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

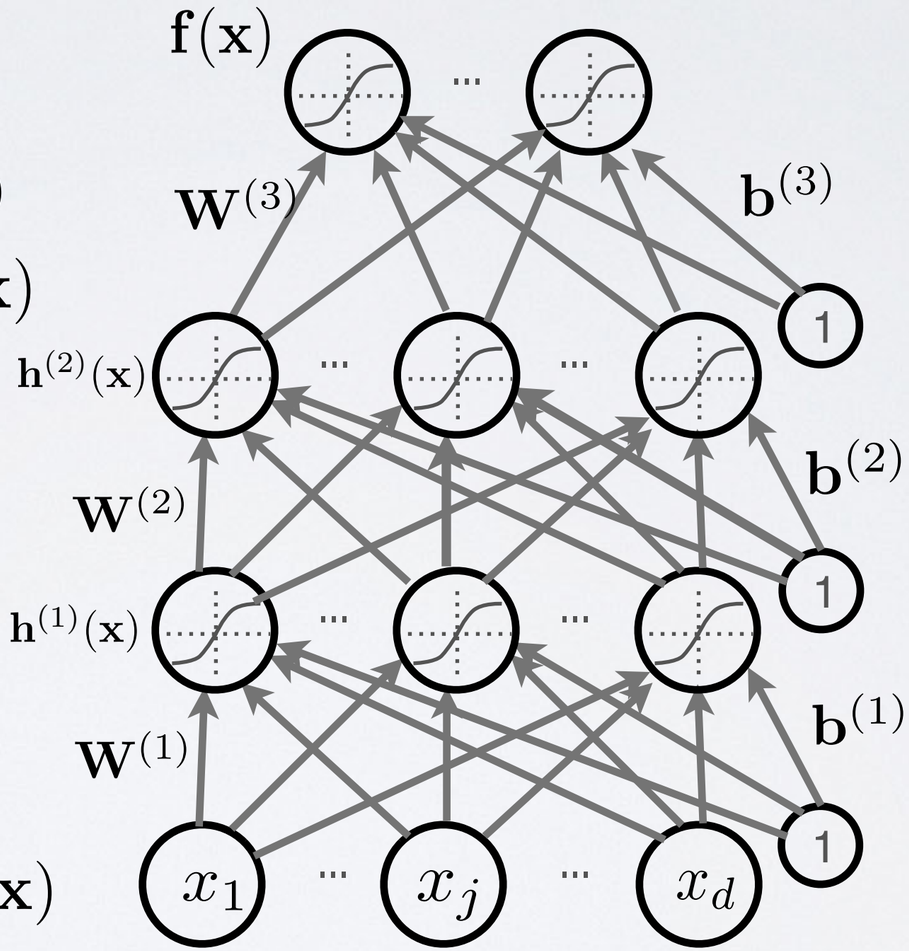
$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

  - 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

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

Adding this term makes it structural risk minimization

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

GRADIENT COMPUTATION

Topics: loss gradient at output

- Partial derivative:

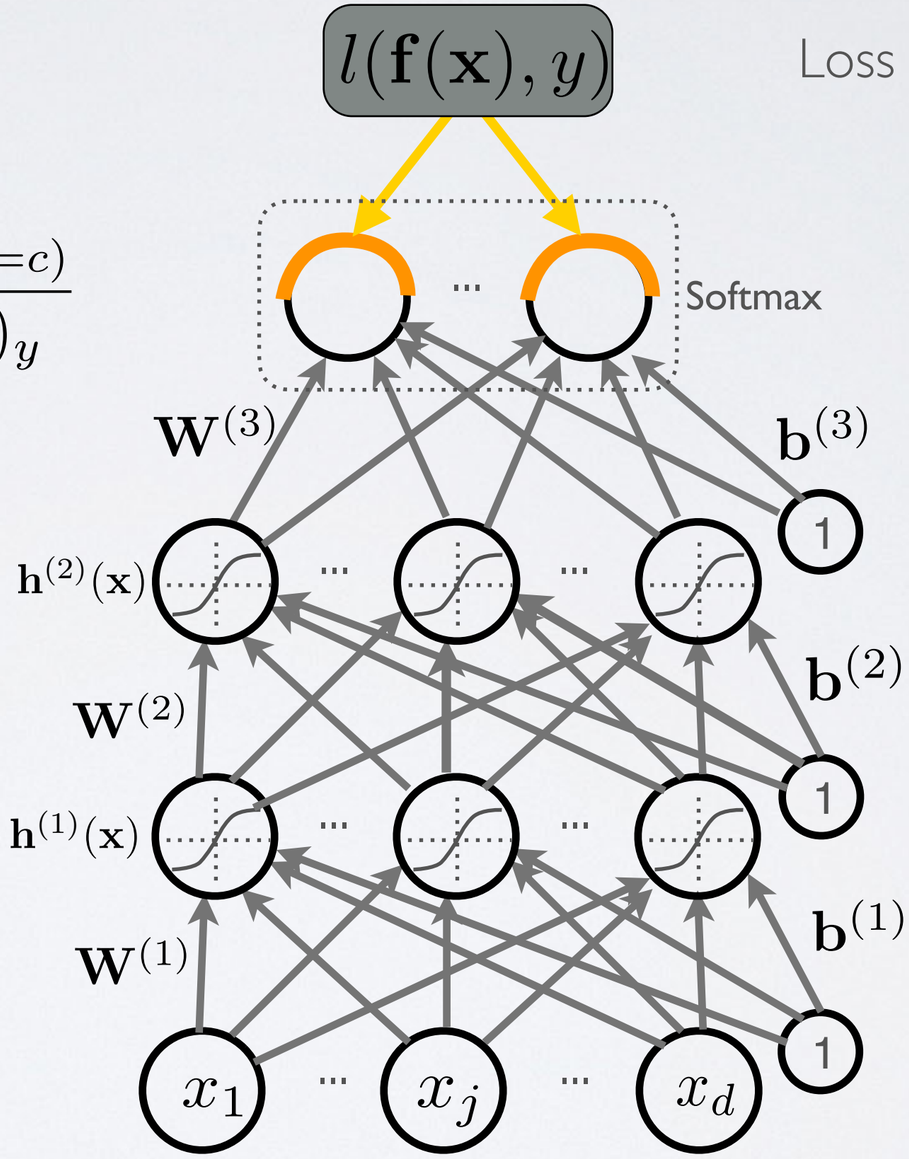
$$\frac{\partial}{\partial f(\mathbf{x})_c} - \log f(\mathbf{x})_y = \frac{-1_{(y=c)}}{f(\mathbf{x})_y}$$

- Gradient:

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

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

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



Loss function = $-\log f(\mathbf{x})_y$

This is known as the **Cross Entropy** loss function. It is by far the most popular loss function for classification tasks with class label $\boldsymbol{y}$. It also corresponds to the negative of the **log likelihood** for a multinomial.

GRADIENT COMPUTATION

Topics: loss gradient at output pre-activation

- Partial derivative:

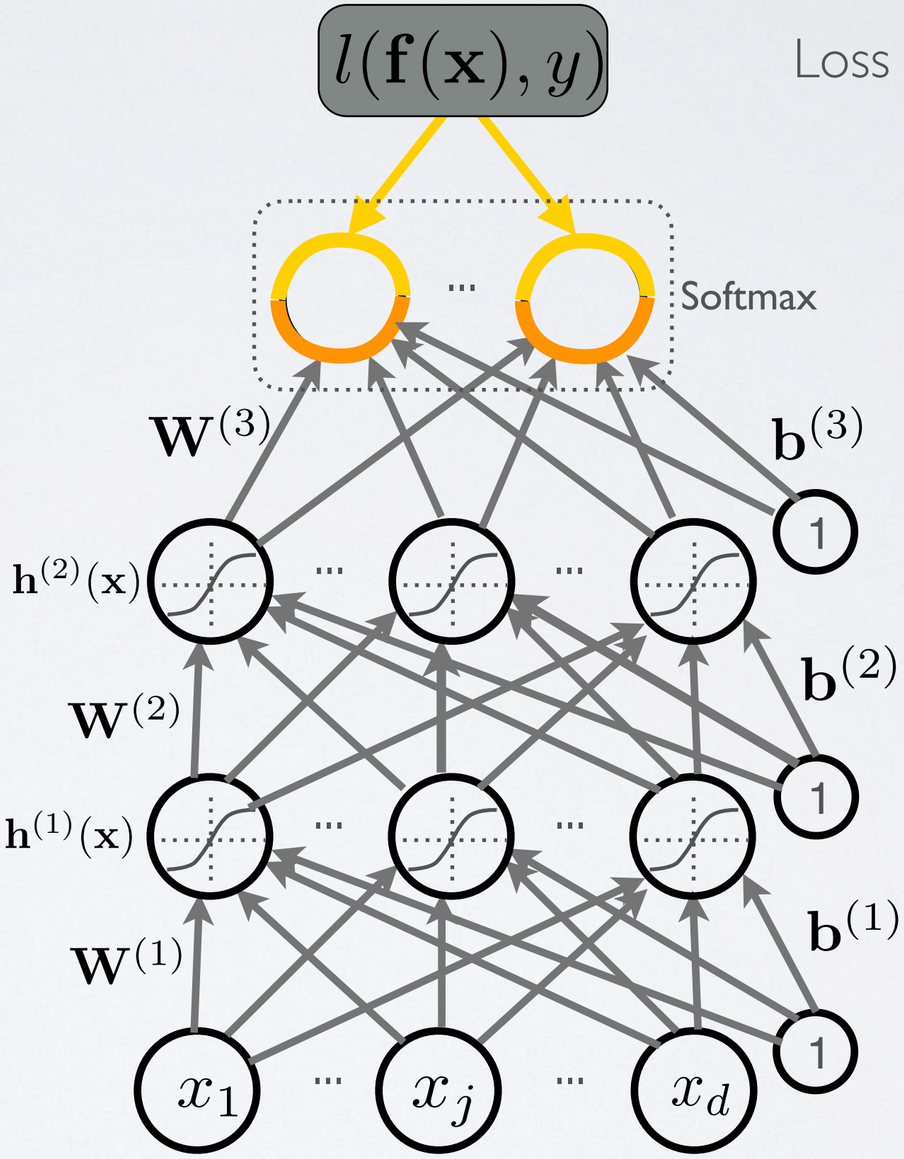
$$\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} - \log f(\mathbf{x})_y$$

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

- Gradient:

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

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



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

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

GRADIENT COMPUTATION

Topics: loss gradient at output pre-activation

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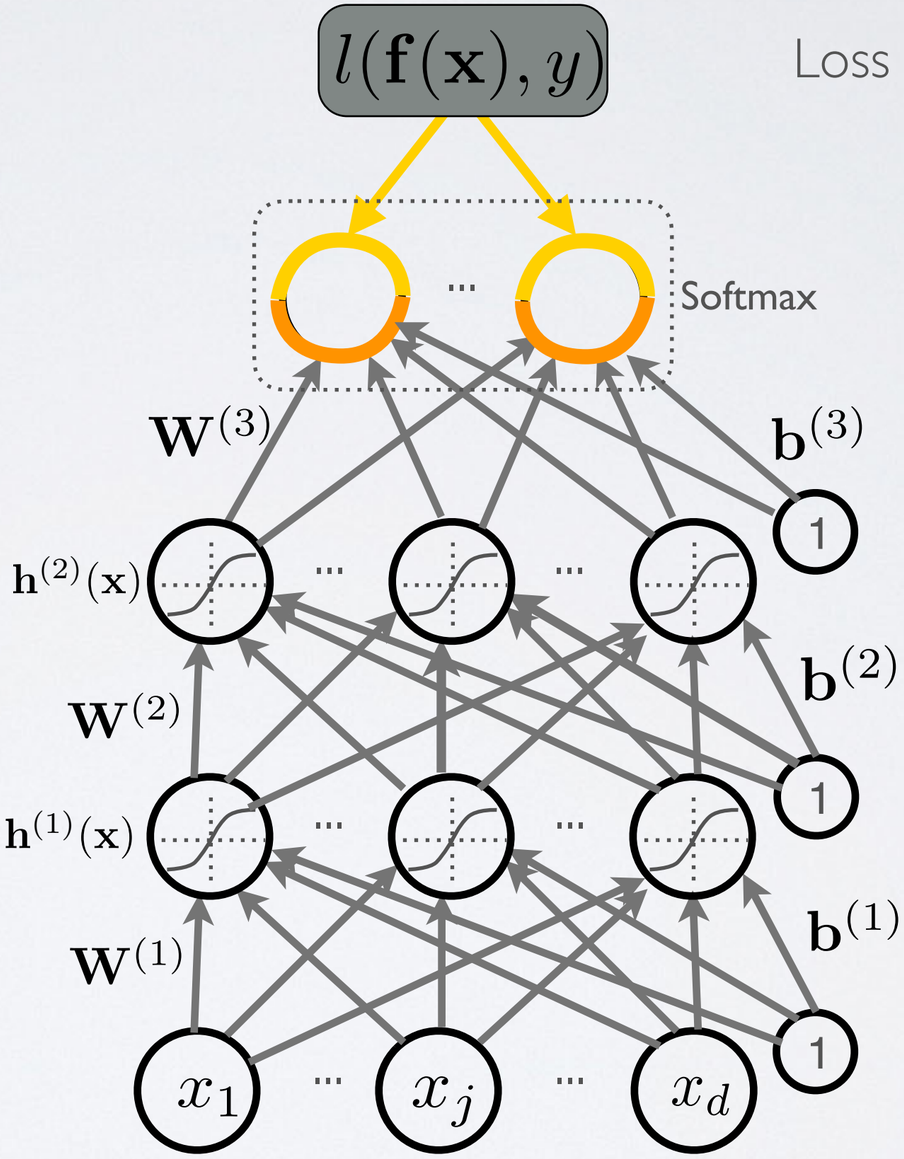
$$= \quad -\left(\mathbf{e}(y) - \mathbf{f}(\mathbf{x})\right)$$



