10417/10617
Intermediate Deep Learning: Fall2020

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Neural Networks I

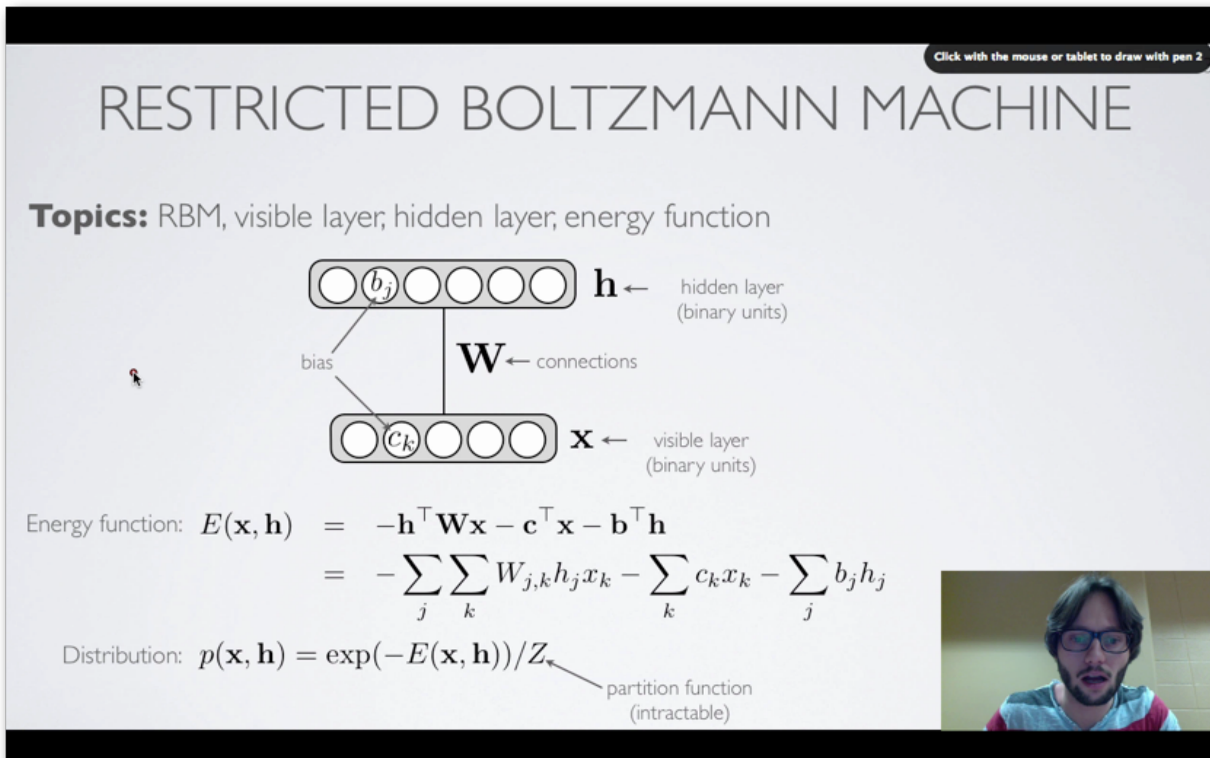
Neural Networks Online Course

• **Disclaimer**: Much of the material and slides for this lecture were borrowed from Hugo Larochelle's class on Neural Networks: https://sites.google.com/site/deeplearningsummerschool2016/

http://info.usherbrooke.ca/hlarochelle/neural_networks

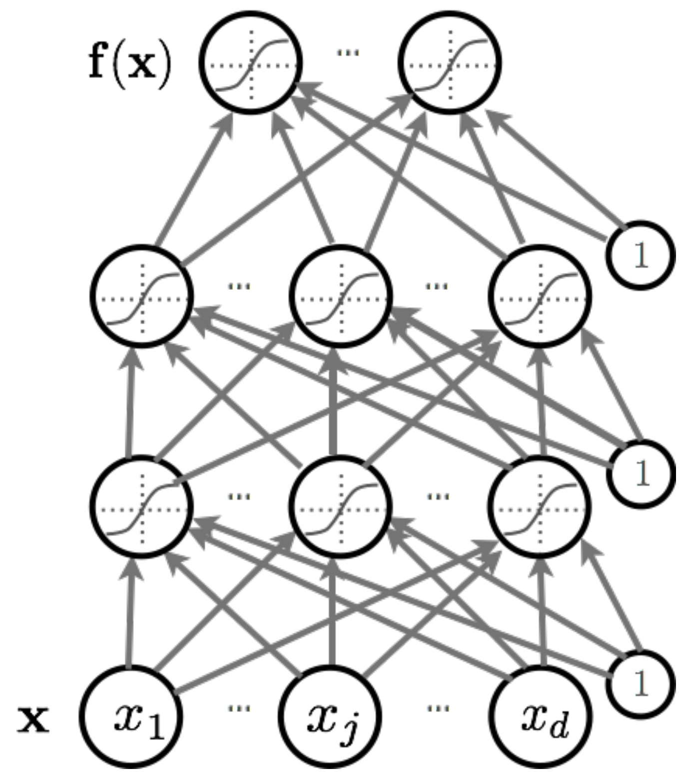
• Hugo's class covers many other topics: convolutional networks, neural language model, Boltzmann machines, autoencoders, sparse coding, etc.

• We will use his material for some of the other lectures.



Feedforward Neural Networks

- How neural networks predict f(x) given an input x:
  - Forward propagation
  - Types of units
  - Capacity of neural networks
- How to train neural nets:
  - Loss function
  - Backpropagation with gradient descent
- More recent techniques:
  - Dropout
  - Batch normalization
  - Unsupervised Pre-training



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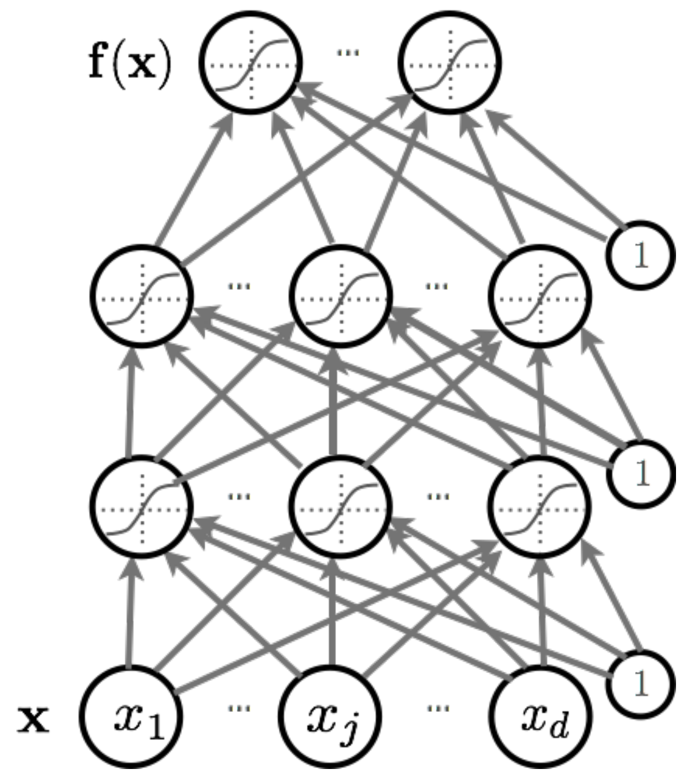


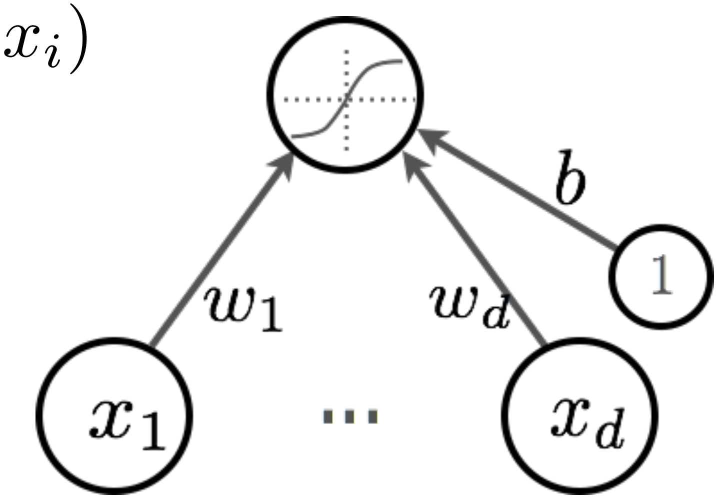
Artificial Neuron

- Neuron pre-activation (or input activation):

$$a(\mathbf{x}) = b + \sum_i w_i x_i = b + \mathbf{w}^\top \mathbf{x}$$

- Neuron output activation:

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$



where

$\mathbf{w}$ are the weights (parameters)

b is the bias term

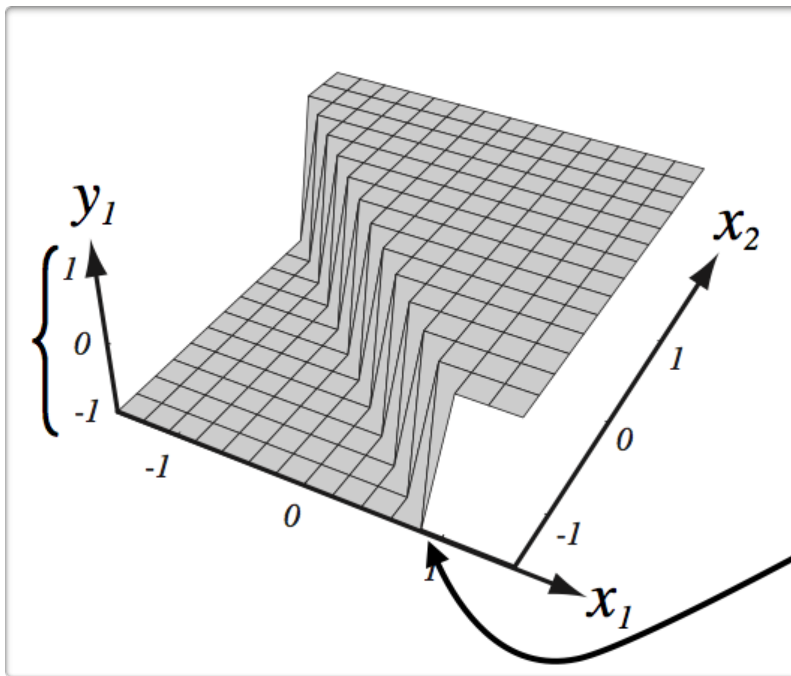
$g(\cdot)$ is called the activation function

Artificial Neuron

- Output activation of the neuron:

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \textstyle\sum_i w_i x_i)$$

Range is determined by $g(\cdot)$



Bias only changes the position of the riff

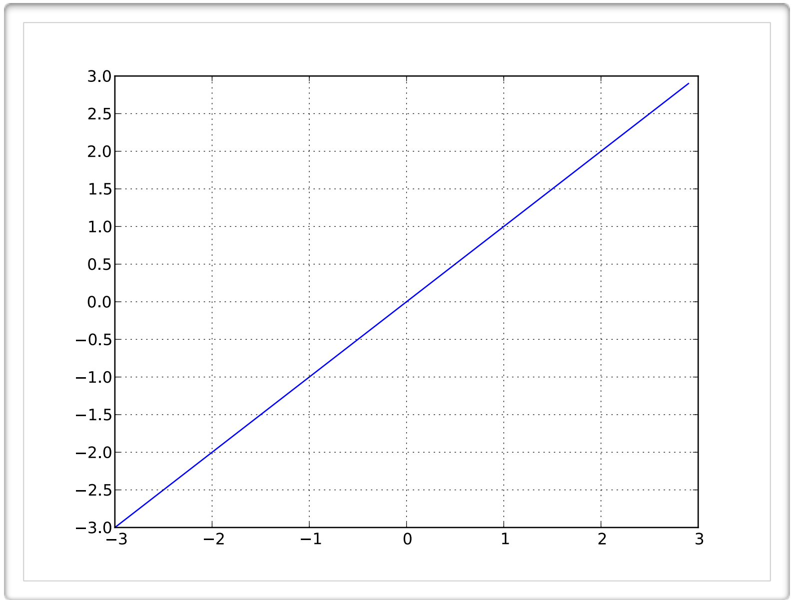
(from Pascal Vincent's slides)

Activation Function

- Linear activation function:

$$g(a) = a$$

  - No nonlinear transformation
  - No input squashing

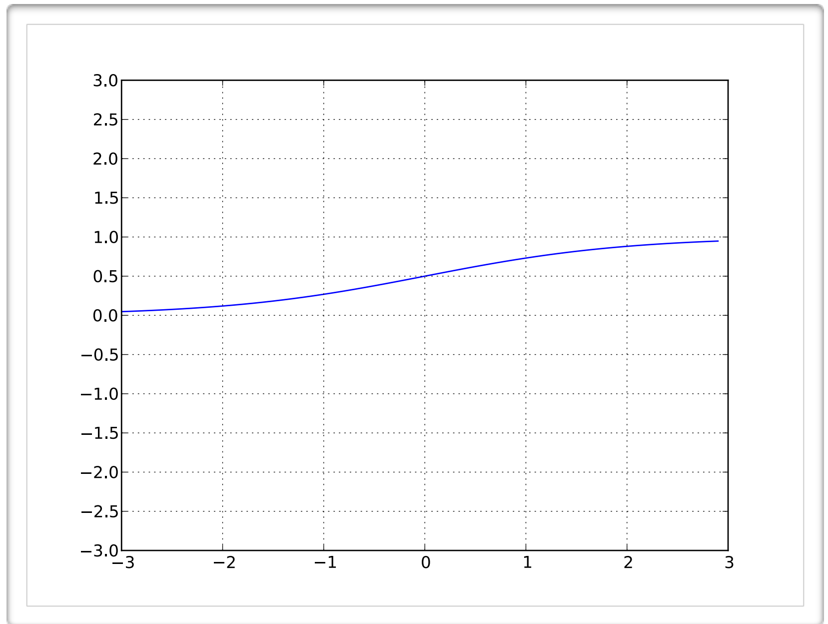


Activation Function

- Sigmoid activation function:

  - Squashes the neuron's output between 0 and 1
  - Always positive
  - Bounded
  - Strictly Increasing

$$g(a) = \mathrm{sigm}(a) = \frac{1}{1+\exp(-a)}$$



Activation Function

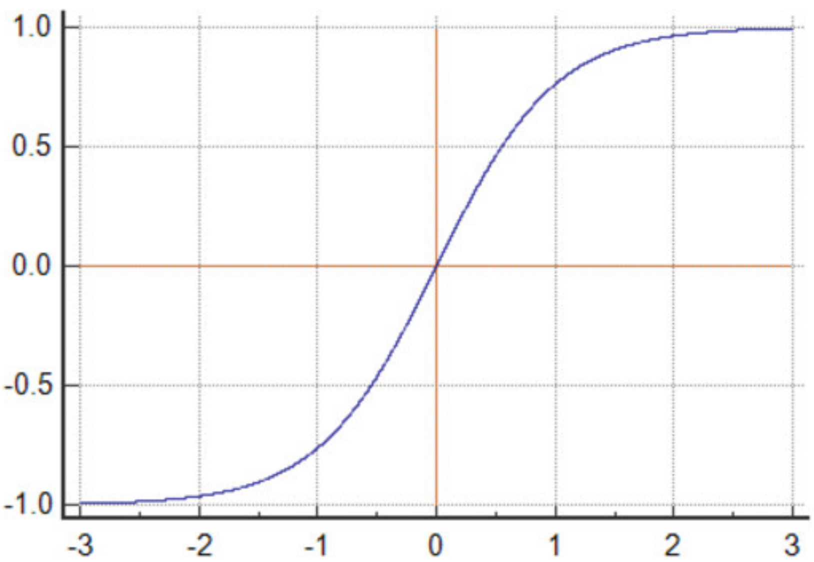
- Hyperbolic tangent (“tanh”) activation function:

$$g(a) = \tanh(a) =$$

$$= \frac{\exp(a)-\exp(-a)}{\exp(a)+\exp(-a)} = \frac{\exp(2a)-1}{\exp(2a)+1}$$

- Squashes the neuron’s activation between -1 and 1
- Can be positive or negative
- Bounded
- Strictly increasing

