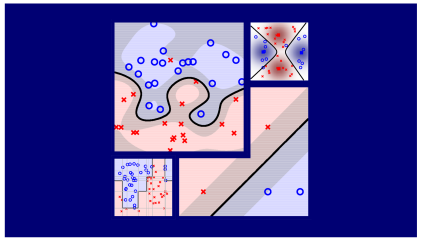
# Machine Learning Techniques
# (機器學習技法)



## 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**

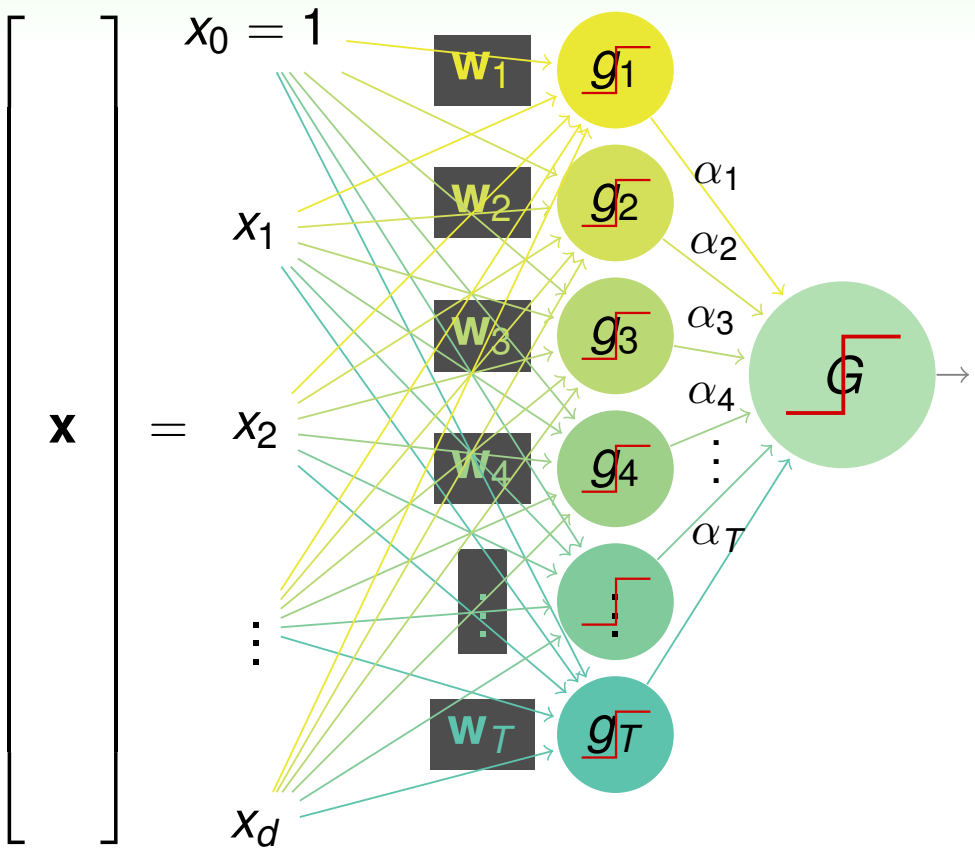
aggregating trees from **functional gradient** and **steepest descent** subject to **any error measure**

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

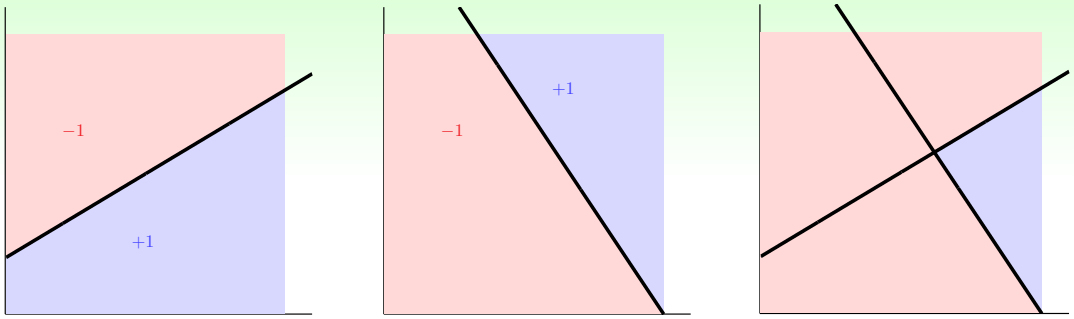



$$G(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t \underbrace{\text{sign}\left(\mathbf{w}_t^T \mathbf{x}\right)}_{g_t(\mathbf{x})}\right)$$