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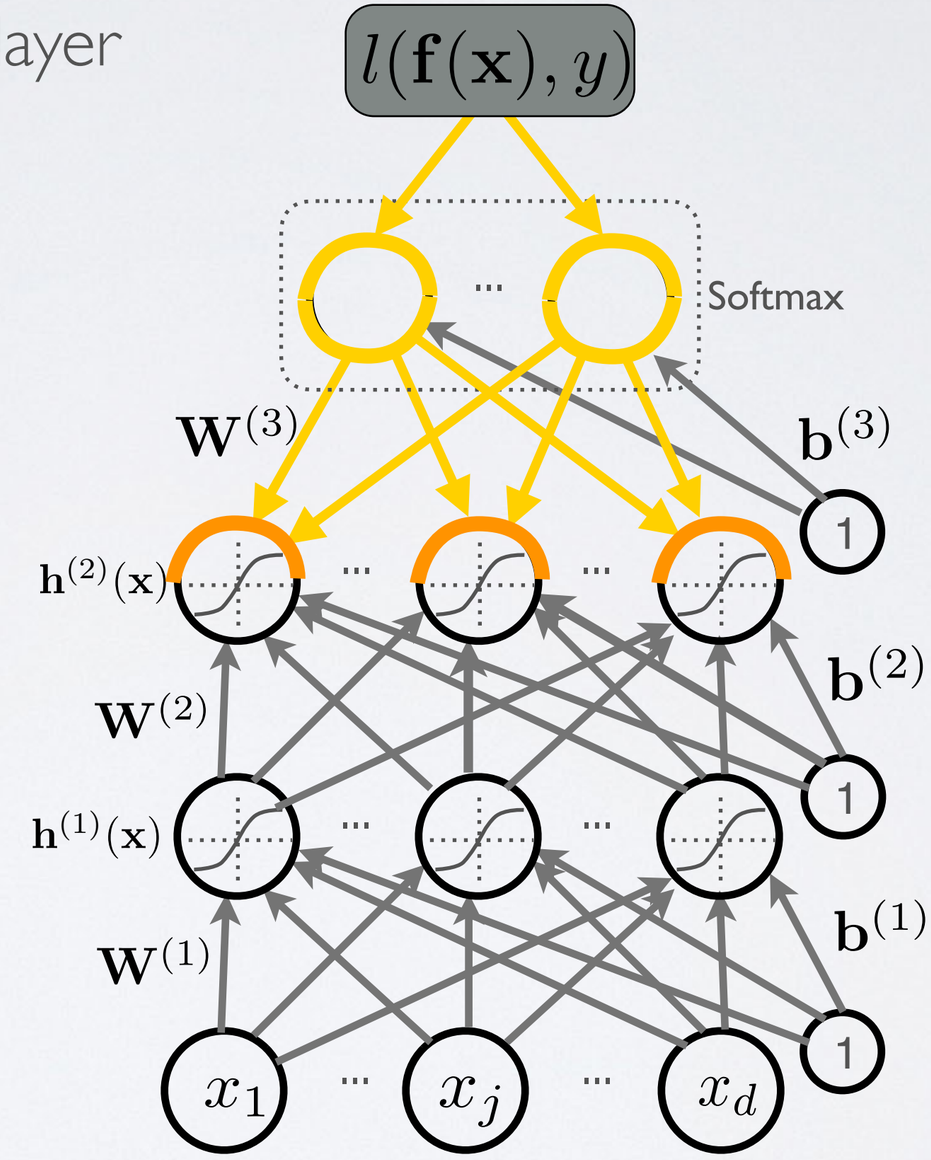
GRADIENT COMPUTATION

Topics: loss gradient at hidden layer

- ... this is getting complicated!!



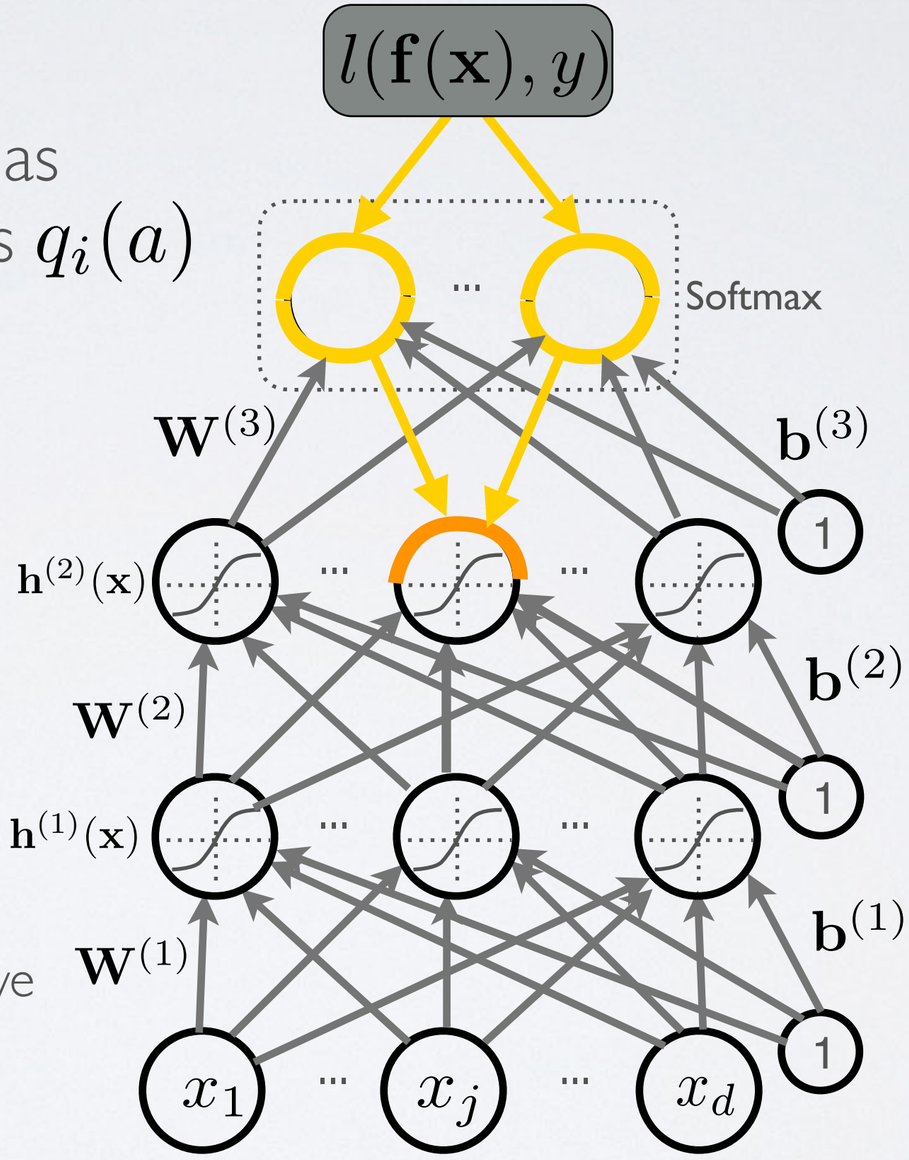
GRADIENT COMPUTATION

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:

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

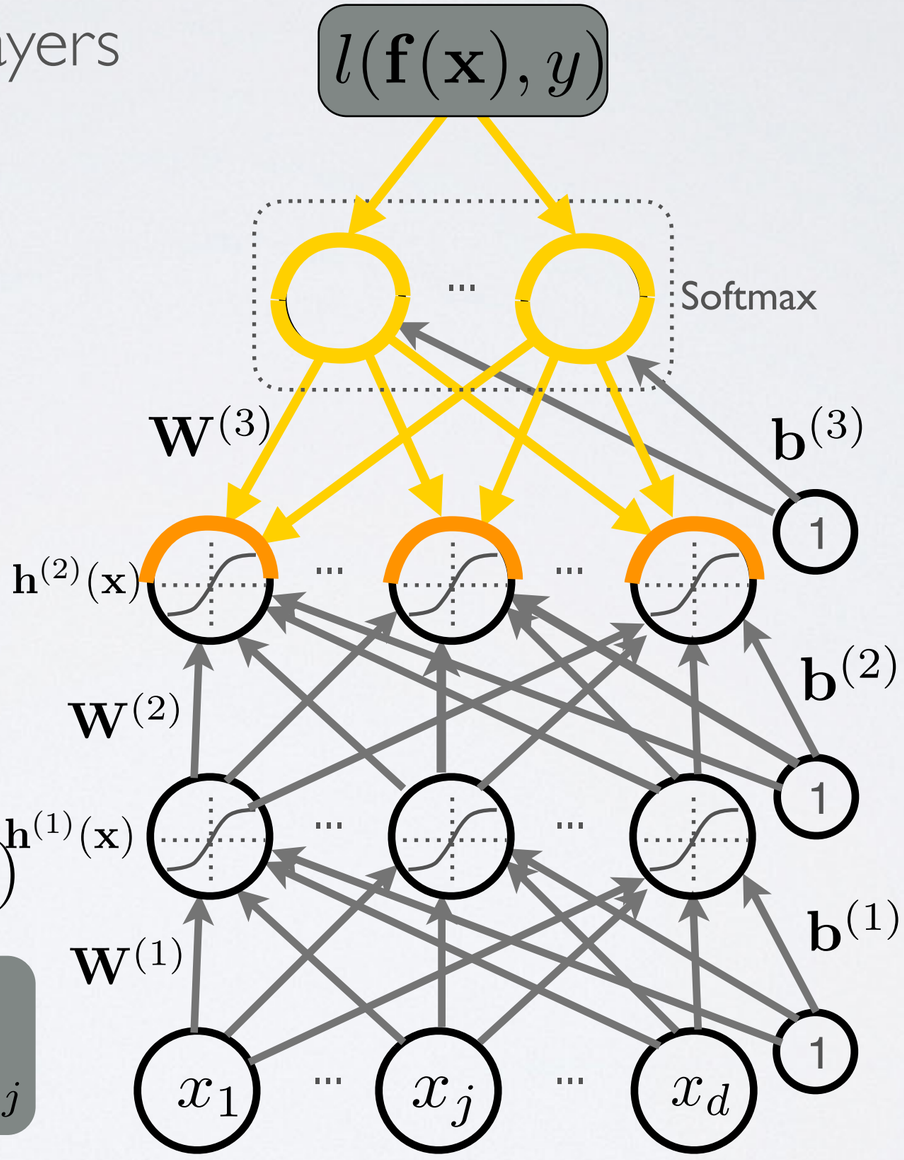
$$= \sum_i \frac{\partial - \log f(\mathbf{x})_y}{\partial a^{(k+1)}(\mathbf{x})_i} \frac{\partial a^{(k+1)}(\mathbf{x})_i}{\partial h^{(k)}(\mathbf{x})_j}$$

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

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

REMINDER

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



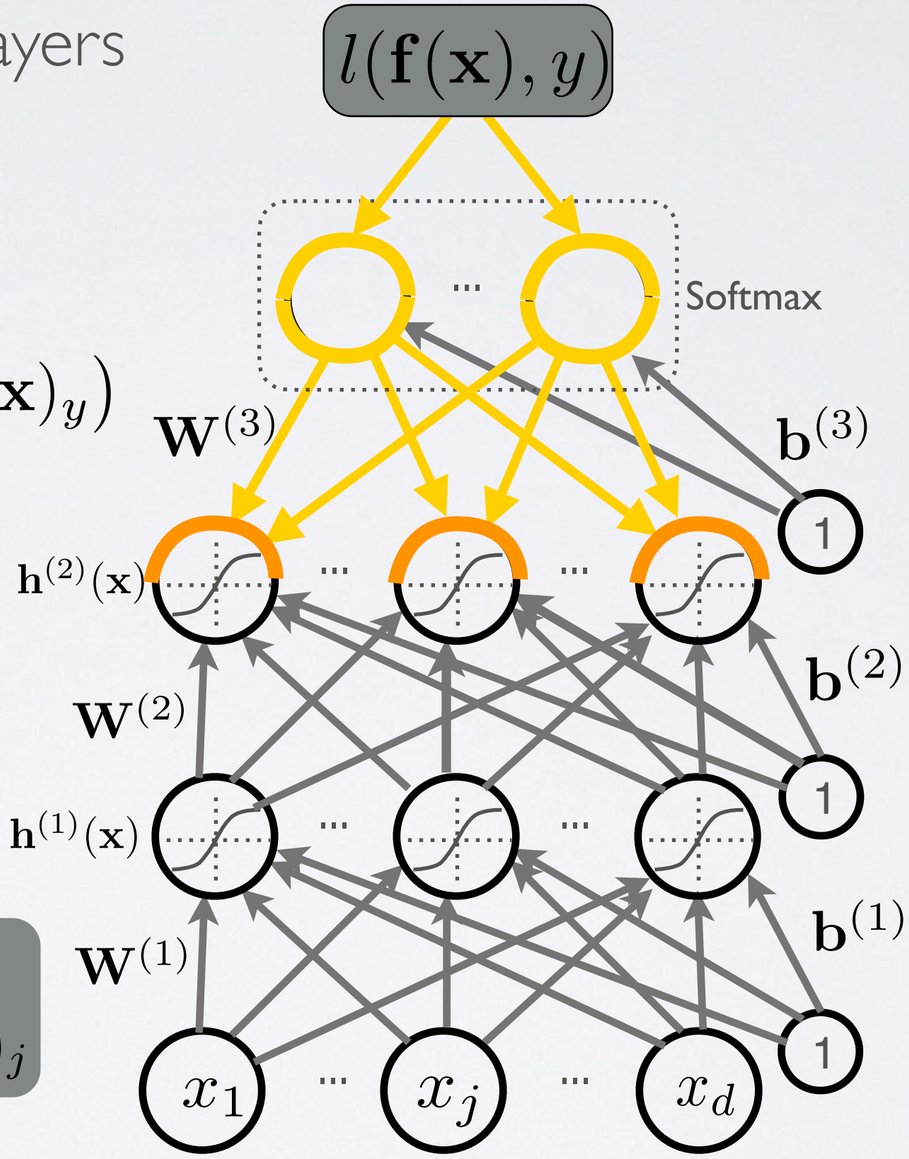
GRADIENT COMPUTATION

Topics: loss gradient at hidden layers

- Gradient:

