Neural networks

Training neural networks - empirical risk minimization

NEURAL NETWORK

Topics: multilayer neural network

- Could have L hidden layers:
  - layer input activation for $k>0$ $\quad (\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$

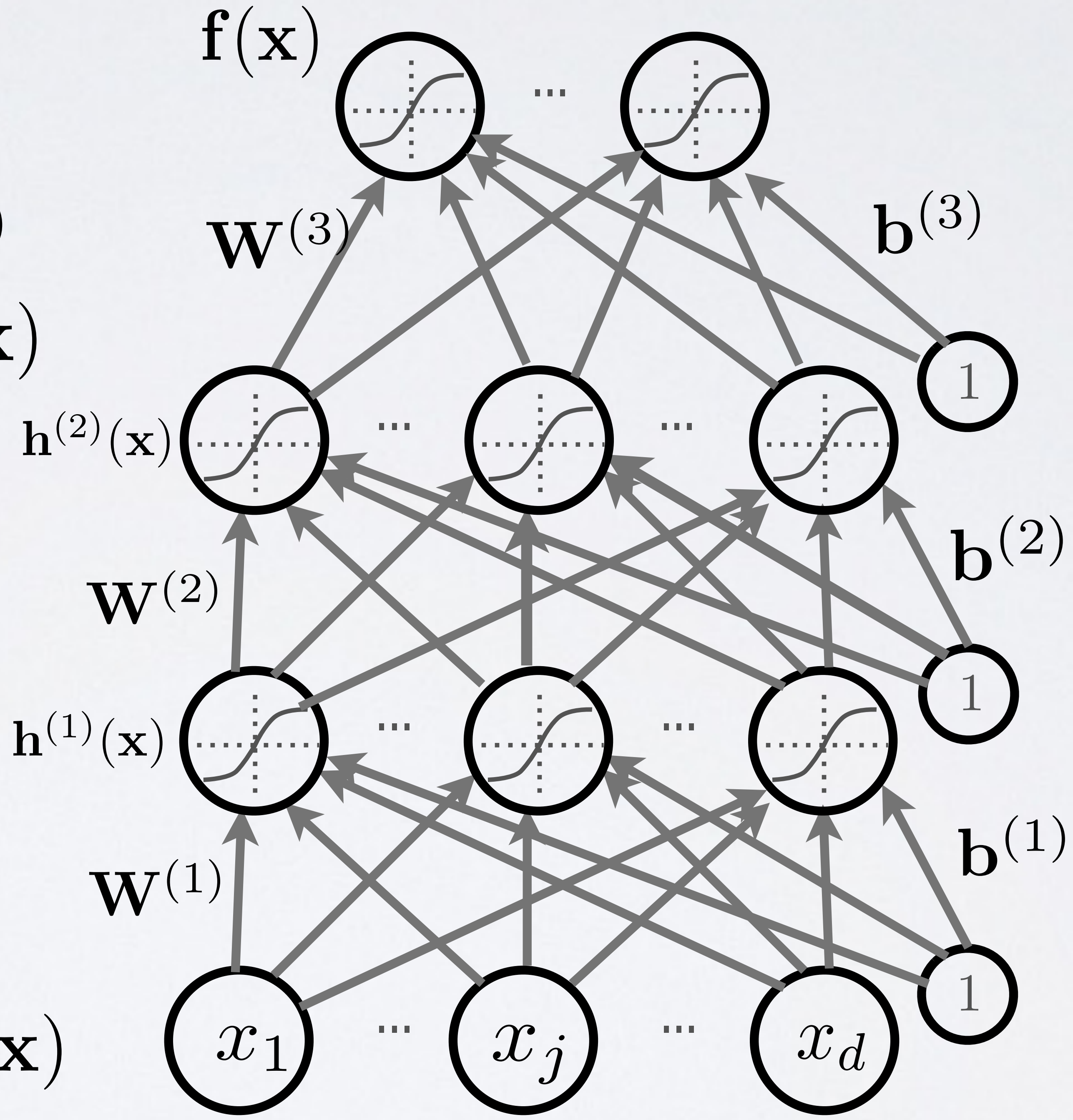
$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

  - hidden layer activation (k from 1 to L):

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

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

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



MACHINE LEARNING

Topics: empirical risk minimization, regularization

- Empirical risk minimization
  - framework to design learning algorithms

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

  - $l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$ is a loss function
  - $\Omega(\boldsymbol{\theta})$ is a regularizer (penalizes certain values of $\boldsymbol{\theta}$)
- Learning is cast as optimization
  - ideally, we'd optimize classification error, but it's not smooth
  - loss function is a surrogate for what we truly should optimize (e.g. upper bound)

MACHINE LEARNING

Topics: stochastic gradient descent (SGD)

- Algorithm that performs updates after each example
  - initialize $\boldsymbol{\theta}$ ($\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$)
  - for N iterations
    - 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 over **all** examples

- To apply this algorithm to neural network training, we need
  - the loss function $l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - a procedure to compute the parameter gradients $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - the regularizer $\Omega(\boldsymbol{\theta})$ (and the gradient $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)

GRADIENT COMPUTATION

Topics: loss gradient at output

- Partial derivative:

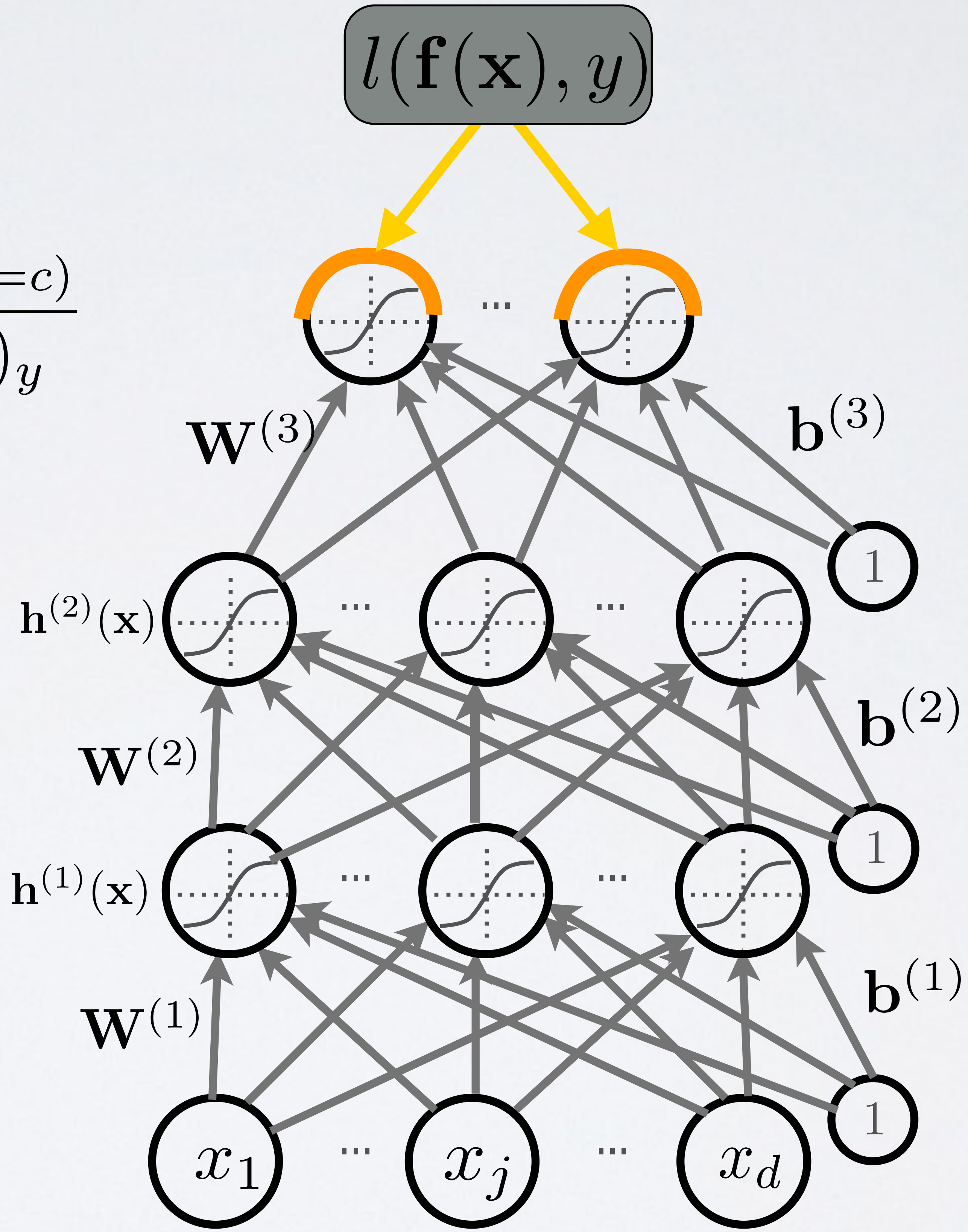
$$\frac{\partial}{\partial f(\mathbf{x})_c} - \log f(\mathbf{x})_y \quad = \quad \frac{-1_{(y=c)}}{f(\mathbf{x})_y}$$

- Gradient:

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

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

$$= \quad \frac{-\mathbf{e}(y)}{f(\mathbf{x})_y}$$



GRADIENT COMPUTATION

Topics: loss gradient at output pre-activation

- Partial derivative:

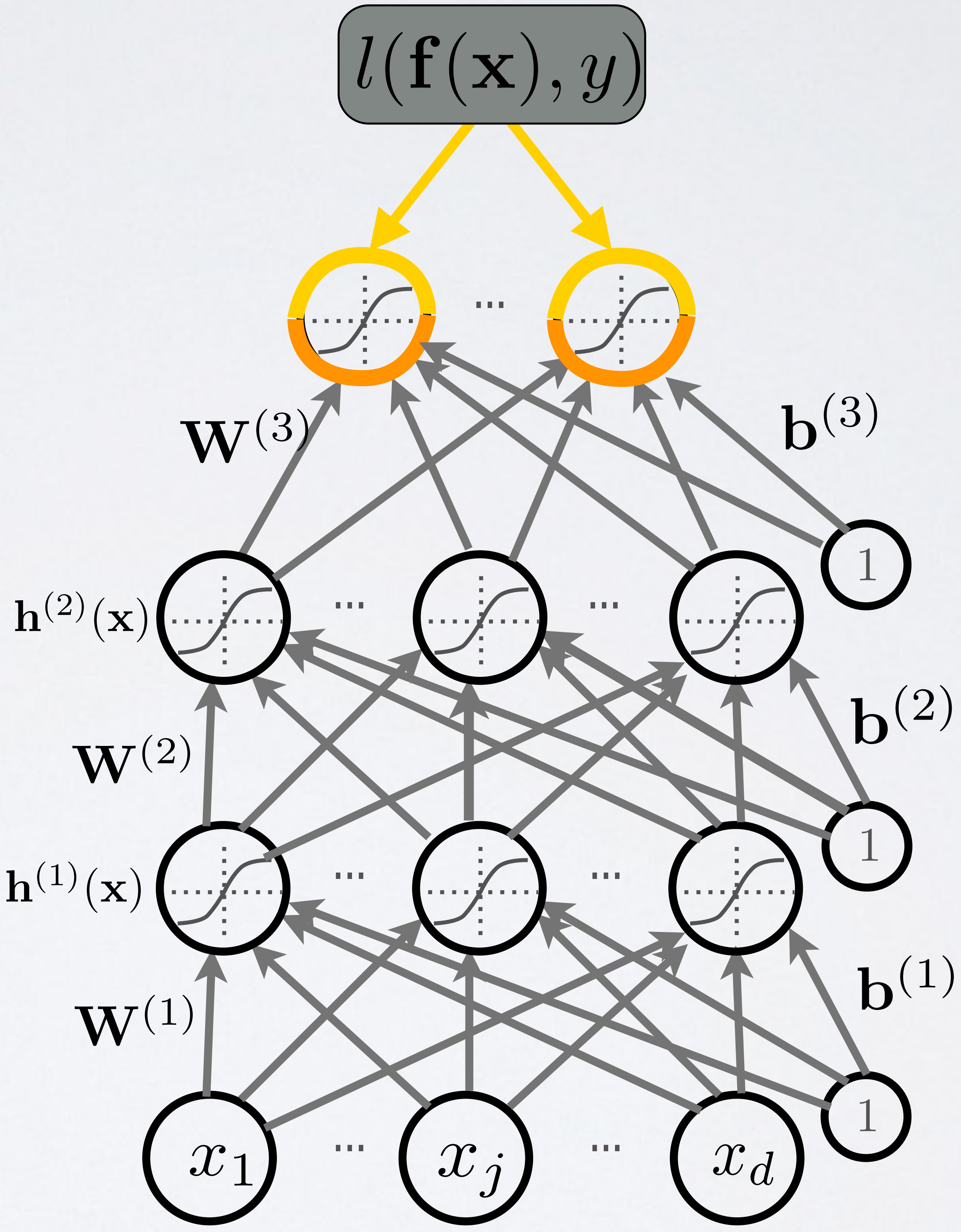
$$\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} - \log f(\mathbf{x})_y$$

$$= \quad -\left(1_{(y=c)} - f(\mathbf{x})_c\right)$$

- Gradient:

