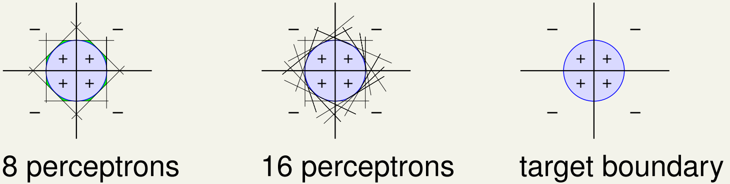


target boundary

- 'convex set' hypotheses implemented:

Powerfulness and Limitation



- ‘convex set’ hypotheses implemented: $d_{\mathrm{VC}} \to \infty$, **remember? :-)**

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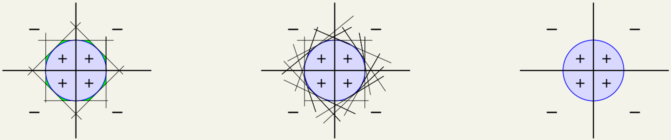

8 perceptrons 16 perceptrons target boundary

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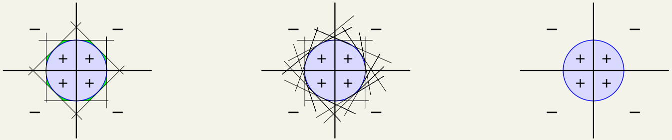
- powerfulness: enough perceptrons $\approx$ **smooth boundary**

Powerfulness and Limitation



8 perceptrons | 16 perceptrons | target boundary

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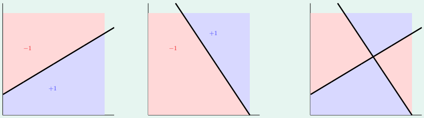
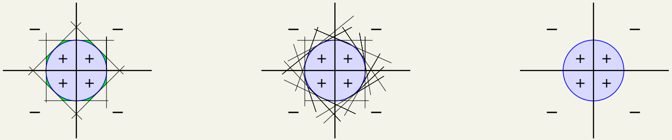


g_1 | g_2 | $\text{XOR}(g_1, g_2)$

Powerfulness and Limitation



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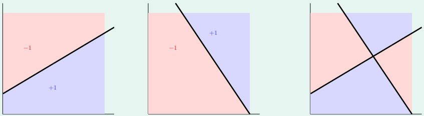

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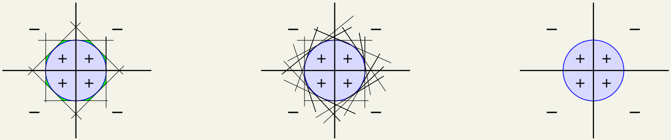

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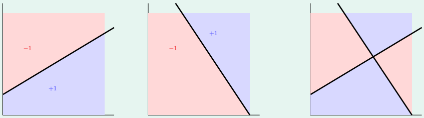

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how to implement $\mathrm{XOR}(g_1, g_2)$?

Multi-Layer Perceptrons: Basic Neural Network

- non-separable data:

Multi-Layer Perceptrons: Basic Neural Network

- non-separable data: can use more **transform**

Multi-Layer Perceptrons: Basic Neural Network

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- how about one more layer of **AND** **transform**?

$$\mathrm{XOR}(g_1, g_2) = \mathrm{OR}(\mathrm{AND}(-g_1, g_2), \mathrm{AND}(g_1, -g_2))$$

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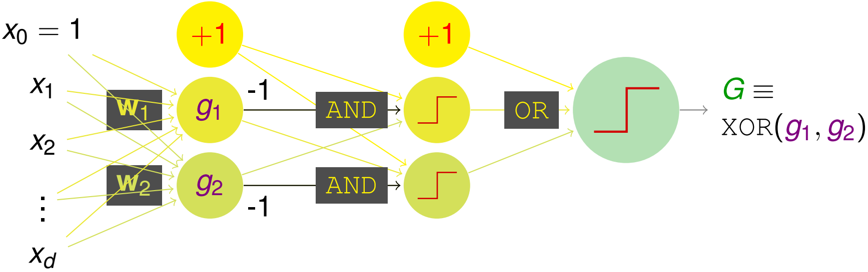

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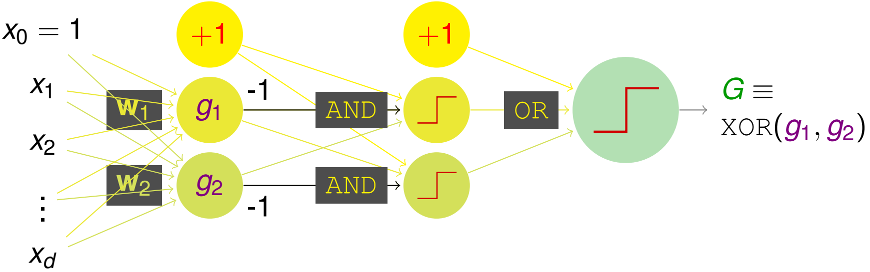

perceptron (simple)

