Advanced Machine Learning from Theory to Practice
Lecture 08
Introduction to Neural Networks

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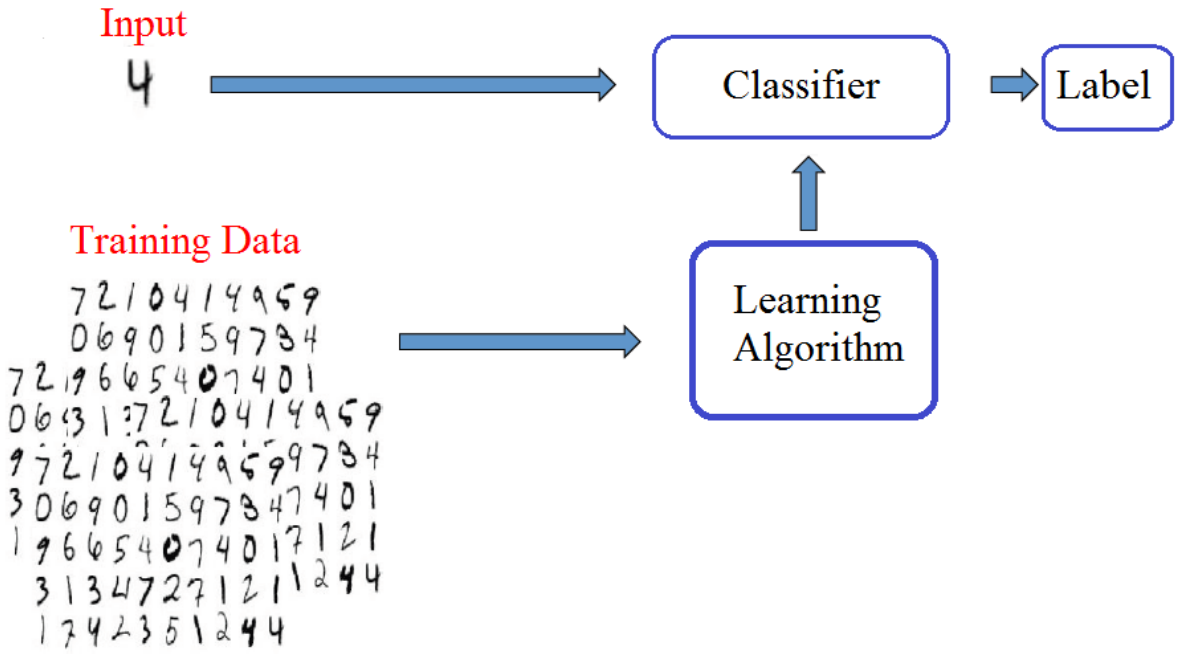
Machine Learning



A definition by Tom Mitchell (http://www.cs.cmu.edu/~tom/)

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

Outline

1. Supervised Learning
2. (Deep) Neural Networks
3. Perceptron
4. Multilayer Perceptron
5. Backprop Algorithm

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2. (Deep) Neural Networks
3. Perceptron
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5. Backprop Algorithm

Supervised Learning

Supervised Learning Framework

- Input measurement $\mathbf{X} = (X^{(1)}, X^{(2)}, \ldots, X^{(d)}) \in \mathcal{X}$
- Output measurement $Y \in \mathcal{Y}$.
- $(\mathbf{X}, Y) \sim \mathbf{P}$ with $\mathbf{P}$ unknown.
- Training data : $\mathcal{D}_n = \{(\mathbf{X}_1, Y_1), \ldots, (\mathbf{X}_n, Y_n)\}$ (i.i.d. $\sim \mathbf{P}$)
- Often
  - $\mathbf{X} \in \mathbb{R}^d$ and $Y \in \{-1, 1\}$ (classification)
  - or $\mathbf{X} \in \mathbb{R}^d$ and $Y \in \mathbb{R}$ (regression).

- A classifier is a function in $\mathcal{F} = \{f : \mathcal{X} \to \mathcal{Y} \text{ measurable}\}$

Goal

- Construct a good classifier $\widehat{f}$ from the training data.

- Need to specify the meaning of good.
- Formally, classification and regression are the same problem!

Loss and Probabilistic Framework

Loss function

- Loss function : $\ell(y, f(x))$ measure how well $f(x)$ "predicts" y.
- Examples:
  - Prediction loss: $\ell(Y, f(\mathbf{X})) = \mathbf{1}_{Y \neq f(\mathbf{X})}$
  - Quadratic loss: $\ell(Y, \mathbf{X}) = |Y - f(\mathbf{X})|^2$

Risk of a generic classifier

- Risk measured as the average loss for a new couple:

$$\mathcal{R}(f) = \mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] = \mathbb{E}_X\left[\mathbb{E}_{Y|\mathbf{X}}\left[\ell(Y, f(\mathbf{X}))\right]\right]$$

- Examples:
  - Prediction loss: $\mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] = \mathbb{P}\left\{Y \neq f(\mathbf{X})\right\}$
  - Quadratic loss: $\mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] = \mathbb{E}\left[|Y - f(\mathbf{X})|^2\right]$

- **Beware:** As $\widehat{f}$ depends on $\mathcal{D}_n$, $\mathcal{R}(\widehat{f})$ is a random variable!

Supervised Learning

Experience, Task and Performance measure

- Training data : $\mathcal{D} = \{(\mathbf{X}_1, Y_1), \ldots, (\mathbf{X}_n, Y_n)\}$ (i.i.d. $\sim \mathbf{P}$)
- Predictor: $f : \mathcal{X} \to \mathcal{Y}$ measurable
- Cost/Loss function : $\ell(Y, f(\mathbf{X}))$ measure how well $f(\mathbf{X})$ "predicts" Y
- Risk:

$$\mathcal{R}(f) = \mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] = \mathbb{E}_X\left[\mathbb{E}_{Y|\mathbf{X}}\left[\ell(Y, f(\mathbf{X}))\right]\right]$$

- Often $\ell(Y, f(\mathbf{X})) = |f(\mathbf{X}) - Y|^2$ or $\ell(Y, f(\mathbf{X})) = \mathbf{1}_{Y \neq f(\mathbf{X})}$

Goal

- Learn a rule to construct a classifier $\widehat{f} \in \mathcal{F}$ from the training data $\mathcal{D}_n$ s.t. the risk $\mathcal{R}(\widehat{f})$ is small on average or with high probability with respect to $\mathcal{D}_n$.