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

$$= \quad -\left(\mathbf{e}(y) - \mathbf{f}(\mathbf{x})\right)$$



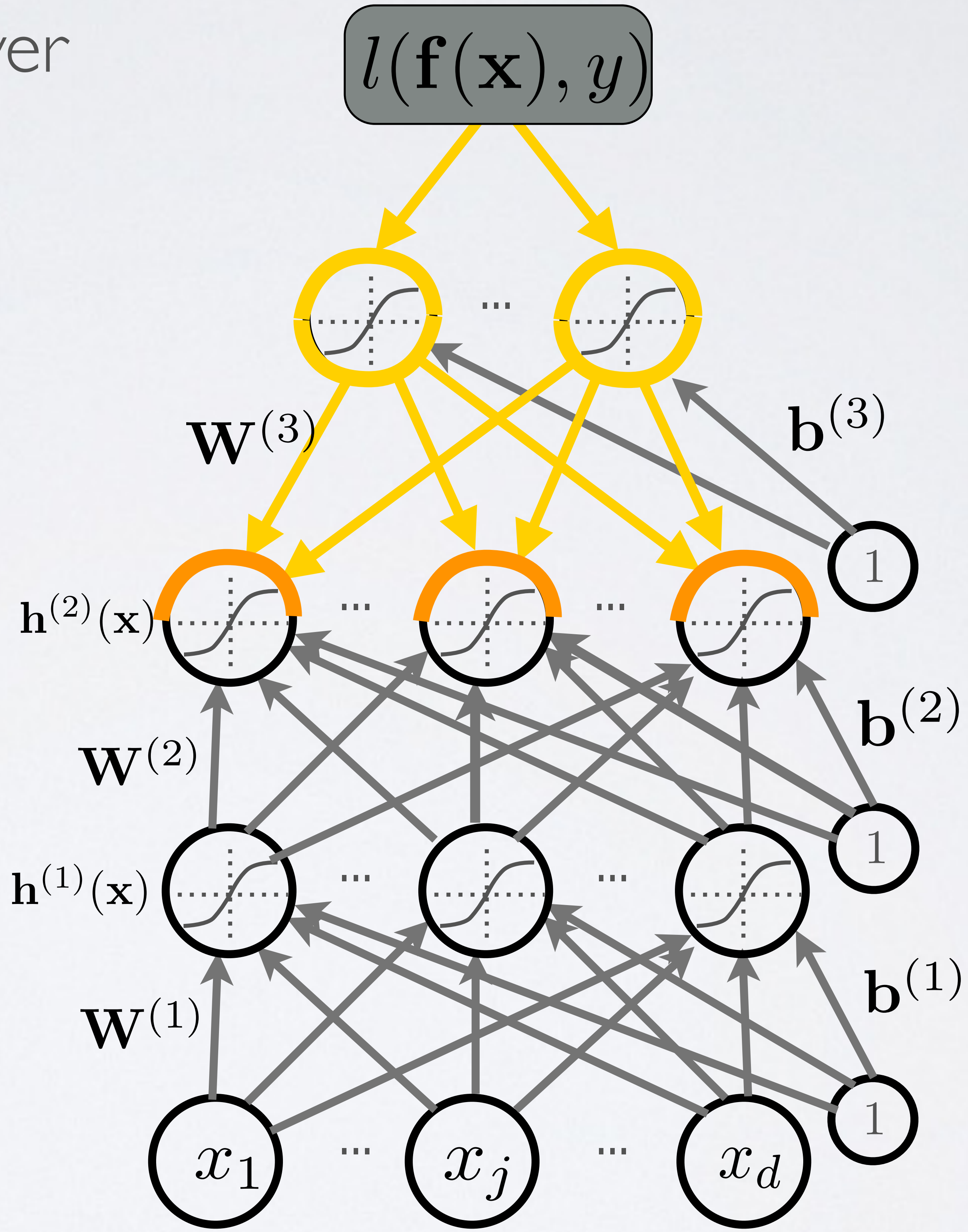
$$\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} - \log f(\mathbf{x})_y$$

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

GRADIENT COMPUTATION

Topics: loss gradient at hidden layer

- ... this is getting complicated!!



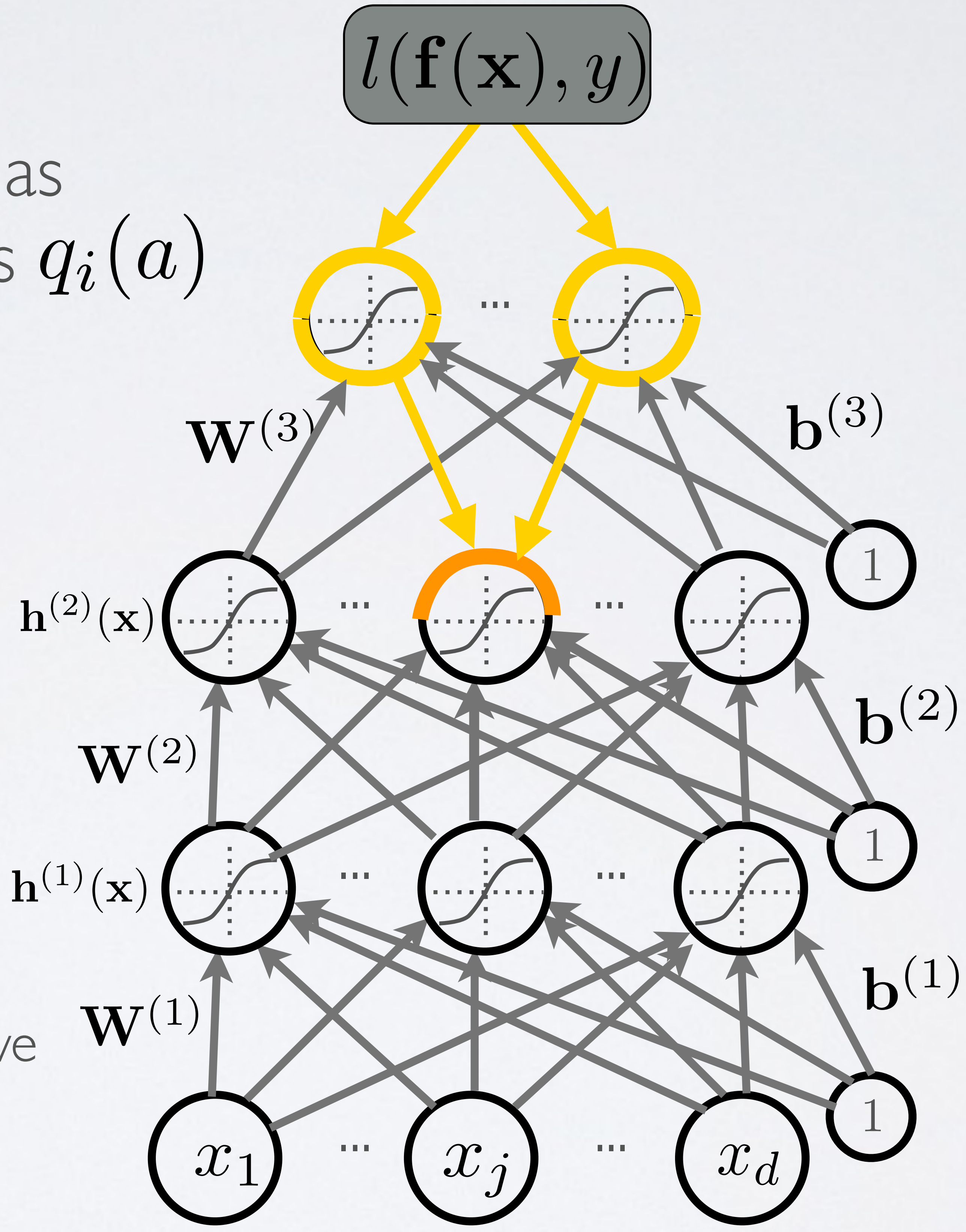
GRADIENT COMPUTATION

Topics: chain rule

- If a function $p(a)$ can be written as a function of intermediate results $q_i(a)$ then we have:

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

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



GRADIENT COMPUTATION

Topics: loss gradient at hidden layers

- Partial derivative:

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

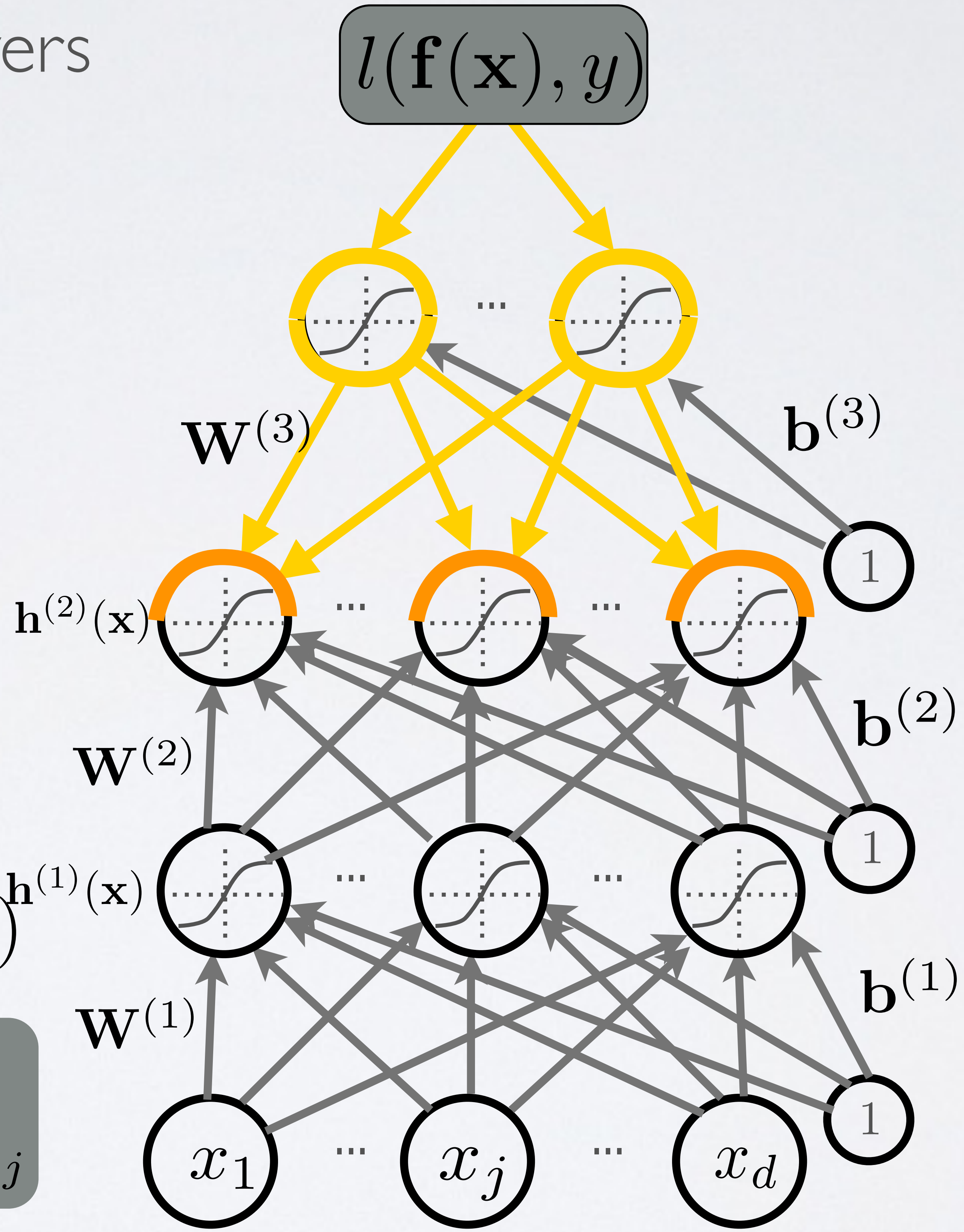
$$= \sum_i \frac{\partial - \log f(\mathbf{x})_y}{\partial a^{(k+1)}(\mathbf{x})_i} \frac{\partial a^{(k+1)}(\mathbf{x})_i}{\partial h^{(k)}(\mathbf{x})_j}$$