Multi-Layer Perceptrons: Basic Neural Network

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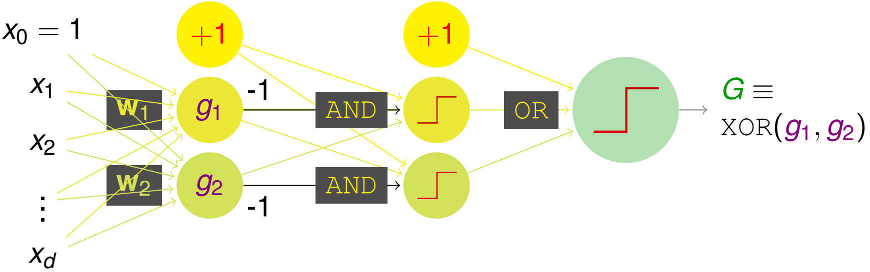

perceptron (simple)
$\Longrightarrow$ aggregation of perceptrons (powerful)

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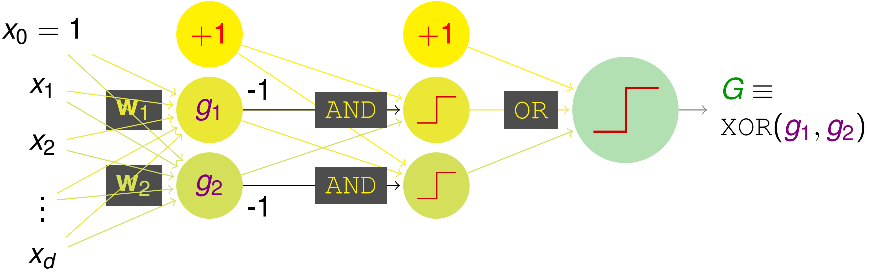
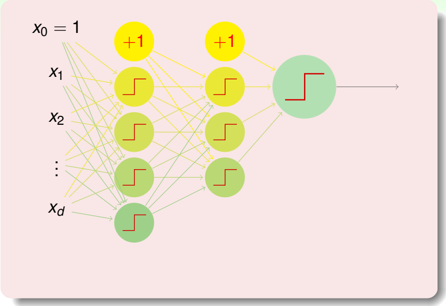


perceptron (simple)
$\Longrightarrow$ aggregation of perceptrons (powerful)
$\Longrightarrow$ **multi-layer perceptrons** (**more powerful**)

Connection to Biological Neurons



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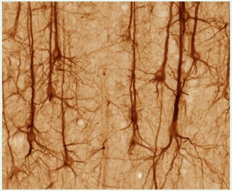

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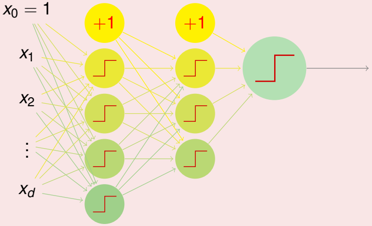

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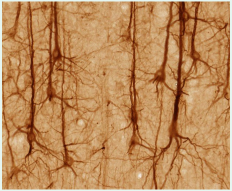

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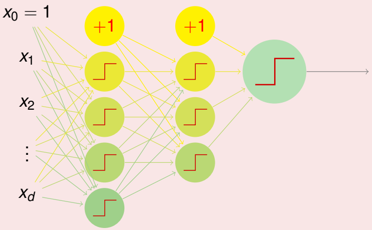

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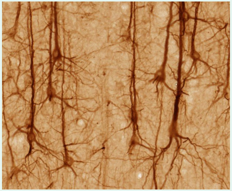

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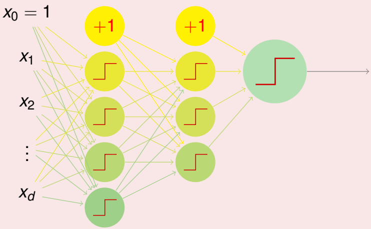

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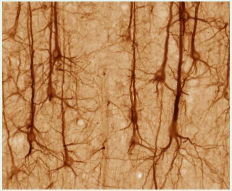
Connection to Biological Neurons



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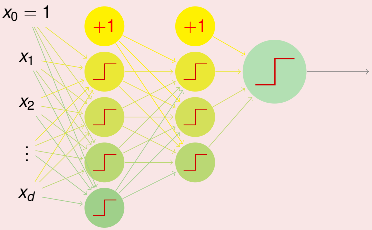

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neural network: **bio-inspired** model

Fun Time

Let $g_0(\mathbf{x}) = +1$. Which of the following $(\alpha_0, \alpha_1, \alpha_2)$ allows $G(\mathbf{x}) = \text{sign}\left(\sum_{t=0}^{2} \alpha_t g_t(\mathbf{x})\right)$ to implement $\text{OR}(g_1, g_2)$?

1. $(-3, +1, +1)$
2. $(-1, +1, +1)$
3. $(+1, +1, +1)$
4. $(+3, +1, +1)$

Fun Time

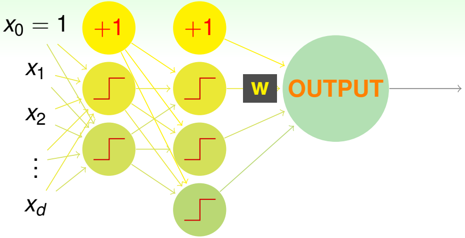
Let $g_0(\mathbf{x}) = +1$. Which of the following $(\alpha_0, \alpha_1, \alpha_2)$ allows $G(\mathbf{x}) = \text{sign}\left(\sum_{t=0}^{2} \alpha_t g_t(\mathbf{x})\right)$ to implement $\text{OR}(g_1, g_2)$?