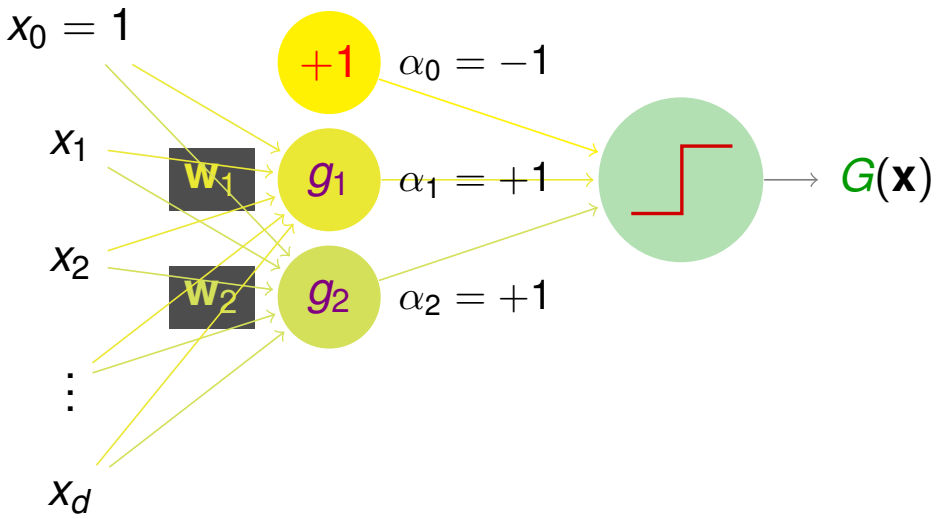
- two layers of weights: $\mathbf{w}_t$ and $\alpha$
- two layers of sign functions: in $g_t$ and in $G$

what boundary can $G$ **implement**?

# Logic Operations with Aggregation




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

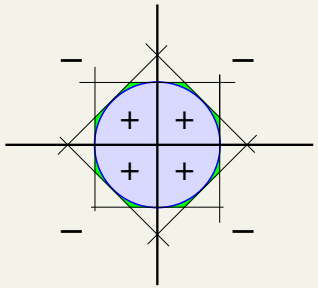



$G(\mathbf{x}) = \text{sign}\left(-1 + g_1(\mathbf{x}) + g_2(\mathbf{x})\right)$

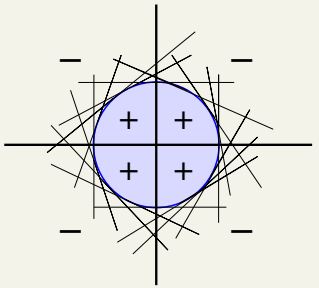
- $g_1(\mathbf{x}) = g_2(\mathbf{x}) = +1$ (TRUE): $G(\mathbf{x}) = +1$ (TRUE)
- otherwise: $G(\mathbf{x}) = -1$ (FALSE)
- $G \equiv \texttt{AND}(g_1, g_2)$

OR, NOT can be **similarly implemented**

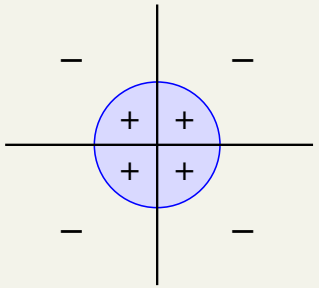
# Powerfulness and Limitation



8 perceptrons

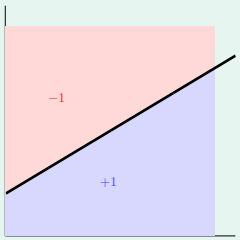


16 perceptrons

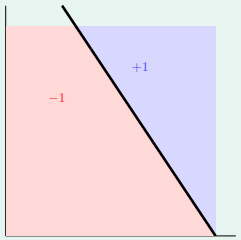


target boundary

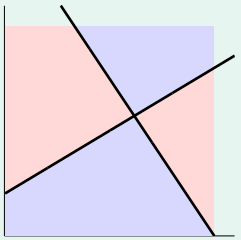
- 'convex set' hypotheses implemented: $d_{VC} \to \infty$, **remember? :-)**
- powerfulness: enough perceptrons $\approx$ **smooth boundary**