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

$$= (\mathbf{W}_{\cdot,j}^{k+1})^\top (\nabla_{\mathbf{a}^{k+1}(\mathbf{x})} - \log f(\mathbf{x})_y)$$

REMINDER

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



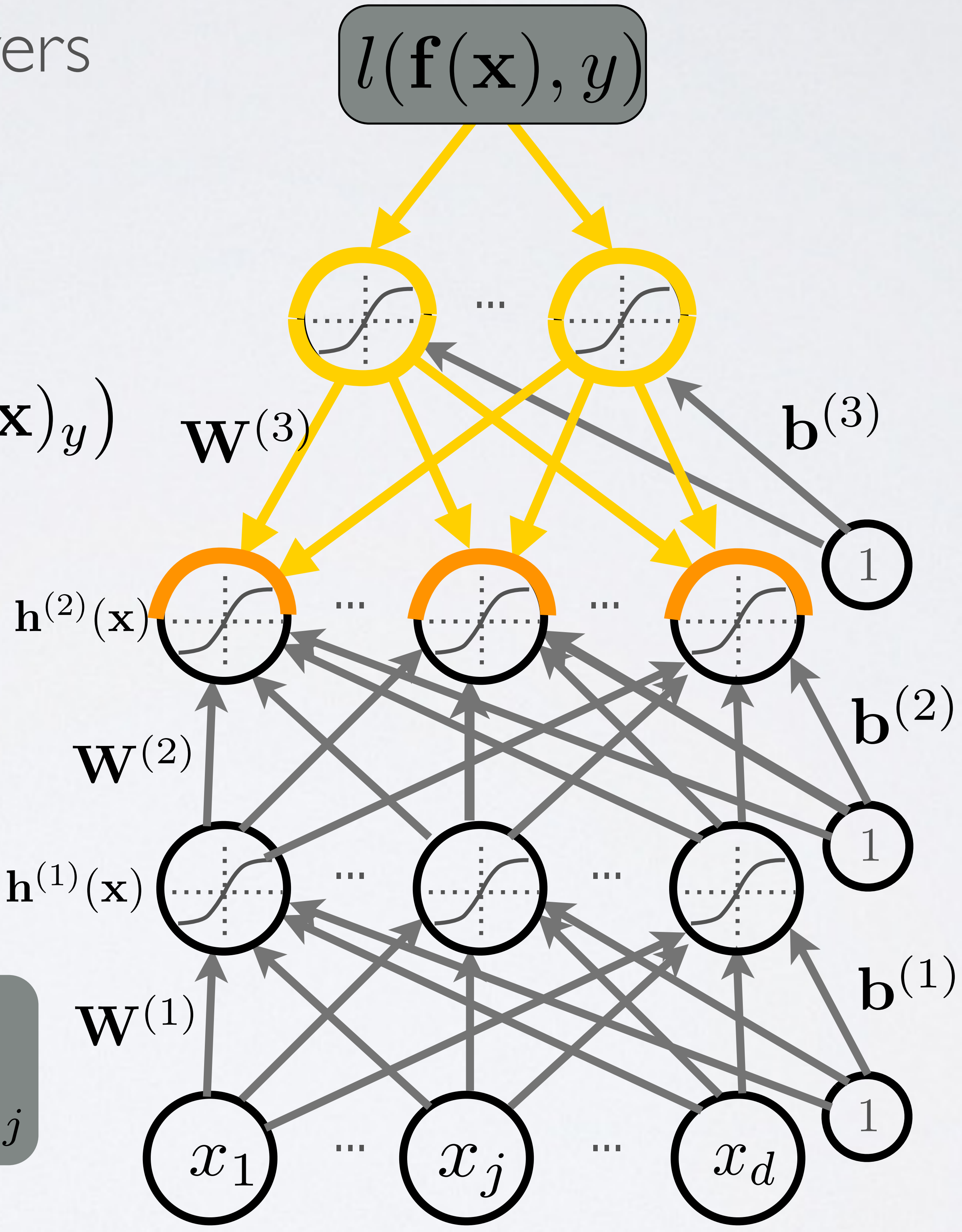
GRADIENT COMPUTATION

Topics: loss gradient at hidden layers

- Gradient:

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

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



REMINDER

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

GRADIENT COMPUTATION

Topics: loss gradient at hidden layers
pre-activation

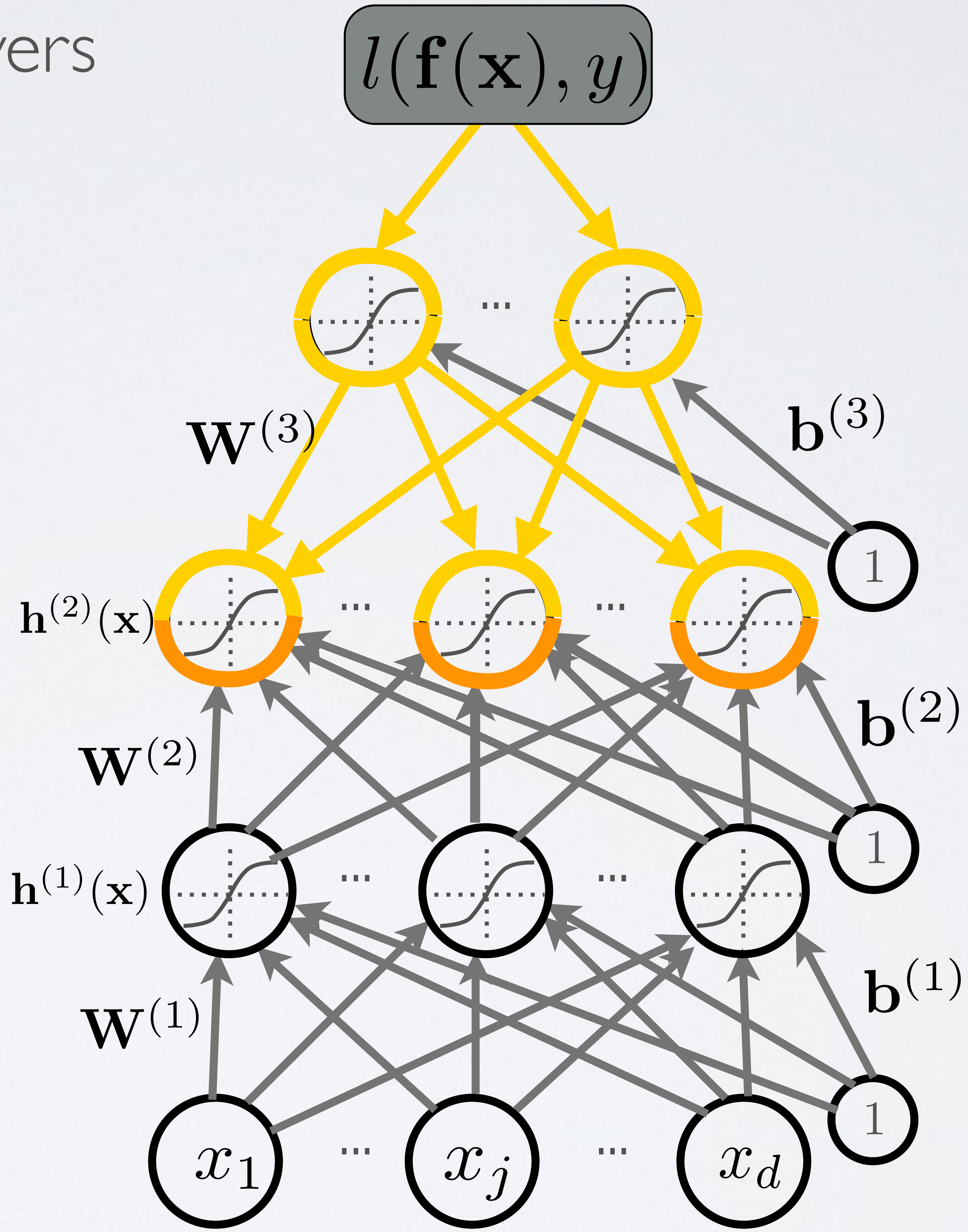
- Partial derivative:

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

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

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

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



GRADIENT COMPUTATION

Topics: loss gradient at hidden layers pre-activation

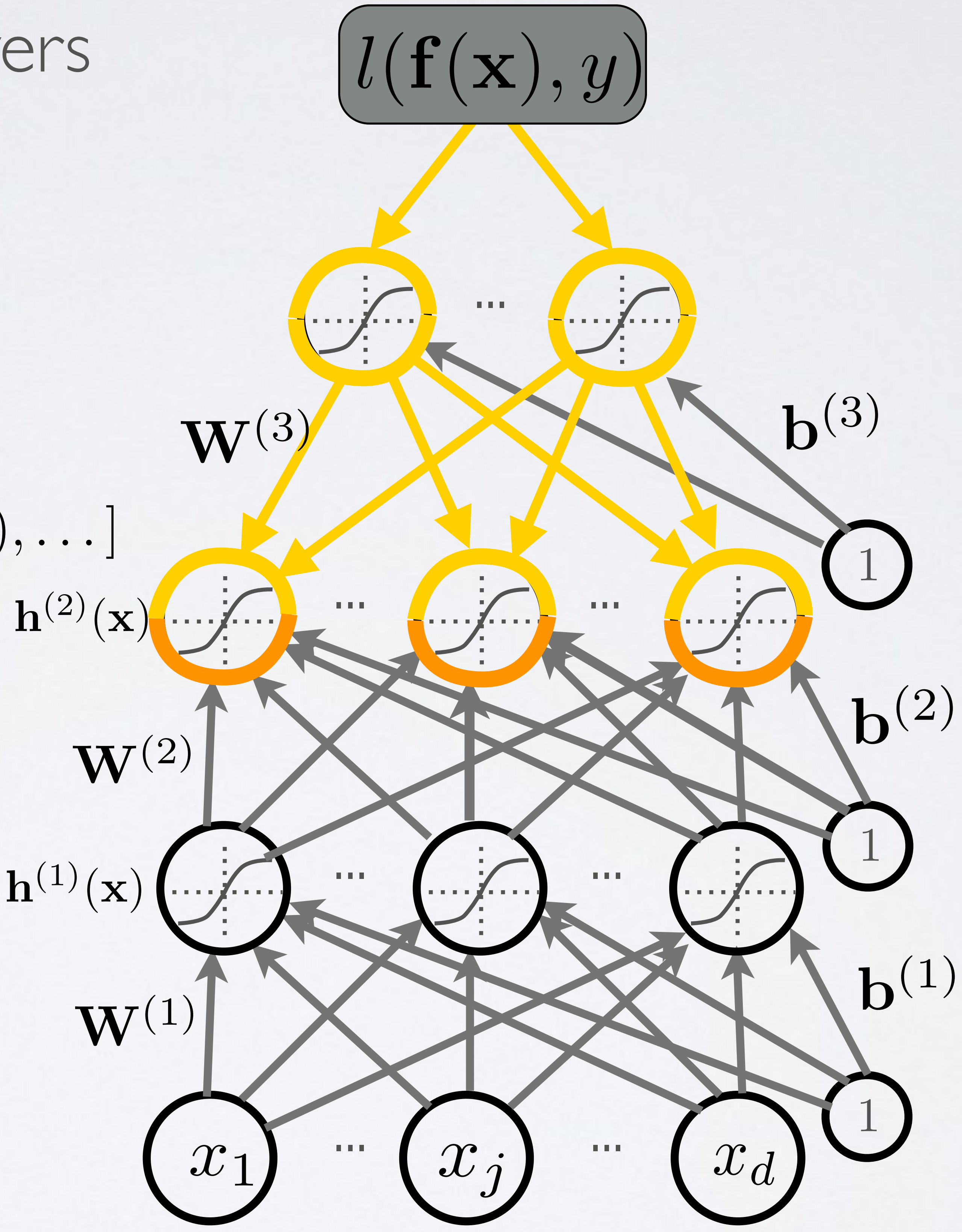
- Gradient:

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

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

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

element-wise product



REMINDER

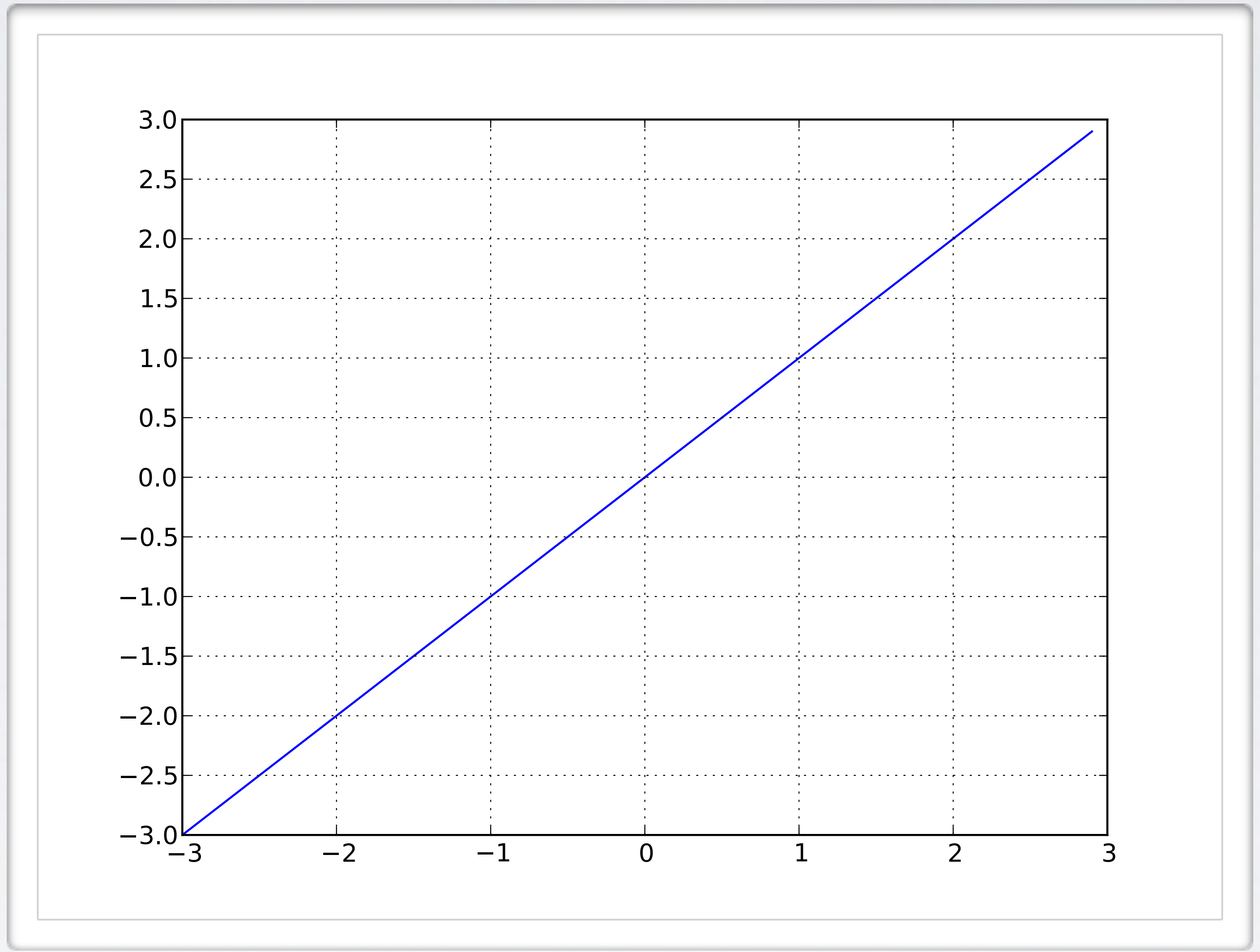
$$h^{(k)}(\mathbf{x})_j = g(a^{(k)}(\mathbf{x})_j)$$

ACTIVATION FUNCTION

Topics: linear activation function gradient

- Partial derivative:

$$g'(a) = 1$$



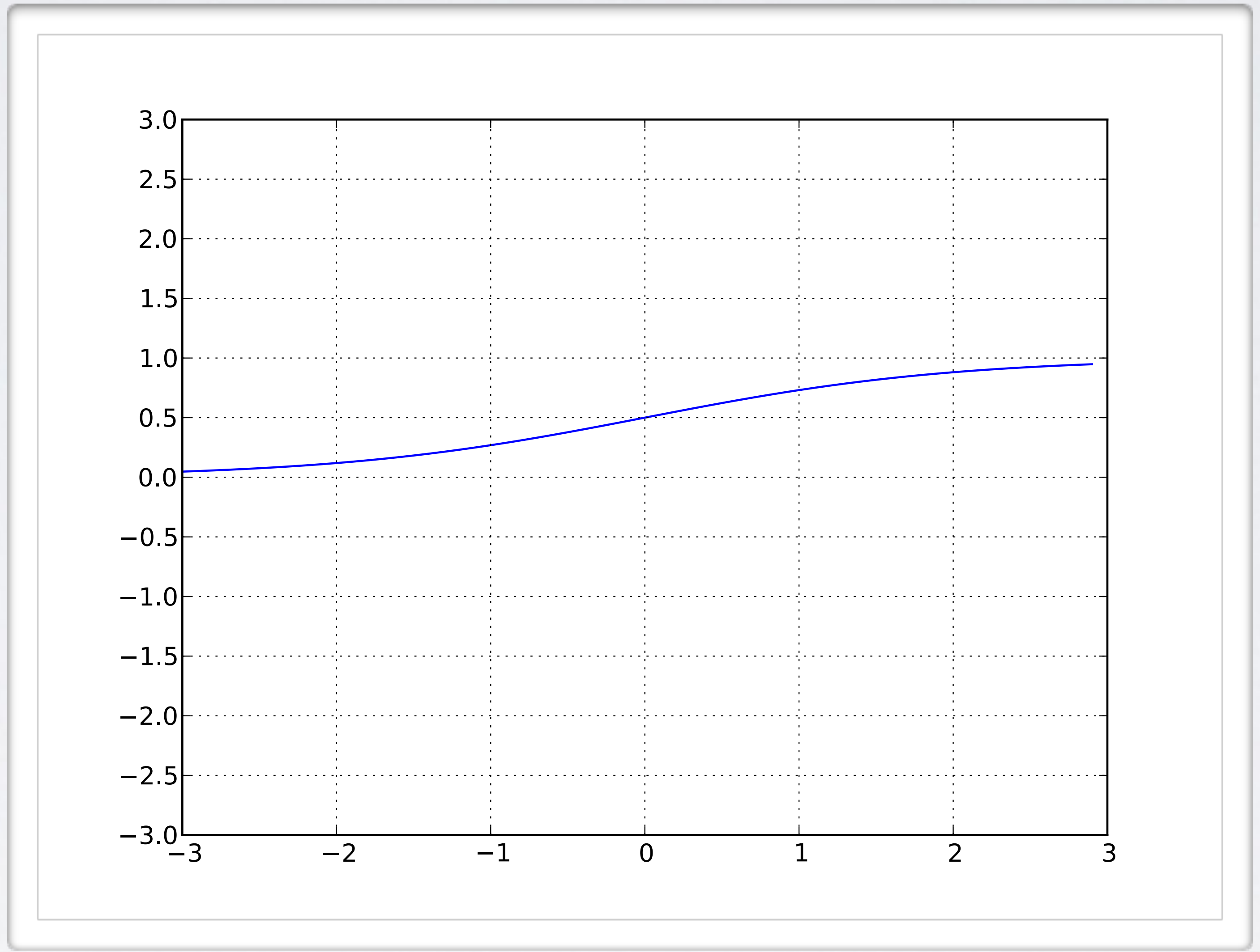
$$g(a) = a$$

ACTIVATION FUNCTION

Topics: sigmoid activation function gradient

- Partial derivative:

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



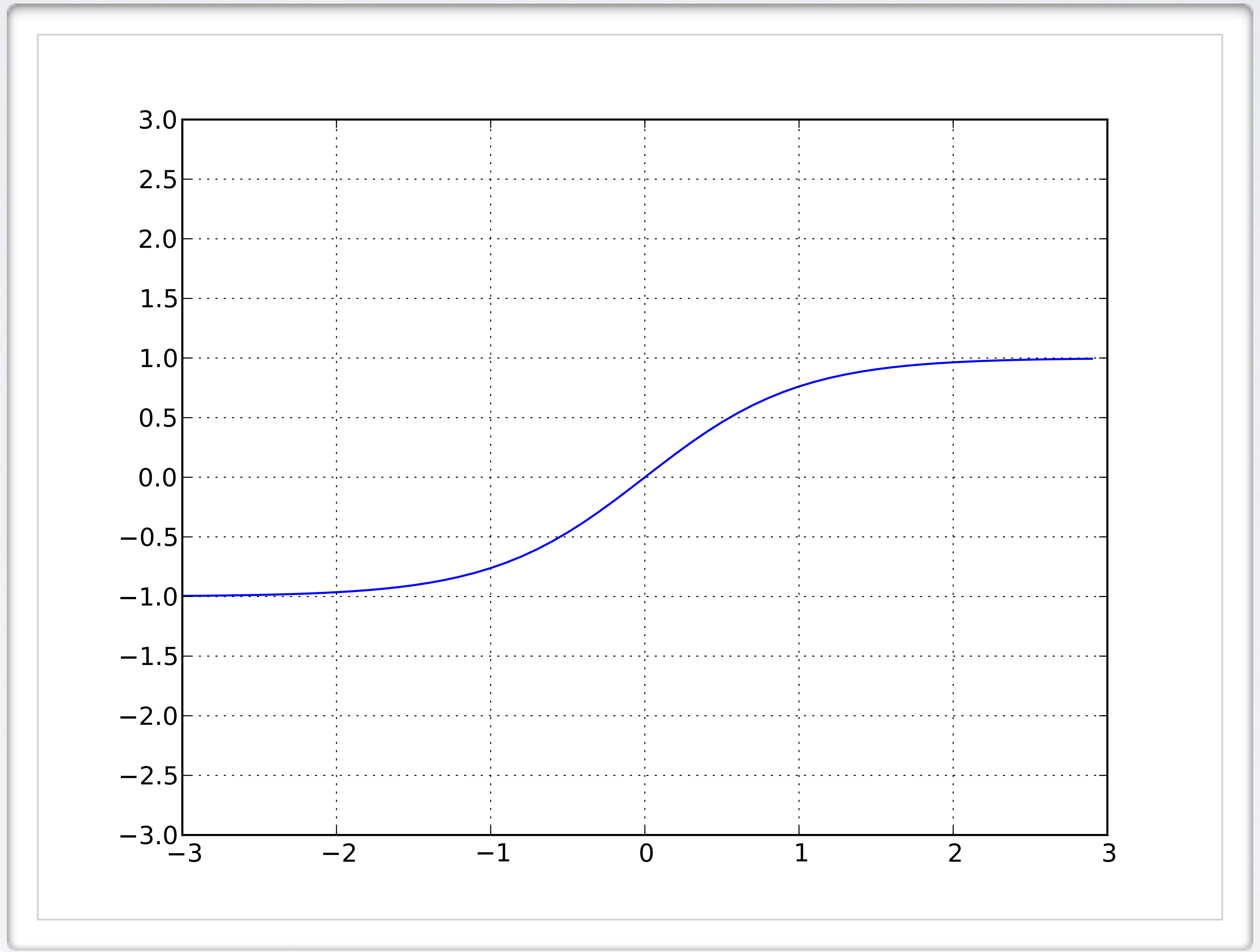
$$g(a) = \mathrm{sigm}(a) = \frac{1}{1+\exp(-a)}$$