1. $(-3, +1, +1)$
2. $(-1, +1, +1)$
3. $(+1, +1, +1)$
4. $(+3, +1, +1)$

Reference Answer: 3

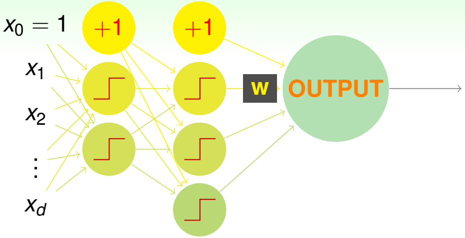
You can easily verify with all four possibilities of $(g_1(\mathbf{x}), g_2(\mathbf{x}))$.

Neural Network Hypothesis: Output



- **OUTPUT**: simply a **linear model** with $s = \mathbf{w}^T \phi^{(2)}(\phi^{(1)}(\mathbf{x}))$

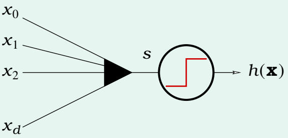
Neural Network Hypothesis: Output



- **OUTPUT**: simply a **linear model** with $s = \mathbf{w}^T \phi^{(2)}(\phi^{(1)}(\mathbf{x}))$
- any linear model can be used—**remember? :-)**

linear classification

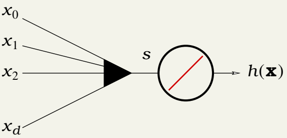
$h(\mathbf{x}) = \text{sign}(s)$



err = 0/1

linear regression

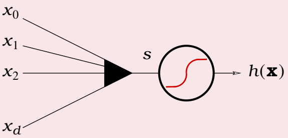
$h(\mathbf{x}) = s$



err = squared

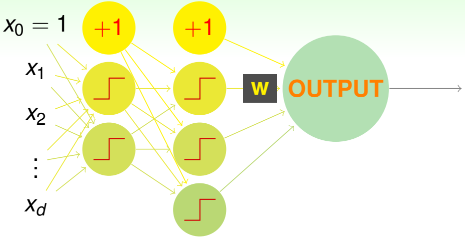
logistic regression

$h(\mathbf{x}) = \theta(s)$



err = cross-entropy

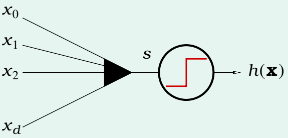
Neural Network Hypothesis: Output



- **OUTPUT**: simply a **linear model** with $s = \mathbf{w}^T \phi^{(2)}(\phi^{(1)}(\mathbf{x}))$
- any linear model can be used—**remember? :-)**

linear classification

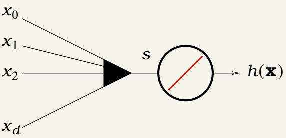
$h(\mathbf{x}) = \text{sign}(s)$



err = 0/1

linear regression

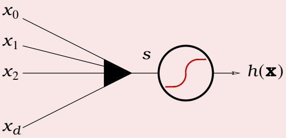
$h(\mathbf{x}) = s$



err = squared

logistic regression

$h(\mathbf{x}) = \theta(s)$

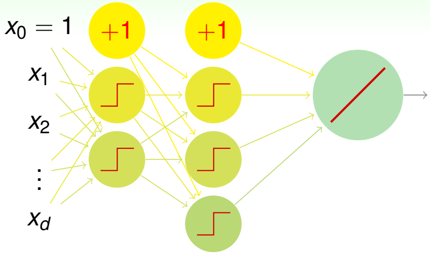


err = cross-entropy

will discuss **'regression' with squared error**

Neural Network Hypothesis: Transformation

- ⌐ : **transformation** function of score (signal) s



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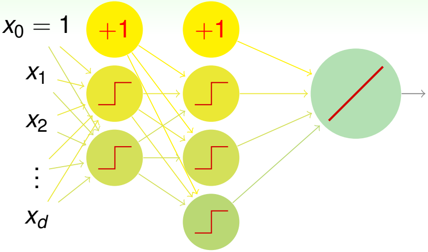

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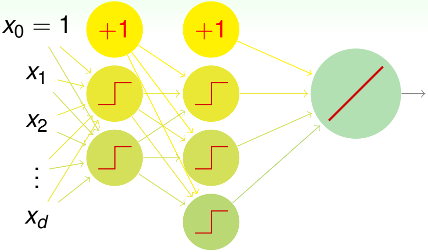

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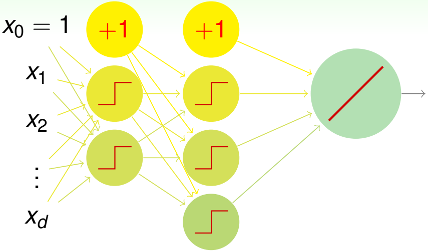

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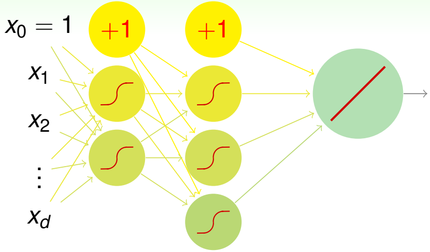