(wrong plot)

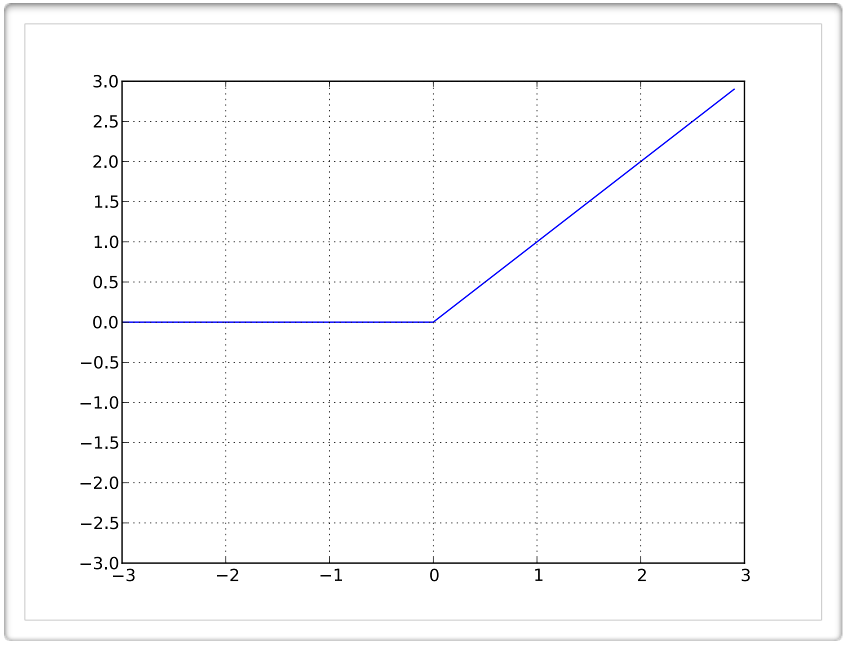


Activation Function

- Rectified linear (ReLU) activation function:

$$g(a) = \mathrm{reclin}(a) = \max(0, a)$$

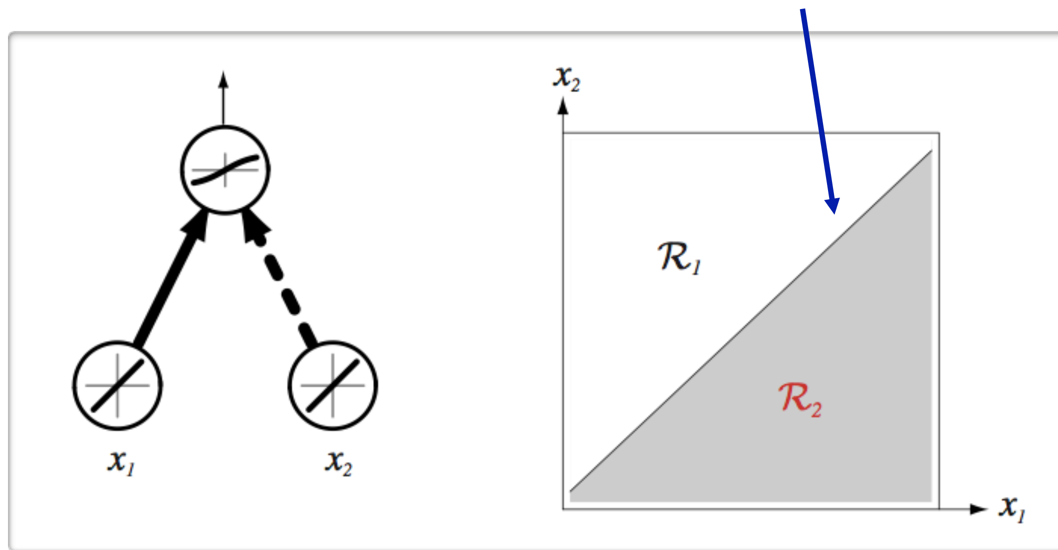
  - Bounded below by 0 (always non-negative)
  - Tends to produce units with sparse activities
  - Not upper bounded
  - Strictly increasing



Decision Boundary of a Neuron

- Binary classification:
  - With sigmoid, one can interpret neuron as estimating $p(y = 1|\mathbf{x})$
  - Interpret as a logistic classifier

Decision boundary



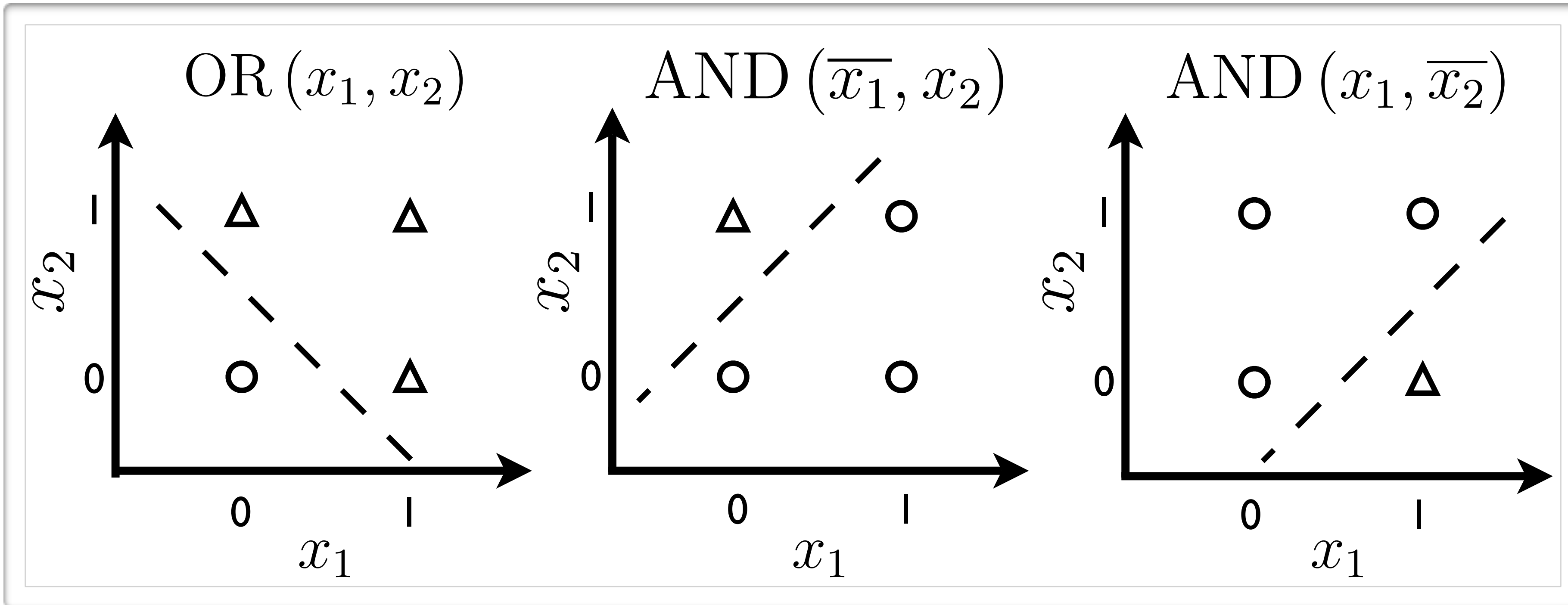
(from Pascal Vincent's slides)

  - If activation is greater than 0.5, predict 1
  - Otherwise predict 0

Same idea can be applied to a tanh activation

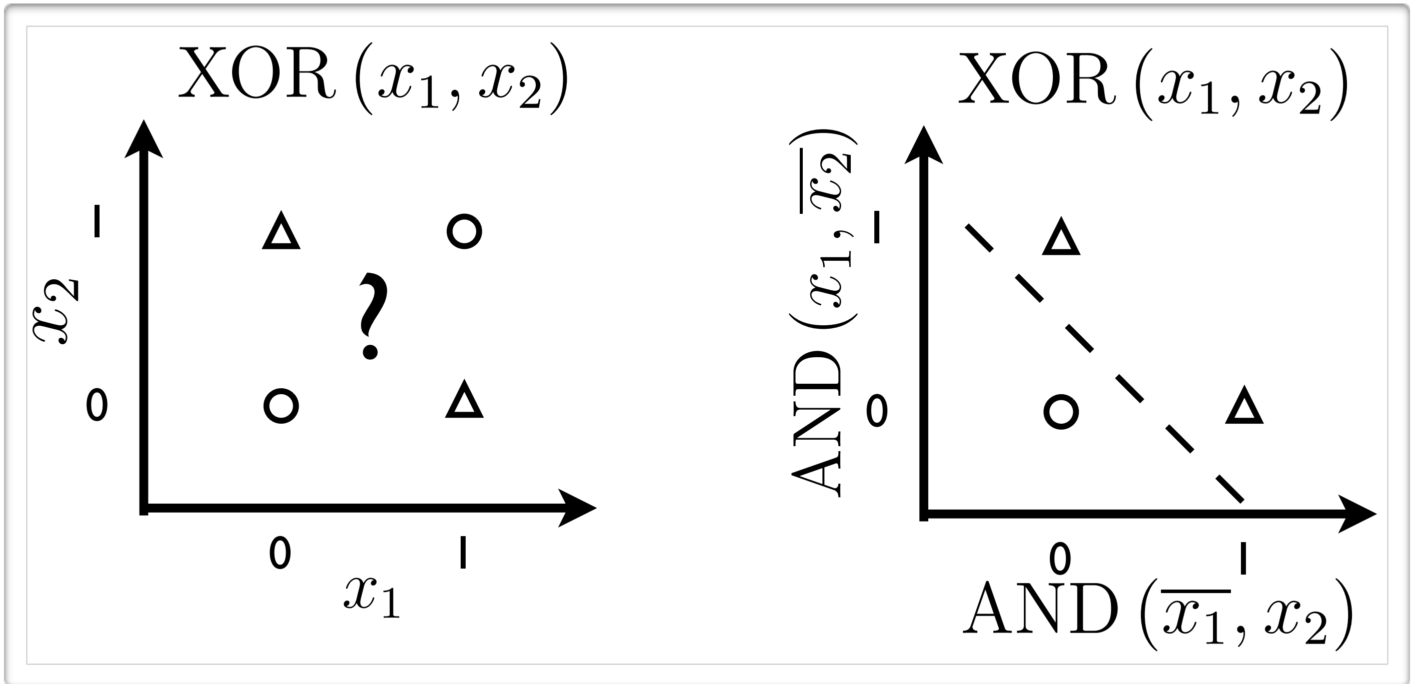
Capacity of a Single Neuron

- Can solve linearly separable problems.



Capacity of a Single Neuron

- Can not solve non-linearly separable problems.



- Need to transform the input into a better representation.
- Remember basis functions!

Single Hidden Layer Neural Net

- Hidden layer pre-activation:

$$\mathbf{a}(\mathbf{x}) = \mathbf{b}^{(1)} + \mathbf{W}^{(1)}\mathbf{x}$$

$$\left(a(\mathbf{x})_i = b_i^{(1)} + \sum_j W_{i,j}^{(1)} x_j\right)$$

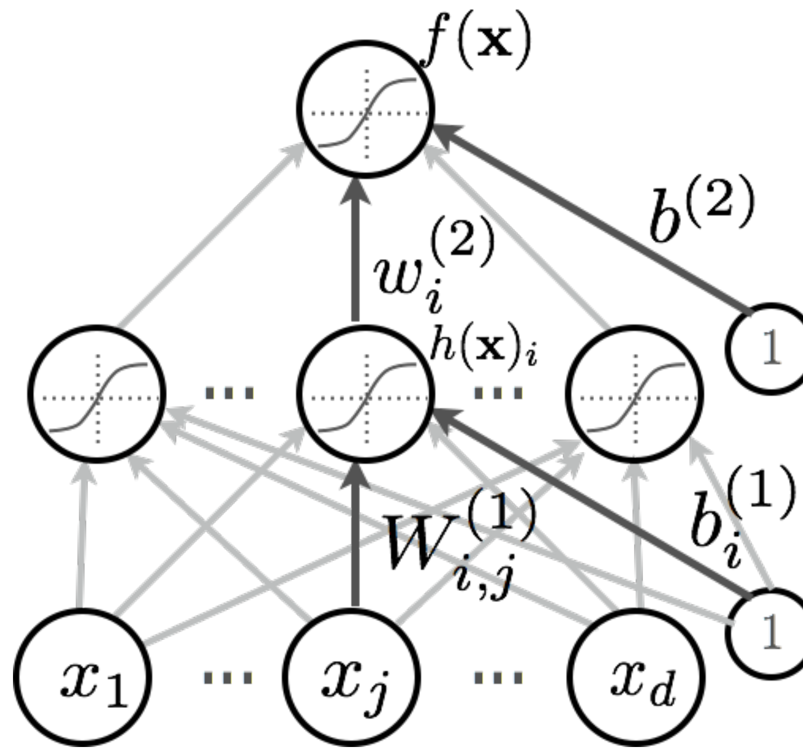
- Hidden layer activation:

$$\mathbf{h}(\mathbf{x}) = \mathbf{g}(\mathbf{a}(\mathbf{x}))$$

- Output layer activation:

$$f(\mathbf{x}) = o\left(b^{(2)} + \mathbf{w}^{(2)}{}^{\top}\mathbf{h}^{(1)}\mathbf{x}\right)$$

Output activation function



Softmax Activation Function

- Remember multi-way classification:
  - We need multiple outputs (1 output per class)
  - We need to estimate conditional probability: $p(y = c|\mathbf{x})$
  - Discriminative Learning

- Softmax activation function at the output

$$\mathbf{o}(\mathbf{a}) = \mathrm{softmax}(\mathbf{a}) = \left[\frac{\exp(a_1)}{\sum_c \exp(a_c)} \cdots \frac{\exp(a_C)}{\sum_c \exp(a_c)} \right]^\top$$

  - strictly positive
  - sums to one

- Predict class with the highest estimated class conditional probability.