$g_1$




$g_2$



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

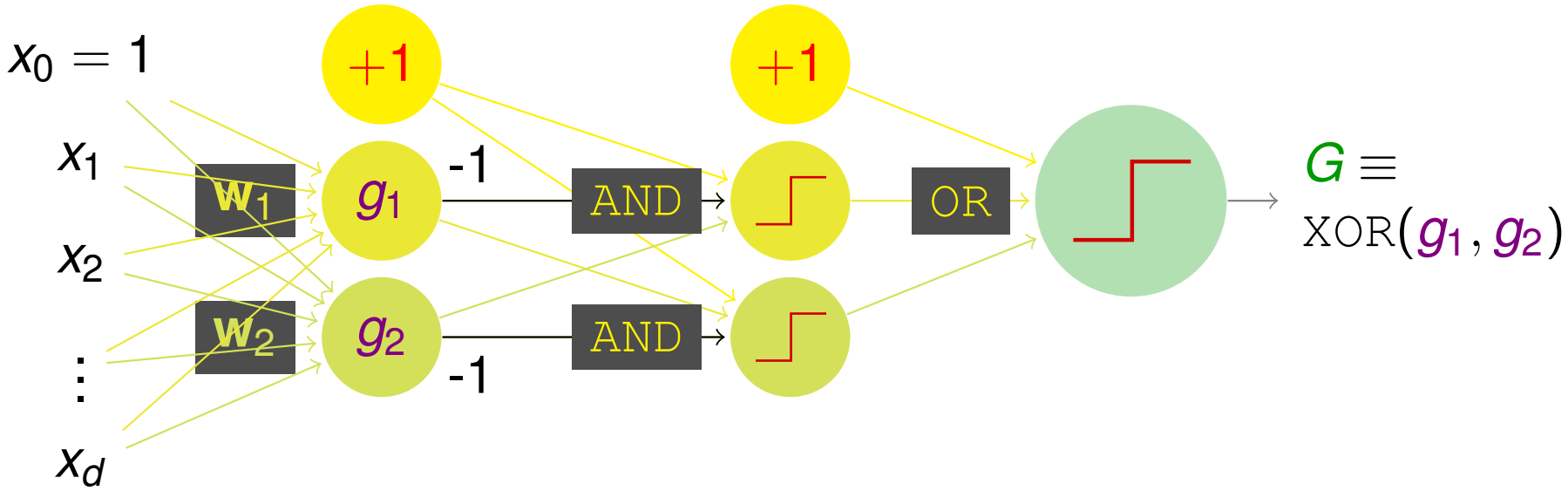
- limitation: XOR **not 'linear separable'** under $\phi(\mathbf{x}) = (g_1(\mathbf{x}), g_2(\mathbf{x}))$

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

# Multi-Layer Perceptrons: Basic Neural Network

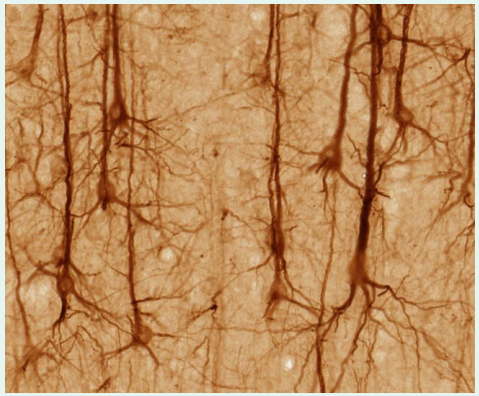
- non-separable data: can use more **transform**
- how about one more layer of **AND transform**?

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




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

# Connection to Biological Neurons



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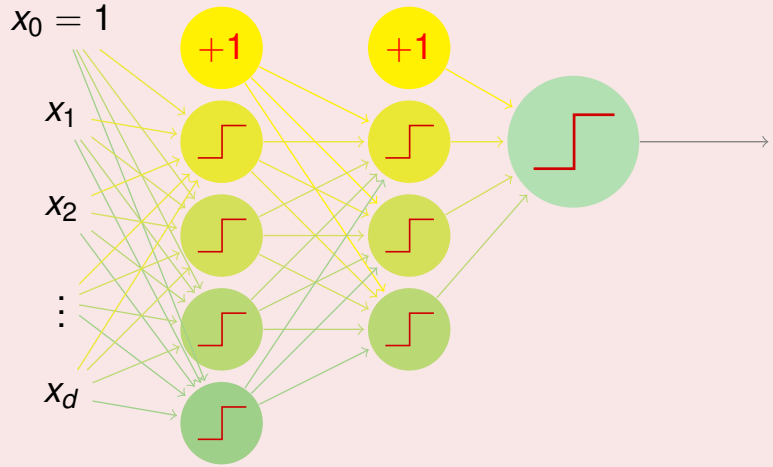


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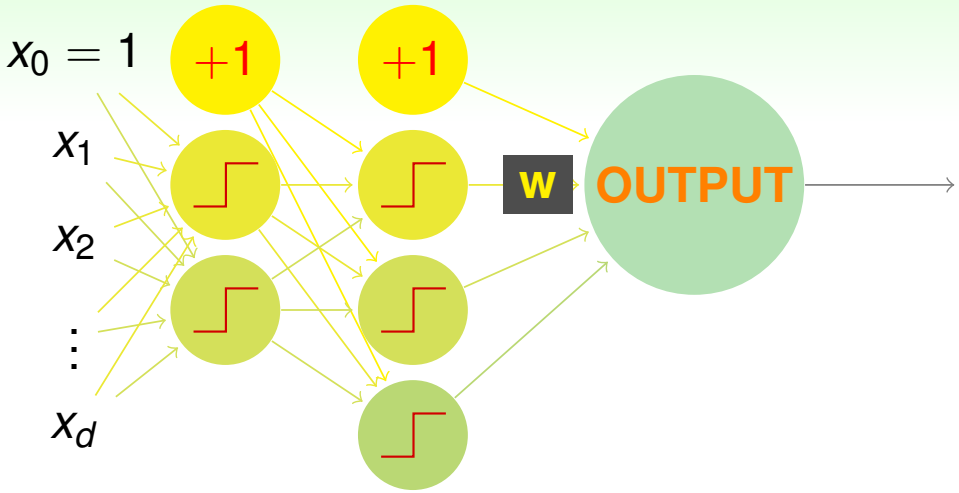
neural network: **bio-inspired** model