ACTIVATION FUNCTION

Topics: tanh activation function gradient

- Partial derivative:

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



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

MACHINE LEARNING

Topics: stochastic gradient descent (SGD)

- Algorithm that performs updates after each example
  - initialize $\boldsymbol{\theta}$ ($\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$)
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training epoch
=
iteration over **all** examples

- To apply this algorithm to neural network training, we need
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  - a procedure to compute the parameter gradients $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - the regularizer $\Omega(\boldsymbol{\theta})$ (and the gradient $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)

GRADIENT COMPUTATION

Topics: loss gradient of parameters

- Partial derivative (weights):

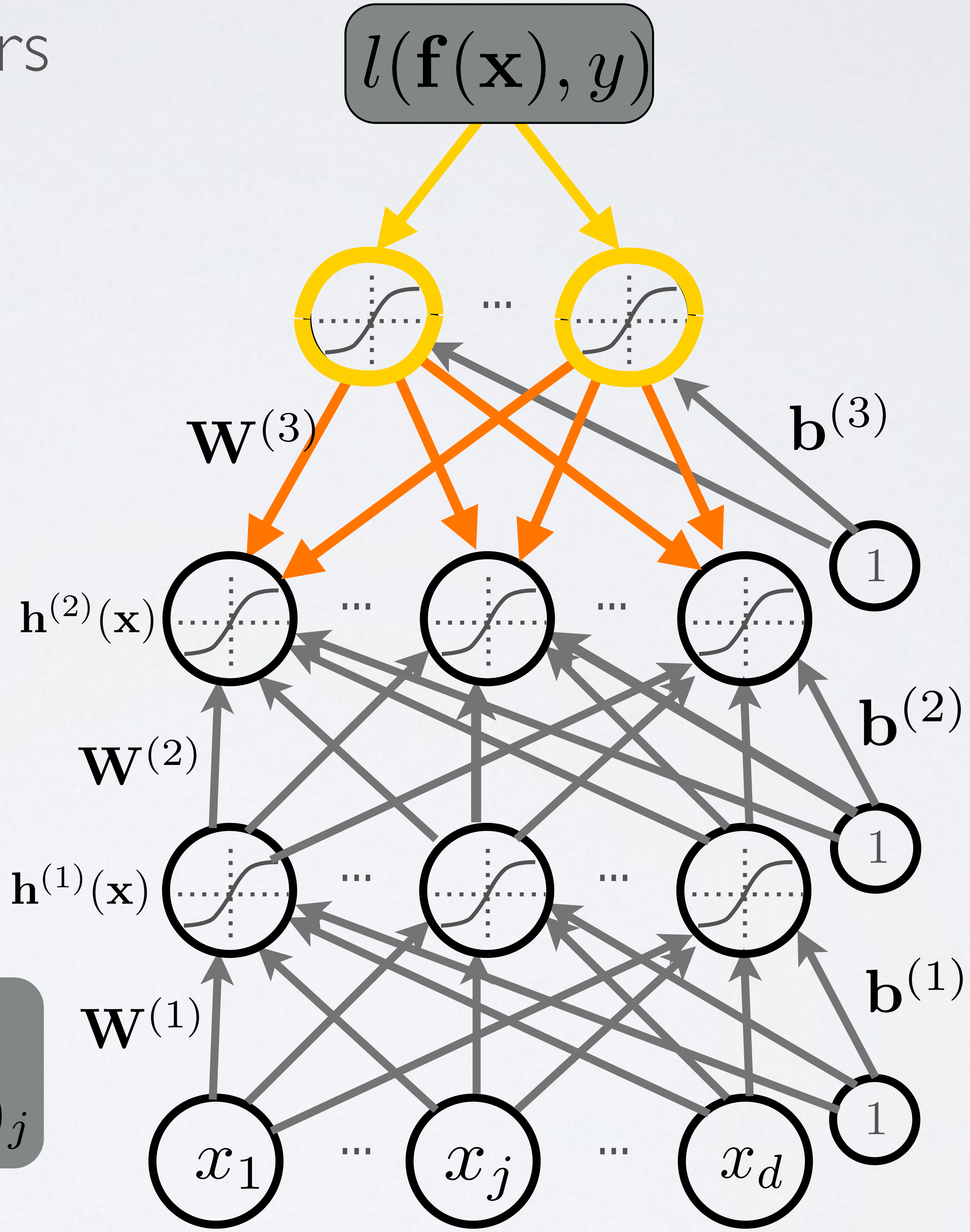
$$\frac{\partial}{\partial W_{i,j}^{(k)}} - \log f(\mathbf{x})_y$$

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

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

REMINDER

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

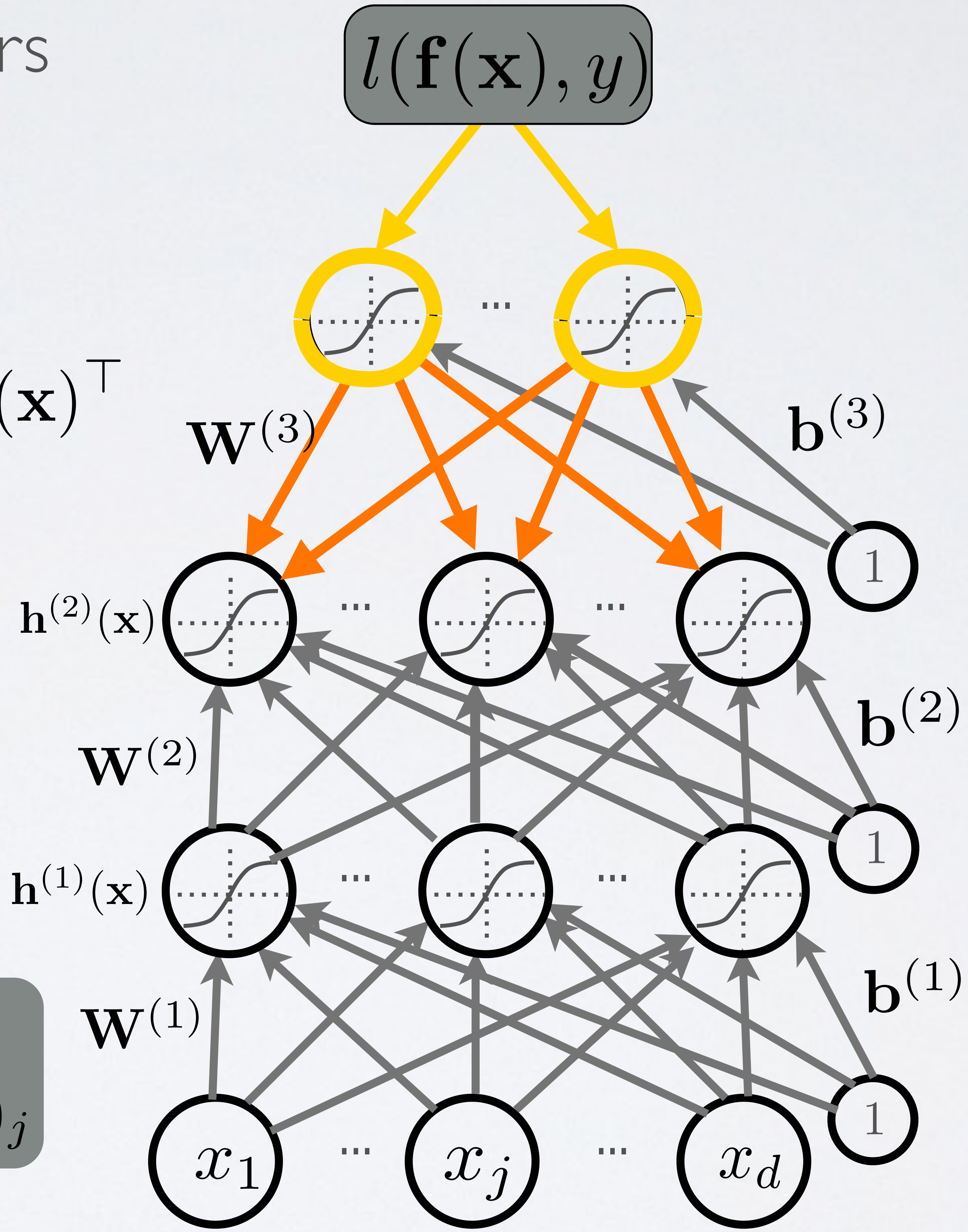


GRADIENT COMPUTATION

Topics: loss gradient of parameters

- Gradient (weights):

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



REMINDER

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

GRADIENT COMPUTATION

Topics: loss gradient of parameters

- Partial derivative (biases):