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

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



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:

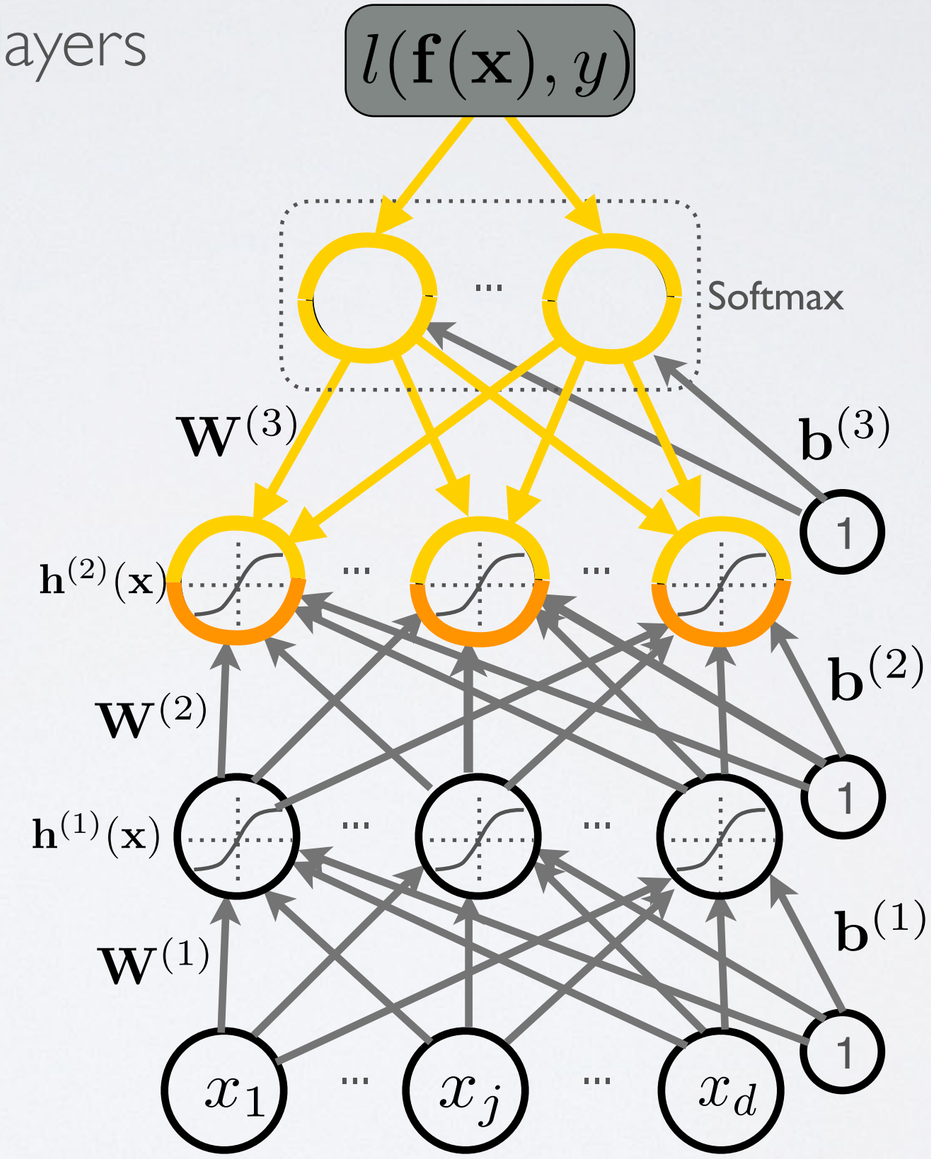
$$\frac{\partial}{\partial a^{(k)}(\mathbf{x})_j} - \log f(\mathbf{x})_y$$

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

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

REMINDER

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



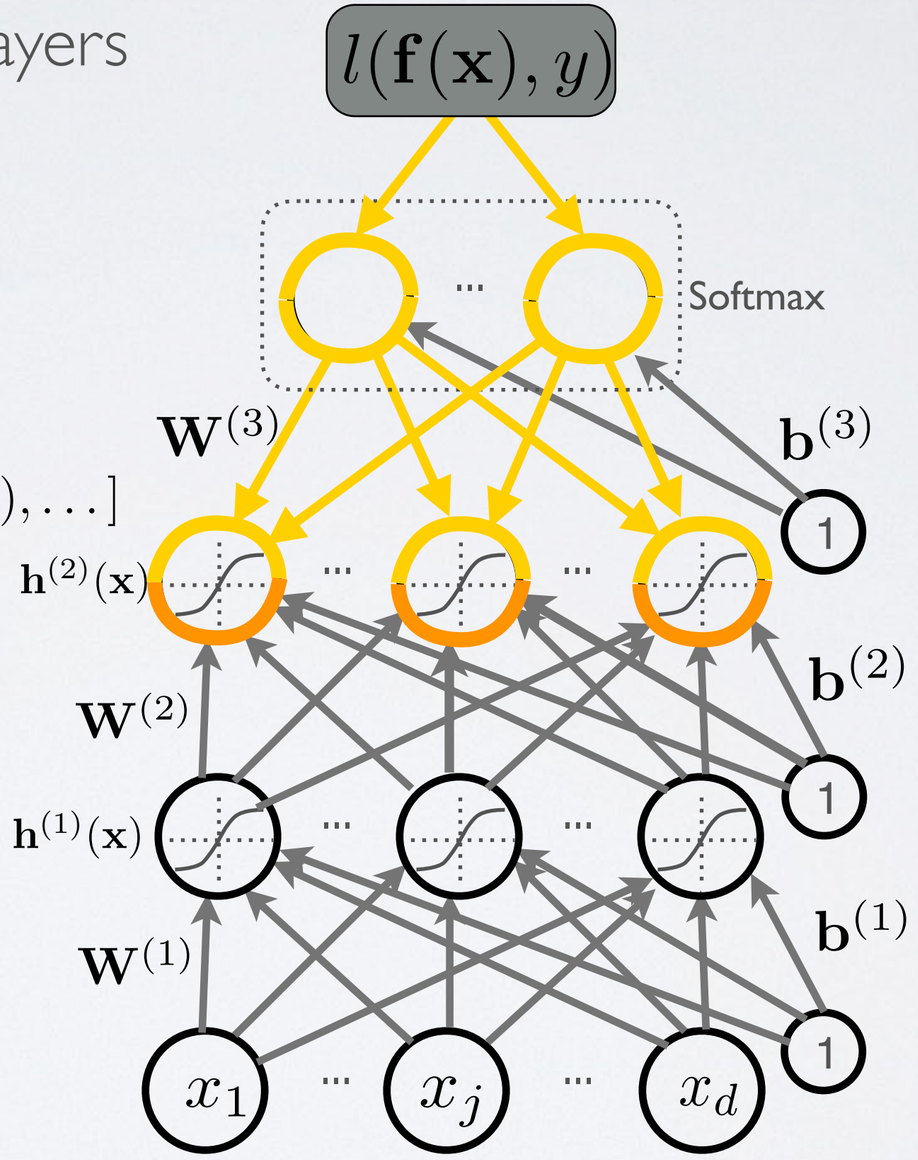
GRADIENT COMPUTATION

Topics: loss gradient at hidden layers pre-activation

- Gradient:

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

element-wise product



REMINDER

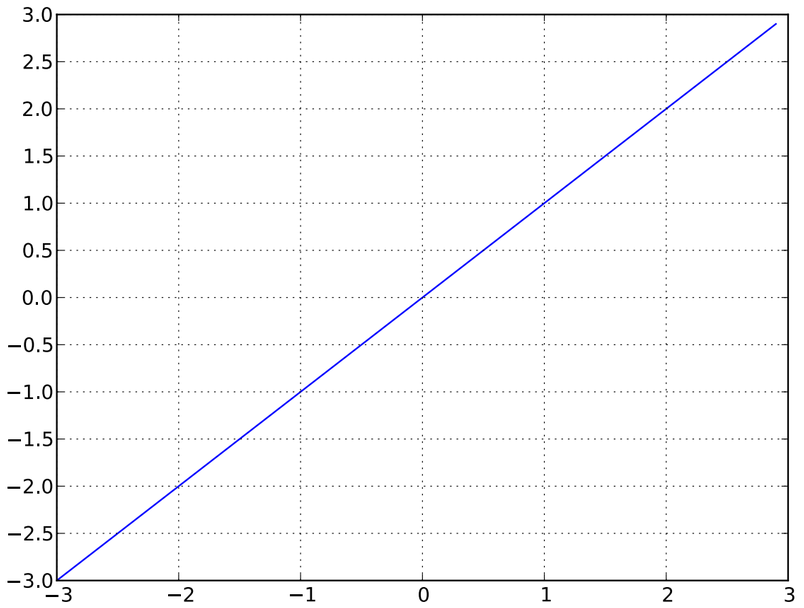
$$h^{(k)}(\mathbf{x})_j = g(a^{(k)}(\mathbf{x})_j)$$

ACTIVATION FUNCTION

Topics: linear activation function gradient

- Partial derivative:

$$g'(a) = 1$$



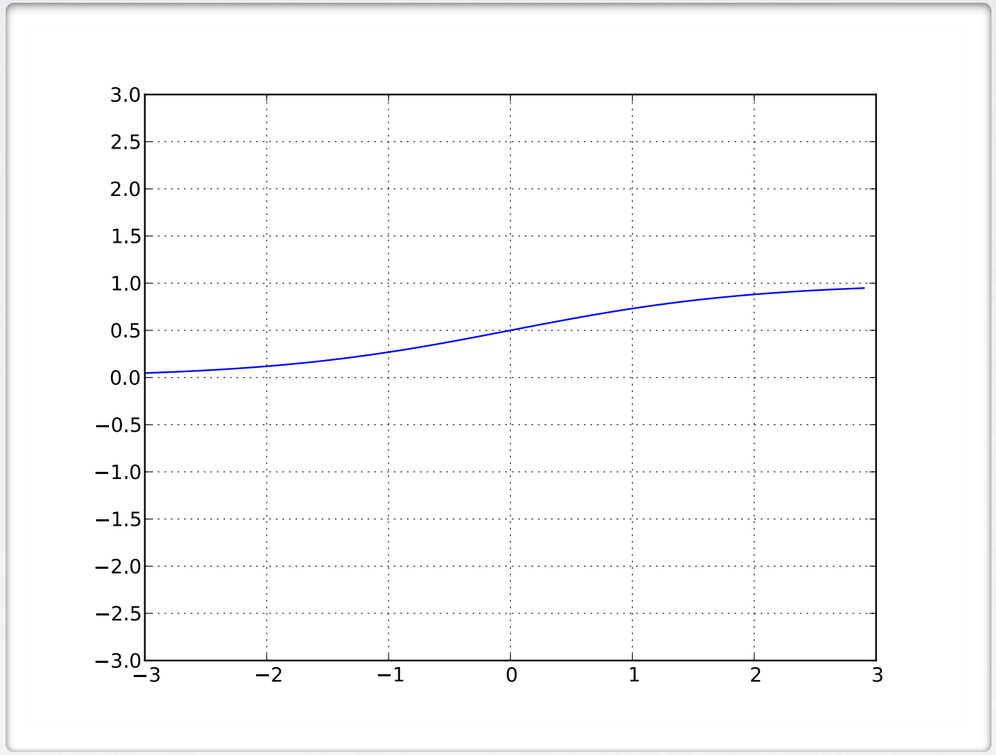
$$g(a) = a$$

ACTIVATION FUNCTION

Topics: sigmoid activation function gradient

- Partial derivative:

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



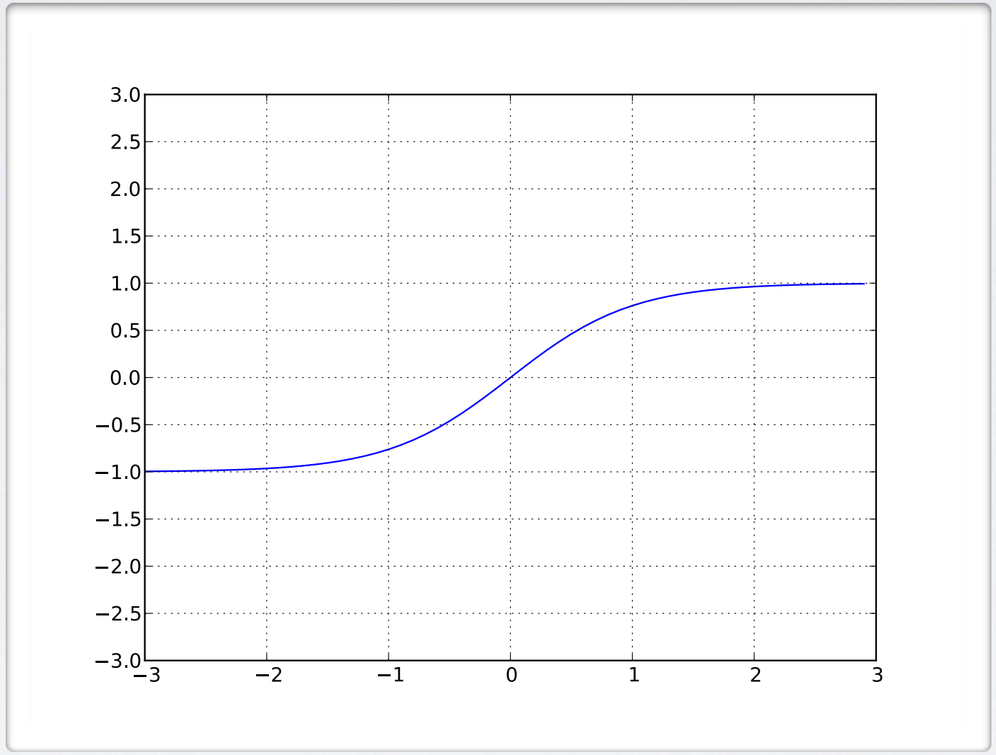
$$g(a) = \text{sigm}(a) = \frac{1}{1+\exp(-a)}$$

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 $\boldsymbol{\theta}$ ($\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$)
  - 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 $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)
  - initialization method

GRADIENT COMPUTATION

Topics: loss gradient of parameters

- Partial derivative (weights):

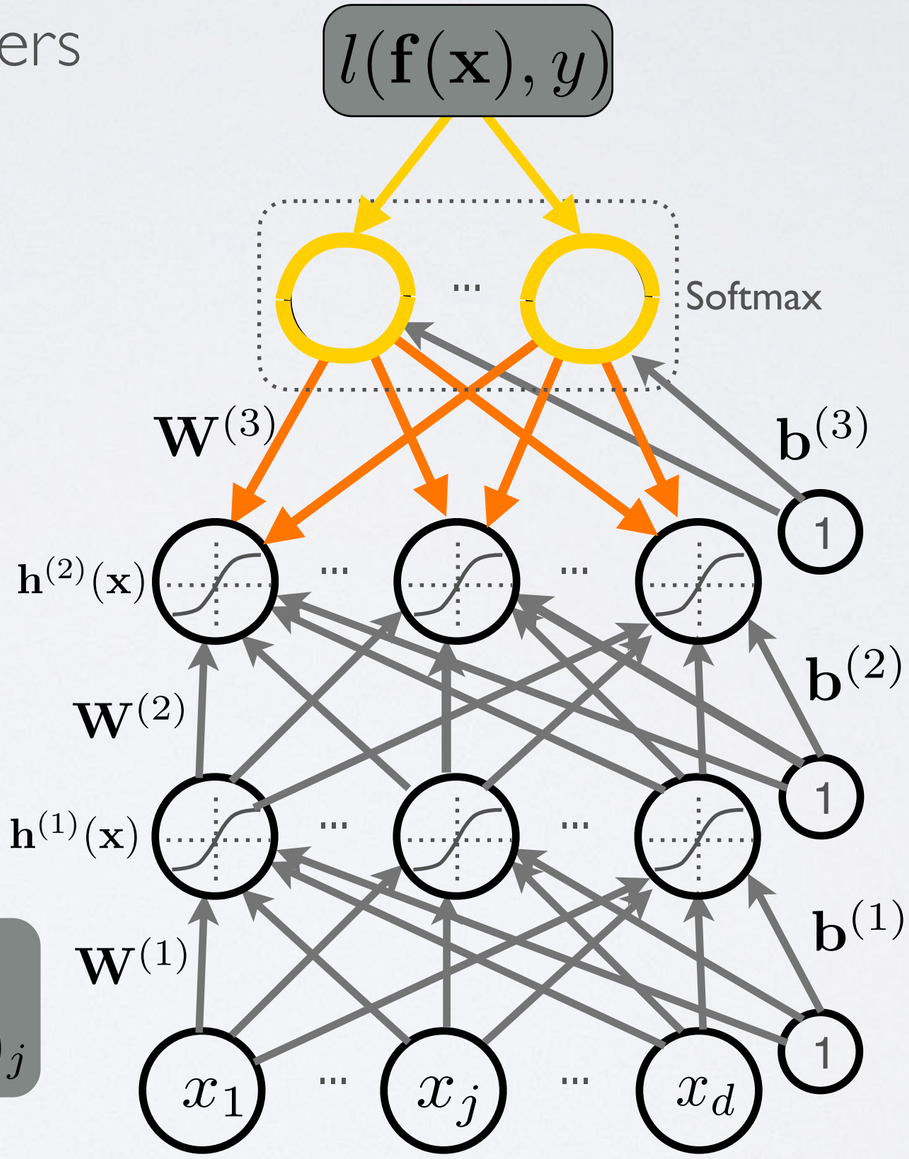
$$\frac{\partial}{\partial W_{i,j}^{(k)}} - \log f(\mathbf{x})_y$$

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

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

REMINDER

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

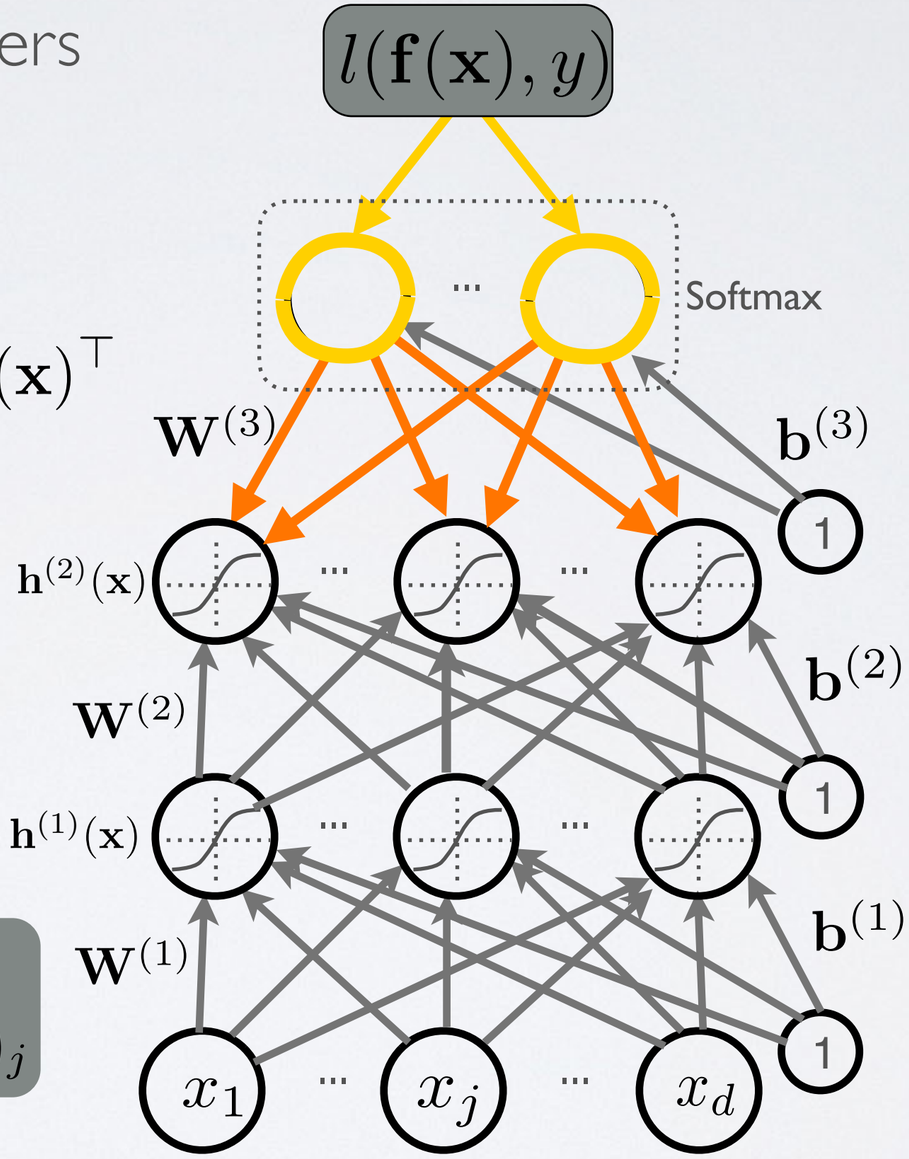


GRADIENT COMPUTATION

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):

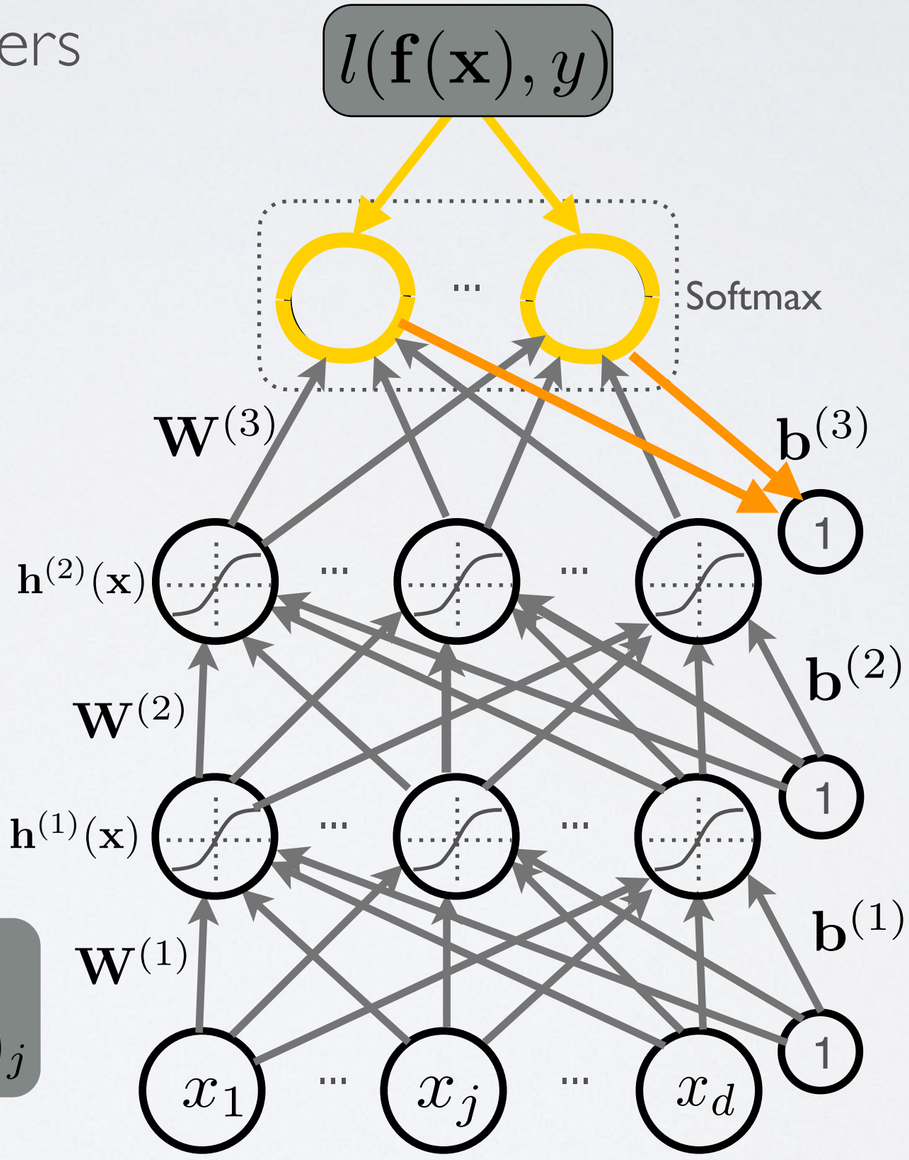
$$\frac{\partial}{\partial b_i^{(k)}} - \log f(\mathbf{x})_y$$