# 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 $\texttt{OR}(g_1, g_2)$?

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

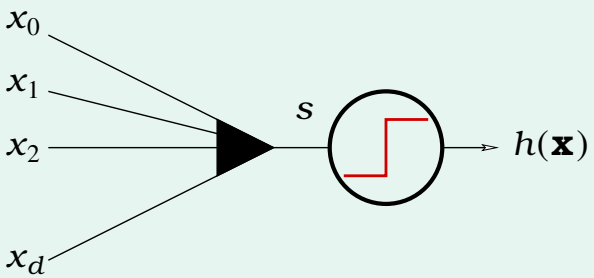
# Neural Network Hypothesis: Output




- **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

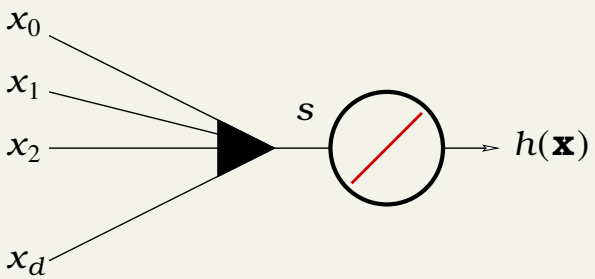
$h(\mathbf{x}) = \text{sign}(s)$




err = 0/1

## linear regression

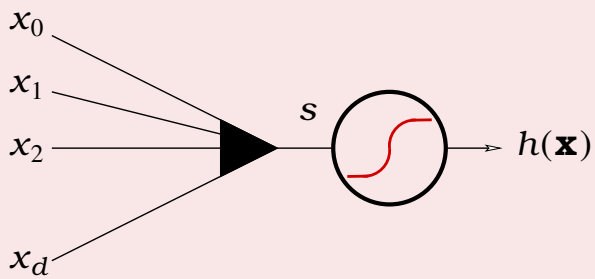
$h(\mathbf{x}) = s$




err = squared

## logistic regression

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

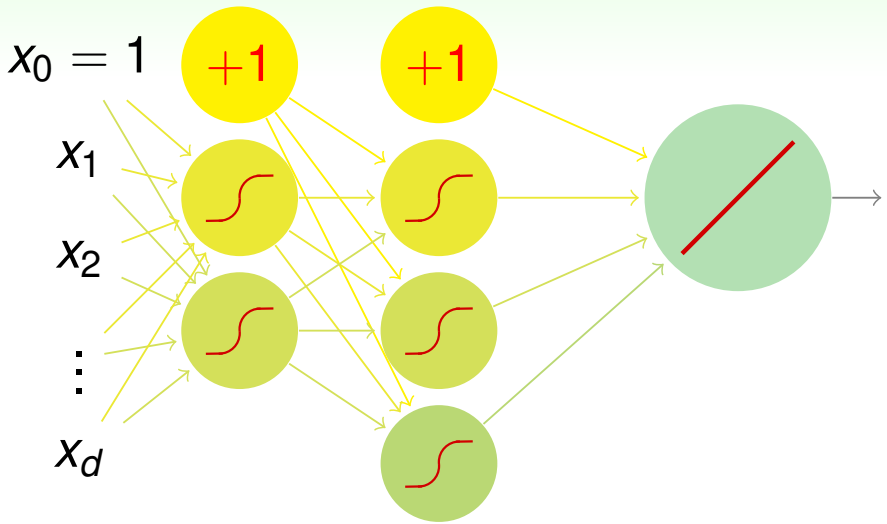


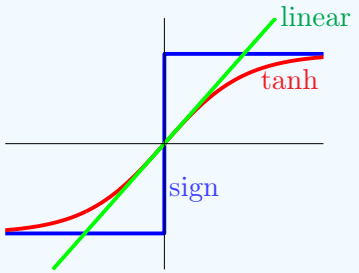

err = cross-entropy

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

# Neural Network Hypothesis: Transformation

- $\sqcap$ : **transformation** function of score (signal) $s$
- any transformation?
  - $/$ : whole network linear & thus **less useful**
  - $\sqcap$ : discrete & thus **hard to optimize** for $\mathbf{w}$
- popular choice of transformation: $\int = \tanh(s)$
  - 'analog' approximation of $\sqcap$ : **easier to optimize**
  - somewhat **closer to biological** neuron
  - **not that new! :-)**