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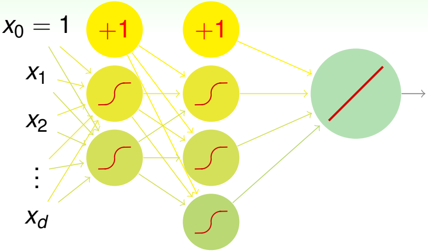

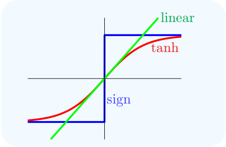

$$\tanh(s) = \frac{\exp(s) - \exp(-s)}{\exp(s) + \exp(-s)}$$

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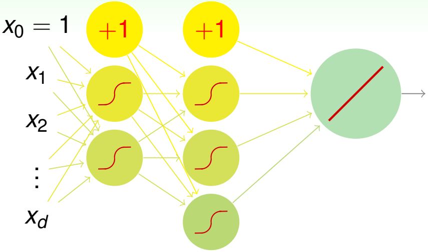

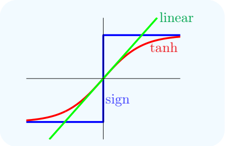

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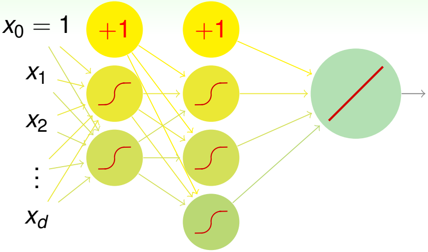

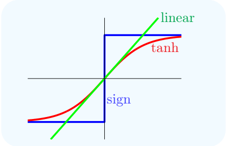

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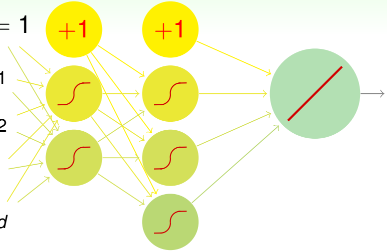

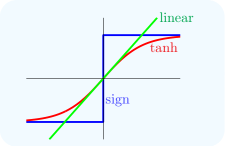

$$\begin{aligned}\tanh(s) &= \frac{\exp(s) - \exp(-s)}{\exp(s) + \exp(-s)} \\ &= 2\theta(2s) - 1\end{aligned}$$

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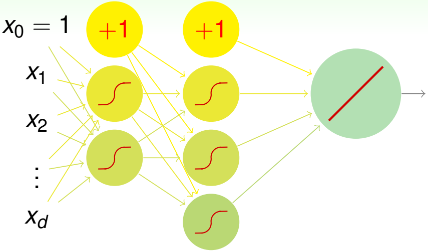

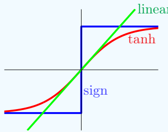

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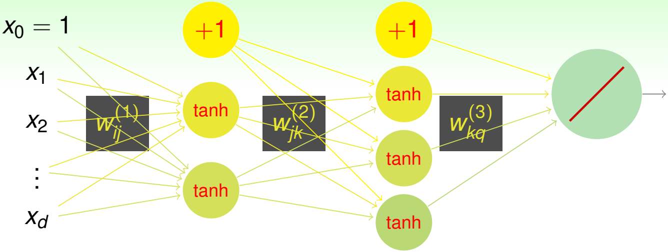
$$

will discuss with tanh as transformation function

Neural Network Hypothesis



$d^{(0)}$-$d^{(1)}$-$d^{(2)}$-$\cdots$-$d^{(L)}$ Neural Network (NNet)

$$w_{ij}^{(\ell)} : \begin{cases} 1 \le \ell \le L & \text{layers} \\ \quad \le i \le d^{(\ell-1)} & \text{inputs} \\ \quad \le j \le d^{(\ell)} & \text{outputs} \end{cases} ,$$

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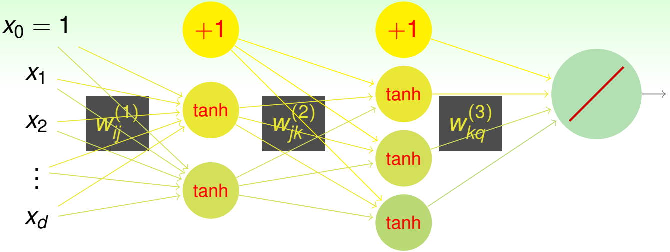

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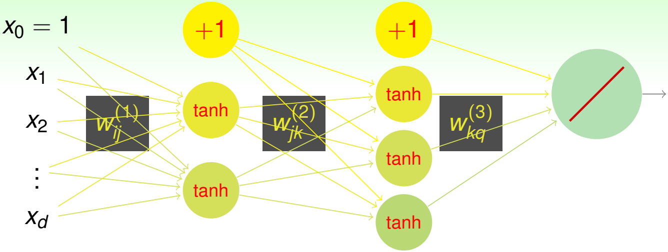

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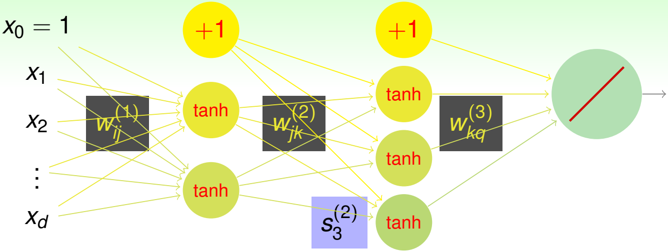