Best Solution

- The best solution f^* (which is independent of $\mathcal{D}_n$) is

$$f^* = \arg\min_{f \in \mathcal{F}} R(f) = \arg\min_{f \in \mathcal{F}} \mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] = \arg\min_{f \in \mathcal{F}} \mathbb{E}_{\mathbf{X}}\left[\mathbb{E}_{Y|\mathbf{X}}\left[\ell(Y, f(\mathbf{x}))\right]\right]$$

Bayes Classifier (explicit solution)

- In binary classification with $0-1$ loss:

$$f^*(\mathbf{X}) = \begin{cases} +1 & \text{if } \mathbb{P}\{Y = +1|\mathbf{X}\} \geq \mathbb{P}\{Y = -1|\mathbf{X}\} \\ & \Leftrightarrow \mathbb{P}\{Y = +1|\mathbf{X}\} \geq 1/2 \\ -1 & \text{otherwise} \end{cases}$$

- In regression with the quadratic loss

$$f^*(\mathbf{X}) = \mathbb{E}[Y|\mathbf{X}]$$

Issue: Explicit solution requires to know $\mathbb{E}[Y|\mathbf{X}]$ for all values of $\mathbf{X}$!

Goal

Machine Learning

- Learn a rule to construct a classifier $\widehat{f} \in \mathcal{F}$ from the training data $\mathcal{D}_n$ s.t. the risk $\mathcal{R}(\widehat{f})$ is small on average or with high probability with respect to $\mathcal{D}_n$.

Canonical example: Empirical Risk Minimizer

- One restricts f to a subset of functions $\mathcal{S} = \{f_\theta, \theta \in \Theta\}$
- One replaces the minimization of the average loss by the minimization of the empirical loss

$$\widehat{f} = f_{\widehat{\theta}} = \underset{f_\theta, \theta \in \Theta}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i, f_\theta(\mathbf{X}_i))$$

- Examples:
  - Linear regression
  - Linear discrimination with

$$\mathcal{S} = \{\mathbf{x} \mapsto \mathtt{sign}\{\beta^T \mathbf{x} + \beta_0\} / \beta \in \mathbb{R}^d, \beta_0 \in \mathbb{R}\}$$

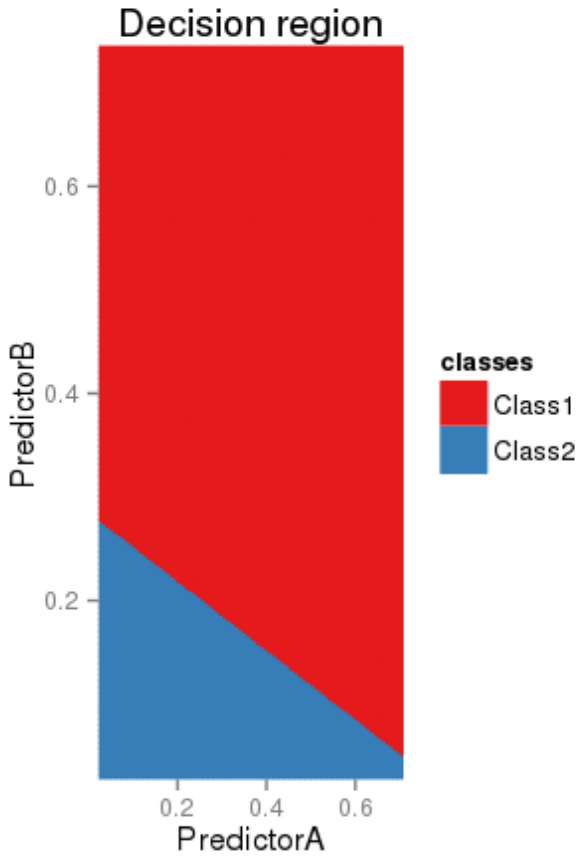
Example: TwoClass Dataset

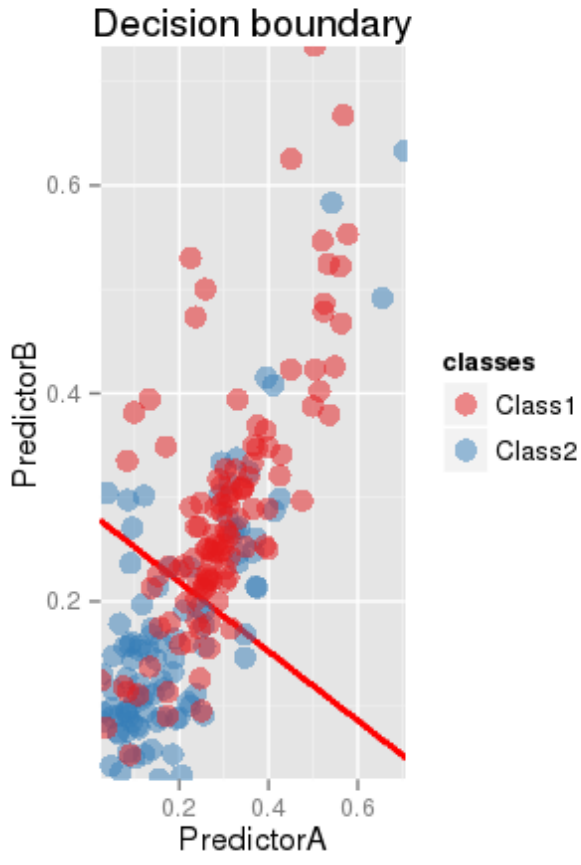
Synthetic Dataset

- Two features/covariates.
- Two classes.