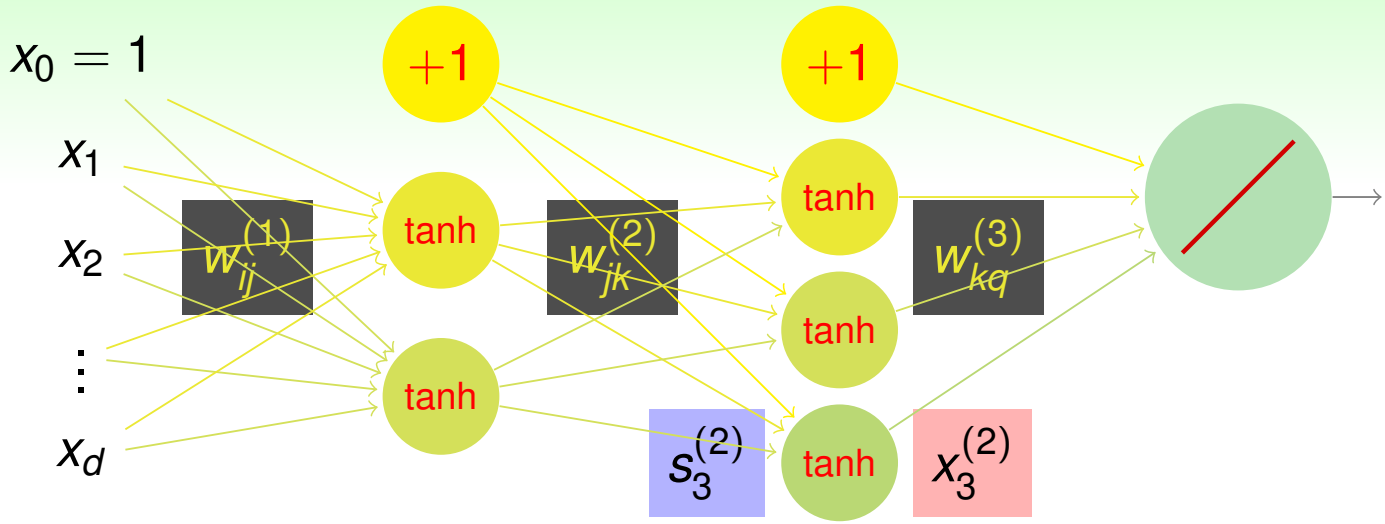



$$\tanh(s) = \frac{\exp(s) - \exp(-s)}{\exp(s) + \exp(-s)} = 2\theta(2s) - 1$$

will discuss with tanh as transformation function

# Neural Network Hypothesis



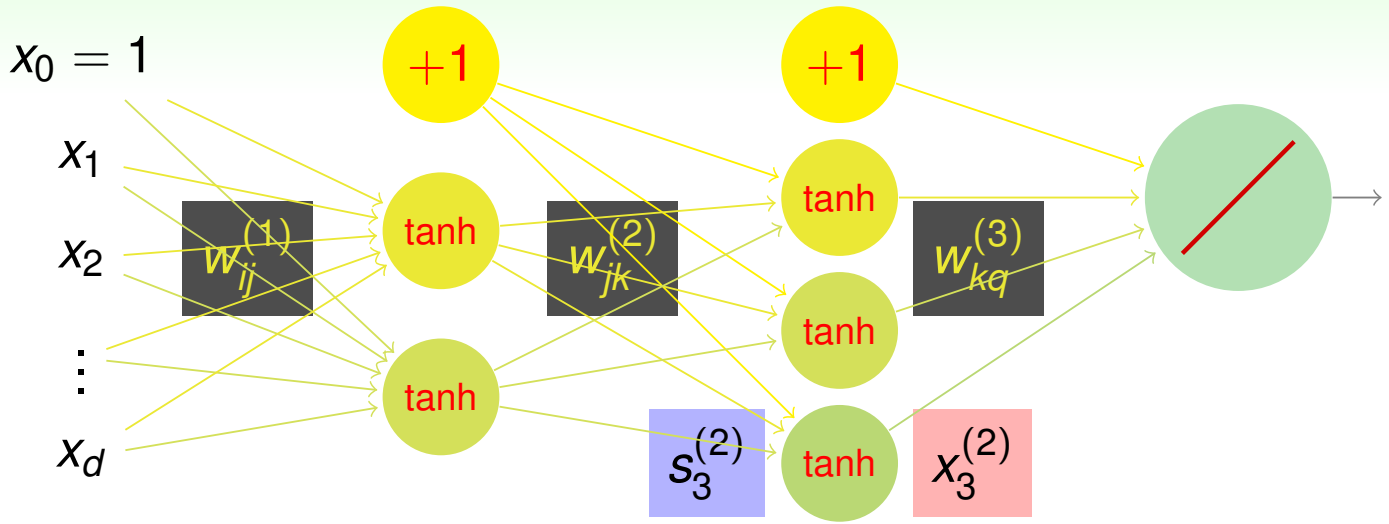

## $d^{(0)}$-$d^{(1)}$-$d^{(2)}$-$\cdots$-$d^{(L)}$ Neural Network (NNet)

$w_{ij}^{(\ell)}$ : $\begin{cases} 1 \le \ell \le L & \text{layers} \\ 0 \le i \le d^{(\ell-1)} & \text{inputs} \\ 1 \le j \le d^{(\ell)} & \text{outputs} \end{cases}$, score $s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{ij}^{(\ell)} x_i^{(\ell-1)}$,