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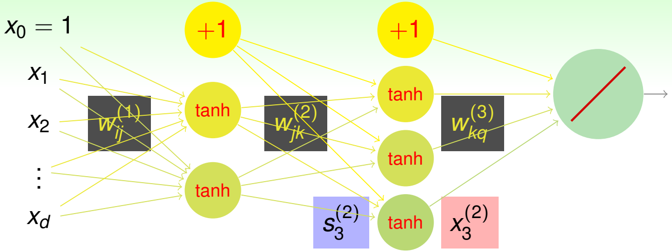

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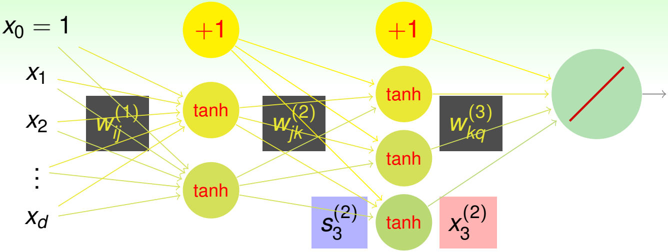

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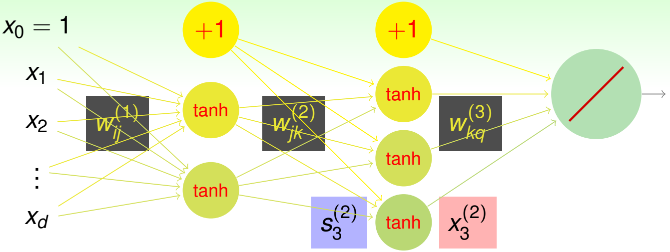

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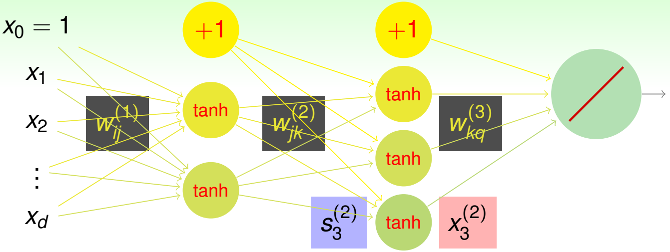

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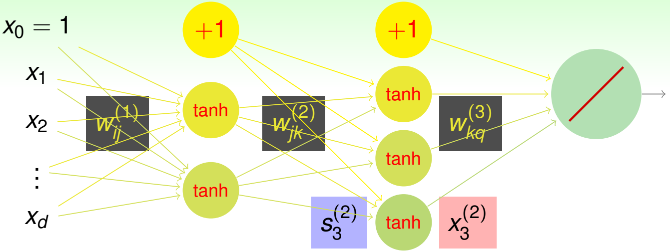

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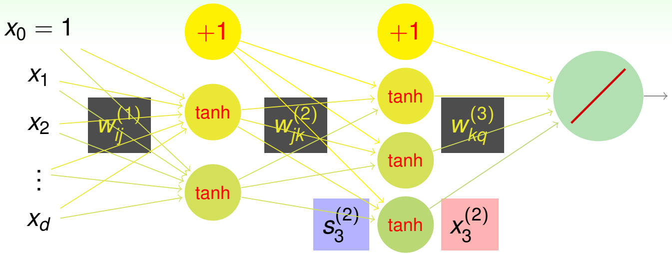
Physical Interpretation



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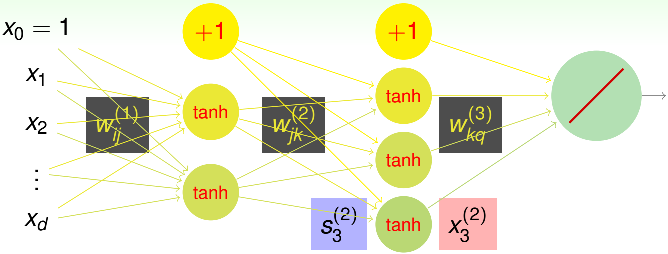

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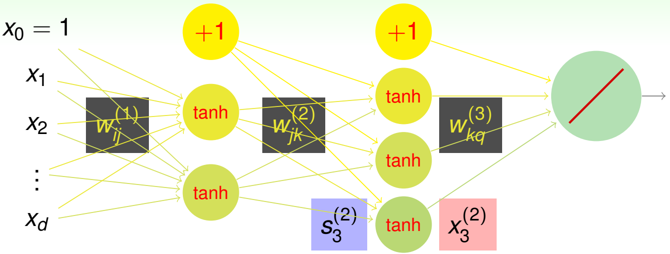

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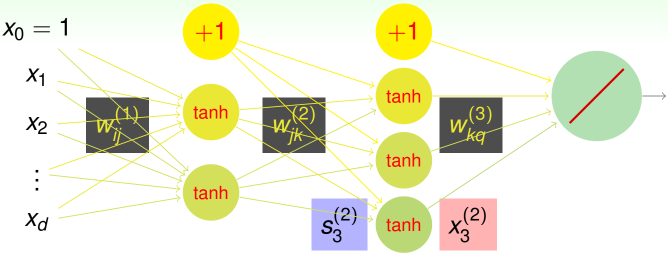

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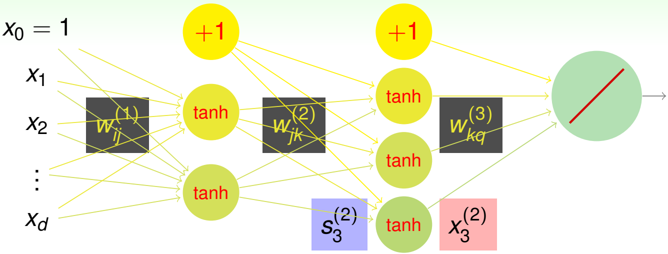

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NNet: **pattern extraction** with
layers of connection weights

Fun Time

How many weights $\{w_{ij}^{(\ell)}\}$ are there in a 3-5-1 NNet?