Multilayer Neural Net

- Consider a network with L hidden layers.
  - layer pre-activation for k>0

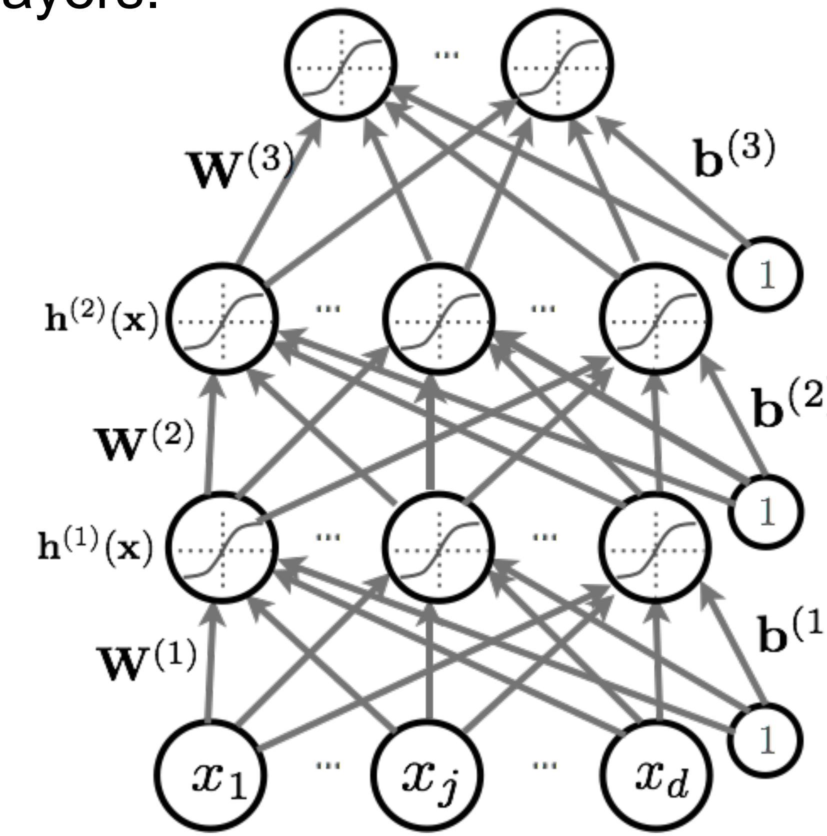
$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

  - hidden layer activation from 1 to L:

$$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x}))$$

  - output layer activation (k=L+1):

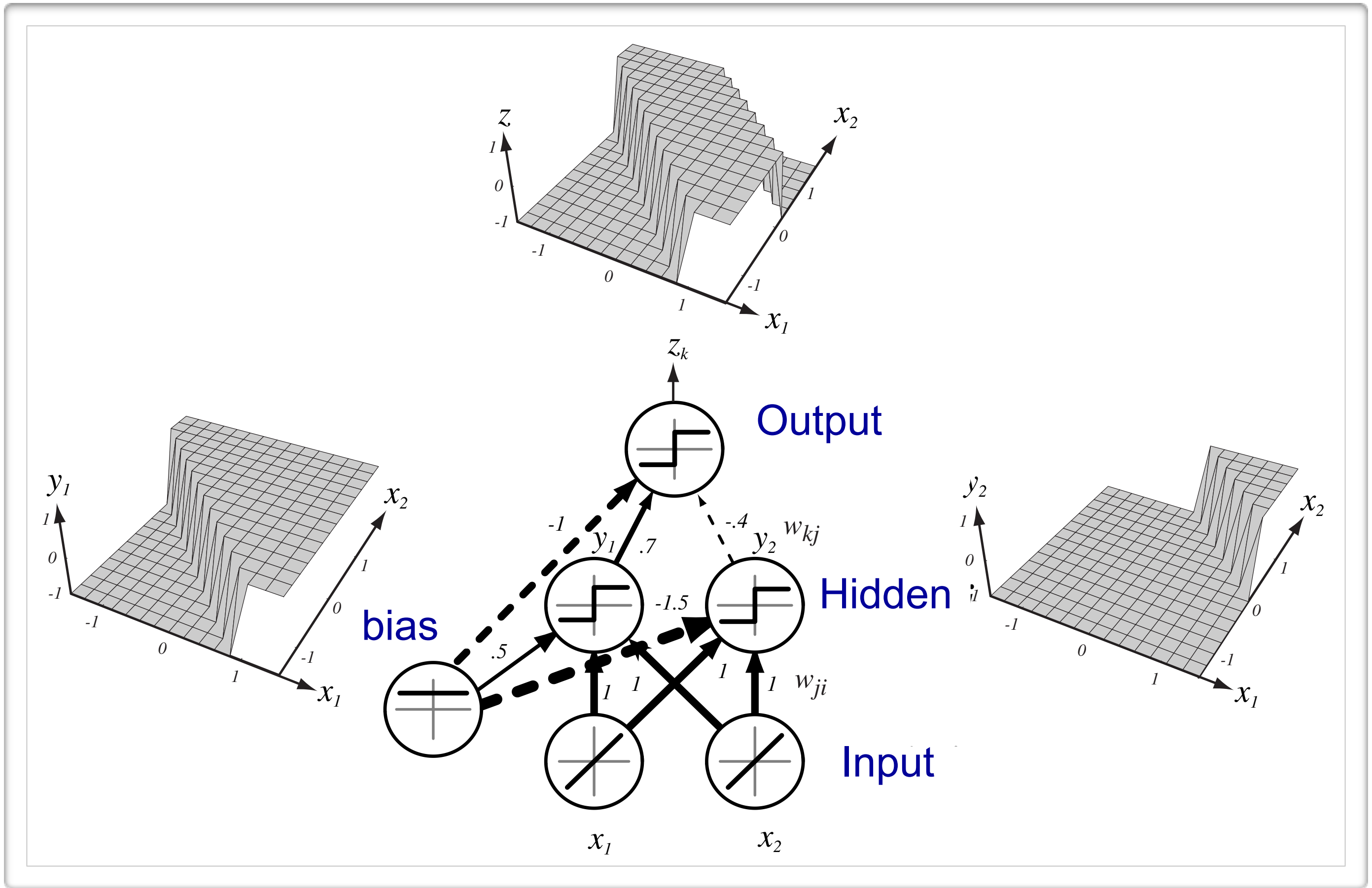
$$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$



$$(\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$$

Capacity of Neural Nets

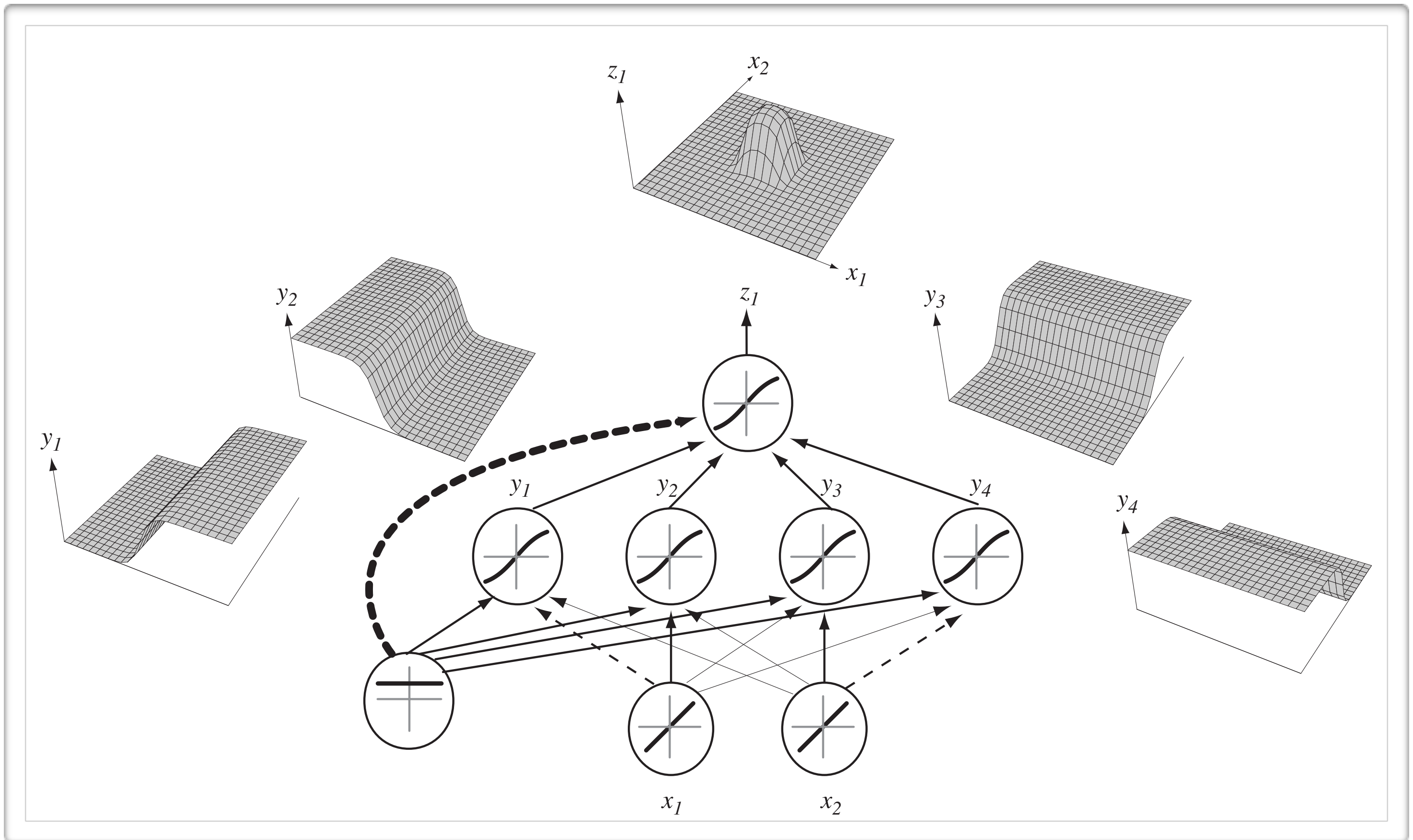
- Consider a single layer neural network



(from Pascal Vincent's slides)

Capacity of Neural Nets

- Consider a single layer neural network



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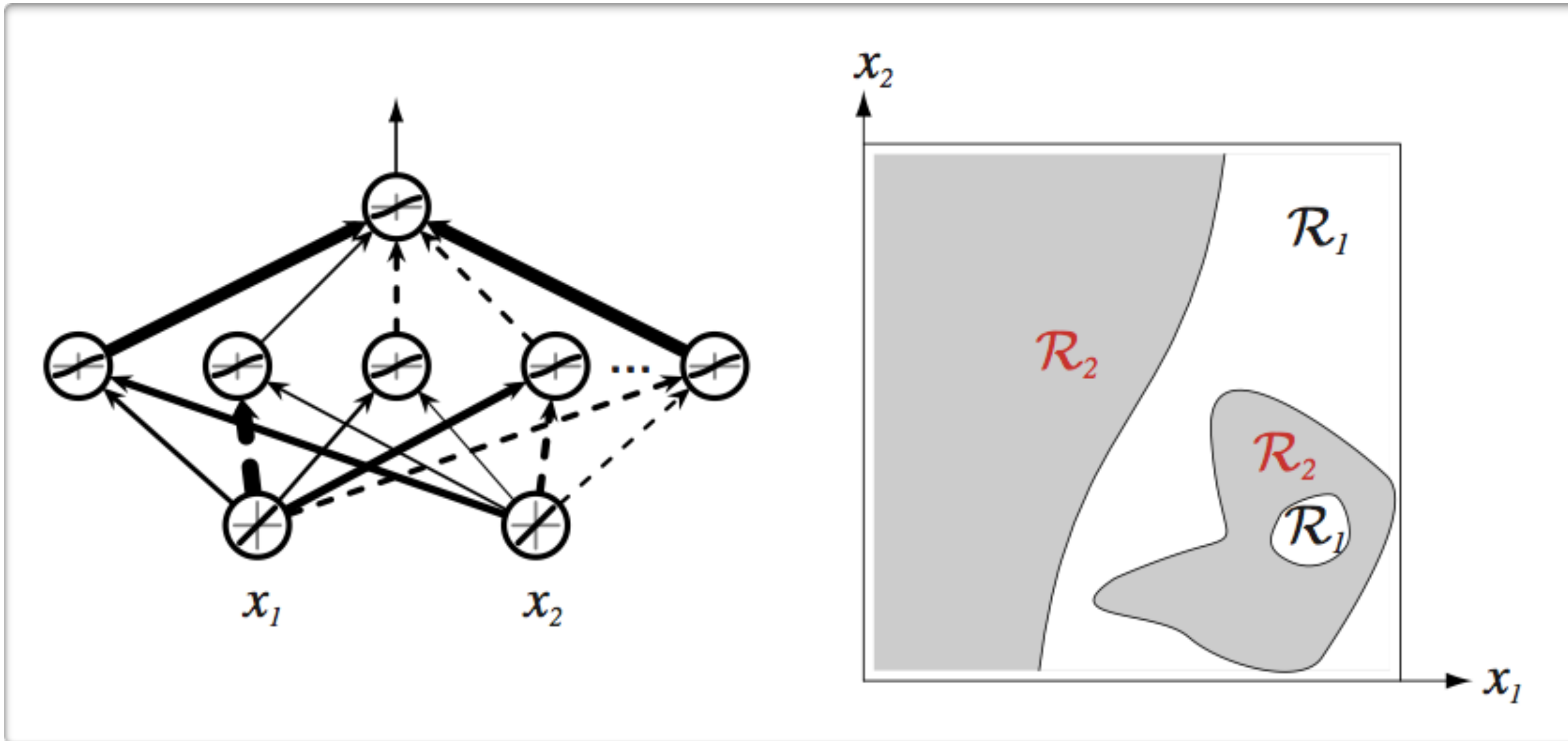
Capacity of Neural Nets

- Consider a single layer neural network



(from Pascal Vincent's slides)

Universal Approximation

- Universal Approximation Theorem (Hornik, 1991):
  - “a single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units”

- This applies for sigmoid, tanh and many other activation functions.

- However, this does not mean that there is learning algorithm that can find the necessary parameter values.

Feedforward Neural Networks

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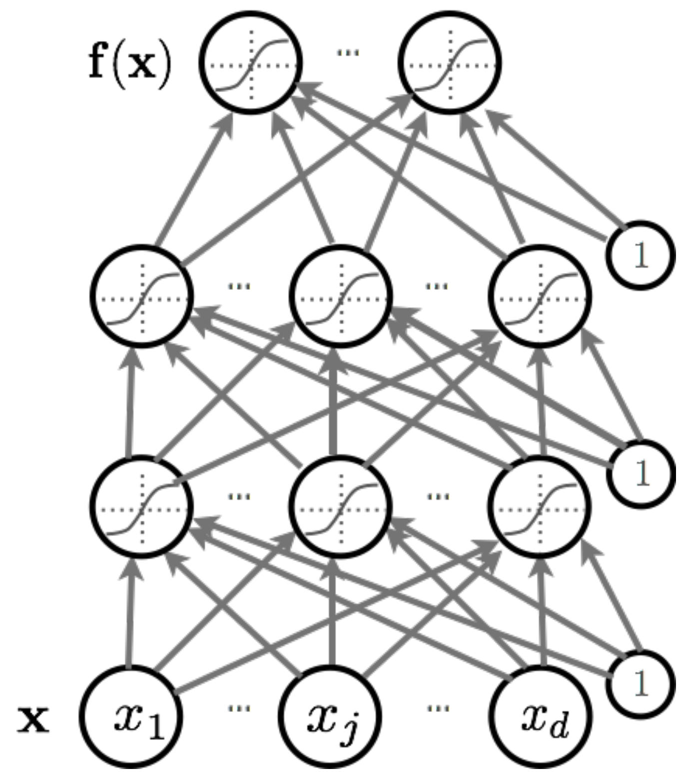

Training

- Empirical Risk Minimization:

$$\arg\min_{\boldsymbol{\theta}} \frac{1}{T} \sum_t \underbrace{l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})}_{\text{Loss function}} + \underbrace{\lambda \Omega(\boldsymbol{\theta})}_{\text{Regularizer}}$$

- Learning is cast as optimization.