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

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

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

REMINDER

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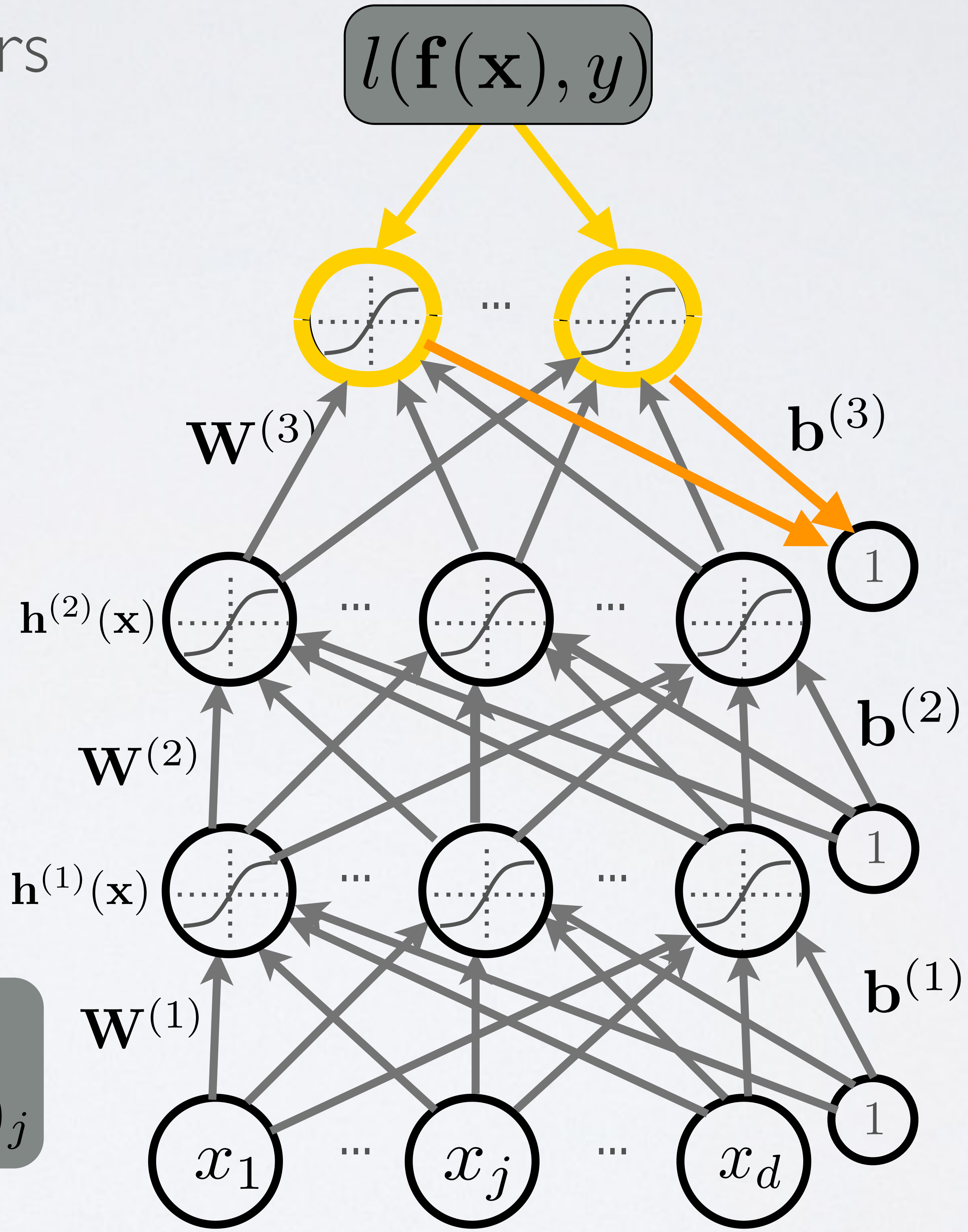
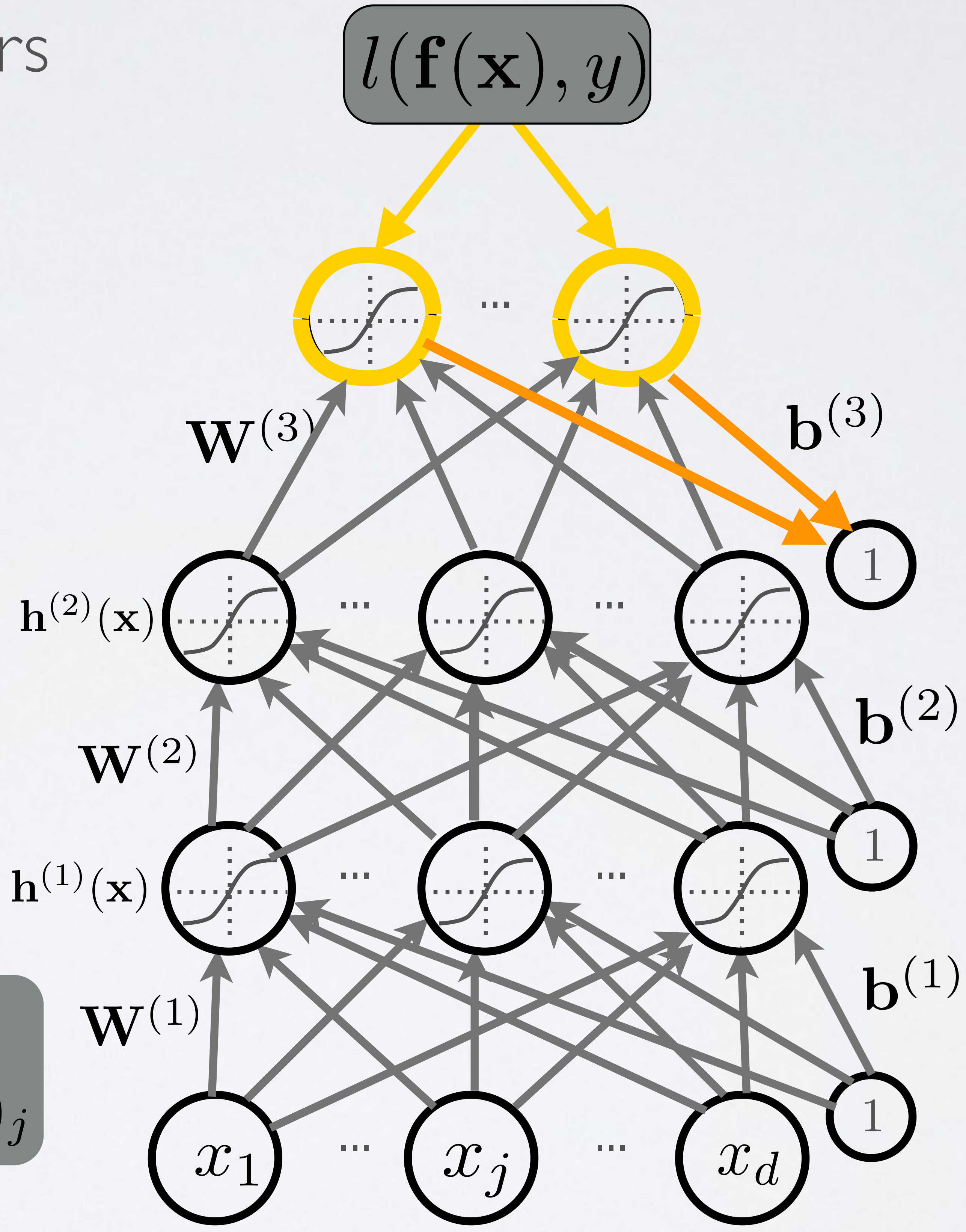


GRADIENT COMPUTATION

Topics: loss gradient of parameters

- Gradient (biases):

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



REMINDER

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

BACKPROPAGATION

Topics: backpropagation algorithm

- This assumes a forward propagation has been made before
  - compute output gradient (before activation)

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

  - for k from $L{+}1$ to 1
    - compute gradients of hidden layer parameter

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

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

    - compute gradient of hidden layer below

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

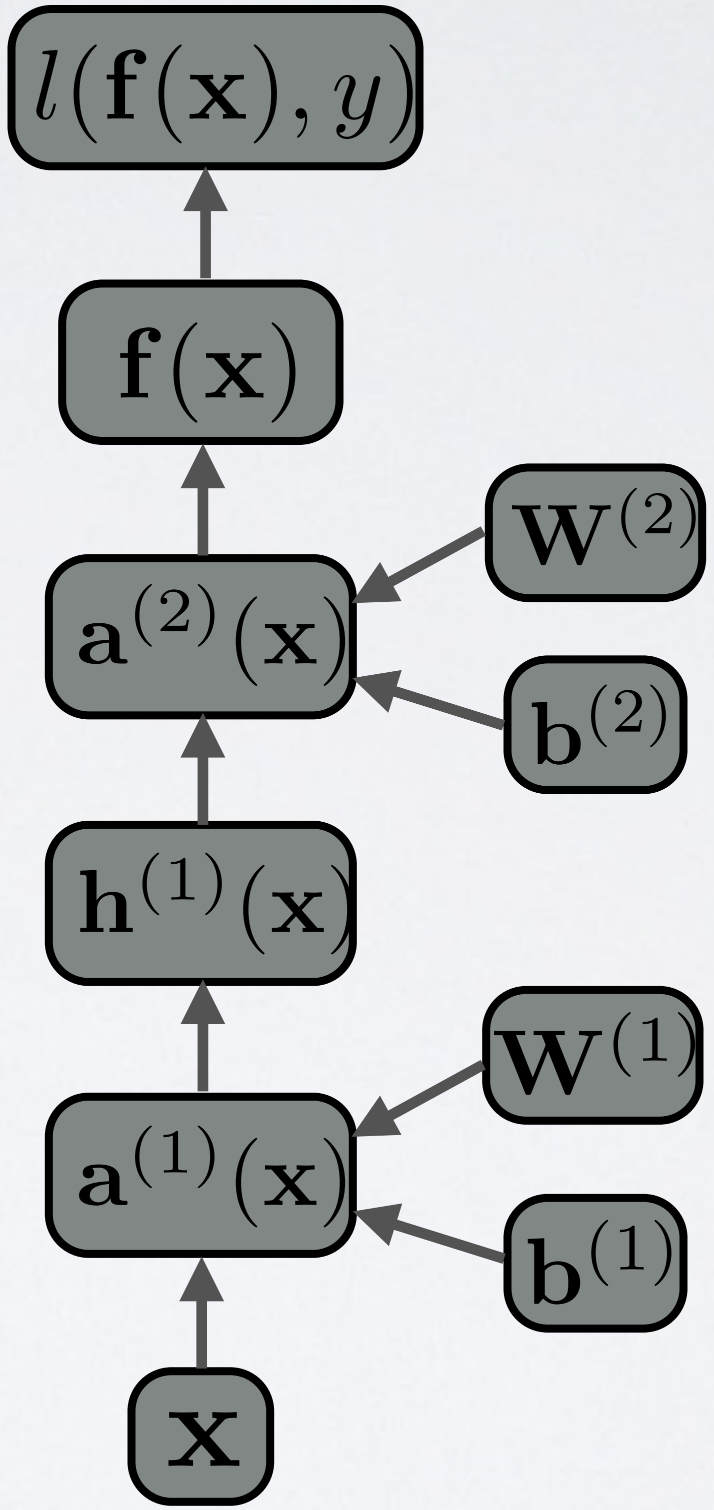
    - compute gradient of hidden layer below (before activation)

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

FLOW GRAPH

Topics: flow graph

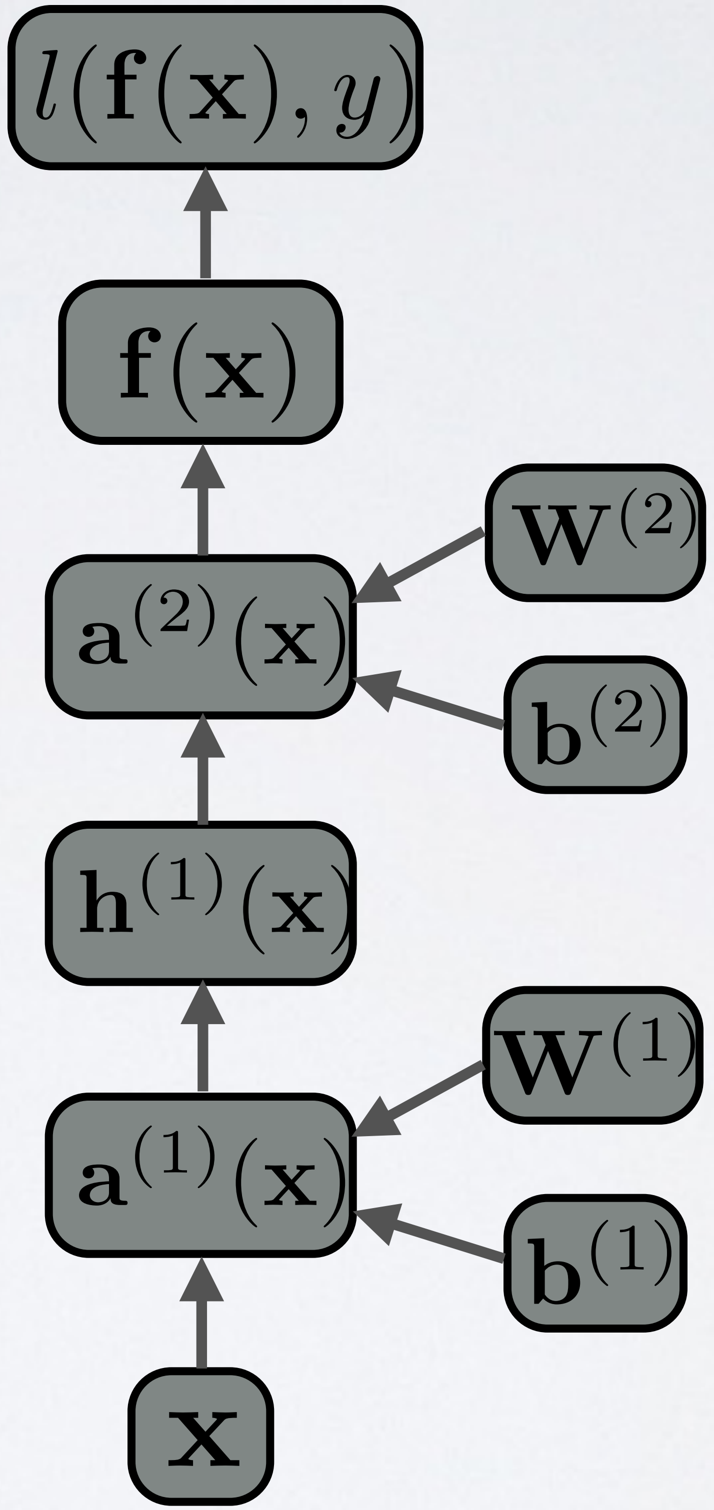
- Forward propagation can be represented as an acyclic flow graph
- It's a nice way of implementing forward propagation in a modular way
  - each box could be an object with an fprop method, that computes the value of the box given its children
  - calling the fprop method of each box in the right order yield forward propagation



FLOW GRAPH

Topics: automatic differentiation

- Each object also has a bprop method
  - it computes the gradient of the loss with respect to each children
  - fprop depends on the fprop of a box's children, while bprop depends the bprop of a box's parents
- By calling bprop in the reverse order, we get backpropagation
  - only need to reach the parameters



GRADIENT CHECKING

Topics: finite difference approximation

- 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

MACHINE LEARNING

Topics: stochastic gradient descent (SGD)