1. 9
2. 15
3. 20
4. 26

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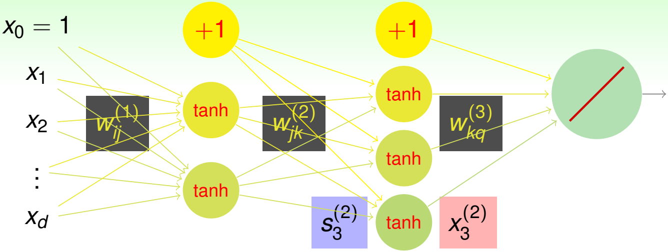
Reference Answer: ④

There are $(3+1) \times 5$ weights in $w_{ij}^{(1)}$, and $(5+1) \times 1$ weights in $w_{jk}^{(2)}$.

How to Learn the Weights?



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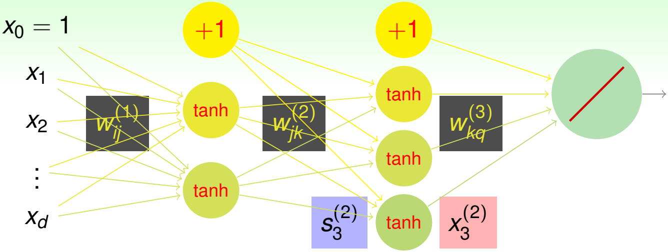

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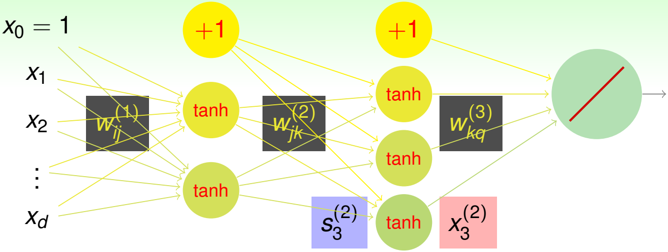

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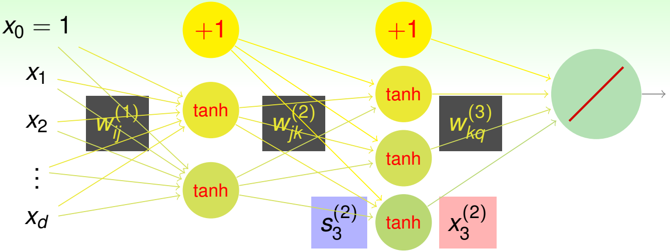

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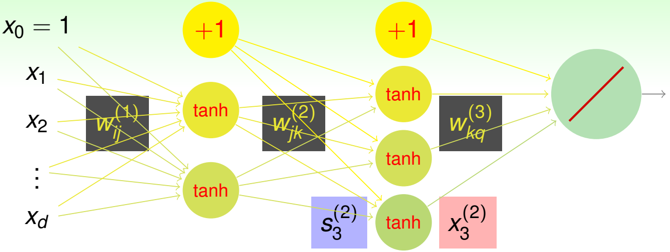

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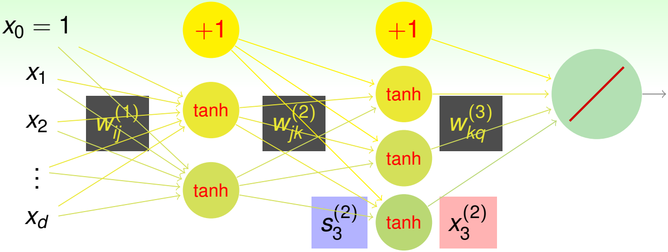

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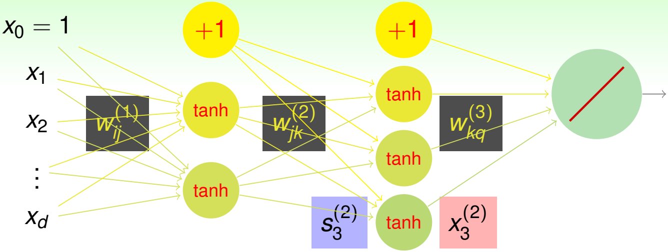

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- multiple hidden layers? **not easy**
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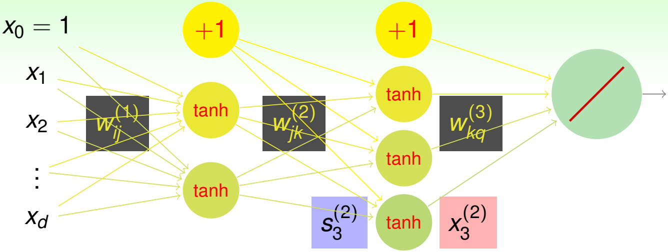