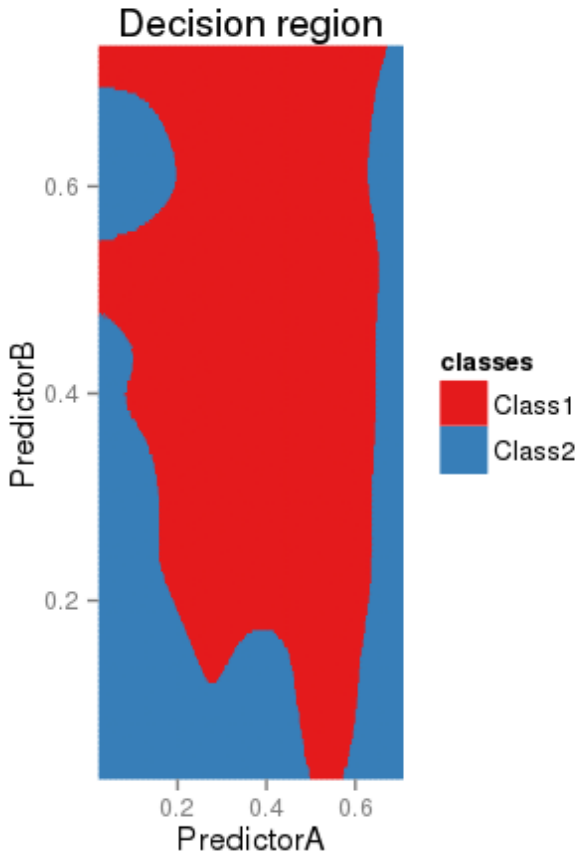
- Dataset from *Applied Predictive Modeling*, M. Kuhn and K. Johnson, Springer
- Numerical experiments with **R** and the **caret** package.

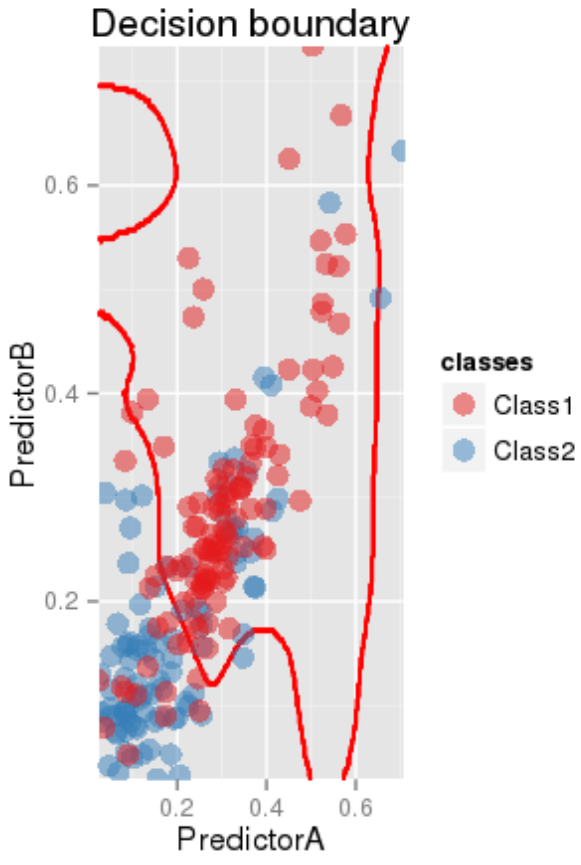
Example: Linear Discrimination





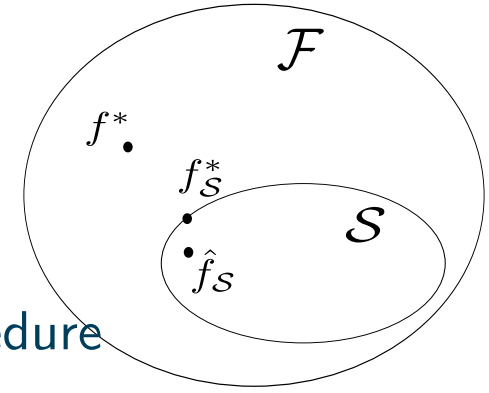
Example: More complex model





Bias-Variance Dilemna

- General setting:
  - $\mathcal{F} = \{\text{measurable fonctions } \mathcal{X} \to \mathcal{Y}\}$
  - Best solution: $f^* = \text{argmin}_{f \in \mathcal{F}} \mathcal{R}(f)$
  - Class $\mathcal{S} \subset \mathcal{F}$ of functions
  - Ideal target in $\mathcal{S}$: $f_{\mathcal{S}}^* = \text{argmin}_{f \in \mathcal{S}} \mathcal{R}(f)$
  - Estimate in $\mathcal{S}$: $\widehat{f}_{\mathcal{S}}$ obtained with some procedure



Approximation error and estimation error (Bias/Variance)

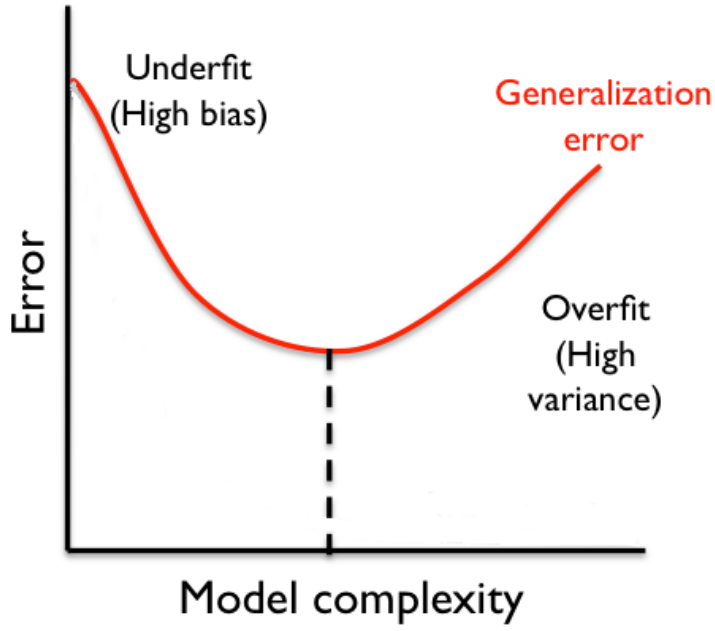
$$\mathcal{R}(\widehat{f}_{\mathcal{S}}) - \mathcal{R}(f^*) = \underbrace{\mathcal{R}(f_{\mathcal{S}}^*) - \mathcal{R}(f^*)}_{\text{Approximation error}} + \underbrace{\mathcal{R}(\widehat{f}_{\mathcal{S}}) - \mathcal{R}(f_{\mathcal{S}}^*)}_{\text{Estimation error}}$$

- Approx. error can be large if the model $\mathcal{S}$ is not suitable.
- Estimation error can be large if the model is complex.