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

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

REMINDER

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

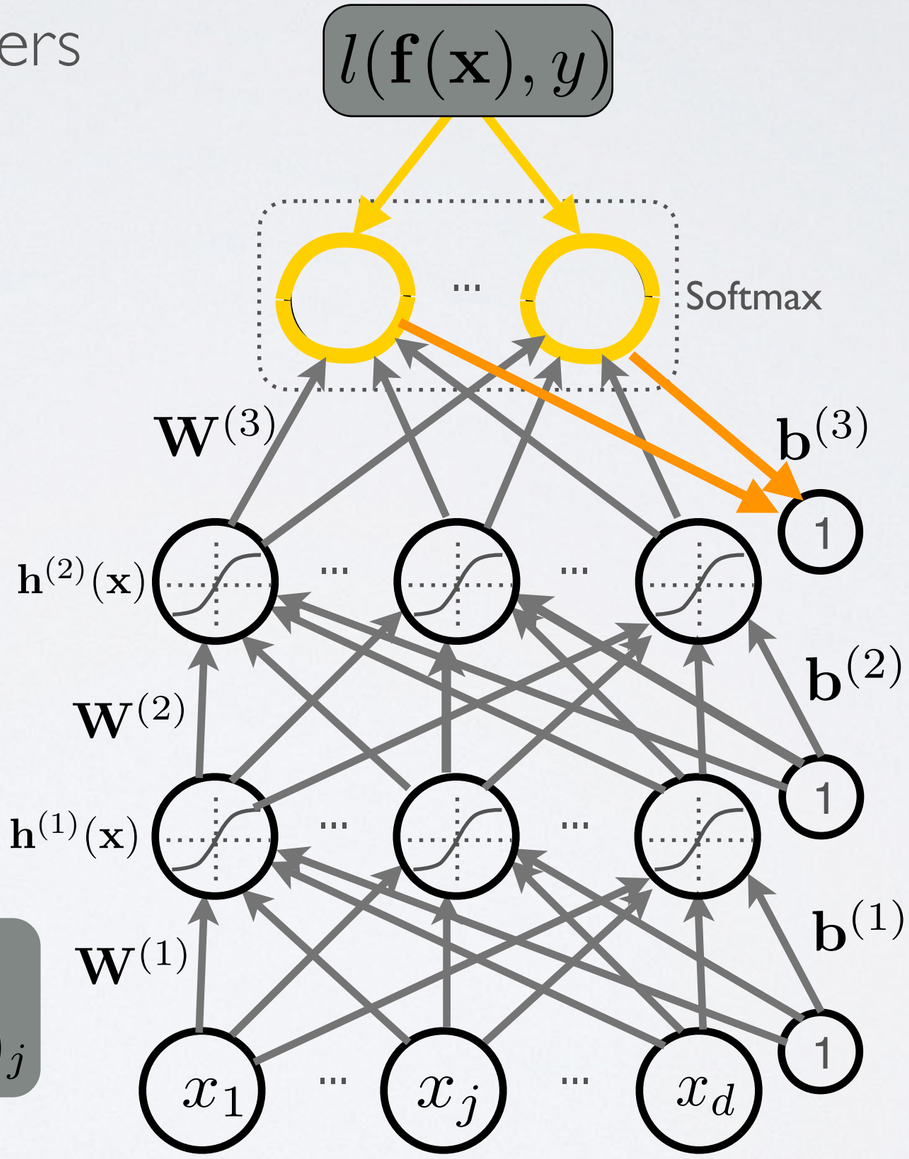


GRADIENT COMPUTATION

Topics: loss gradient of parameters

- Gradient (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)

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

  - for *k* from *L*+1 to 1
    - compute gradients of hidden layer parameter

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

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

    - compute gradient of hidden layer below

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

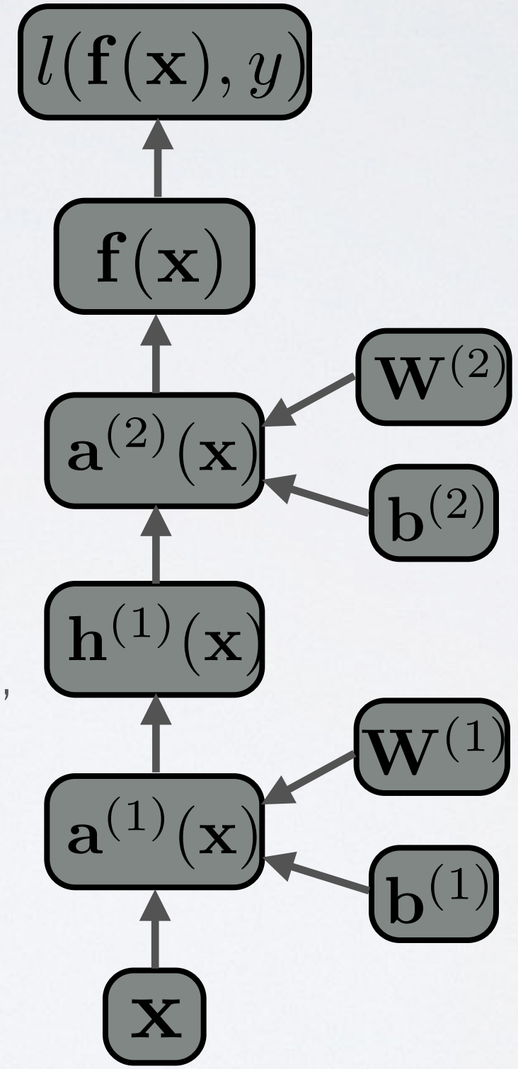
    - compute gradient of hidden layer below (before activation)

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

FLOW GRAPH

Topics: *flow graph*

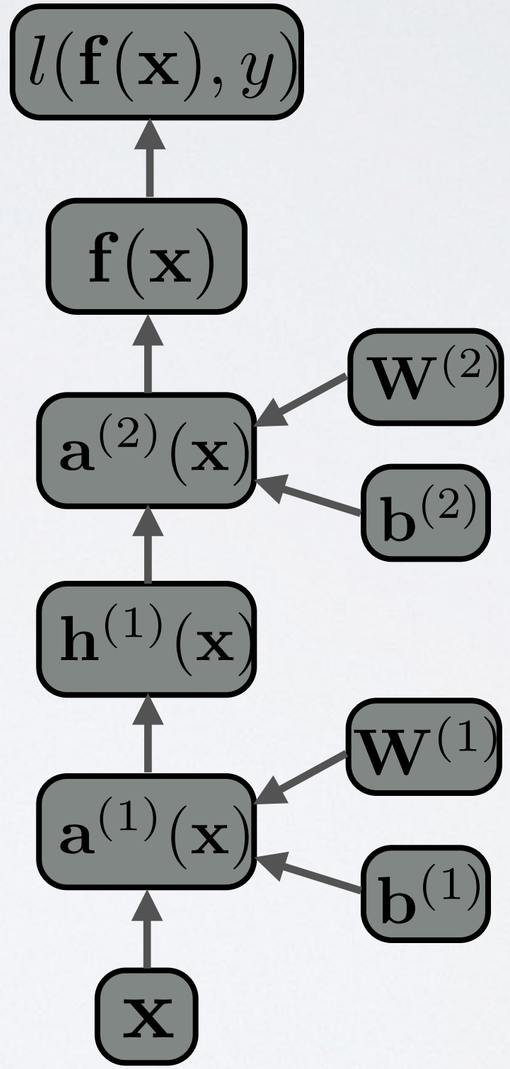
- Forward propagation can be represented as an acyclic flow graph
- It's a nice way of implementing forward propagation in a modular way
  - each box could be an object with an fprop method, that computes the value of the box given its children
  - calling the fprop method of each box in the right order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



OPTIMIZATION

Topics: local optimum, global optimum, plateau

Neural network training demo
(by Andrej Karpathy)

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

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 $\boldsymbol{\theta}$ ($\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$)
  - for N iterations
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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 $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)
  - initialization method

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"

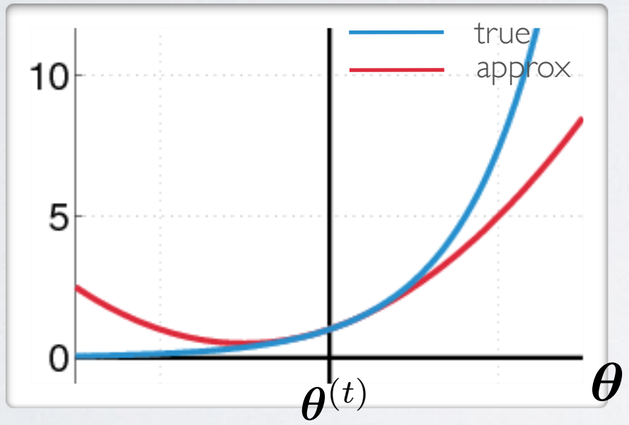
GRADIENT DESCENT

Topics: Newton's method

- If we locally approximate the loss through Taylor expansion:

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

$l(\mathbf{f}(\mathbf{x};\boldsymbol{\theta}),y)$



- 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 strictly convex (so the Hessian is invertible)

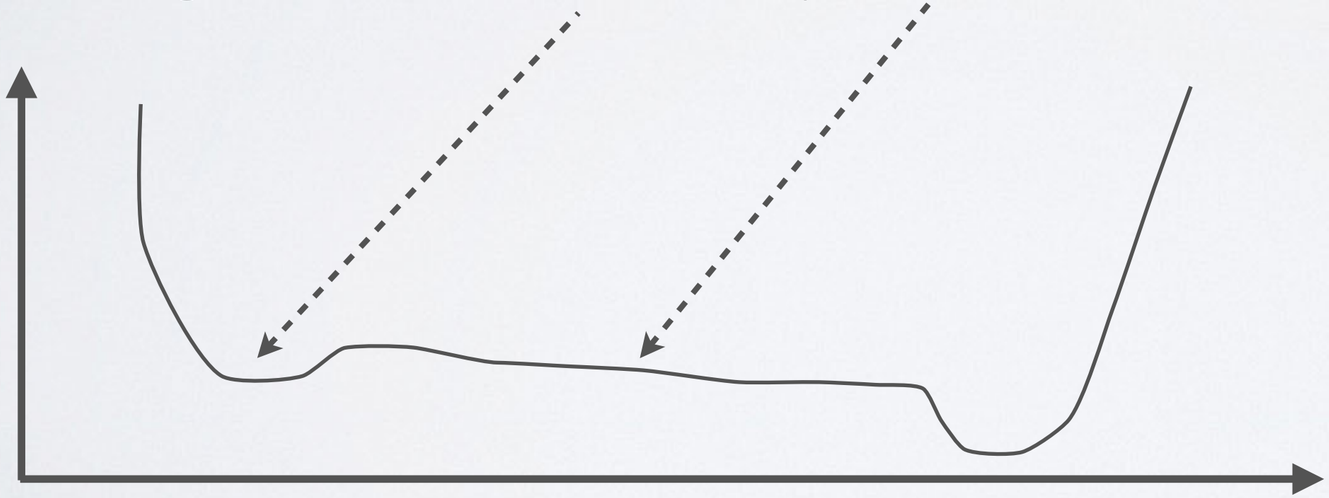
- See Deep Learning, Chap. 8 for more on optimization of neural networks

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

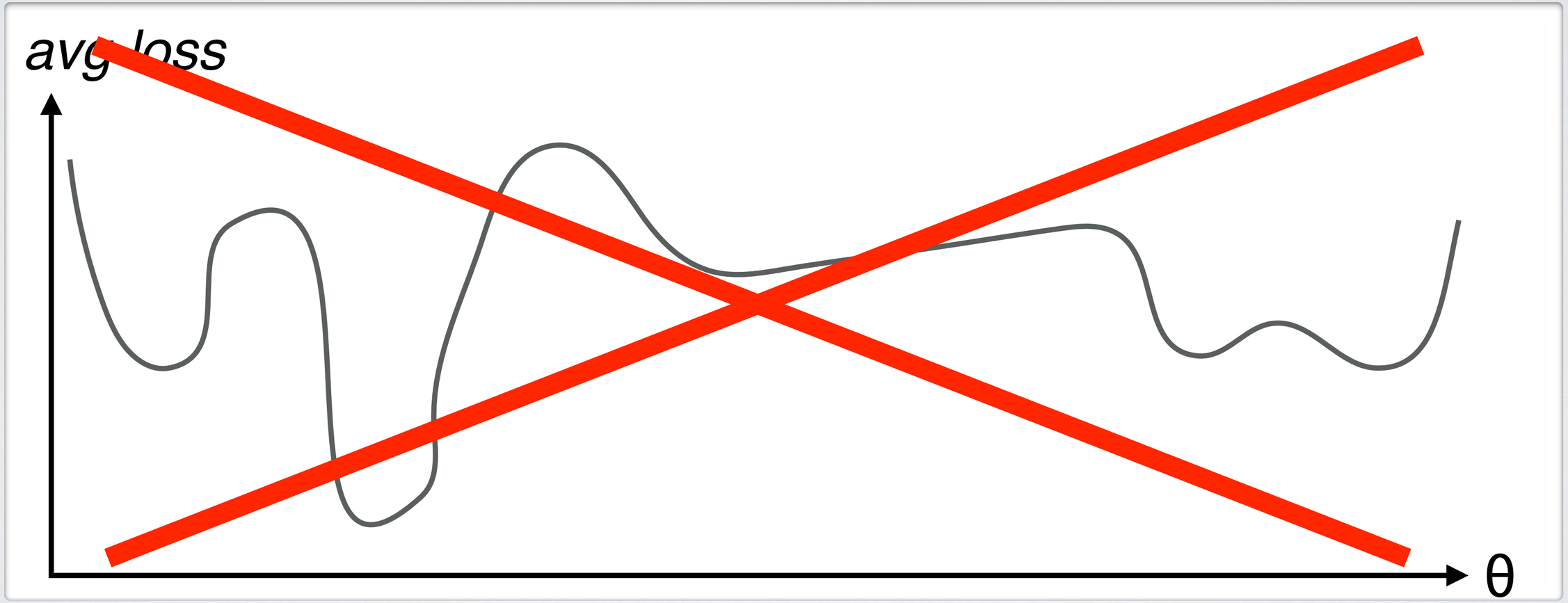
- Optimization can get stuck in local minimum or plateaus



THEY ARE STRANGELY NON-CONVEX

Topics: non-convexity, saddle points

- *Identifying and attacking the saddle point problem in high-dimensional non-convex optimization*
  Dauphin, Pascanu, Gulcehre, Cho, Ganguli, Bengio, NIPS 2014