  ➢ For classification problems, we would like to minimize classification error.

  ➢ Loss function can sometimes be viewed as a surrogate for what we want to optimize (e.g. upper bound)

Stochastic Gradient Descend

- Perform updates after seeing each example:
  - Initialize: $\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$
  - For t=1:T
    - for each training example $(\mathbf{x}^{(t)}, y^{(t)})$

$$\Delta = -\nabla_{\boldsymbol{\theta}} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$$

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha\, \Delta$$

Training epoch
=
Iteration of all examples

- To train a neural net, we need:
  - Loss function: $l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - A procedure to compute gradients: $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - Regularizer and its gradient: $\Omega(\boldsymbol{\theta})$, $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$

Loss Function

- Let us start by considering a classification problem with a softmax output layer.

- We need to estimate: $f(\mathbf{x})_c = p(y = c|\mathbf{x})$
  - We can maximize the log-probability of the correct class given an input: $\log p(y^{(t)} = c|x^{(t)})$

- Alternatively, we can minimize the negative log-likelihood:

$$l(\mathbf{f}(\mathbf{x}), y) = -\sum_c 1_{(y=c)} \log f(\mathbf{x})_c = -\log f(\mathbf{x})_y$$

- As seen before, this is also known as a cross-entropy entropy function for multi-class classification problem.

Stochastic Gradient Descend

- Perform updates after seeing each example:
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Multilayer Neural Net: Reminder

- Consider a network with L hidden layers.
  - layer pre-activation for k>0

$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

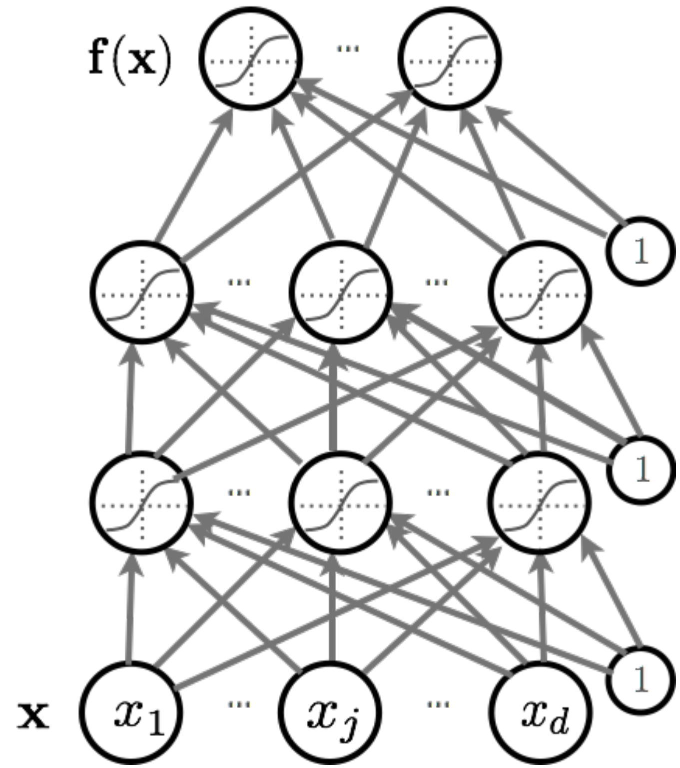
  - hidden layer activation from 1 to L:

$$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x}))$$

  - output layer activation (k=L+1):

$$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$

Softmax activation function



$$(\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$$

Gradient Computation

- Loss gradient at output
  - Partial derivative:

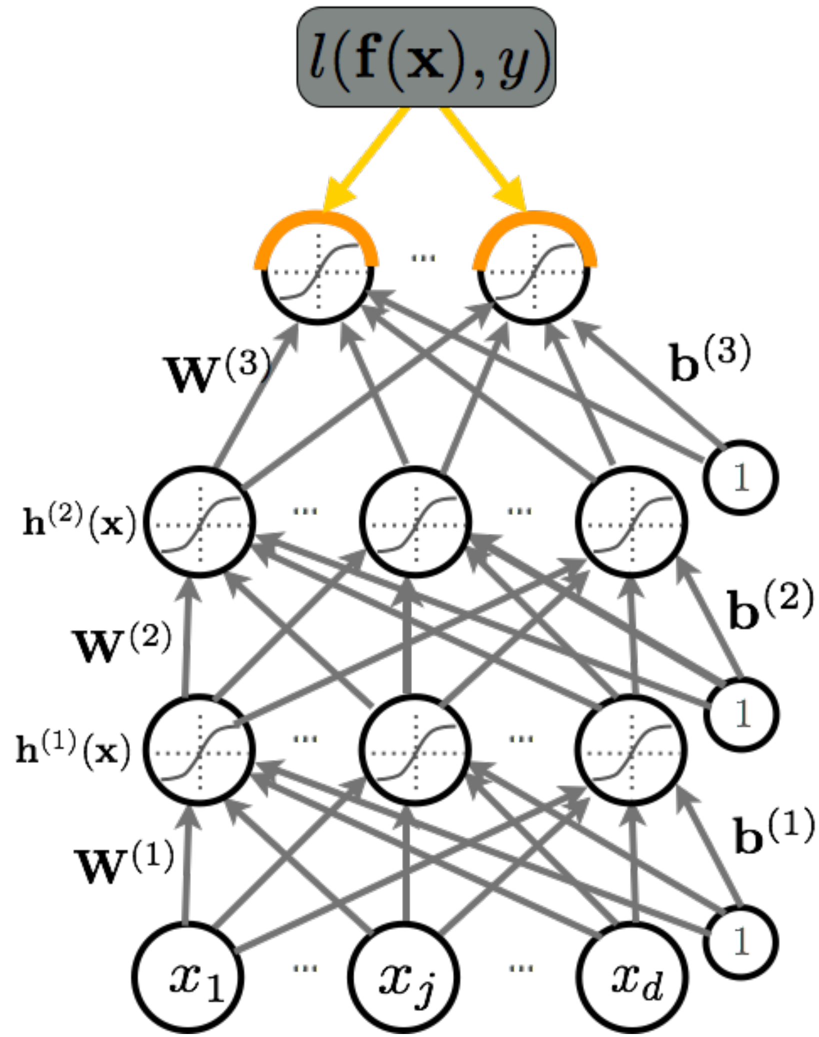
$$\frac{\partial}{\partial f(\mathbf{x})_c} - \log f(\mathbf{x})_y \quad = \quad \frac{-1_{(y=c)}}{f(\mathbf{x})_y}$$

  - Gradient:

$$\begin{aligned} & \nabla_{\mathbf{f}(\mathbf{x})} - \log f(\mathbf{x})_y \\ = \quad & \frac{-1}{f(\mathbf{x})_y} \begin{bmatrix} 1_{(y=0)} \\ \vdots \\ 1_{(y=C-1)} \end{bmatrix} \\ = \quad & \frac{-\mathbf{e}(y)}{f(\mathbf{x})_y} \end{aligned}$$

Indicator function

Remember: $f(\mathbf{x})_c = p(y = c|\mathbf{x})$



Gradient Computation

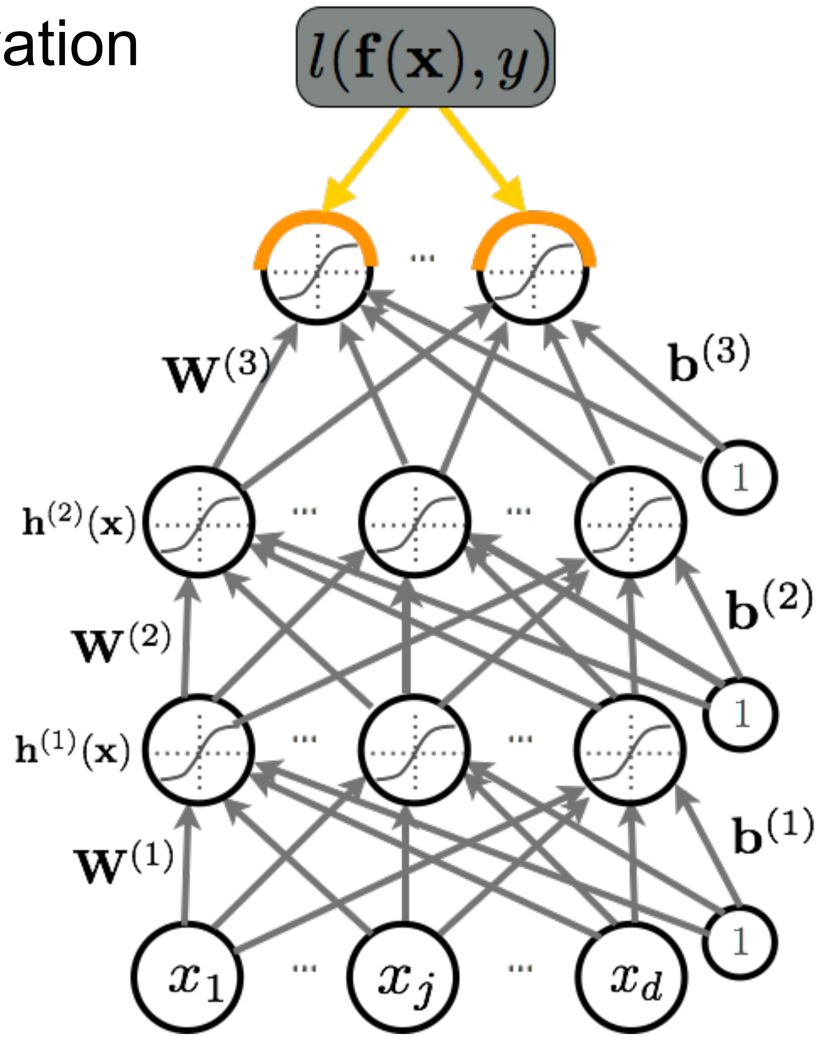
- Loss gradient at output pre-activation
  - Partial derivative:

$$\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} - \log f(\mathbf{x})_y$$
$$= \quad -\left(1_{(y=c)} - f(\mathbf{x})_c\right)$$

  - Gradient:

$$\nabla_{\mathbf{a}^{(L+1)}(\mathbf{x})} - \log f(\mathbf{x})_y$$
$$= \quad -\left(\mathbf{e}(y) - \mathbf{f}(\mathbf{x})\right)$$

Indicator function



Derivation

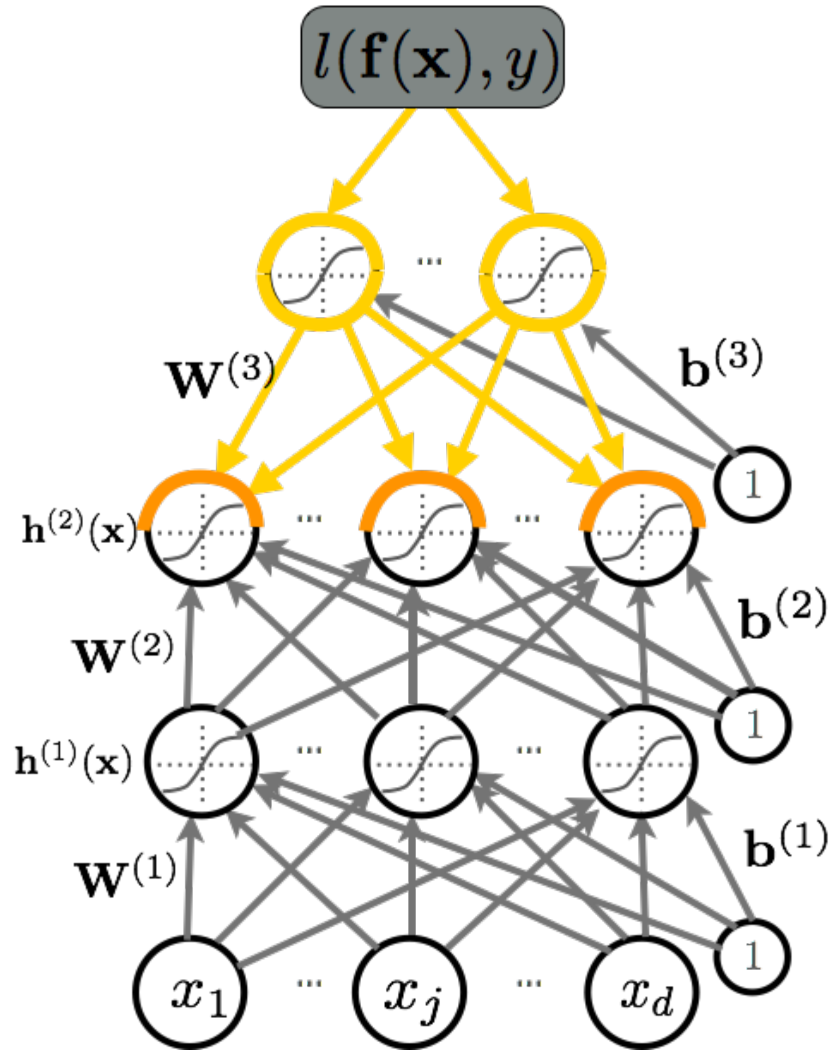
$$\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} - \log f(\mathbf{x})_y$$

$$\boxed{\frac{\partial \frac{g(x)}{h(x)}}{\partial x} = \frac{\partial g(x)}{\partial x}\frac{1}{h(x)} - \frac{g(x)}{h(x)^2}\frac{\partial h(x)}{\partial x}}$$

$$\begin{aligned}
&= \frac{-1}{f(\mathbf{x})_y}\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} f(\mathbf{x})_y \\
&= \frac{-1}{f(\mathbf{x})_y}\;\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c}\mathrm{softmax}(\mathbf{a}^{(L+1)}(\mathbf{x}))_y \\
&= \frac{-1}{f(\mathbf{x})_y}\;\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c}\frac{\exp(a^{(L+1)}(\mathbf{x})_y)}{\sum_{c'}\exp(a^{(L+1)}(\mathbf{x})_{c'})} \\
&= \frac{-1}{f(\mathbf{x})_y}\left(\frac{\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c}\exp(a^{(L+1)}(\mathbf{x})_y)}{\sum_{c'}\exp(a^{(L+1)}(\mathbf{x})_{c'})} - \frac{\exp(a^{(L+1)}(\mathbf{x})_y)\left(\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c}\sum_{c'}\exp(a^{(L+1)}(\mathbf{x})_{c'})\right)}{\left(\sum_{c'}\exp(a^{(L+1)}(\mathbf{x})_{c'})\right)^2}\right) \\
&= \frac{-1}{f(\mathbf{x})_y}\left(\frac{1_{(y=c)}\exp(a^{(L+1)}(\mathbf{x})_y)}{\sum_{c'}\exp(a^{(L+1)}(\mathbf{x})_{c'})} - \frac{\exp(a^{(L+1)}(\mathbf{x})_y)}{\sum_{c'}\exp(a^{(L+1)}(\mathbf{x})_{c'})}\;\frac{\exp(a^{(L+1)}(\mathbf{x})_c)}{\sum_{c'}\exp(a^{(L+1)}(\mathbf{x})_{c'})}\right) \\
&= \frac{-1}{f(\mathbf{x})_y}\left(1_{(y=c)}\mathrm{softmax}(\mathbf{a}^{(L+1)}(\mathbf{x}))_y - \mathrm{softmax}(\mathbf{a}^{(L+1)}(\mathbf{x}))_y\,\mathrm{softmax}(\mathbf{a}^{(L+1)}(\mathbf{x}))_c\right) \\
&= \frac{-1}{f(\mathbf{x})_y}\left(1_{(y=c)}f(\mathbf{x})_y - f(\mathbf{x})_y\, f(\mathbf{x})_c\right) \\
&= -\left(1_{(y=c)} - f(\mathbf{x})_c\right)
\end{aligned}$$

Gradient Computation

- Loss gradient for hidden layers
  - This is getting complicated!