Agnostic approach

- No assumption (so far) on the law of $(\mathbf{X}, Y)$.

Under-fitting / Over-fitting Issue



- Different behavior for different model complexity
- Low complexity model are easily learned but the approximation error ("bias") may be large (Under-fit).
- High complexity model may contains a good ideal target but the estimation error ("variance") can be large (Over-fit)

Bias-variance trade-off $\Longleftrightarrow$ avoid overfitting and underfitting

Statistical and Optimization Point of View Framework

How to find a good function f with a *small* risk

$$R(f) = \mathbb{E}\left[\ell(Y, f(X))\right] \quad ?$$

Canonical approach: $\widehat{f}_{\mathcal{S}} = \text{argmin}_{f \in \mathcal{S}} \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i, f(\mathbf{X}_i))$

Problems

- How to choose $\mathcal{S}$?
- How to compute the minimization?

A Statistical Point of View

Solution: For $\mathbf{X}$, estimate $Y|\mathbf{X}$ plug this estimate in the Bayes classifier: (Generalized) Linear Models, Kernel methods, k-nn, Naive Bayes, Tree, Bagging...

An Optimization Point of View

Solution: If necessary replace the loss ℓ by an upper bound ℓ' and minimize the empirical loss: SVR, SVM, **Neural Network**,Tree, Boosting

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1 Supervised Learning

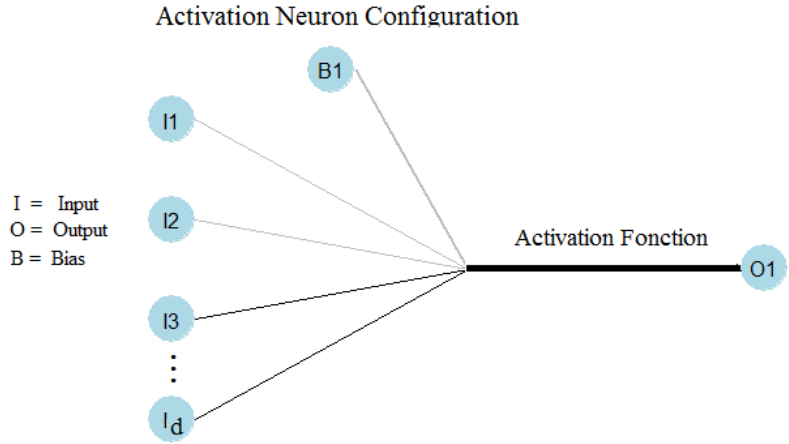
2 (Deep) Neural Networks

3 Perceptron

4 Multilayer Perceptron

5 Backprop Algorithm

Artificial Neuron and Logistic Regression



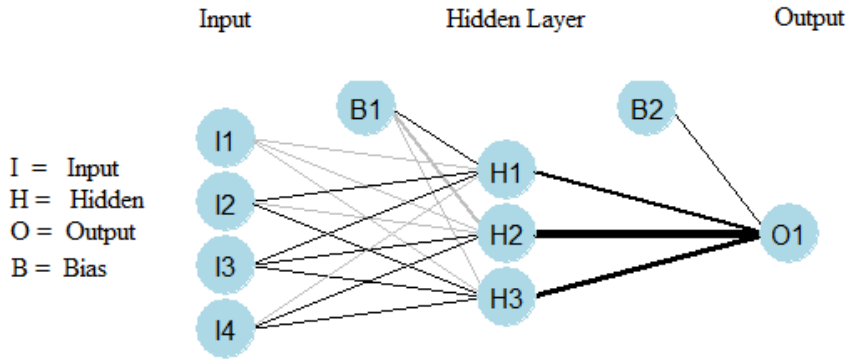
Artificial neuron

- Structure:
  - Mix inputs with a weighted sum,
  - Apply a (non linear) activation function to this sum,
  - Eventually threshold the result to make a decision.
- Weights learned by minimizing a loss function.

Logistic unit

- Structure:
  - Mix inputs with a weighted sum,
  - Apply the logistic function $\sigma(t) = e^t/(1 + e^t)$,
  - Threshold at $1/2$ to make a decision!
- Logistic weights learned by minimizing the -log-likelihood.