- Algorithm that performs updates after each example
  - initialize $\boldsymbol{\theta}$ ($\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$)
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      - ✓ $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha\, \Delta$

training epoch
=
iteration over **all** examples

- To apply this algorithm to neural network training, we need
  - the loss function $l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - a procedure to compute the parameter gradients $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - the regularizer $\Omega(\boldsymbol{\theta})$ (and the gradient $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)

REGULARIZATION

Topics: 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 applied on weights, not on biases (weight decay)
- Can be interpreted as having a Gaussian prior over the weights

REGULARIZATION

Topics: L1 regularization

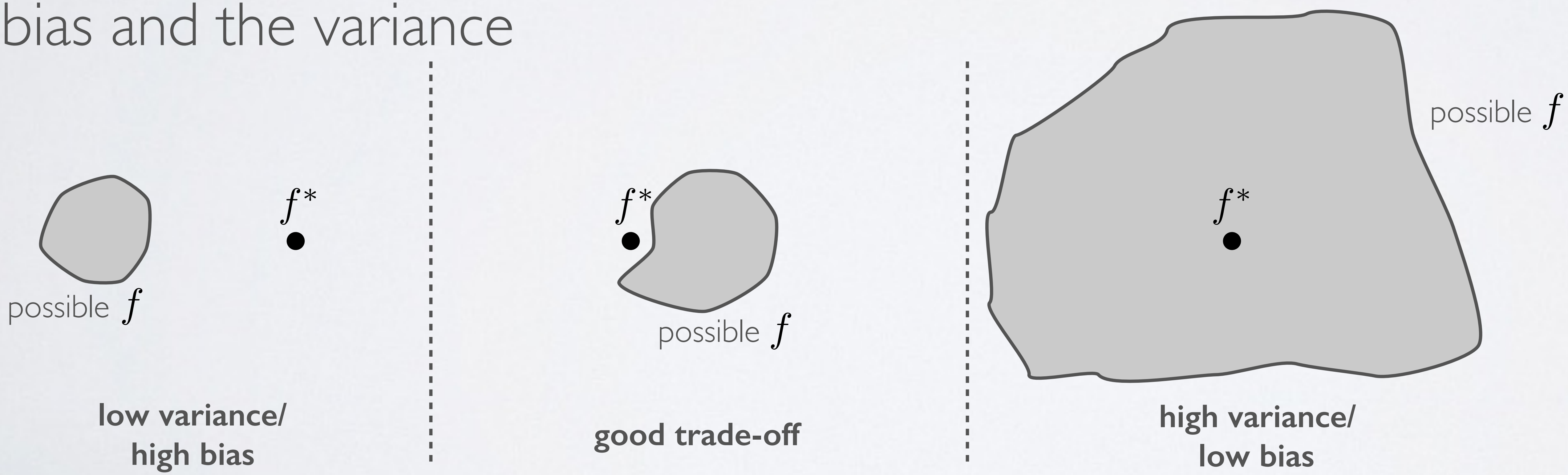
$$\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j |W_{i,j}^{(k)}|$$

- Gradient: $\nabla_{\mathbf{W}^{(k)}} \Omega(\boldsymbol{\theta}) = \operatorname{sign}(\mathbf{W}^{(k)})$
  - where $\operatorname{sign}(\mathbf{W}^{(k)})_{i,j} = 1_{\mathbf{W}_{i,j}^{(k)} > 0} - 1_{\mathbf{W}_{i,j}^{(k)} < 0}$
- Also only applied on weights
- Unlike L2, L1 will push certain weights to be exactly 0
- Can be interpreted as having a Laplacian prior over the weights

REGULARIZATION

Topics: bias-variance trade-off

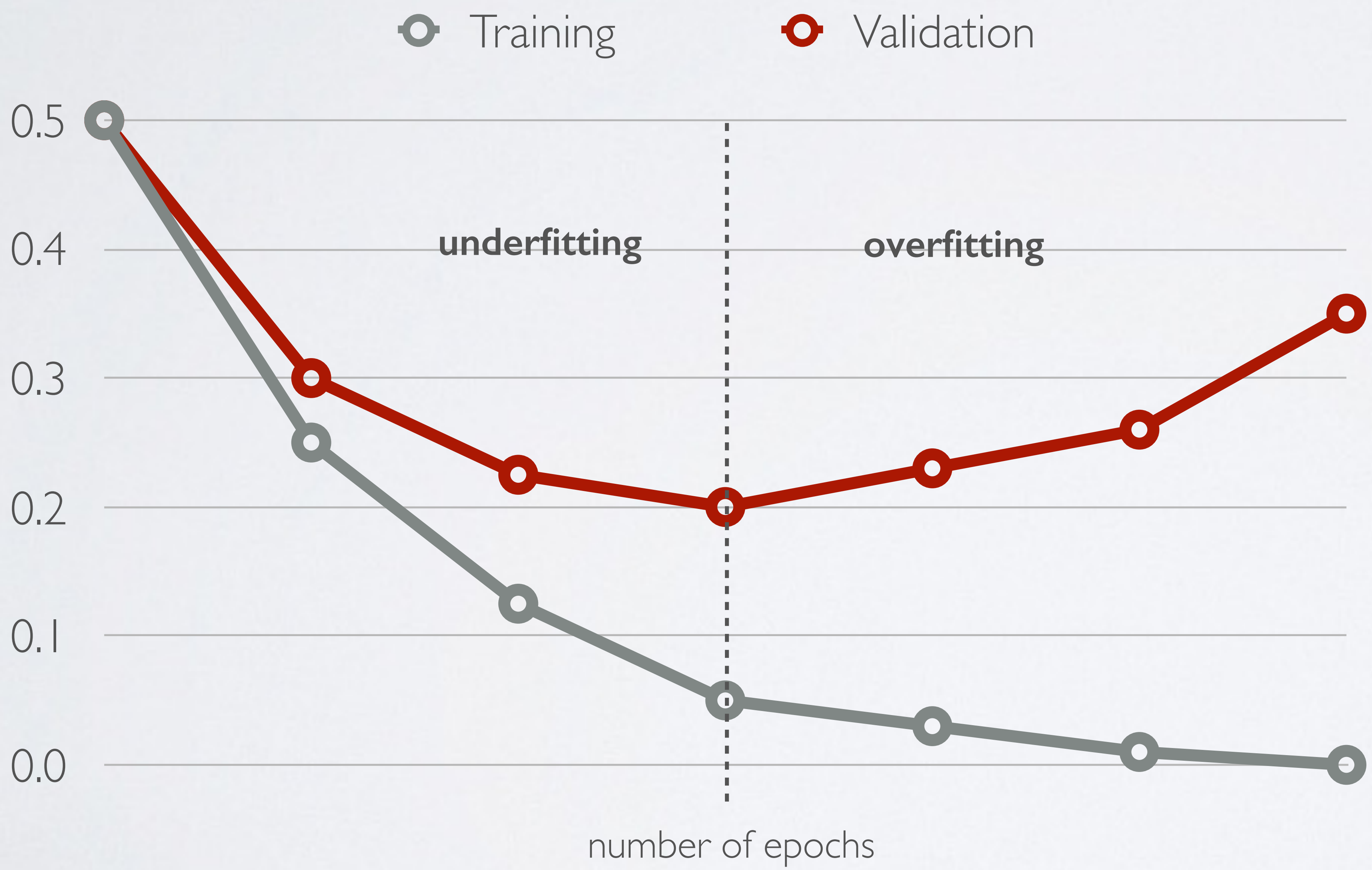
- Variance of trained model: does it vary a lot if the training set changes
- Bias of trained model: is the average model close to the true solution
- Generalization error can be seen as the sum of the (squared) bias and the variance



KNOWING WHEN TO STOP

Topics: early stopping

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



PARAMETER INITIALIZATION

Topics: initialization

- For biases
  - initialize all to 0
- For weights
  - Can't initialize weights to 0 with tanh activation
    - we can show that all gradients would then be 0 (saddle point)
  - Can't initialize all weights to the same value
    - we can show that all hidden units in a layer will always behave the same
    - need to break symmetry
  - Recipe: sample $\mathbf{W}^{(k)}_{i,j}$ from $U\left[-b, b\right]$ where $b = \frac{\sqrt{6}}{\sqrt{H_k + H_{k-1}}}$

    size of $\mathbf{h}^{(k)}(\mathbf{x})$
    - the idea is to sample around 0 but break symmetry
    - other values of b could work well (not an exact science) (see Glorot & Bengio, 2010)

MODEL SELECTION

Topics: training, validation and test sets, generalization

- Training set $\mathcal{D}^{\mathrm{train}}$ serves to train a model
- Validation set $\mathcal{D}^{\mathrm{valid}}$ serves to select hyper-parameters
- Test set $\mathcal{D}^{\mathrm{test}}$ serves to estimate the generalization performance (error)

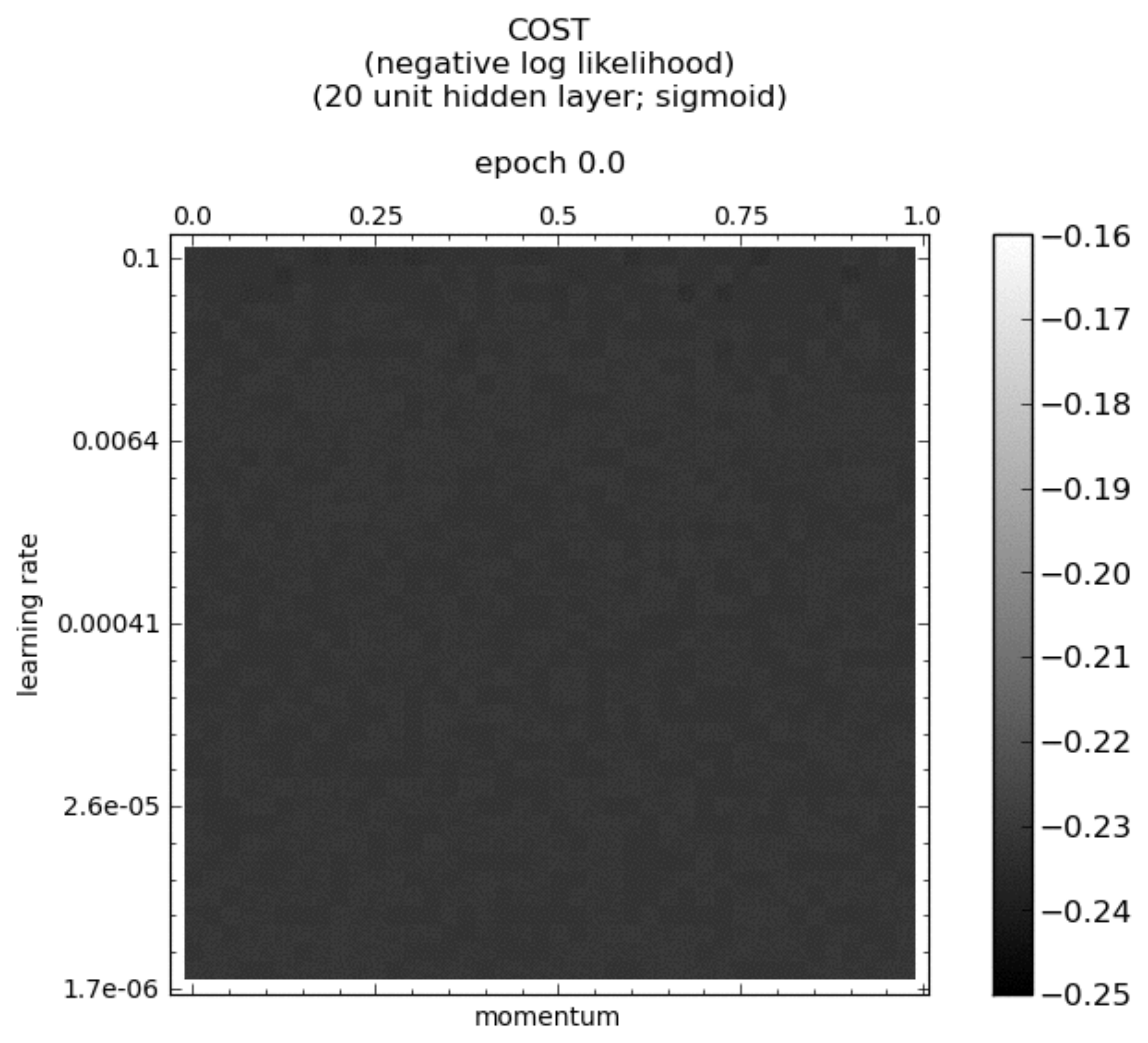
- Generalization is the behavior of the model on **unseen examples**
  - this is what we care about in machine learning!