transformed $x_j^{(\ell)} = \begin{cases} \tanh\left(s_j^{(\ell)}\right) & \text{if } \ell < L \\ s_j^{(\ell)} & \text{if } \ell = L \end{cases}$

apply $\mathbf{x}$ as input layer $\mathbf{x}^{(0)}$, go through hidden layers to get $\mathbf{x}^{(\ell)}$, predict at output layer $x_1^{(L)}$

# Physical Interpretation




- each layer: **transformation** to be **learned** from data
- $\phi^{(\ell)}(\mathbf{x}) = \tanh\left(\begin{bmatrix} \sum_{i=0}^{d^{(\ell-1)}} w_{i1}^{(\ell)} x_i^{(\ell-1)} \\ \vdots \end{bmatrix}\right)$

  —whether $\mathbf{x}$ 'matches' weight vectors in pattern

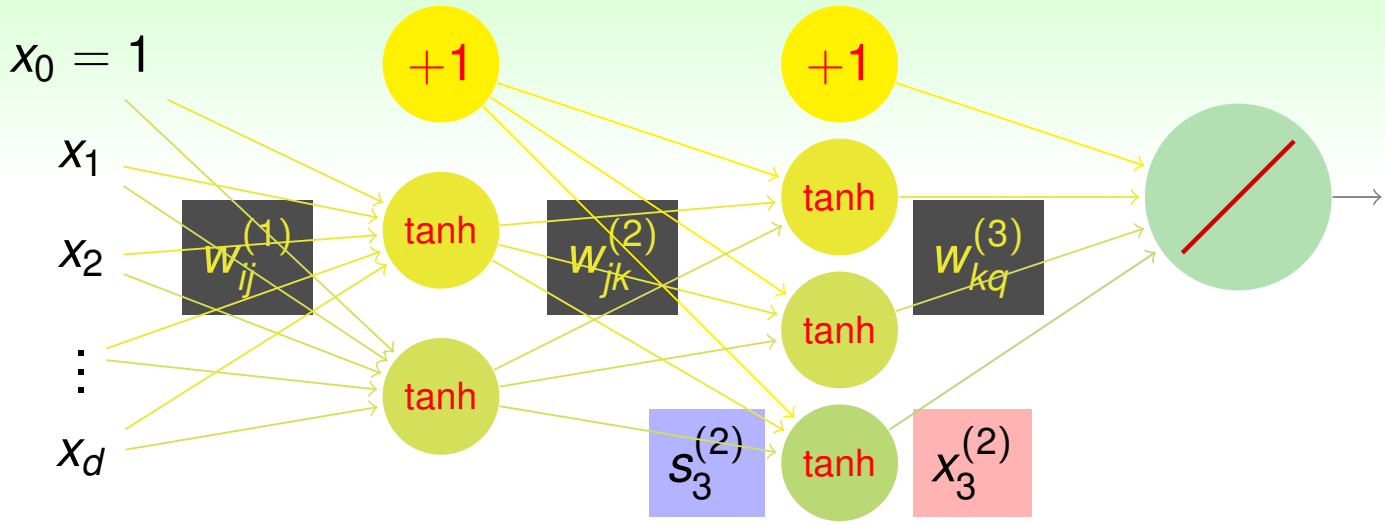
NNet: **pattern extraction** with layers of connection weights

# Fun Time

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

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

# How to Learn the Weights?




- goal: learning all $\{w_{ij}^{(\ell)}\}$ to **minimize** $E_{\text{in}}\left(\{w_{ij}^{(\ell)}\}\right)$
- 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)

$$e_n = (y_n - \text{NNet}(\mathbf{x}_n))^2 = \left(y_n - s_1^{(L)}\right)^2 = \left(y_n - \sum_{i=0}^{d^{(L-1)}} w_{i1}^{(L)} x_i^{(L-1)}\right)^2$$

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

$$\begin{aligned} & \frac{\partial e_n}{\partial w_{i1}^{(L)}} \\ = & \frac{\partial e_n}{\partial s_1^{(L)}} \cdot \frac{\partial s_1^{(L)}}{\partial w_{i1}^{(L)}} \\ = & -2\left(y_n - s_1^{(L)}\right) \cdot \left(x_i^{(L-1)}\right) \end{aligned}$$