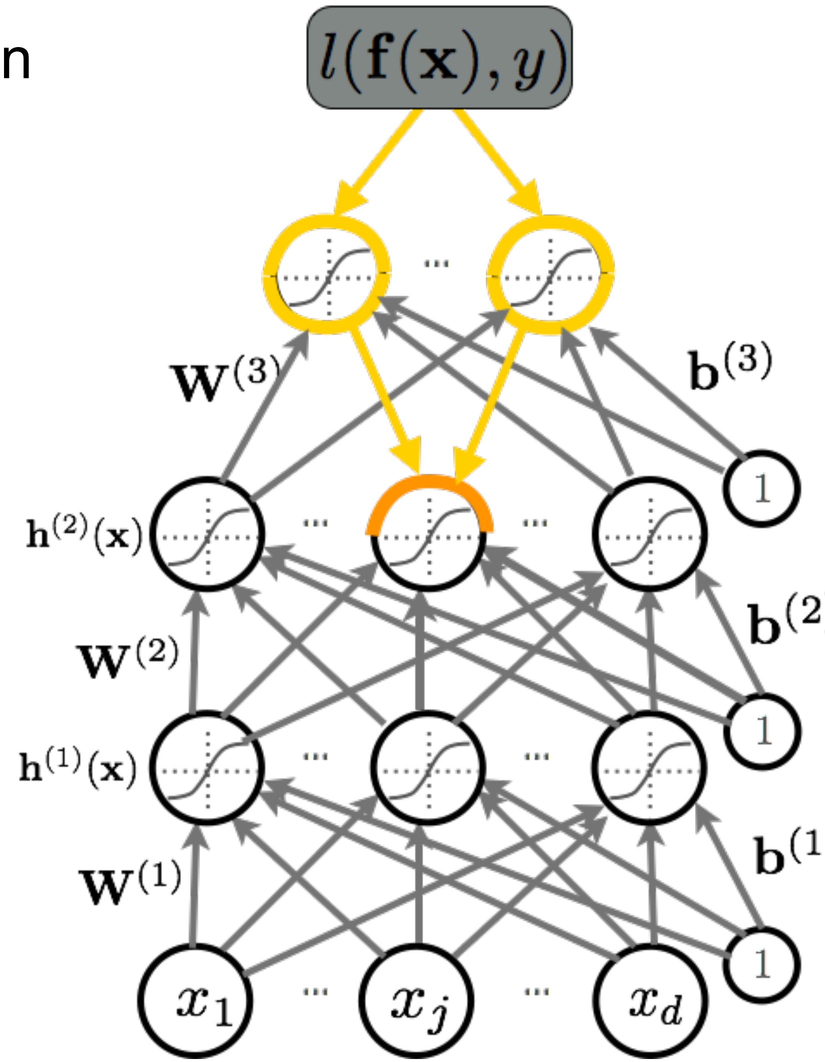


Gradient Computation

- Chain Rule: Assume that a function $p(a)$ can be written as a function of intermediate results $q_i(a)$, then:

$$\frac{\partial p(a)}{\partial a} = \sum_i \frac{\partial p(a)}{\partial q_i(a)} \frac{\partial q_i(a)}{\partial a}$$

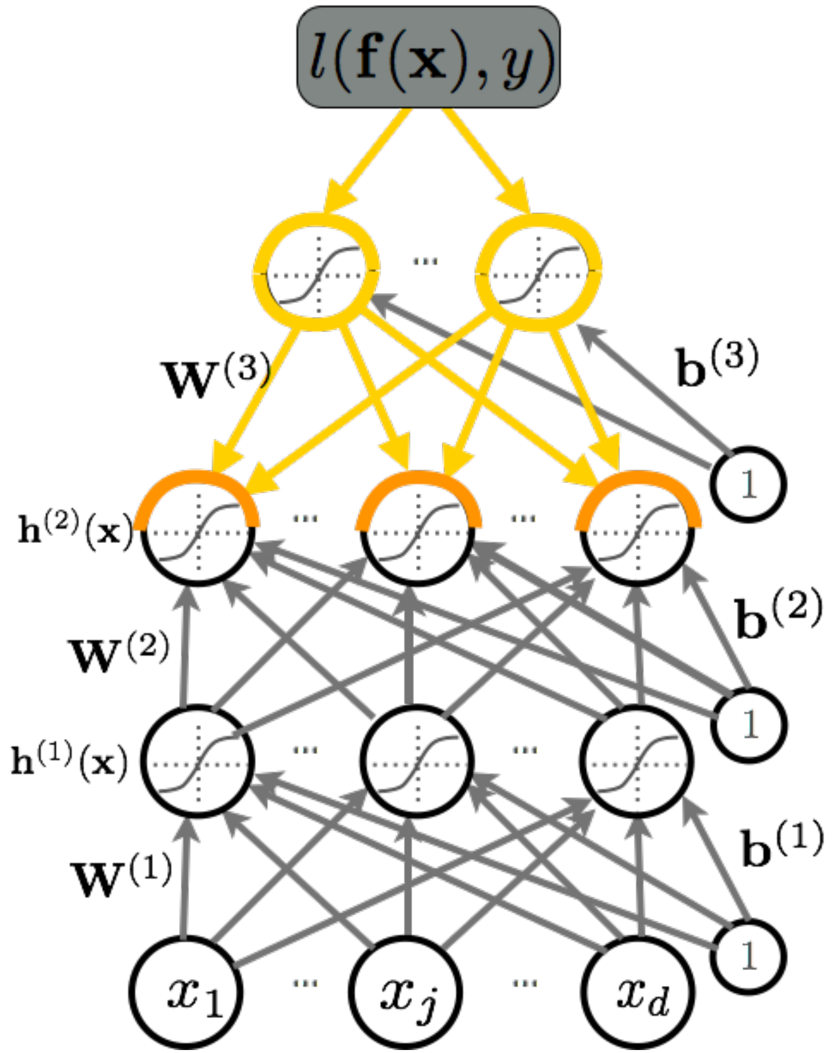
- We can invoke it by setting:
  - a be a hidden unit
  - $q_i(a)$ be a pre-activation in the layer above
  - $p(a)$ be the loss function



Gradient Computation

- Loss gradient at hidden layers
  - Partial derivative:

$$
\begin{aligned}
&\frac{\partial}{\partial h^{(k)}(\mathbf{x})_j} - \log f(\mathbf{x})_y \\
= &\sum_i \frac{\partial - \log f(\mathbf{x})_y}{\partial a^{(k+1)}(\mathbf{x})_i} \frac{\partial a^{(k+1)}(\mathbf{x})_i}{\partial h^{(k)}(\mathbf{x})_j} \\
= &\sum_i \frac{\partial - \log f(\mathbf{x})_y}{\partial a^{(k+1)}(\mathbf{x})_i} W_{i,j}^{(k+1)}
\end{aligned}
$$

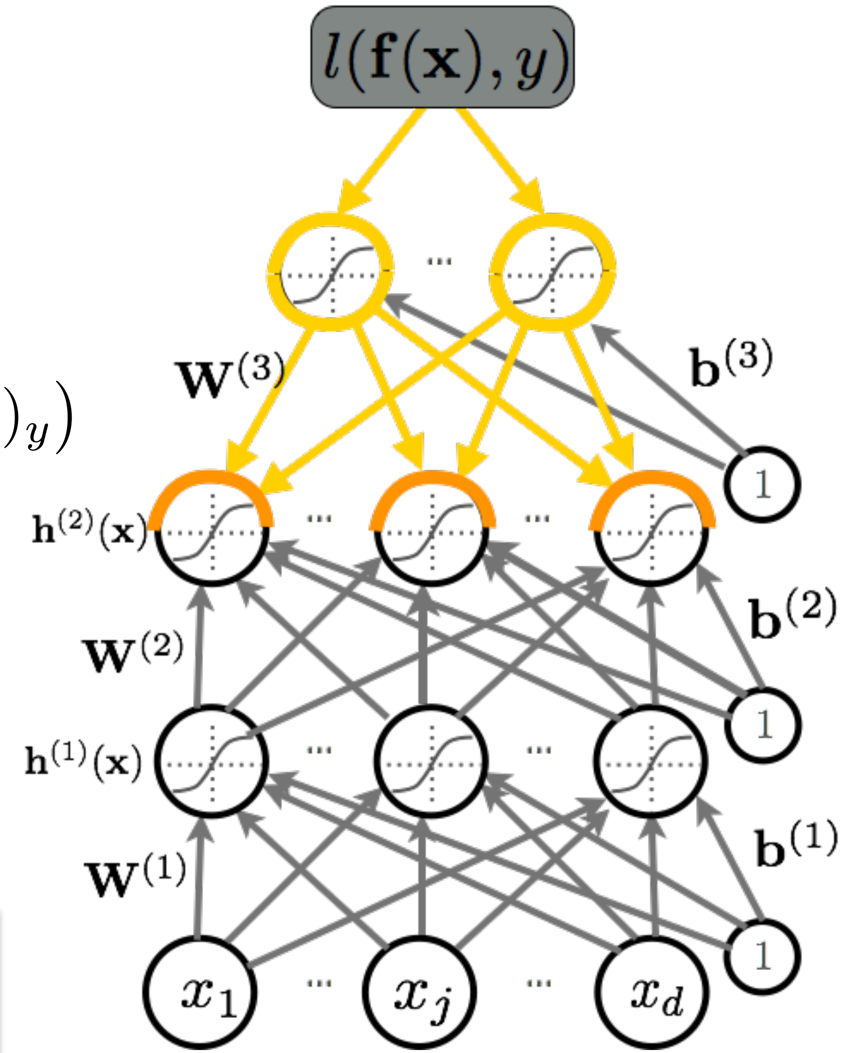


Remember:
$a^{(k)}(\mathbf{x})_i = b_i^{(k)} + \sum_j W_{i,j}^{(k)} h^{(k-1)}(\mathbf{x})_j$

Gradient Computation

- Loss gradient at hidden layers
  - Gradient

$$
\begin{aligned}
& \nabla_{\mathbf{h}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y \\
= \quad & \mathbf{W}^{(k+1)^\top} \underbrace{\left(\nabla_{\mathbf{a}^{(k+1)}(\mathbf{x})} - \log f(\mathbf{x})_y\right)}_{\text{We already know how to compute that}}
\end{aligned}
$$



Remember:
$a^{(k)}(\mathbf{x})_i = b_i^{(k)} + \sum_j W_{i,j}^{(k)} h^{(k-1)}(\mathbf{x})_j$

Gradient Computation

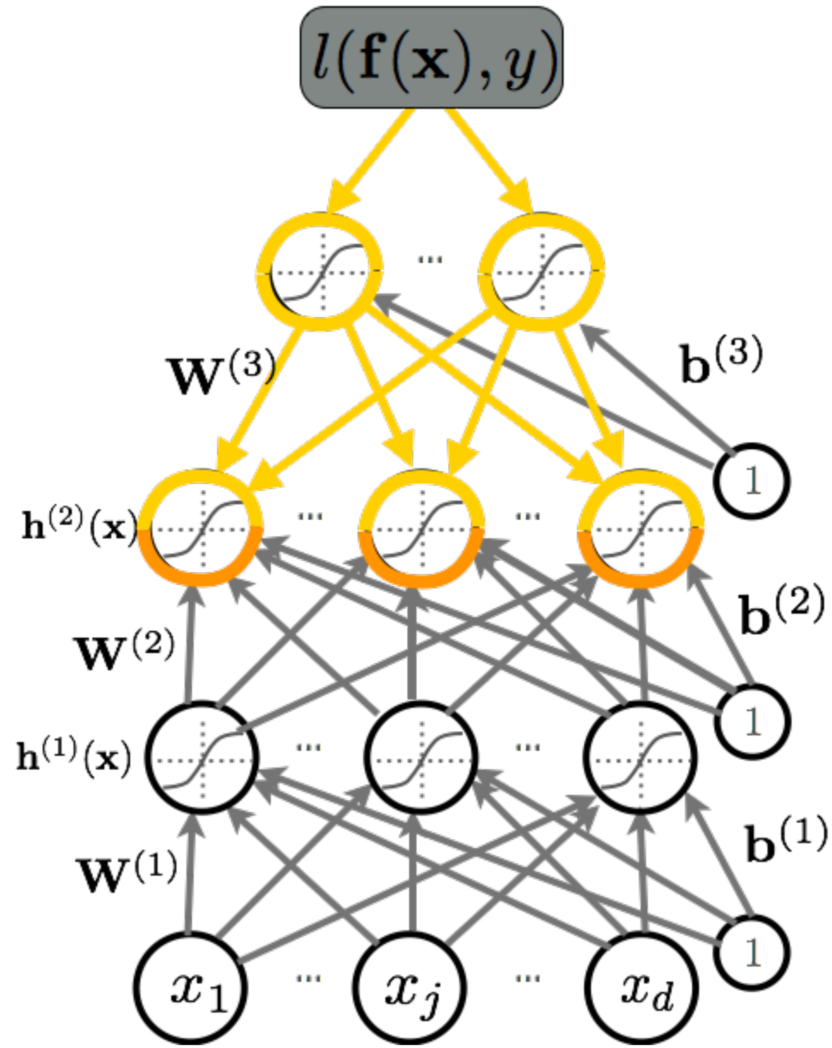
- Loss gradient at hidden layers (pre-activation)
  - Partial derivative:

$$\frac{\partial}{\partial a^{(k)}(\mathbf{x})_j} - \log f(\mathbf{x})_y$$

$$= \frac{\partial - \log f(\mathbf{x})_y}{\partial h^{(k)}(\mathbf{x})_j} \frac{\partial h^{(k)}(\mathbf{x})_j}{\partial a^{(k)}(\mathbf{x})_j}$$

$$= \frac{\partial - \log f(\mathbf{x})_y}{\partial h^{(k)}(\mathbf{x})_j} g'(a^{(k)}(\mathbf{x})_j)$$

Remember:
$h^{(k)}(\mathbf{x})_j = g(a^{(k)}(\mathbf{x})_j)$



Gradient Computation

- Loss gradient at hidden layers (pre-activation)
  - Gradient:

$$
\begin{aligned}
& \nabla_{\mathbf{a}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y \\
= \quad & \left(\nabla_{\mathbf{h}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y\right)^\top \nabla_{\mathbf{a}^{(k)}(\mathbf{x})} \mathbf{h}^{(k)}(\mathbf{x}) \\
= \quad & \left(\nabla_{\mathbf{h}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y\right) \odot [\ldots, g'(a^{(k)}(\mathbf{x})_j), \ldots]
\end{aligned}
$$

Let's look at the gradients of activation functions.