Neural network

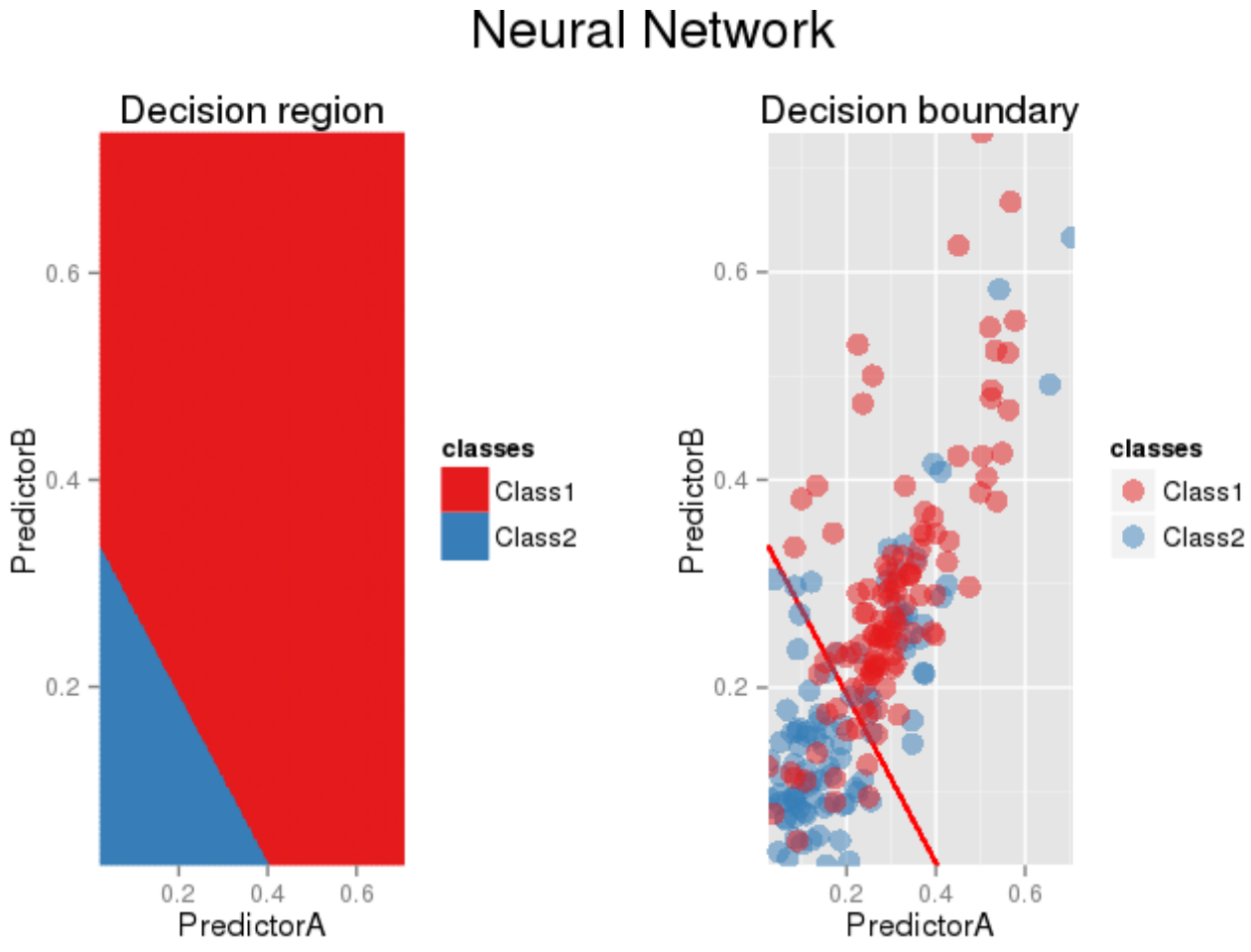


Neural network structure

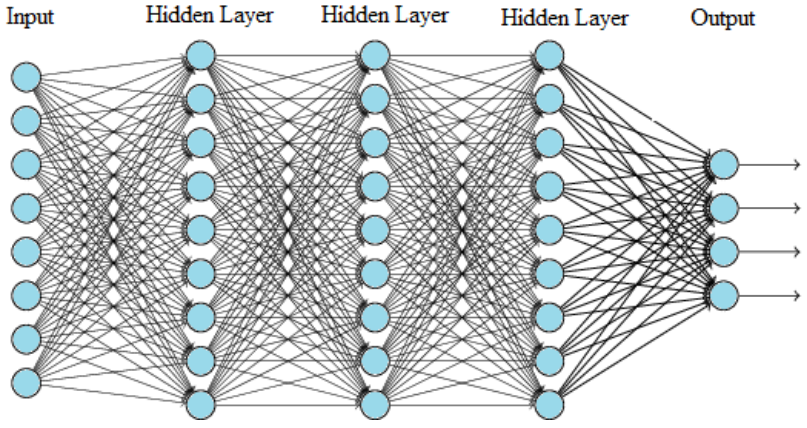
- Cascade of artificial neurons organized in layers
- Thresholding decision only at the output layer

- Most classical case use logistic neurons and the -log-likelihood as the criterion to minimize.
- Classical (stochastic) gradient descent algorithm with a clever implementation (Back propagation)
- Non convex and thus may be trapped in local minima.