## generally $(1 \le \ell < L)$ $(0 \le i \le d^{(\ell-1)}; 1 \le j \le d^{(\ell)})$

$$\begin{aligned} & \frac{\partial e_n}{\partial w_{ij}^{(\ell)}} \\ = & \frac{\partial e_n}{\partial s_j^{(\ell)}} \cdot \frac{\partial s_j^{(\ell)}}{\partial w_{ij}^{(\ell)}} \\ = & \delta_j^{(\ell)} \cdot \left(x_i^{(\ell-1)}\right) \end{aligned}$$

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

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

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

$$\delta_j^{(\ell)} = \frac{\partial e_n}{\partial s_j^{(\ell)}} = \sum_{k=1}^{d^{(\ell+1)}} \frac{\partial e_n}{\partial s_k^{(\ell+1)}} \frac{\partial s_k^{(\ell+1)}}{\partial x_j^{(\ell)}} \frac{\partial x_j^{(\ell)}}{\partial s_j^{(\ell)}}$$

$$= \sum_k \left(\delta_k^{(\ell+1)}\right) \left(w_{jk}^{(\ell+1)}\right) \left(\tanh'\left(s_j^{(\ell)}\right)\right)$$

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

# Backpropagation (Backprop) Algorithm

## Backprop on NNet

initialize all weights $w_{ij}^{(\ell)}$

for $t = 0, 1, \ldots, T$

1. stochastic: randomly pick $n \in \{1, 2, \cdots, N\}$
2. forward: compute all $x_i^{(\ell)}$ with $\mathbf{x}^{(0)} = \mathbf{x}_n$
3. backward: compute all $\delta_j^{(\ell)}$ subject to $\mathbf{x}^{(0)} = \mathbf{x}_n$
4. gradient descent: $w_{ij}^{(\ell)} \leftarrow w_{ij}^{(\ell)} - \eta x_i^{(\ell-1)} \delta_j^{(\ell)}$

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

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**

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

# Neural Network Optimization

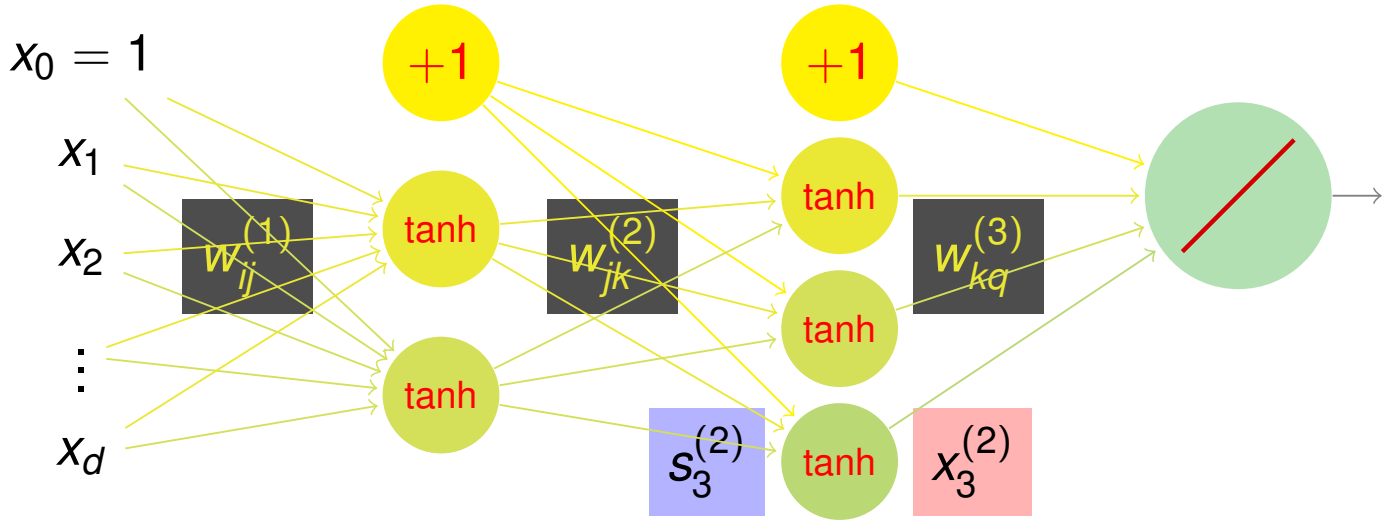
$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \text{err}\left(\left(\cdots \tanh\left(\sum_j w_{jk}^{(2)} \cdot \tanh\left(\sum_i w_{ij}^{(1)} x_{n,i}\right)\right)\right), y_n\right)$$

- generally **non-convex** when multiple hidden layers
  - not easy to reach **global minimum**
  - GD/SGD with **backprop** only gives **local minimum**
- different initial $w_{ij}^{(\ell)} \Longrightarrow$ different **local minimum**
  - somewhat '**sensitive**' to initial weights
  - **large weights** $\Longrightarrow$ **saturate** (small gradient)
  - advice: try **some random** & **small** ones