Gradient of the activation function

Remember:
$h^{(k)}(\mathbf{x})_j = g(a^{(k)}(\mathbf{x})_j)$

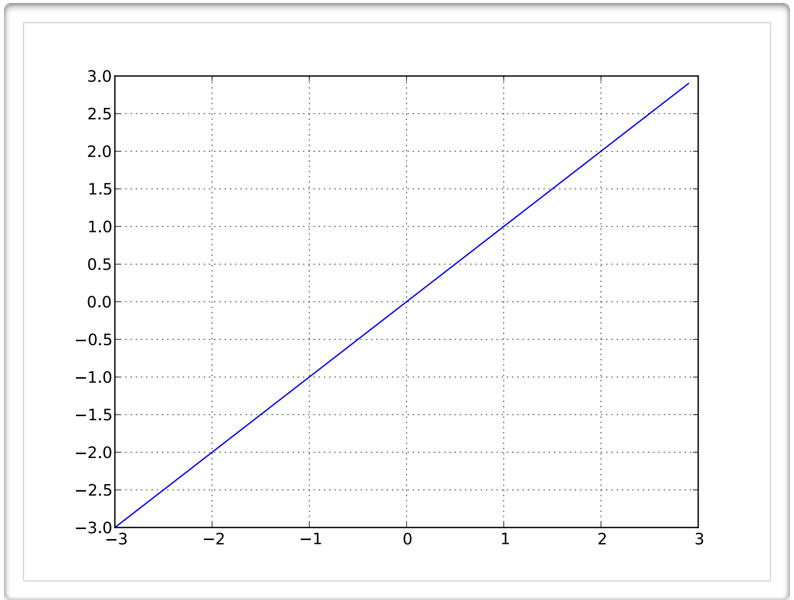
Linear Activation Function Gradient

- Linear activation function:

$$g(a) = a$$

  - Partial derivative

$$g'(a) = 1$$



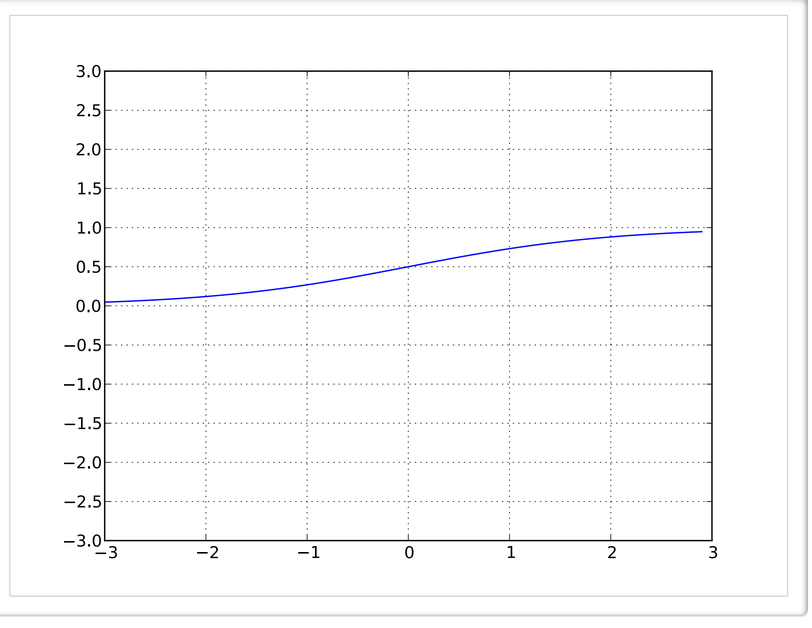
Sigmoid Activation Function Gradient

- Sigmoid activation function:

$$g(a) = \mathrm{sigm}(a) = \frac{1}{1+\exp(-a)}$$

  - Partial derivative

$$g'(a) = g(a)(1 - g(a))$$



Tanh Activation Function Gradient

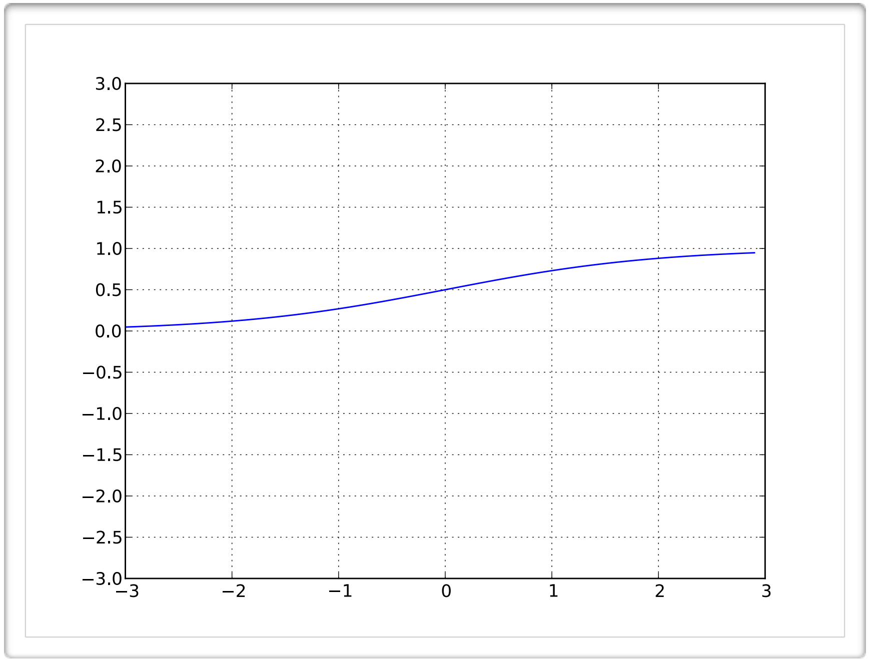
- Hyperbolic tangent (“tanh”) activation function:

$$g(a) = \tanh(a) =$$

$$= \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} = \frac{\exp(2a) - 1}{\exp(2a) + 1}$$

  - Partial derivative

$$g'(a) = 1 - g(a)^2$$



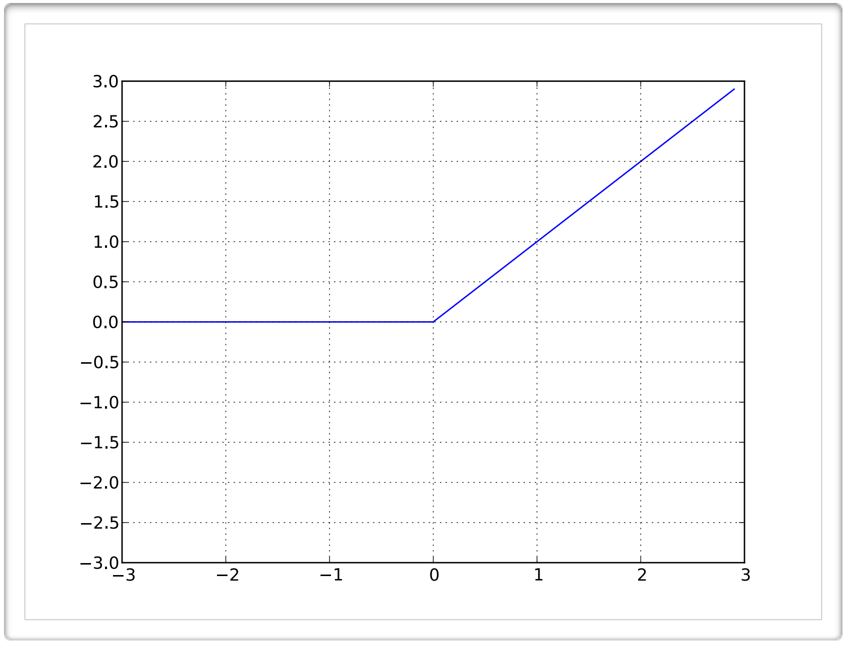
Tanh Activation Function Gradient

- Rectified linear (ReLU) activation function:

$$g(a) = \mathrm{reclin}(a) = \max(0, a)$$

  - Partial derivative

$$g'(a) = 1_{a>0}$$



Stochastic Gradient Descend

- Perform updates after seeing each example:
  - Initialize: $\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$
  - For t=1:T
    - for each training example $(\mathbf{x}^{(t)}, y^{(t)})$

$$\Delta = -\nabla_{\boldsymbol{\theta}} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$$

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha\, \Delta$$

Training epoch
=
Iteration of all examples

- To train a neural net, we need:
  - Loss function: $l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - A procedure to compute gradients: $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - Regularizer and its gradient: $\Omega(\boldsymbol{\theta})$, $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$

Gradient Computation

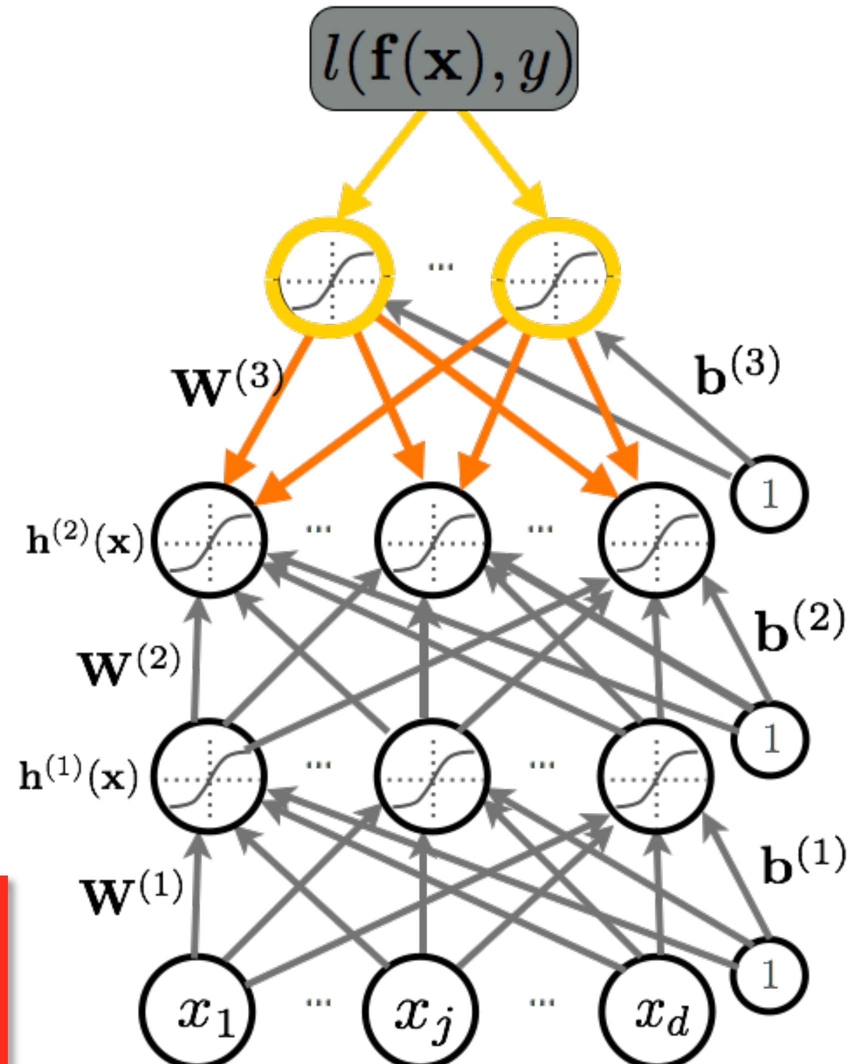
- Loss gradient of parameters
  - Partial derivative (weights):

$$\frac{\partial}{\partial W_{i,j}^{(k)}} - \log f(\mathbf{x})_y$$

$$= \frac{\partial - \log f(\mathbf{x})_y}{\partial a^{(k)}(\mathbf{x})_i} \frac{\partial a^{(k)}(\mathbf{x})_i}{\partial W_{i,j}^{(k)}}$$

$$= \frac{\partial - \log f(\mathbf{x})_y}{\partial a^{(k)}(\mathbf{x})_i} h_j^{(k-1)}(\mathbf{x})$$

Remember:
$a^{(k)}(\mathbf{x})_i = b_i^{(k)} + \sum_j W_{i,j}^{(k)} h^{(k-1)}(\mathbf{x})_j$

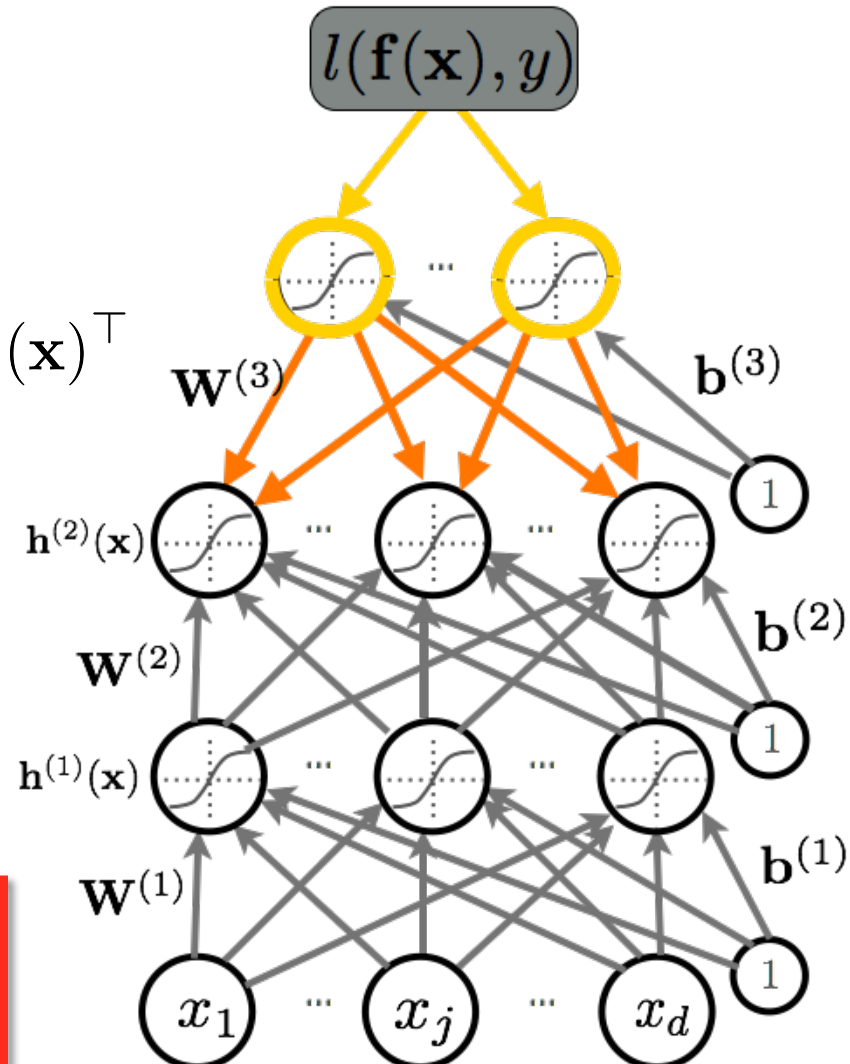


Gradient Computation

- Loss gradient of parameters
  - Gradient (weights):

$$\nabla_{\mathbf{W}^{(k)}} - \log f(\mathbf{x})_y$$

$$= \quad \left(\nabla_{\mathbf{a}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y\right) \quad \mathbf{h}^{(k-1)}(\mathbf{x})^\top$$