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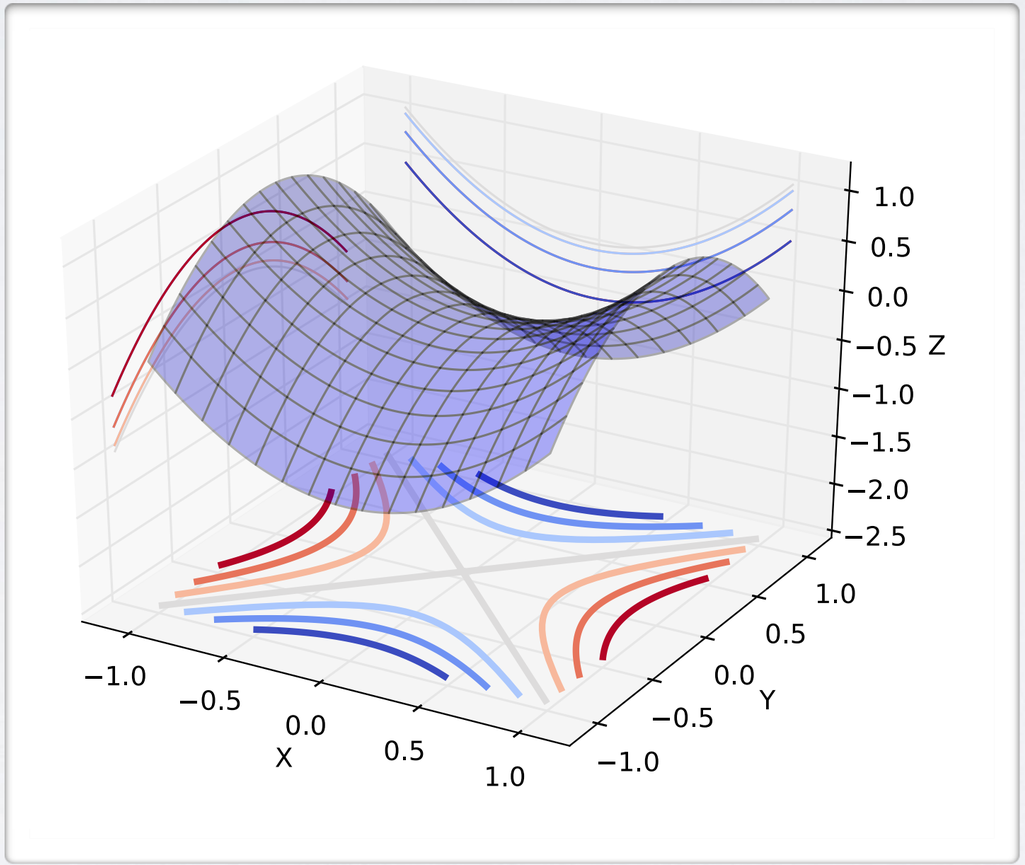
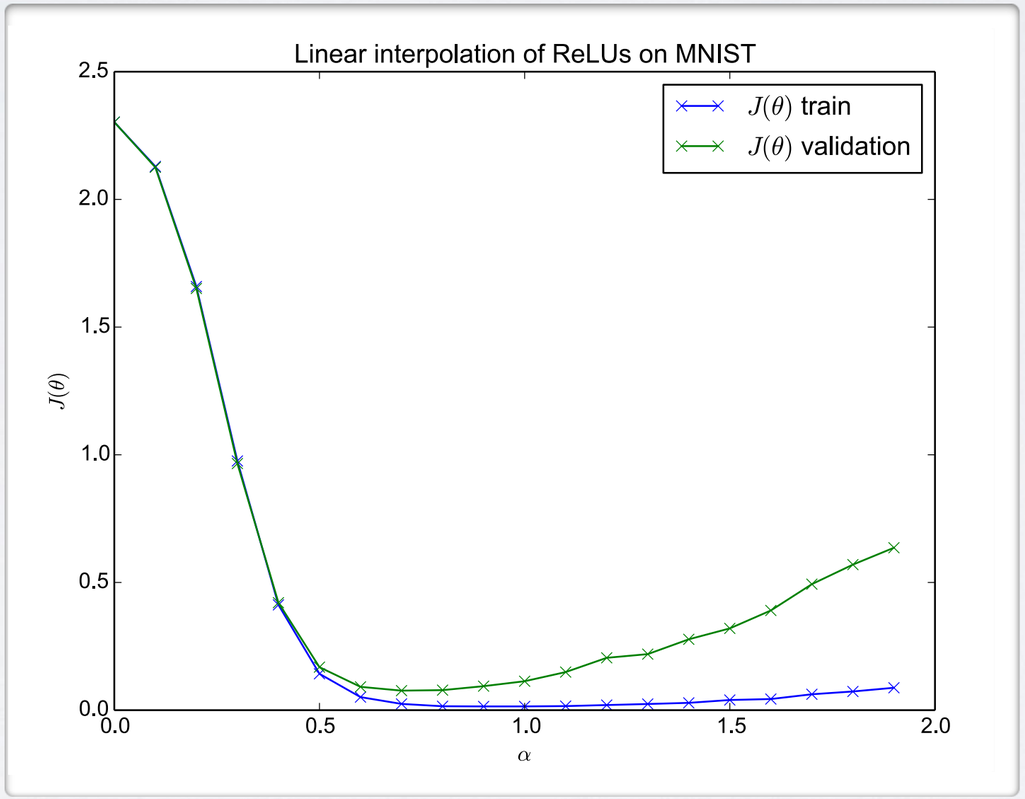


THEY ARE STRANGELY NON-CONVEX

Topics: non-convexity, saddle points

- *Qualitatively Characterizing Neural Network Optimization Problems* Goodfellow, Vinyals, Saxe, ICLR 2015



THEY ARE STRANGELY NON-CONVEX

Topics: Lottery Ticket Hypothesis

- *The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks*
  Frankle, Carbin, ICLR 2019

Algorithm to Identify Winning Tickets (i.e. subnetworks):

1. Randomly initialize a neural network $f(x; \theta_0)$ (where $\theta_0 \sim \mathcal{D}_\theta$).
2. Train the network for j iterations, arriving at parameters θ_j.
3. Prune $p\%$ of the parameters in θ_j, creating a mask m.
4. Reset the remaining parameters to their values in θ_0, creating the winning ticket $f(x; m \odot \theta_0)$.

THEY ARE STRANGELY NON-CONVEX

Topics: Lottery Ticket Hypothesis

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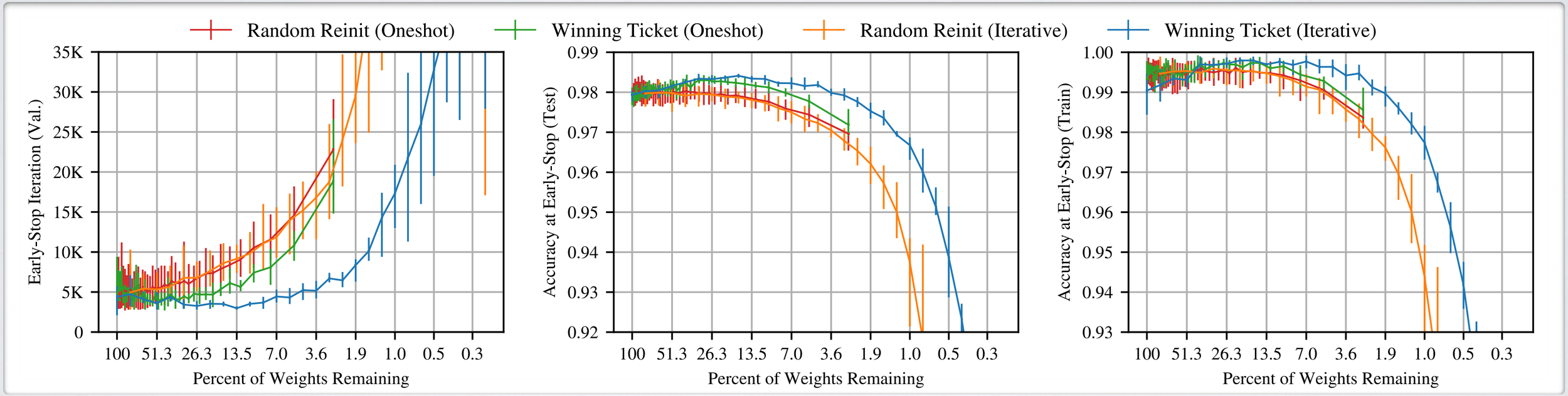
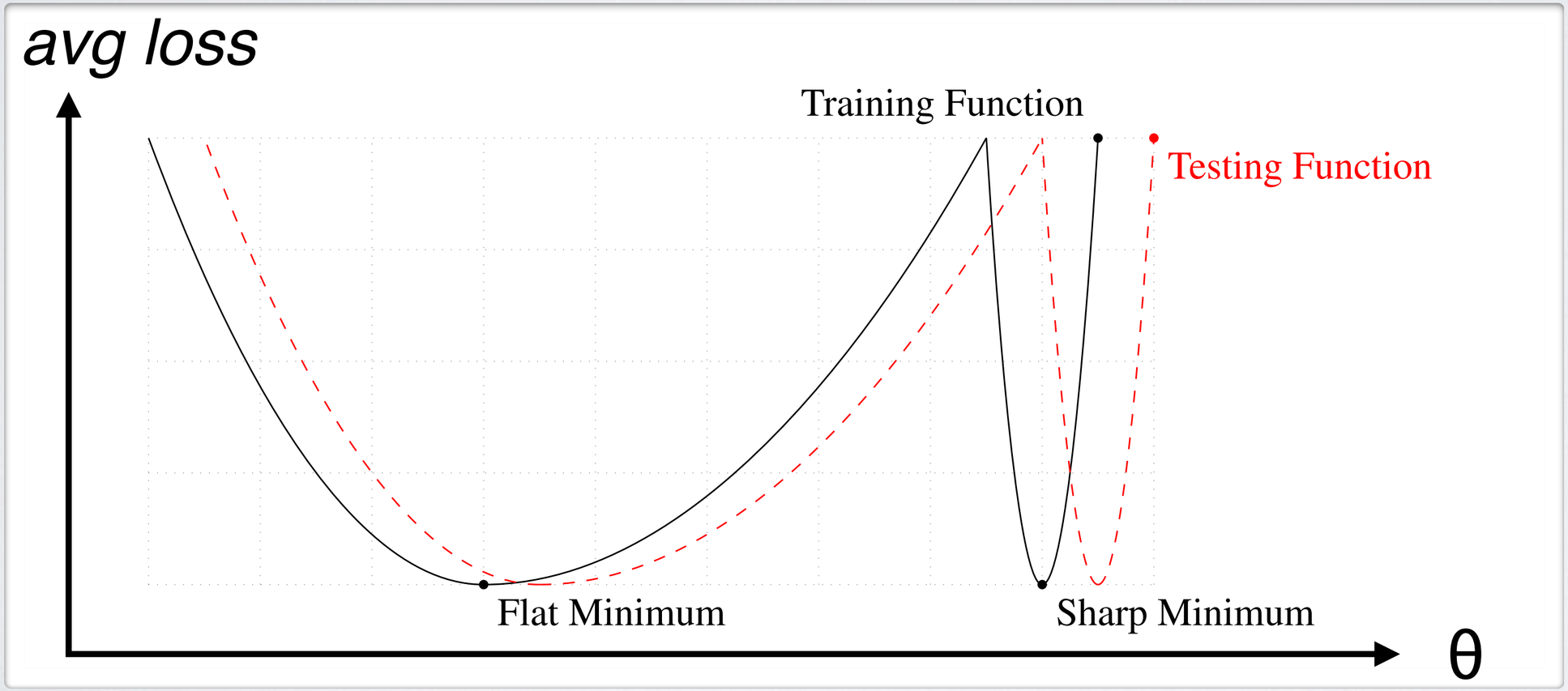


THEY WORK BEST WHEN BADLY TRAINED

Topics: sharp vs. flat minima

- *Flat Minima*
  Hochreiter, Schmidhuber, Neural Computation 1997



THEY WORK BEST WHEN BADLY TRAINED

Topics: sharp vs. flat minima

- *On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima* Keskar, Mudigere, Nocedal, Smelyanskiy, Tang, ICLR 2017
  - found that using large batch sizes tends to find sharper minima and generalize worse

- This means that we can't talk about generalization without taking the training algorithm into account

- **Note:** There are many modern works that show better generalization performance with larger mini-batches.

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 $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)
  - initialization method

What's this?