NNet: **difficult to optimize**,
but **practically works**

# VC Dimension of Neural Network Model

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




- pros: can **approximate 'anything'** if enough neurons ($V$ large)
- cons: can **overfit** if too many neurons

NNet: **watch out for overfitting!**

# Regularization for Neural Network

basic choice:

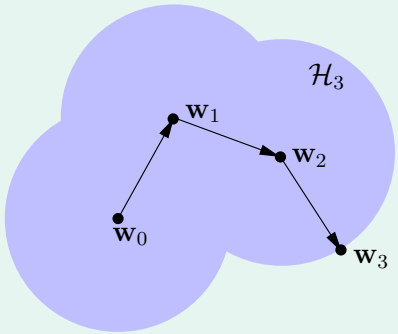
old friend weight-decay (L2) regularizer $\Omega(\mathbf{w}) = \sum \left(w_{ij}^{(\ell)}\right)^2$

- 'shrink' weights:
  large weight $\rightarrow$ large shrink; small weight $\rightarrow$ small shrink
- want $w_{ij}^{(\ell)} = 0$ (sparse) to effectively **decrease** $d_{\text{VC}}$
  - L1 regularizer: $\sum \left|w_{ij}^{(\ell)}\right|$, but **not differentiable**
  - weight-elimination ('scaled' L2) regularizer:
    large weight $\rightarrow$ median shrink; small weight $\rightarrow$ median shrink

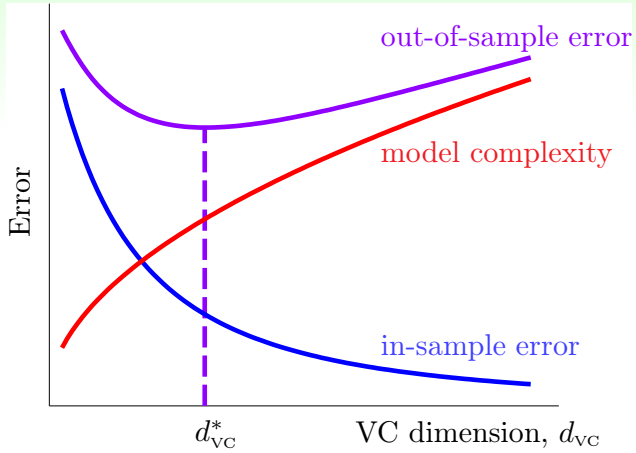
**weight-elimination** regularizer: $\sum \frac{\left(w_{ij}^{(\ell)}\right)^2}{1+\left(w_{ij}^{(\ell)}\right)^2}$

# Yet Another Regularization: Early Stopping

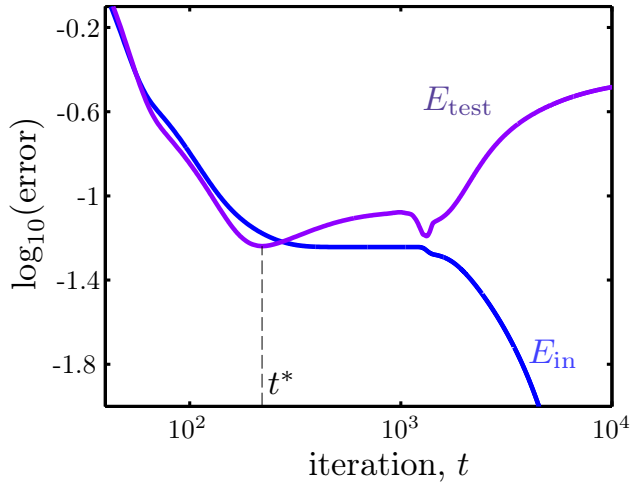
- **GD/SGD (backprop)** visits more weight combinations as $t$ increases




- smaller $t$ effectively decrease $d_{\text{VC}}$
- better 'stop in middle': **early stopping**




($d^*_{\text{VC}}$ **in middle, remember? :-)**)




when to stop? **validation!**

# Fun Time

For the weight elimination regularizer $\sum \frac{\left(w_{ij}^{(\ell)}\right)^2}{1+\left(w_{ij}^{(\ell)}\right)^2}$, what is $\frac{\partial \text{regularizer}}{\partial w_{ij}^{(\ell)}}$?

1. $2w_{ij}^{(\ell)} / \left(1+\left(w_{ij}^{(\ell)}\right)^2\right)^1$
2. $2w_{ij}^{(\ell)} / \left(1+\left(w_{ij}^{(\ell)}\right)^2\right)^2$
3. $2w_{ij}^{(\ell)} / \left(1+\left(w_{ij}^{(\ell)}\right)^2\right)^3$
4. $2w_{ij}^{(\ell)} / \left(1+\left(w_{ij}^{(\ell)}\right)^2\right)^4$

# 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'**