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- one hidden layer: simply **aggregation of perceptrons**
  —**gradient boosting** to determine hidden neuron one by one
- multiple hidden layers? **not easy**
- let $e_n = (y_n - \text{NNet}(\mathbf{x}_n))^2$:
  can apply **(stochastic) GD** after computing $\frac{\partial e_n}{\partial w_{ij}^{(\ell)}}$!

next: efficient computation of $\frac{\partial e_n}{\partial w_{ij}^{(\ell)}}$

Computing $\frac{\partial e_n}{\partial w_{i1}^{(L)}}$ (Output Layer)

$$e_n = (y_n - \text{NNet}(\mathbf{x}_n))^2$$

Computing $\frac{\partial e_n}{\partial w_{i1}^{(L)}}$ (Output Layer)

$$e_n = (y_n - \text{NNet}(\mathbf{x}_n))^2 = \Big(y_n - \qquad \Big)^2$$

Computing $\frac{\partial e_n}{\partial w_{i1}^{(L)}}$ (Output Layer)

$$e_n = (y_n - \text{NNet}(\mathbf{x}_n))^2 = \left(y_n - s_1^{(L)}\right)^2$$

Computing $\frac{\partial e_n}{\partial w_{i1}^{(L)}}$ (Output Layer)

$$e_n = (y_n - \mathrm{NNet}(\mathbf{x}_n))^2 = \left(y_n - s_1^{(L)}\right)^2 = \left(y_n - \sum_{i=0}^{d^{(L-1)}} \qquad x_i^{(L-1)}\right)^2$$

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specially (output layer) $(0 \le i \le d^{(L-1)})$

$$\frac{\partial e_n}{\partial w_{i1}^{(L)}}$$

$$= \frac{\partial e_n}{\partial s_1^{(L)}} \cdot \frac{\partial}{\partial w_{i1}^{(L)}}$$

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$\delta_1^{(L)} = -2\left(y_n - s_1^{(L)}\right)$, how about **others**?

Computing $\delta_j^{(\ell)} = \frac{\partial e_n}{\partial s_j^{(\ell)}}$

$s_j^{(\ell)}$

Computing $\delta_j^{(\ell)} = \frac{\partial e_n}{\partial s_j^{(\ell)}}$

$$s_j^{(\ell)} \overset{\tanh}{\Longrightarrow} x_j^{(\ell)}$$

Computing $\delta_j^{(\ell)} = \frac{\partial e_n}{\partial s_j^{(\ell)}}$

$$s_j^{(\ell)} \overset{\tanh}{\Longrightarrow} x_j^{(\ell)} \overset{w_{jk}^{(\ell+1)}}{\Longrightarrow} \begin{bmatrix} s_1^{(\ell+1)} \\ \vdots \\ s_k^{(\ell+1)} \\ \vdots \end{bmatrix}$$

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$\delta_j^{(\ell)}$ can be computed **backwards** from $\delta_k^{(\ell+1)}$

Backpropagation (Backprop) Algorithm

Backprop on NNet

initialize all weights $w_{ij}^{(\ell)}$
for $t = 0, 1, \ldots, T$

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4. gradient descent: $w_{ij}^{(\ell)} \leftarrow w_{ij}^{(\ell)} - \eta x_i^{(\ell-1)} \delta_j^{(\ell)}$

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return $g_{\text{NNET}}(\mathbf{x}) = \left(\cdots \tanh \left(\sum_j w_{jk}^{(2)} \cdot \tanh \left(\sum_i w_{ij}^{(1)} x_i \right) \right) \right)$

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sometimes (1) to (3) is (parallelly) done many times and average$(x_i^{(\ell-1)}\delta_j^{(\ell)})$ taken for update in (4), called **mini-batch**

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basic NNet algorithm: backprop to compute the gradient **efficiently**

Fun Time

According to $\frac{\partial e_n}{\partial w_{i1}^{(L)}} = -2\left(y_n - s_1^{(L)}\right) \cdot \left(x_i^{(L-1)}\right)$ when would $\frac{\partial e_n}{\partial w_{i1}^{(L)}} = 0$?

1. $y_n = s_1^{(L)}$
2. $x_i^{(L-1)} = 0$
3. $s_i^{(L-1)} = 0$
4. all of the above

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4. all of the above

Reference Answer: 4

Note that $x_i^{(L-1)} = \tanh(s_i^{(L-1)}) = 0$ if and only if $s_i^{(L-1)} = 0$.

Neural Network Optimization

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \text{err}\left(\left(\cdots \tanh\left(\sum_j w_{jk}^{(2)} \cdot \tanh\left(\sum_i w_{ij}^{(1)} x_{n,i}\right)\right)\right), y_n\right)$$

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- generally **non-convex** when multiple hidden layers

Neural Network Optimization

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NNet: **difficult to optimize**,
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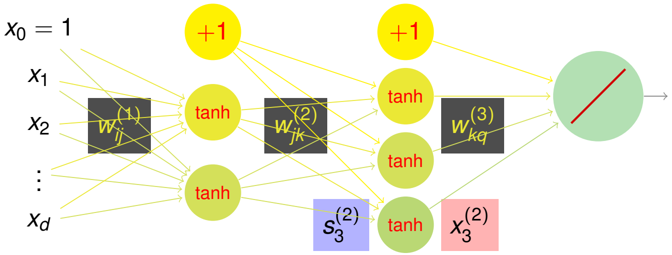
VC Dimension of Neural Network Model

roughly, with tanh-**like transfer functions**:
$d_{VC} = O(VD)$ where V = # of neurons, D = # of weights