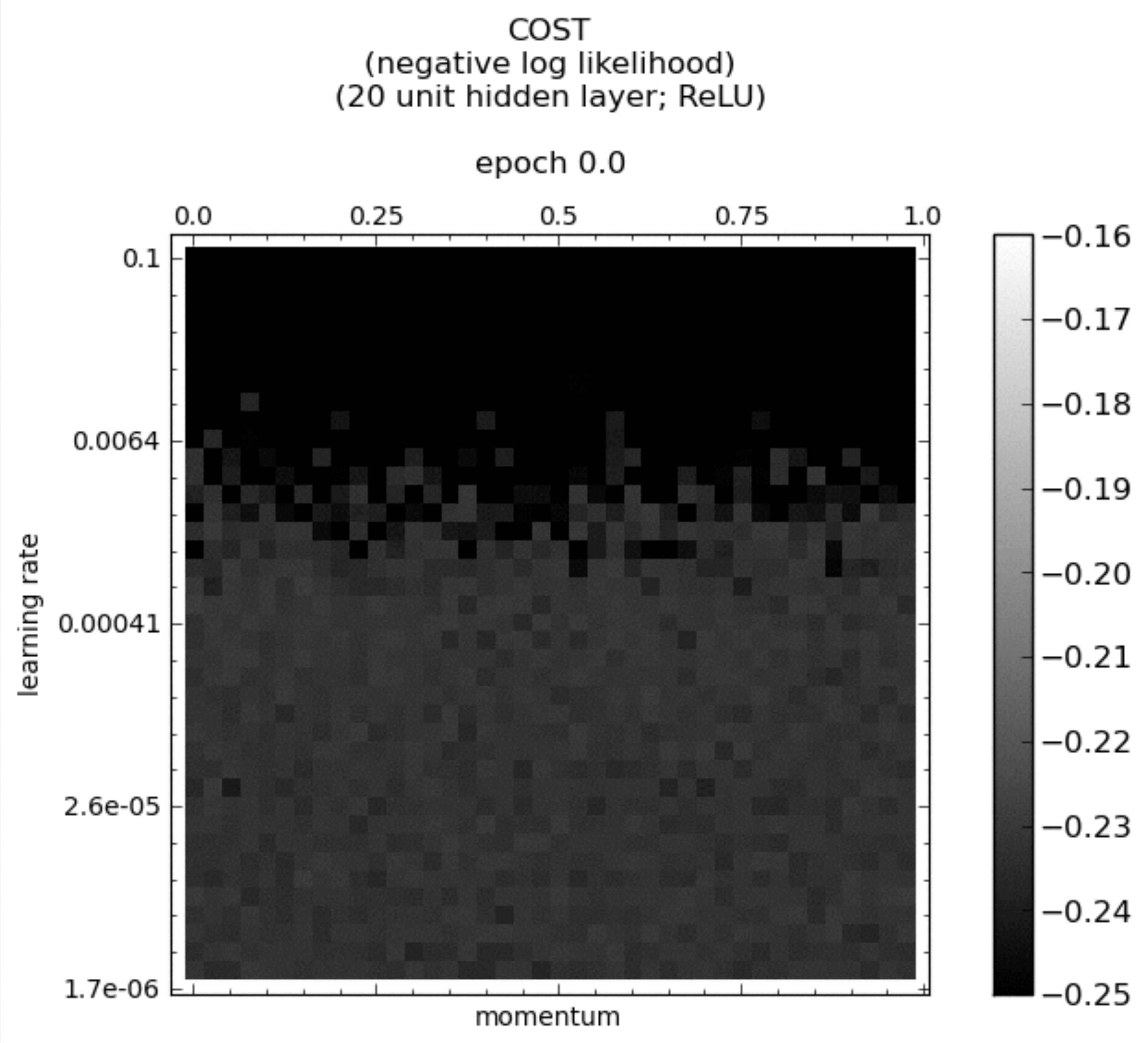
MODEL SELECTION

Topics: grid search

- To search for the best configuration of the hyper-parameters:
  - you can perform a grid search
    - specify a set of values you want to test for each hyper-parameter
    - try all possible configurations of these values
  - you can perform a random search
    - specify a distribution over the values of each hyper-parameters (e.g. uniform in some range)
    - sample independently each hyper-parameter to get a configuration, and repeat as many times as wanted
- Use a validation set performance to select the best configuration
- You can go back and refine the grid/distributions if needed

DISCUSSION: MODEL SELECTION



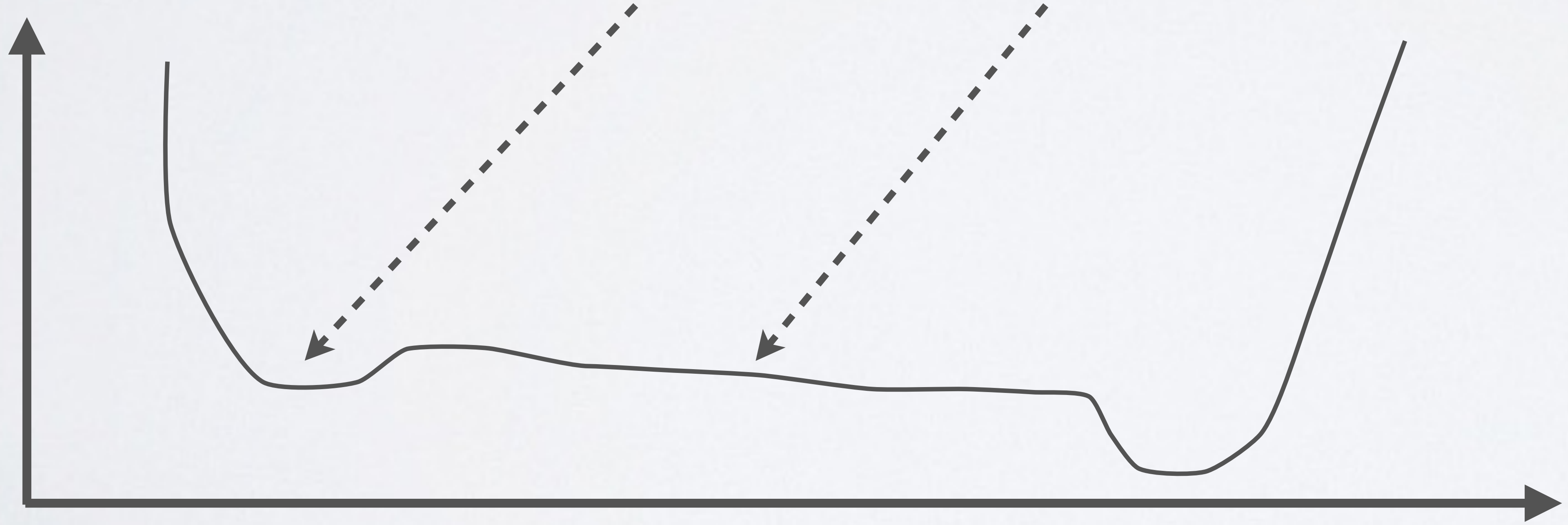


OPTIMIZATION

Topics: local optimum, global optimum, plateau

- Notes on the optimization problem
  - there isn't a single global optimum (non-convex optimization)
    - we can permute the hidden units (with their connections) and get the same function
    - we say that the hidden unit parameters are not identifiable

- Optimization can get stuck in <u>local minimum</u> or <u>plateaus</u>



OPTIMIZATION

Topics: local optimum, global optimum, plateau

Neural network training demo
(by Andrej Karpathy)

http://cs.stanford.edu/~karpathy/svmjs/demo/demonn.html

GRADIENT DESCENT

Topics: convergence conditions, decrease constant

- Stochastic gradient descent will converge if
  - $\sum_{t=1}^{\infty} \alpha_t = \infty$
  - $\sum_{t=1}^{\infty} \alpha_t^2 < \infty$

  where α_t is the learning rate of the t^{th} update

- Decreasing strategies: (δ is the decrease constant)
  - $\alpha_t = \frac{\alpha}{1+\delta t}$
  - $\alpha_t = \frac{\alpha}{t^\delta}$ (où $0.5 < \delta \leq 1$)
- Better to use a fixed learning rate for the first few updates

GRADIENT DESCENT

Topics: mini-batch, momentum

- Can update based on a mini-batch of example (instead of 1 example):
  - the gradient is the average regularized loss for that mini-batch
  - can give a more accurate estimate of the risk gradient
  - can leverage matrix/matrix operations, which are more efficient

- Can use an **exponentially decaying** average of previous gradients:

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

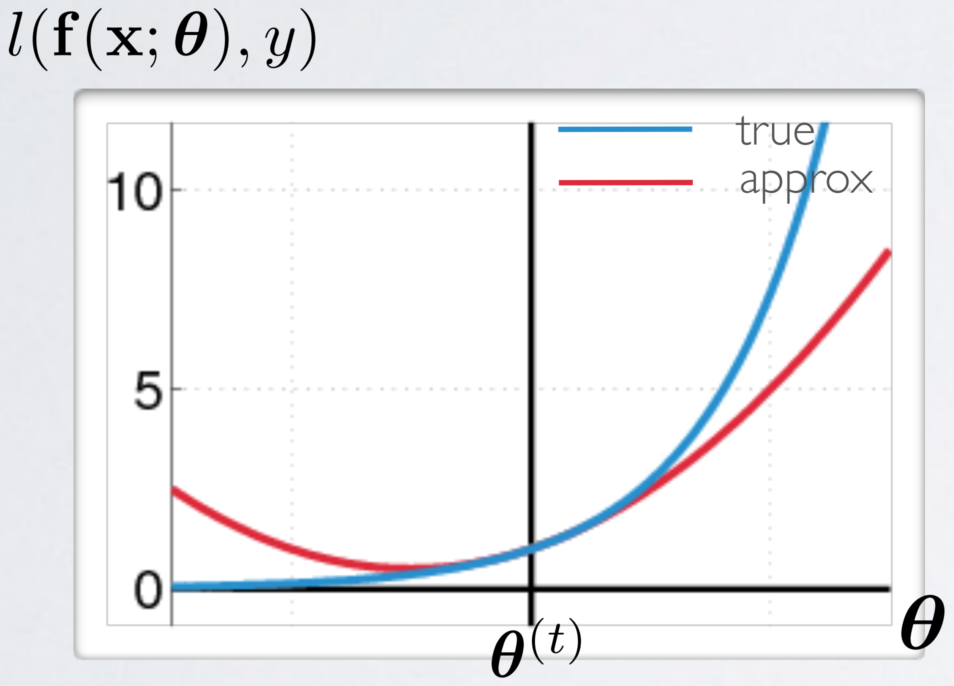
  - can get through plateaus more quickly, by "gaining momentum"

GRADIENT DESCENT

Topics: Newton's method

- If we locally approximate the loss through Taylor expansion:

$$
\begin{aligned}
l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}),y) \quad \approx \quad & l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}^{(t)}),y) + \nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}^{(t)}),y)^\top (\boldsymbol{\theta} - \boldsymbol{\theta}^{(t)}) \\
& + 0.5(\boldsymbol{\theta} - \boldsymbol{\theta}^{(t)})^\top \underbrace{\left(\nabla^2_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}^{(t)}),y)\right)}_{\text{Hessian}} (\boldsymbol{\theta} - \boldsymbol{\theta}^{(t)})
\end{aligned}
$$



- We could minimize that approximation, by solving:

$$
0 = \nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}^{(t)}),y) + \left(\nabla^2_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}^{(t)}),y)\right)(\boldsymbol{\theta} - \boldsymbol{\theta}^{(t)})
$$

GRADIENT DESCENT

Topics: Newton's method

- We can show that the minimum is:

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \left(\nabla^2_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}^{(t)}), y)\right)^{-1} \left(\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}^{(t)}), y)\right)$$

- Only practical if:
  - few parameters (so we can invert Hessian)
  - locally convex (so the Hessian is invertible)

- See recommended readings for more on optimization of neural networks