Neural network



Deep Neural Network

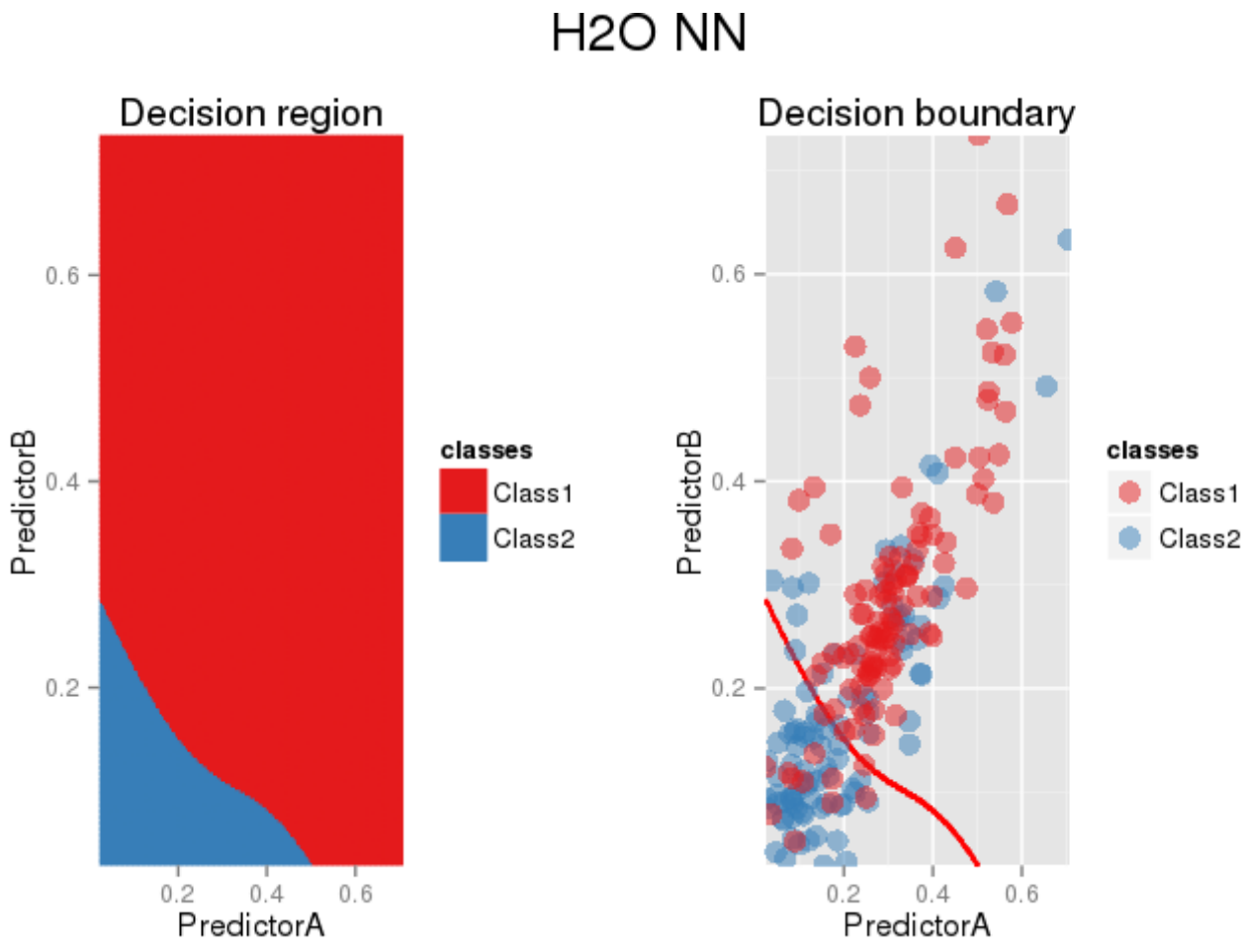


Deep Neural Network structure

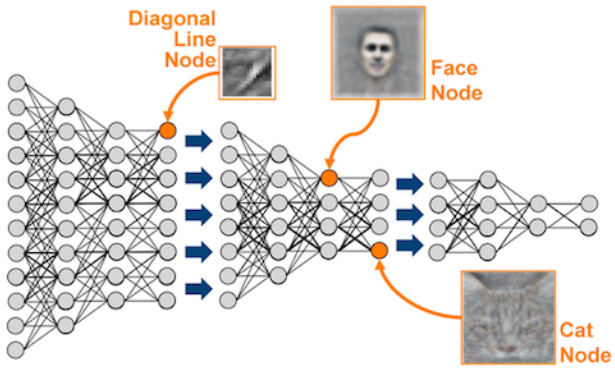
- Deep cascade of layers!

- No conceptual novelty...
- But a lot of details that enabled to obtain a good solution: clever initialization, better activation function, weight regularization, accelerated stochastic gradient descent, early stopping...
- Use of GPU...
- Very impressive results!

Deep Neural Network



Deep Learning



Family of Machine Learning algorithm combining:

- a (deep) multilayered structure,
- a clever optimization including initialization and regularization.

- Examples: Deep Neural Network, Deep (Restricted) Boltzman Machine, Stacked Encoder, Recursive Neural Network...
- Transfer learning: use as initialization a pretrained deep structure.
- Appears to be very efficient but lack of theoretical fundation!

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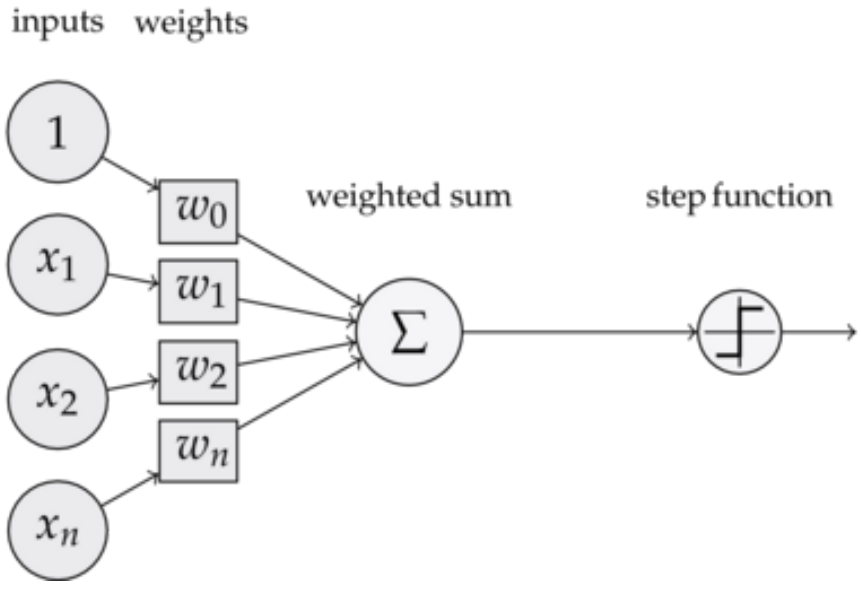
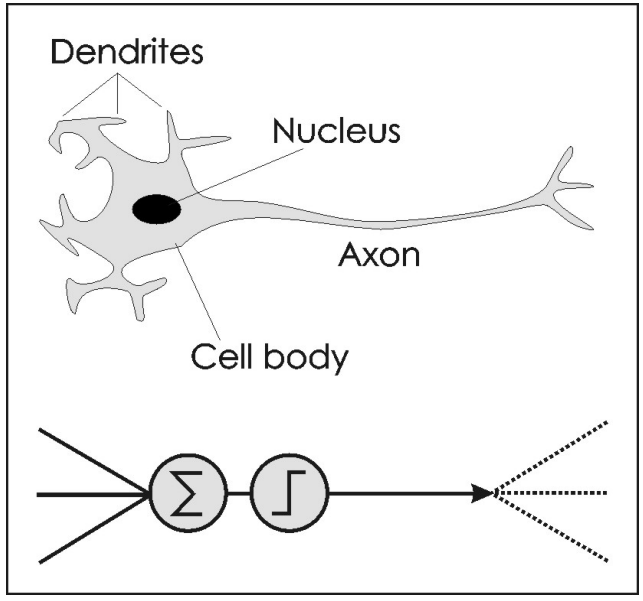
Perceptron



Perceptron (Rosenblatt 1957)

- Inspired from biology.
- Very simple (linear) model!
- Physical implementation and proof of concept.