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

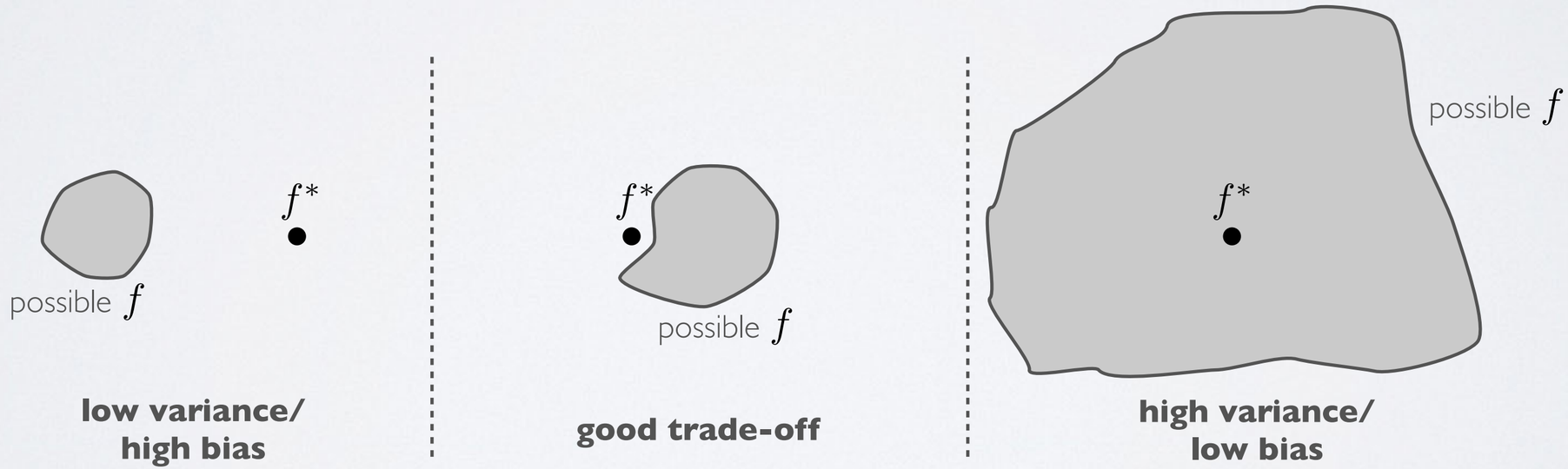
$$\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j |W_{i,j}^{(k)}|$$

- Gradient: $\nabla_{\mathbf{W}^{(k)}} \Omega(\boldsymbol{\theta}) = \text{sign}(\mathbf{W}^{(k)})$
  - where $\text{sign}(\mathbf{W}^{(k)})_{i,j} = 1_{\mathbf{W}_{i,j}^{(k)} > 0} - 1_{\mathbf{W}_{i,j}^{(k)} < 0}$
- 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

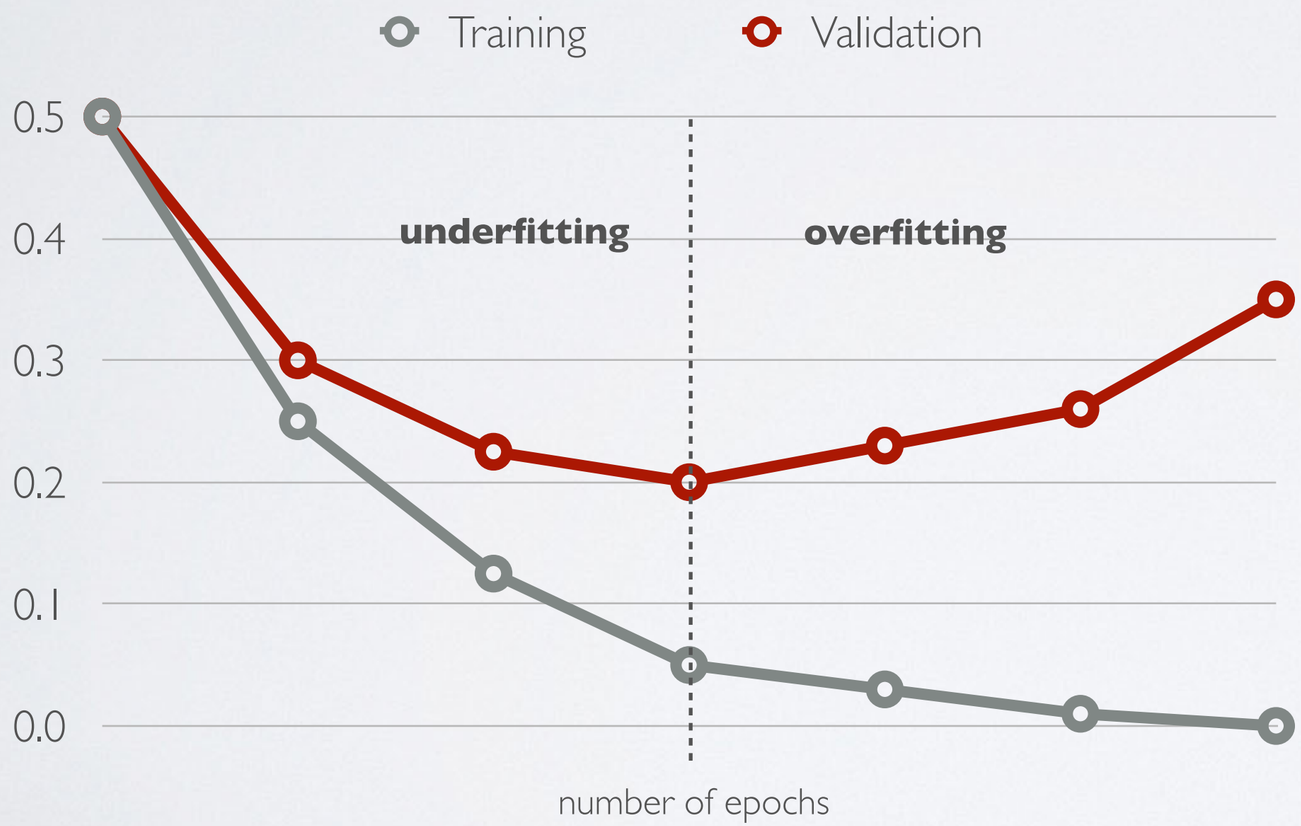
- **Variance** of trained model: does it vary a lot if the training set changes
- **Bias** of trained model: is the average model close to the true solution
- **Generalization error** can be seen as the sum of the (squared) **bias** and the **variance**



KNOWING WHEN TO STOP

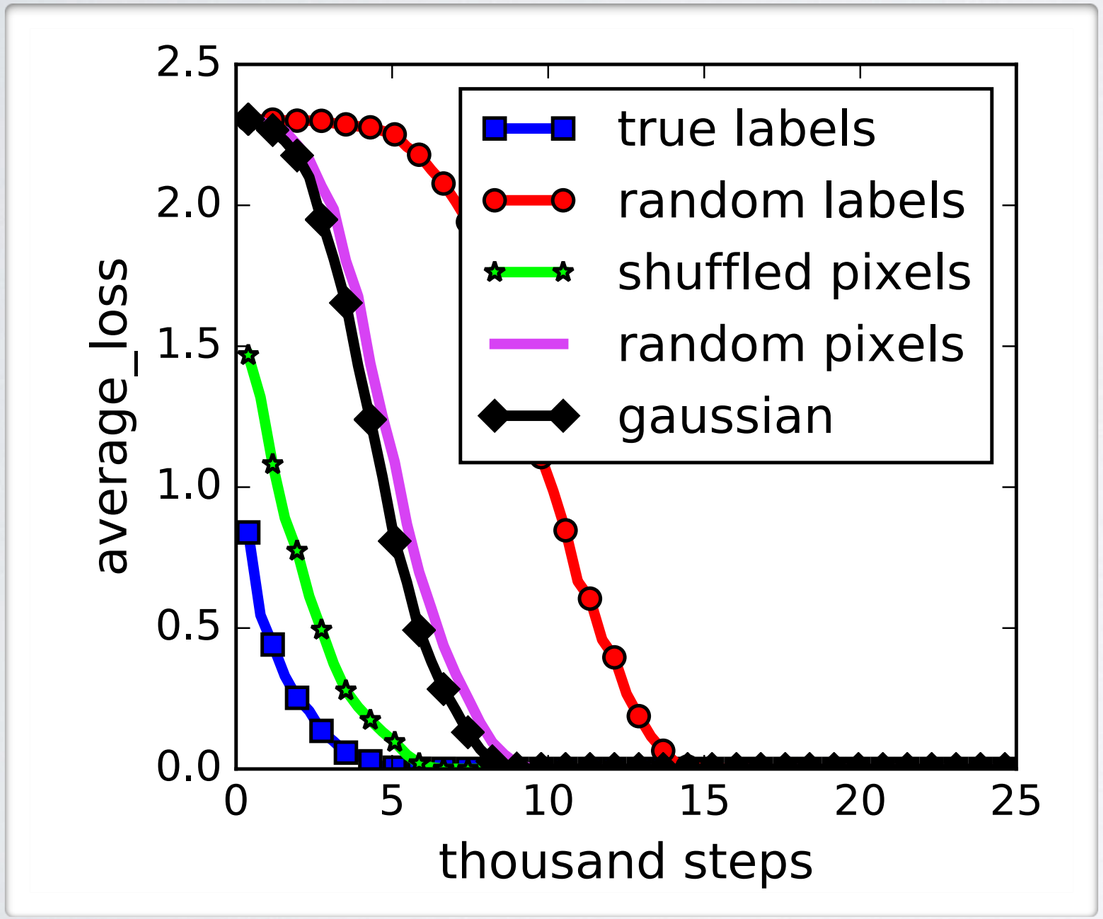
Topics: early stopping

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



NEURAL NETS CAN EASILY MEMORIZE

Understanding Deep Learning Requires Rethinking Generalization
Zhang, Bengio, Hardt, Recth, Vinyals, ICLR 2017



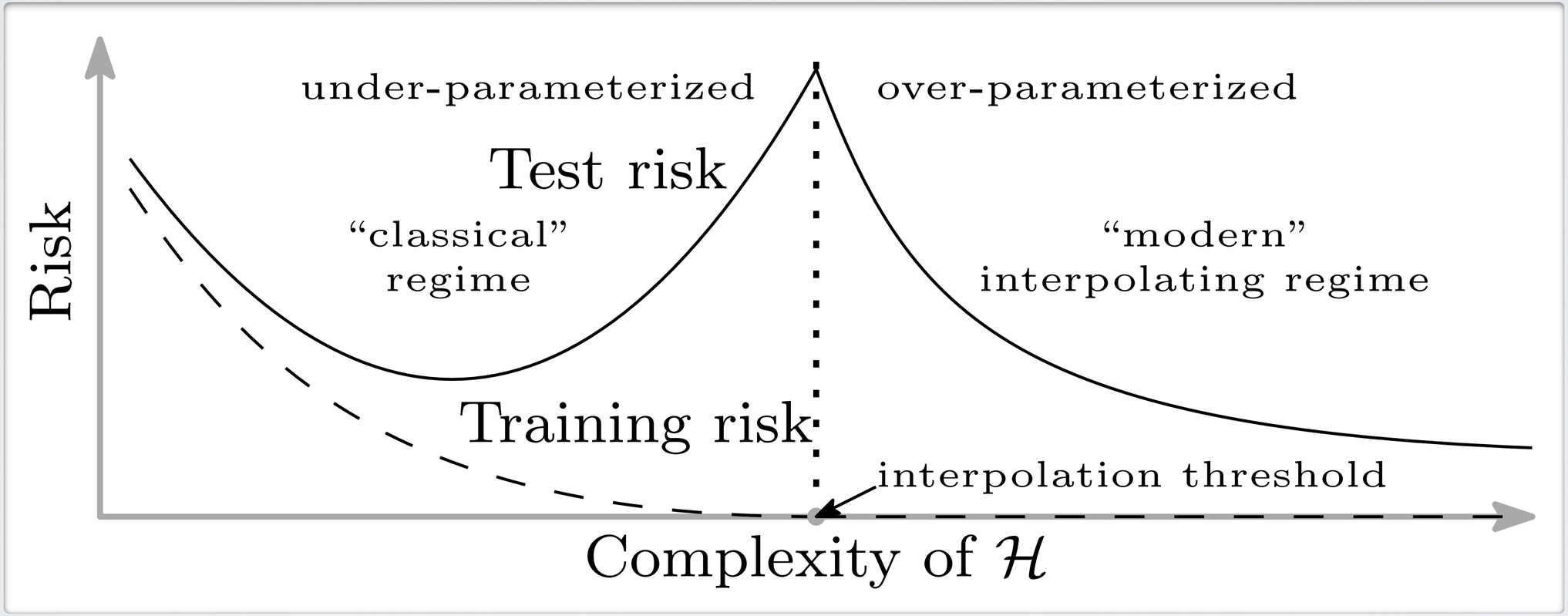
Inception model on the CIFAR10 dataset

- **True labels**: the original dataset without modification.
- **Random labels**: all the labels are replaced with random ones.
- **Shuffled pixels**: a random permutation of the pixels is chosen and then the same permutation is applied to all the images in both training and test set.
- **Random pixels**: a different random permutation is applied to each image independently.
- **Gaussian**: A Gaussian distribution (with matching mean and variance to the original image dataset) is used to generate random pixels for each image.

THEY UNDERFIT/OVERFIT STRANGELY

Topics: bias/variance trade-off, interpolation threshold

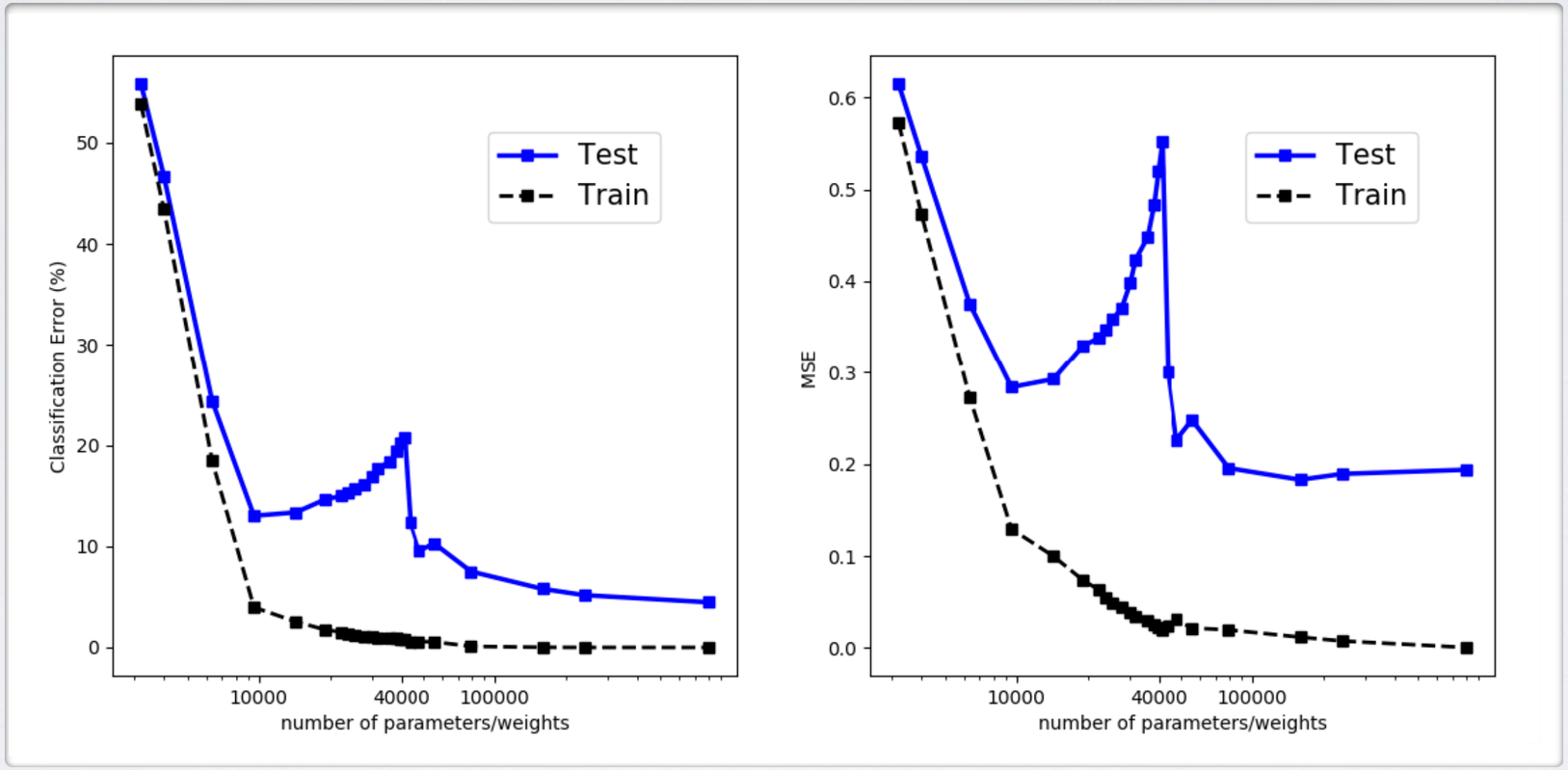
- *Reconciling modern machine learning and the bias-variance trade-off*
  Belkin et al. arXiv 2018