Remember:

$$a^{(k)}(\mathbf{x})_i = b_i^{(k)} + \sum_j W_{i,j}^{(k)} h^{(k-1)}(\mathbf{x})_j$$

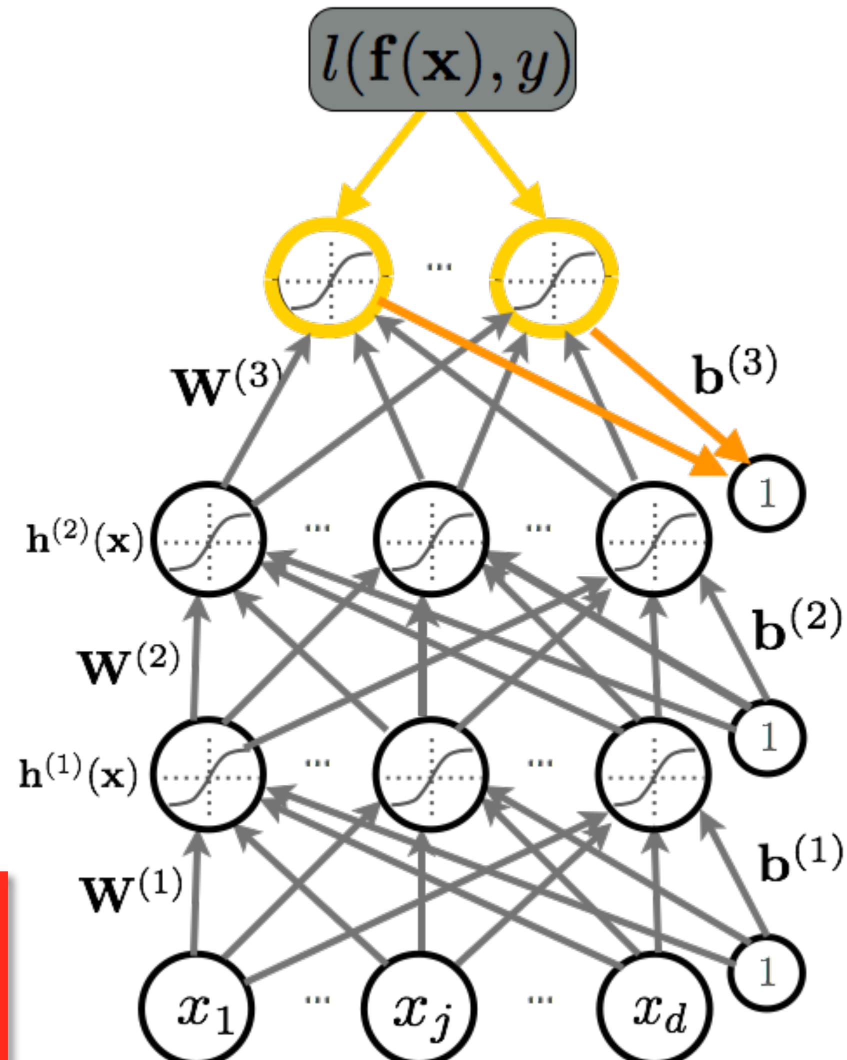
Gradient Computation

- Loss gradient of parameters
  - Partial derivative (biases):

$$\frac{\partial}{\partial b_i^{(k)}} - \log f(\mathbf{x})_y$$

$$= \frac{\partial - \log f(\mathbf{x})_y}{\partial a^{(k)}(\mathbf{x})_i} \frac{\partial a^{(k)}(\mathbf{x})_i}{\partial b_i^{(k)}}$$

$$= \frac{\partial - \log f(\mathbf{x})_y}{\partial a^{(k)}(\mathbf{x})_i}$$

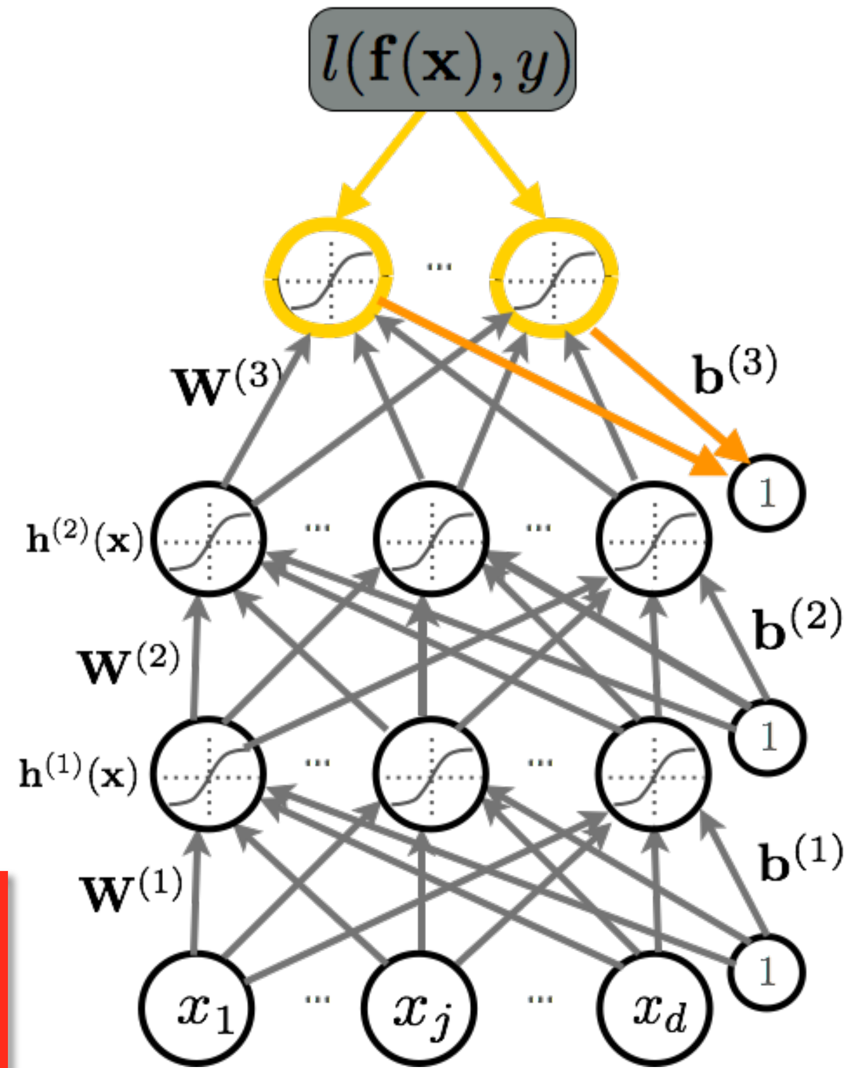


Remember:
$a^{(k)}(\mathbf{x})_i = b_i^{(k)} + \sum_j W_{i,j}^{(k)} h^{(k-1)}(\mathbf{x})_j$

Gradient Computation

- Loss gradient of parameters
  - Gradient (biases):

$$
\begin{aligned}
& \nabla_{\mathbf{b}^{(k)}} - \log f(\mathbf{x})_y \\
= \quad & \nabla_{\mathbf{a}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y
\end{aligned}
$$



Remember:

$a^{(k)}(\mathbf{x})_i = b_i^{(k)} + \sum_j W_{i,j}^{(k)} h^{(k-1)}(\mathbf{x})_j$

Backpropagation Algorithm

- Perform forward propagation
- Compute output gradient (before activation):

$$\nabla_{\mathbf{a}^{(L+1)}(\mathbf{x})} - \log f(\mathbf{x})_y \quad \Longleftarrow \quad -\left(\mathbf{e}(y) - \mathbf{f}(\mathbf{x})\right)$$

- For k=L+1 to 1
  - Compute gradients w.r.t. the hidden layer parameters:

$$\nabla_{\mathbf{W}^{(k)}} - \log f(\mathbf{x})_y \quad \Longleftarrow \quad \left(\nabla_{\mathbf{a}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y\right) \;\; \mathbf{h}^{(k-1)}(\mathbf{x})^\top$$

$$\nabla_{\mathbf{b}^{(k)}} - \log f(\mathbf{x})_y \quad \Longleftarrow \quad \nabla_{\mathbf{a}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y$$

  - Compute gradients w.r.t. the hidden layer below:

$$\nabla_{\mathbf{h}^{(k-1)}(\mathbf{x})} - \log f(\mathbf{x})_y \quad \Longleftarrow \quad \mathbf{W}^{(k)^\top} \left(\nabla_{\mathbf{a}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y\right)$$

  - Compute gradients w.r.t. the hidden layer below (before activation):

$$\nabla_{\mathbf{a}^{(k-1)}(\mathbf{x})} - \log f(\mathbf{x})_y \quad \Longleftarrow \quad \left(\nabla_{\mathbf{h}^{(k-1)}(\mathbf{x})} - \log f(\mathbf{x})_y\right) \odot [\ldots, g'(a^{(k-1)}(\mathbf{x})_j), \ldots]$$

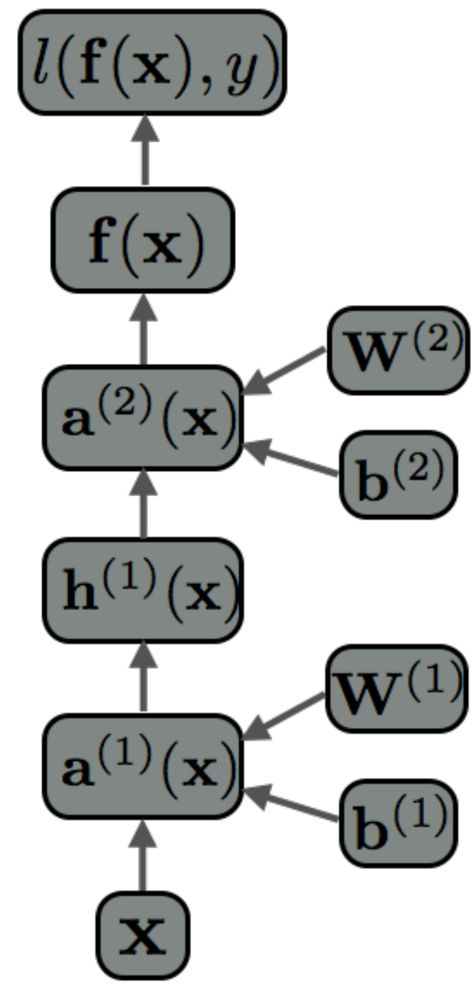
Computational Flow Graph

- Forward propagation can be represented as an acyclic flow graph

- Forward propagation can be implemented in a modular way:

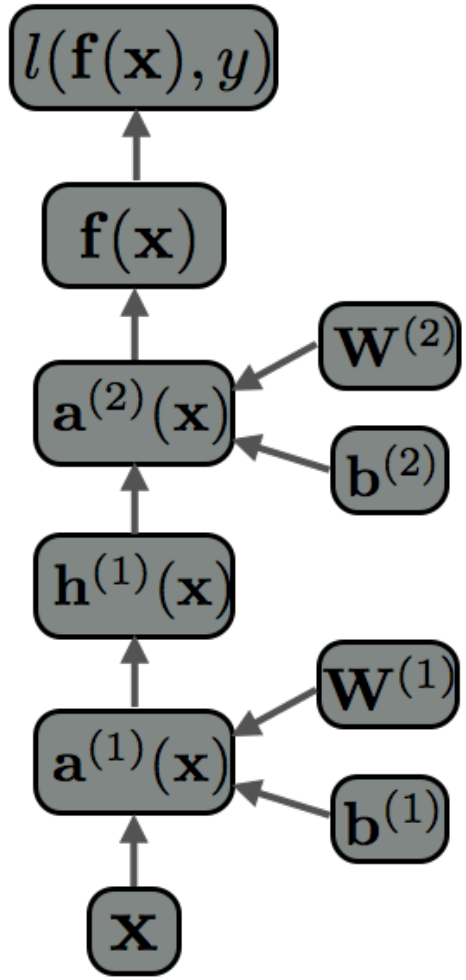
  - ➢ Each box can be an object with an fprop method, that computes the value of the box given its children

  - ➢ Calling the fprop method of each box in the right order yields forward propagation



Computational Flow Graph

- Each object also has a bprop method
  - it computes the gradient of the loss with respect to each child box.
  - fprop depends on the fprop output of box's children, while bprop depends on the bprop of box's parents
- By calling bprop in the reverse order, we obtain backpropagation



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Training epoch
=
Iteration of all examples

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  - A procedure to compute gradients: $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - Regularizer and its gradient: $\Omega(\boldsymbol{\theta})$, $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$

Weight Decay

- L2 regularization:

$$\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j \left(W_{i,j}^{(k)}\right)^2 = \sum_k ||\mathbf{W}^{(k)}||_F^2$$

- Gradient:

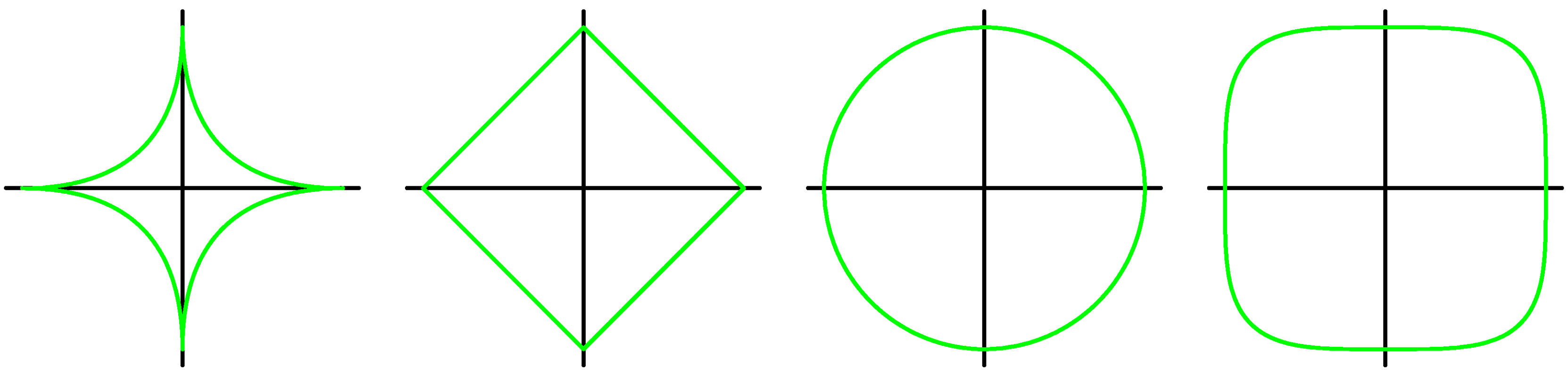
$$\nabla_{\mathbf{W}^{(k)}} \Omega(\boldsymbol{\theta}) = 2\mathbf{W}^{(k)}$$

  - Only applies to weights, not biases (weigh decay)
  - Can be interpreted as having a Gaussian prior over the weights, while performing MAP estimation.
  - We will later look at Bayesian methods.