Perceptron



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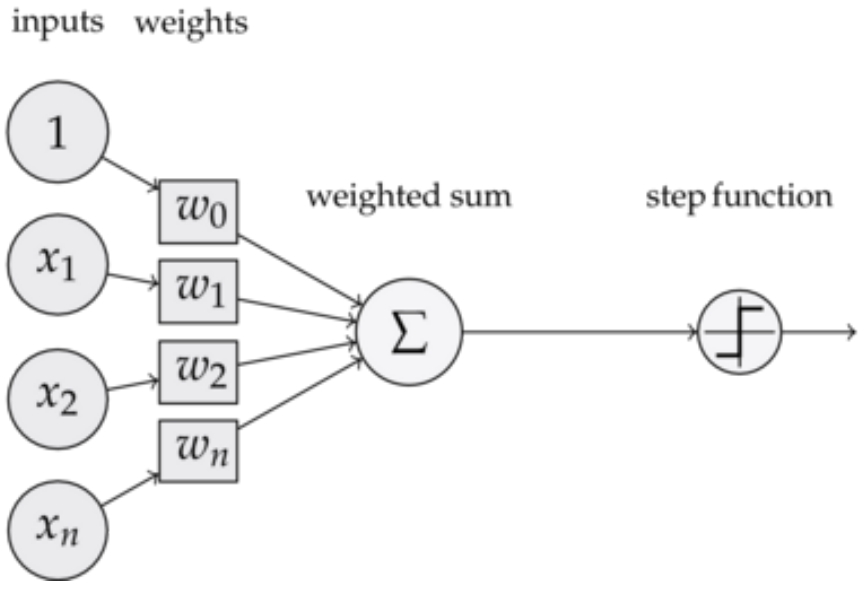

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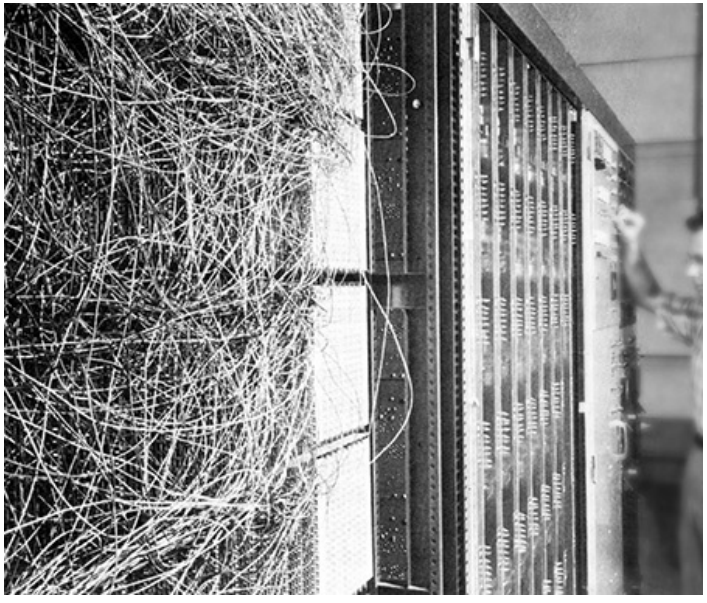

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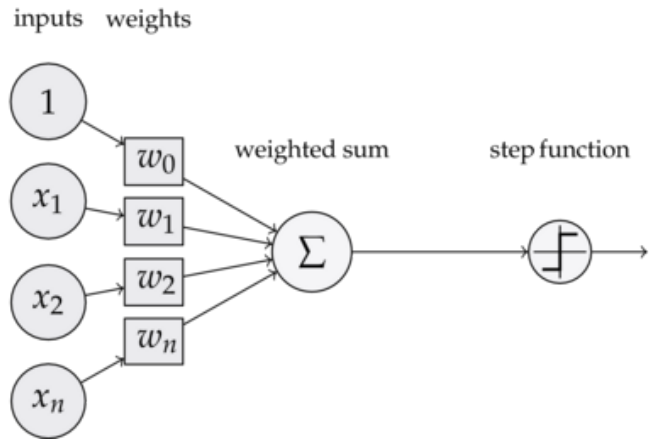
The Perceptron Algorithm



- Key contribution: first (iterative) learning algorithm!

Algorithm

- Start with $w = 0$.
- Repeat over all samples:
  - if $< w, \mathbf{X}_i > Y_i < 0$ modify w into $w + Y_i \mathbf{X}_i$,
  - otherwise do not modify w.

- Convergence to a solution in a finite number of steps if the examples are linearly separable! (1962)

Proof

Linear separability: It exists w^* such that $Y_i\langle w^*, X_i\rangle > 0$.
Proof: Let $C = \max_{X_i} \|C_i\|$ and $\rho = \min Y_i\langle w^*, X_i\rangle > 0$.
Let w_t be the weight at step t. If $\min Y_i\langle w_t, X_i\rangle > 0$ then we are done.
Otherwise, let (X_i, Y_i) be the first example such that $Y_i(\langle w_t, X_i\rangle) \leq 0$
and let $w_{t+1} = w_t + \alpha Y_i X_i$. By construction,

$$\begin{aligned}\langle w^*, w_{t+1}\rangle &= \langle w^*, w_t\rangle + Y_i\langle w^*, W_i\rangle \\ &\geq \langle w^*, w_t\rangle + Y_i\langle w^*, W_i\rangle \\ &\geq \langle w^*, w_t\rangle + \rho \geq \langle w^*, w_0\rangle + t\rho\end{aligned}$$

while

$$\begin{aligned}\|w_{t+1}\|^2 &= \|w_t\|^2 + \|X_i\|^2 + 2\langle w_t, Y_i X_i\rangle \\ &\leq \|w_t\|^2 + \|X_i\|^2 \leq \|w_t\|^2 + C^2 \leq \|w_0\|^2 + tC^2.\end{aligned}$$

this term <0

Now $\langle w^*, w_{t+1}\rangle \leq \|w^*\|\|w_{t+1}\|$ so that we have

$$\langle w^*, w_0\rangle + t\rho \leq \|w^*\| \left(\|w_0\|^2 + tC^2\right)^{1/2}$$

which implies that such a t is upperbounded and hence the algorithm converges.