THEY OVERFIT STRANGELY

Topics: bias/variance trade-off, interpolation threshold

- *Reconciling modern machine learning and the bias-variance trade-off* Belkin et al. arXiv 2018



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 $\mathbf{W}_{i,j}^{(k)}$ 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 $\mathcal{D}^{\text{train}}$ serves to train a model
- Validation set $\mathcal{D}^{\text{valid}}$ serves to select hyper-parameters
- Test set $\mathcal{D}^{\text{test}}$ serves to estimate the generalization performance (error)

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

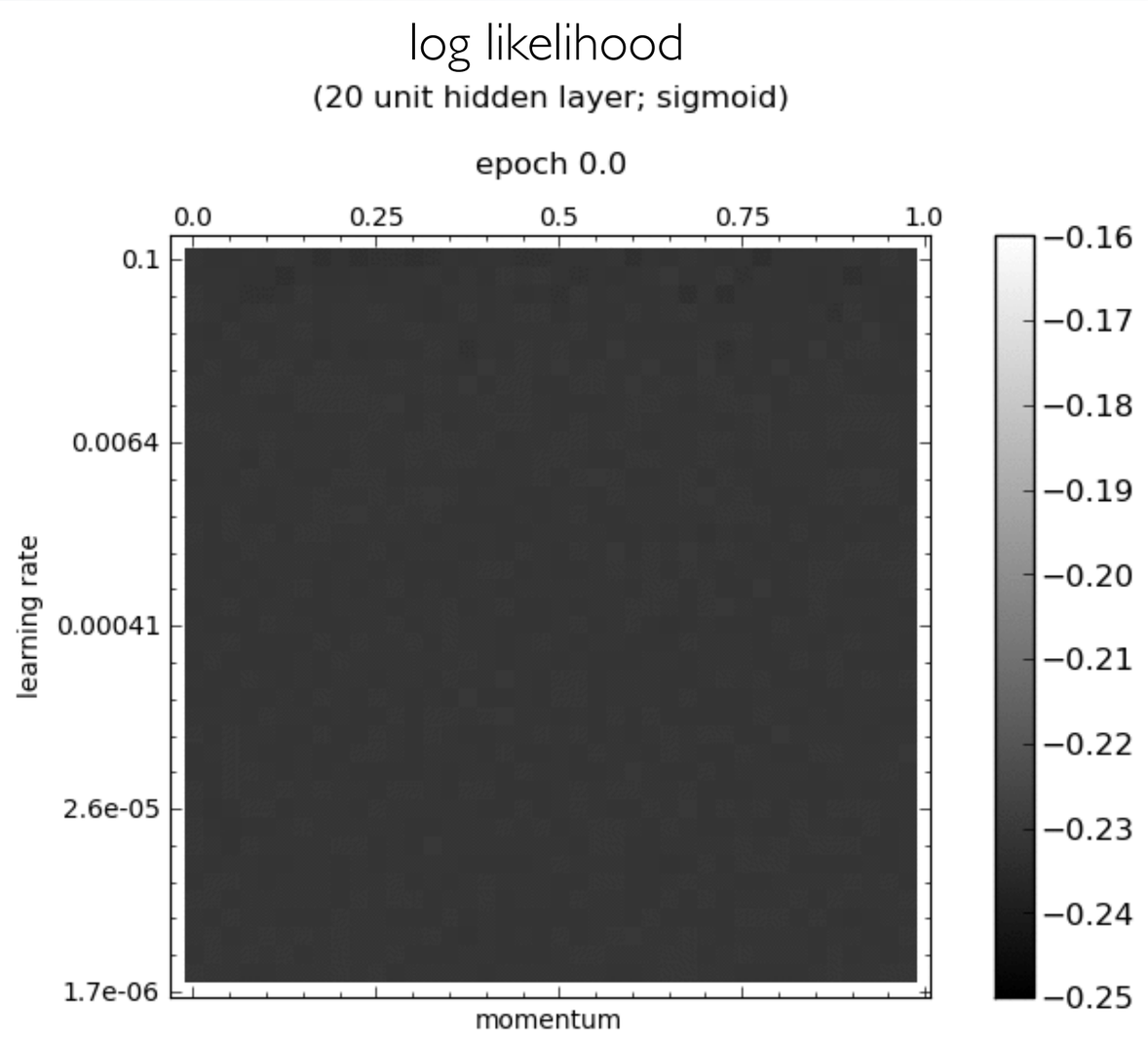
MODEL SELECTION

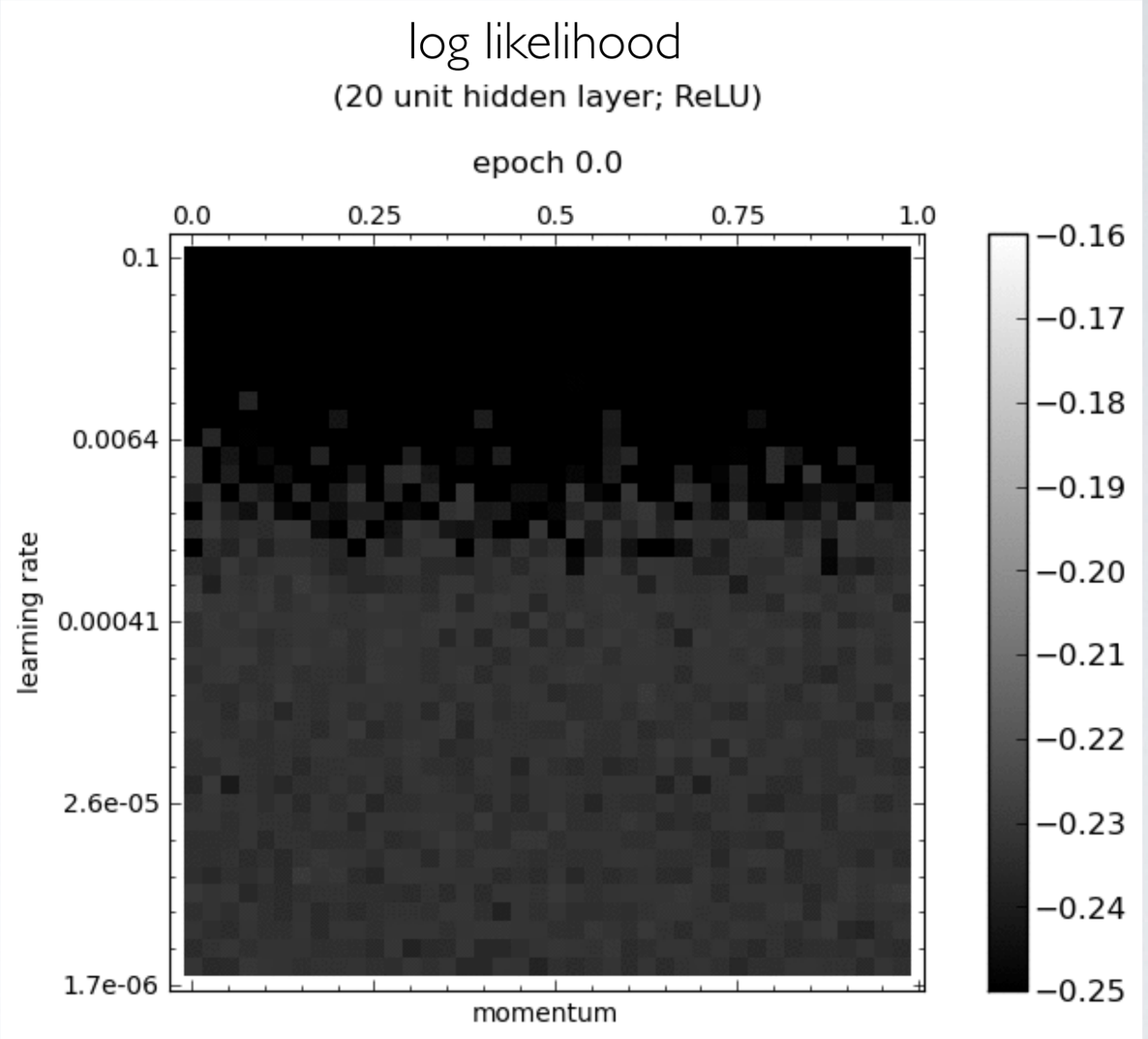
Topics: grid search

- 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 **Validation Set** performance to select the best configuration
- You can go back and refine the grid/distributions if needed

DISCUSSION: MODEL SELECTION





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)
  - $\alpha_t = \frac{\alpha}{1+\delta t}$
  - $\alpha_t = \frac{\alpha}{t^\delta}$ (where $0.5 < \delta \leq 1$)
- Better to use a fixed learning rate for the first few updates

Neural networks

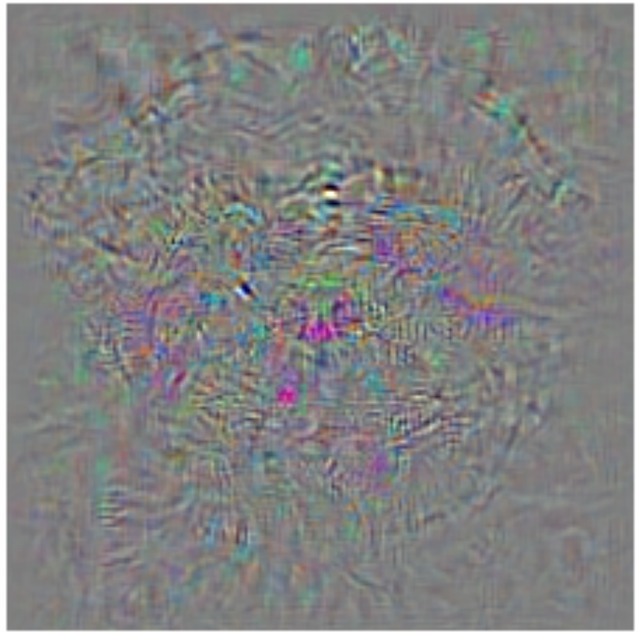
Unintuitive properties of neural networks

THEY CAN MAKE DUMB ERRORS

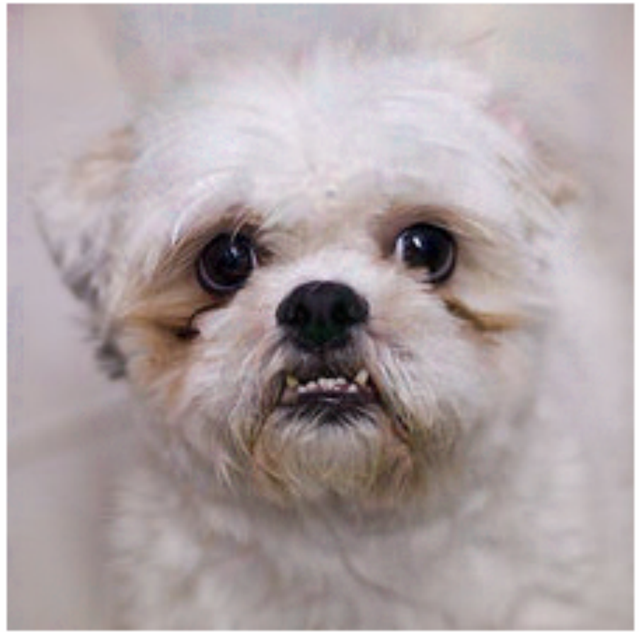
Topics: adversarial examples

- *Intriguing Properties of Neural Networks*
  Szegedy, Zaremba, Sutskever, Bruna, Erhan, Goodfellow, Fergus, ICLR 2014

Correctly classified



Difference



Badly classified

THEY CAN MAKE DUMB ERRORS

Topics: adversarial examples

- Humans have adversarial examples too

- However they don't match those of neural networks

THEY CAN MAKE DUMB ERRORS

Topics: adversarial examples

- Humans have adversarial examples too

- However they don't match those of neural networks