Other Regularizers

- Using a more general regularizer, we get:

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$



$q = 0.5$ $q = 1$ $q = 2$ $q = 4$

Lasso Quadratic

L1 Regularization

- L1 regularization:

$$\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j |W_{i,j}^{(k)}|$$

- Gradient:

$$\nabla_{\mathbf{W}^{(k)}} \Omega(\boldsymbol{\theta}) = \operatorname{sign}(\mathbf{W}^{(k)})$$

$$\operatorname{sign}(\mathbf{W}^{(k)})_{i,j} = 1_{\mathbf{W}_{i,j}^{(k)} > 0} - 1_{\mathbf{W}_{i,j}^{(k)} < 0}$$

  - Only applies to weights, not biases (weigh decay)
  - Can be interpreted as having a Laplace prior over the weights, while performing MAP estimation.
  - Unlike L2, L1 will push some weights to be exactly 0.

Bias-Variance Trade-off

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

Average predictions over all datasets differ from the optimal regression function.

Solutions for individual datasets vary around their averages -- how sensitive is the function to the particular choice of the dataset.

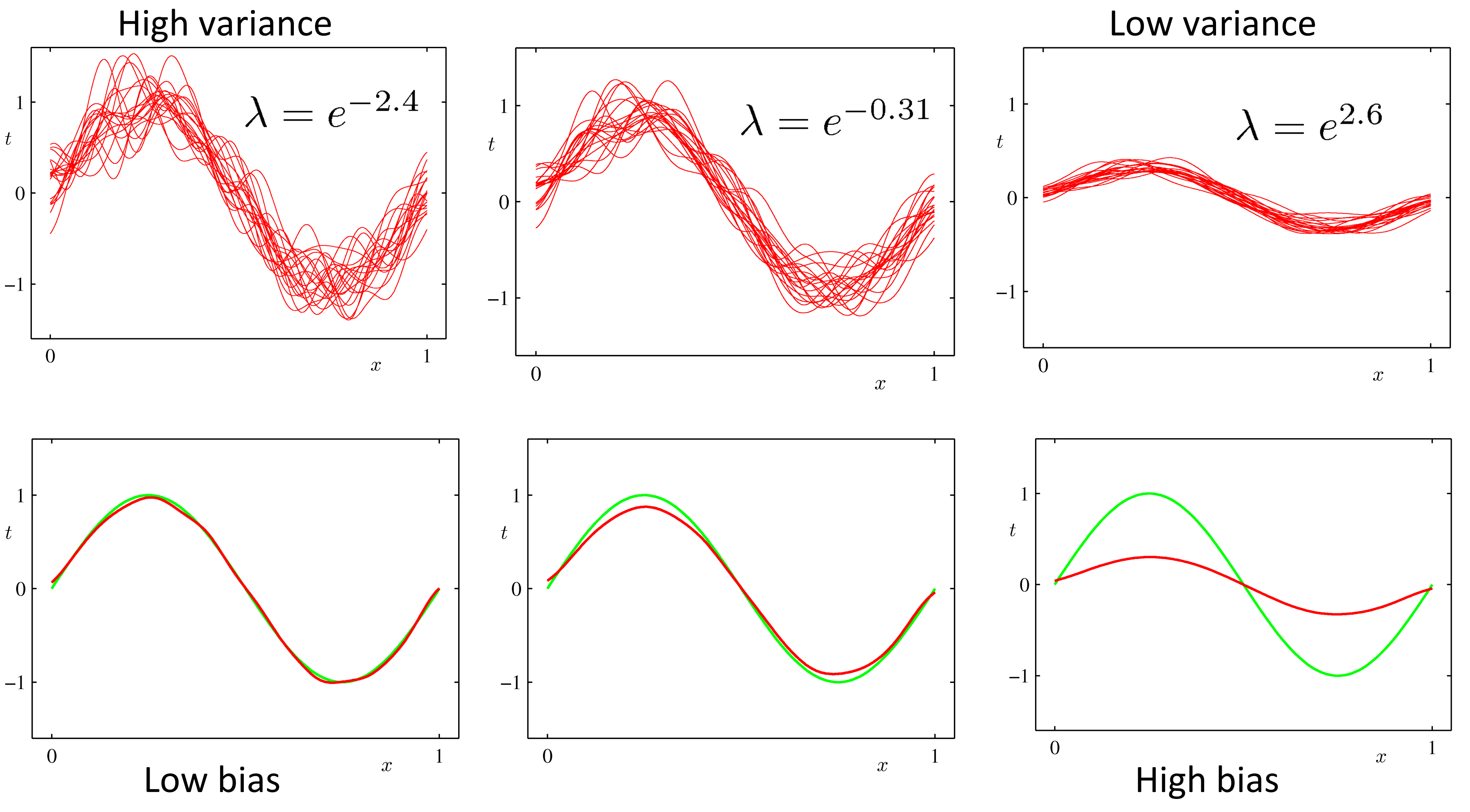
Intrinsic variability of the target values.

$$\begin{aligned}
(\text{bias})^2 &= \int \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x} \\
\text{variance} &= \int \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right] p(\mathbf{x})\,\mathrm{d}\mathbf{x} \\
\text{noise} &= \iint \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t
\end{aligned}$$

- Trade-off between bias and variance: With very flexible models (high complexity) we have low bias and high variance; With relatively rigid models (low complexity) we have high bias and low variance.
- The model with the optimal predictive capabilities has to balance between bias and variance.

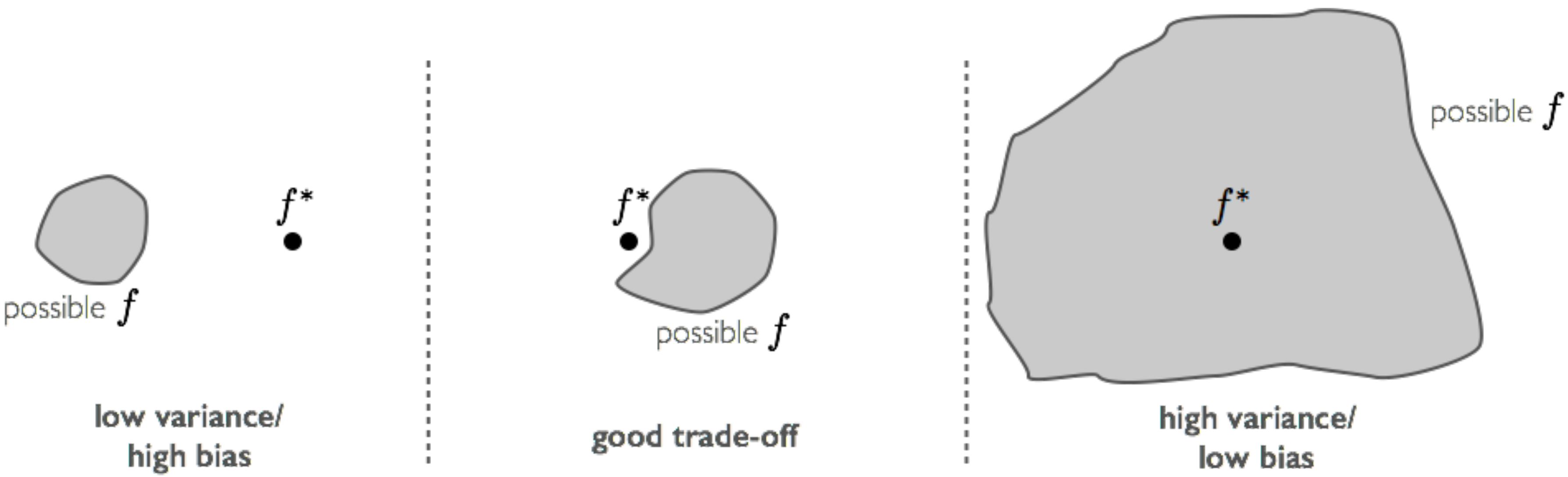
Bias-Variance Trade-off

- Consider the sinusoidal dataset. We generate 100 datasets, each containing N=25 points, drawn independently from $h(x) = \sin 2\pi x$.



Bias-Variance Trade-off

- Generalization error can be seen as the sum of the (squared) bias and the variance



Initialization

- Initialize biases to 0
- For weights
  - Can not initialize weights to 0 with tanh activation
    - All gradients would be zero (saddle point)
  - Can not initialize all weights to the same value
    - All hidden units in a layer will always behave the same
    - Need to break symmetry
  - Sample $\mathbf{W}_{i,j}^{(k)}$ from $U\left[-b, b\right]$, where

$$b = \frac{\sqrt{6}}{\sqrt{H_k + H_{k-1}}}$$

Sample around 0 and break symmetry

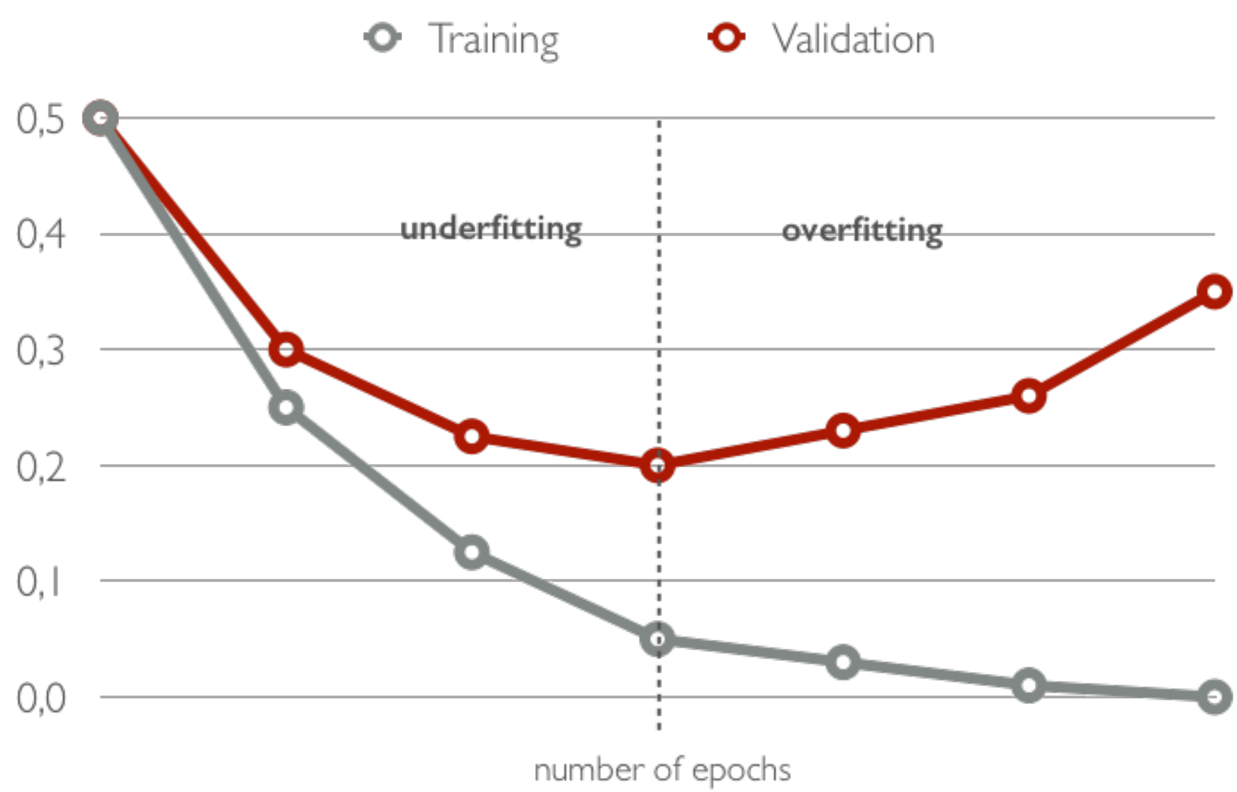
Size of $\mathbf{h}^{(k)}(\mathbf{x})$

Model Selection

- Training Protocol:
  - Train your model on the Training Set $\mathcal{D}^{\mathrm{train}}$
  - For model selection, use Validation Set $\mathcal{D}^{\mathrm{valid}}$
    - Hyper-parameter search: hidden layer size, learning rate, number of iterations/epochs, etc.
  - Estimate generalization performance using the Test Set $\mathcal{D}^{\mathrm{test}}$
- Remember: Generalization is the behavior of the model on **unseen examples**.

Early Stopping

- To select the number of epochs, stop training when validation set error increases (with some look ahead).



Tricks of the Trade:

• Normalizing your (real-valued) data:

- for each dimension x_i subtract its training set mean
- divide each dimension x_i by its training set standard deviation
- this can speed up training

• Decreasing the learning rate: As we get closer to the optimum, take smaller update steps:

i. start with large learning rate (e.g. 0.1)
ii. maintain until validation error stops improving
iii. divide learning rate by 2 and go back to (ii)

Mini-batch, Momentum

- Make updates based on a mini-batch of examples (instead of a single example):
  - the gradient is the average regularized loss for that mini-batch
  - can give a more accurate estimate of the gradient
  - can leverage matrix/matrix operations, which are more efficient

- Momentum: Can use an exponential average of previous gradients:

$$\overline{\nabla}_{\boldsymbol{\theta}}^{(t)} = \nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)}) + \beta \overline{\nabla}_{\boldsymbol{\theta}}^{(t-1)}$$

  - can get pass plateaus more quickly, by “gaining momentum”

Adapting Learning Rates

- Updates with adaptive learning rates ("one learning rate per parameter")

  - Adagrad: learning rates are scaled by the square root of the cumulative sum of squared gradients

$$\gamma^{(t)} = \gamma^{(t-1)} + \left(\nabla_\theta l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)})\right)^2 \qquad \overline{\nabla}_\theta^{(t)} = \frac{\nabla_\theta l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)})}{\sqrt{\gamma^{(t)} + \epsilon}}$$

  - RMSProp: instead of cumulative sum, use exponential moving average

$$\gamma^{(t)} = \beta\gamma^{(t-1)} + (1-\beta)\left(\nabla_\theta l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)})\right)^2$$

$$\overline{\nabla}_\theta^{(t)} = \frac{\nabla_\theta l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)})}{\sqrt{\gamma^{(t)} + \epsilon}}$$

  - Adam: essentially combines RMSProp with momentum

Gradient Checking

- To debug your implementation of fprop/bprop, you can compare with a finite-difference approximation of the gradient:

$$\frac{\partial f(x)}{\partial x} \approx \frac{f(x+\epsilon)-f(x-\epsilon)}{2\epsilon}$$

  - $f(x)$ would be the loss
  - x would be a parameter
  - $f(x+\epsilon)$ would be the loss if you add ϵ to the parameter
  - $f(x-\epsilon)$ would be the loss if you subtract ϵ to the parameter

Debugging on Small Dataset

- Next, make sure your model can overfit on a smaller dataset (~ 500-1000 examples)
- If not, investigate the following situations:
  - Are some of the units saturated, even before the first update?
    - scale down the initialization of your parameters for these units
    - properly normalize the inputs
  - Is the training error bouncing up and down?
    - decrease the learning rate
- This does not mean that you have computed gradients correctly:
  - You could still overfit with some of the gradients being wrong