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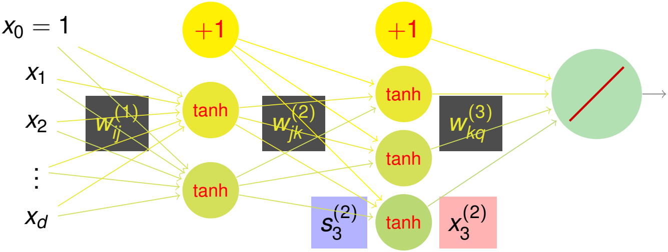

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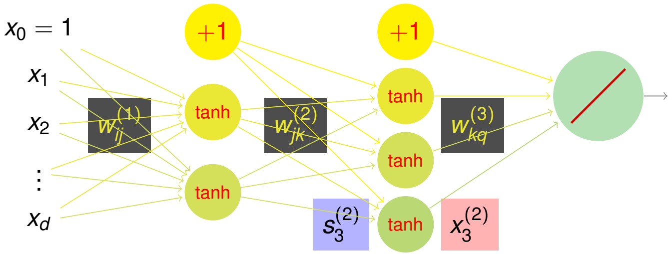

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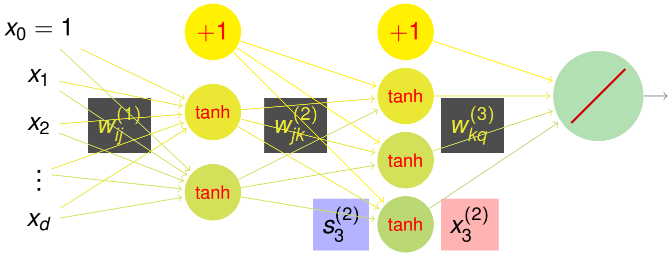

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Yet Another Regularization: Early Stopping

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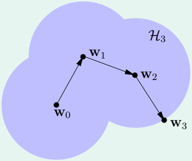

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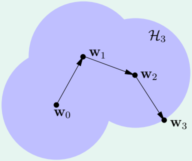

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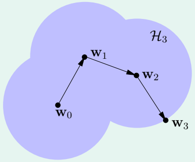

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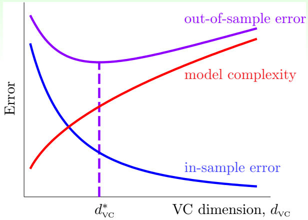

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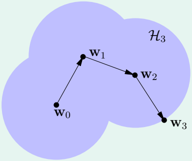

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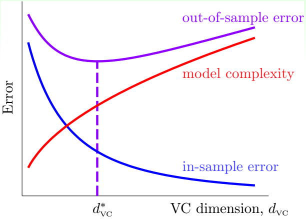

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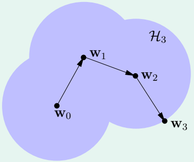

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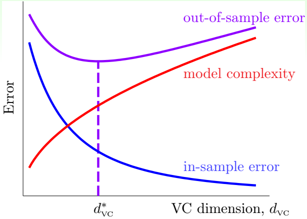

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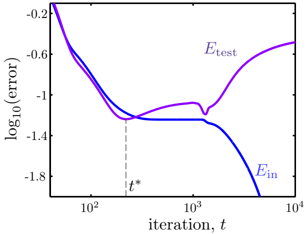

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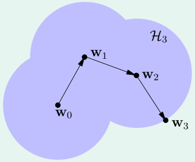

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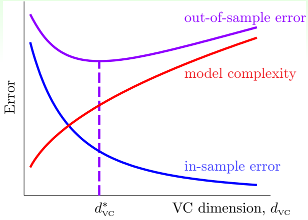

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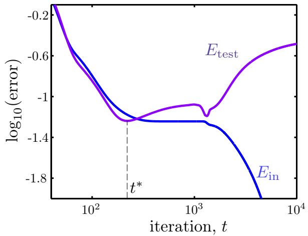

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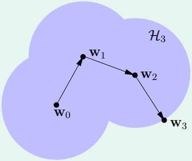

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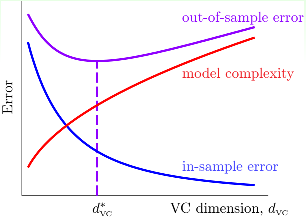

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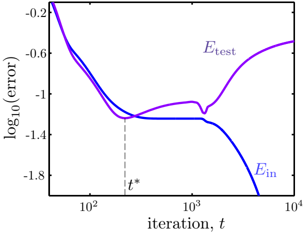

when to stop? **validation!**

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Reference Answer: ②

Too much calculus in this class, huh? :-)

Summary

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models

Lecture 12: Neural Network

- Motivation
  multi-layer for power with biological inspirations
- Neural Network Hypothesis
  layered pattern extraction until linear hypothesis
- Neural Network Learning
  backprop to compute gradient efficiently
- Optimization and Regularization
  tricks on initialization, regularizer, early stopping

- **next: making neural network 'deeper'**