Neural Networks

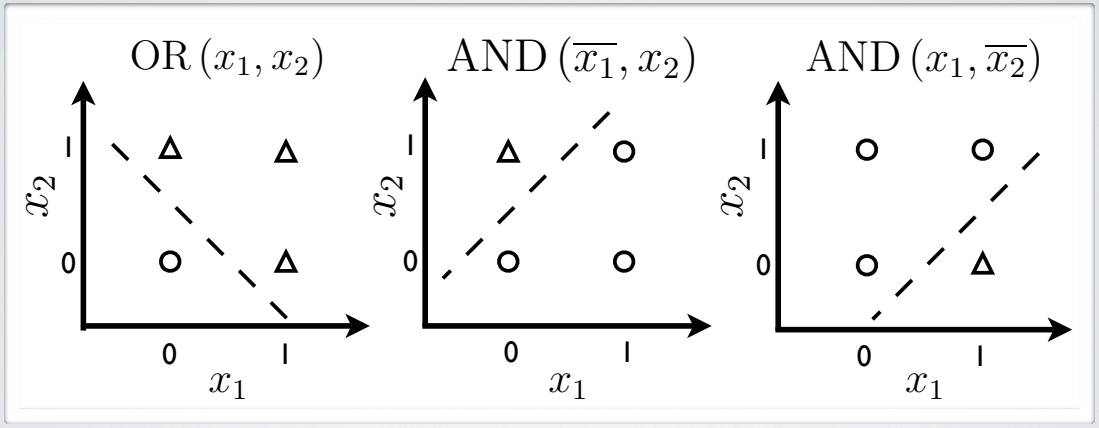
- Slides *shamelessly* stolen from Hugo Larochelle (Sherbrooke)
  `http://www.dmi.usherb.ca/~larocheh/`
- Tremendous website!

Perceptron Limitations

ARTIFICIAL NEURON

Topics: capacity of single neuron

- Can solve linearly separable problems



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Limitations

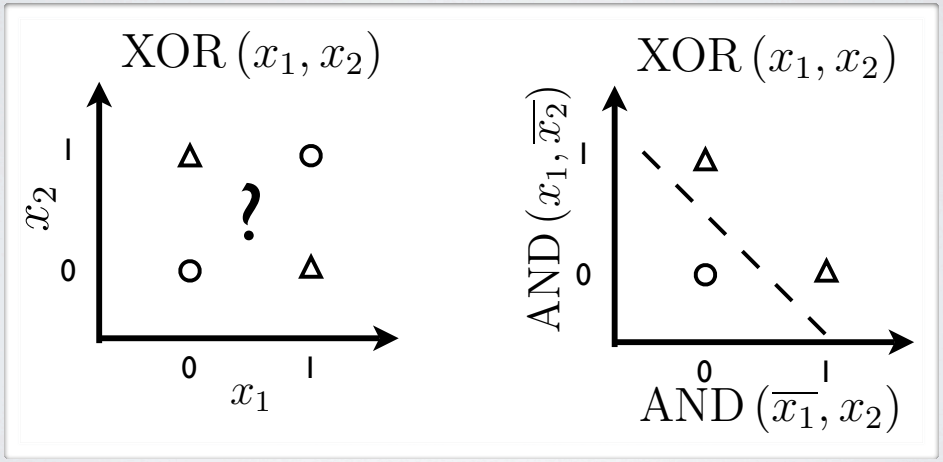
- Can't solve non linearly separable problems... (by design)
- Algorithm not robust to non linear separability!

Perceptron Limitations

ARTIFICIAL NEURON

Topics: capacity of single neuron

- Can't solve non linearly separable problems...



- ... unless the input is transformed in a better representation

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Limitations

- Can't solve non linearly separable problems... (by design)
- Algorithm not robust to non linear separability!

Activation

- Prediction by $f(\mathbf{X}) = \phi(\langle w, \mathbf{X} \rangle)$ (or its sign).

Activation function ϕ

- Hard threshold (non smooth)
- Sigmoid (logistic), tanh (smooth)
- Rectified Linear Unit (almost smooth, sparsification effect)

ARTIFICIAL NEURON

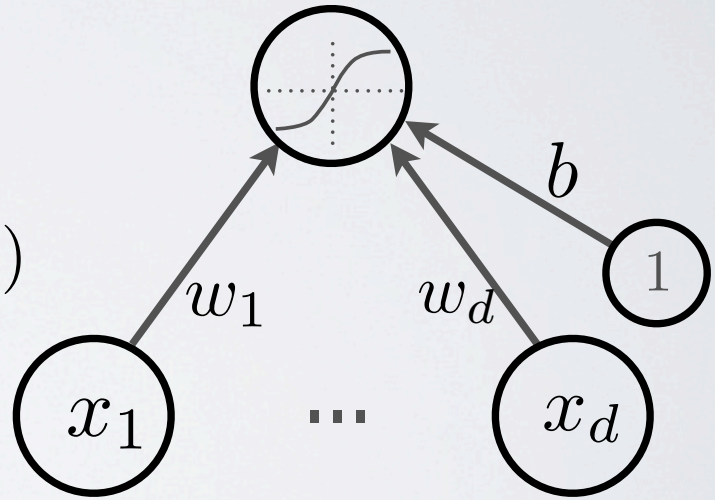
Topics: connection weights, bias, activation function

- Neuron input activation:

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

- Neuron (output) activation

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

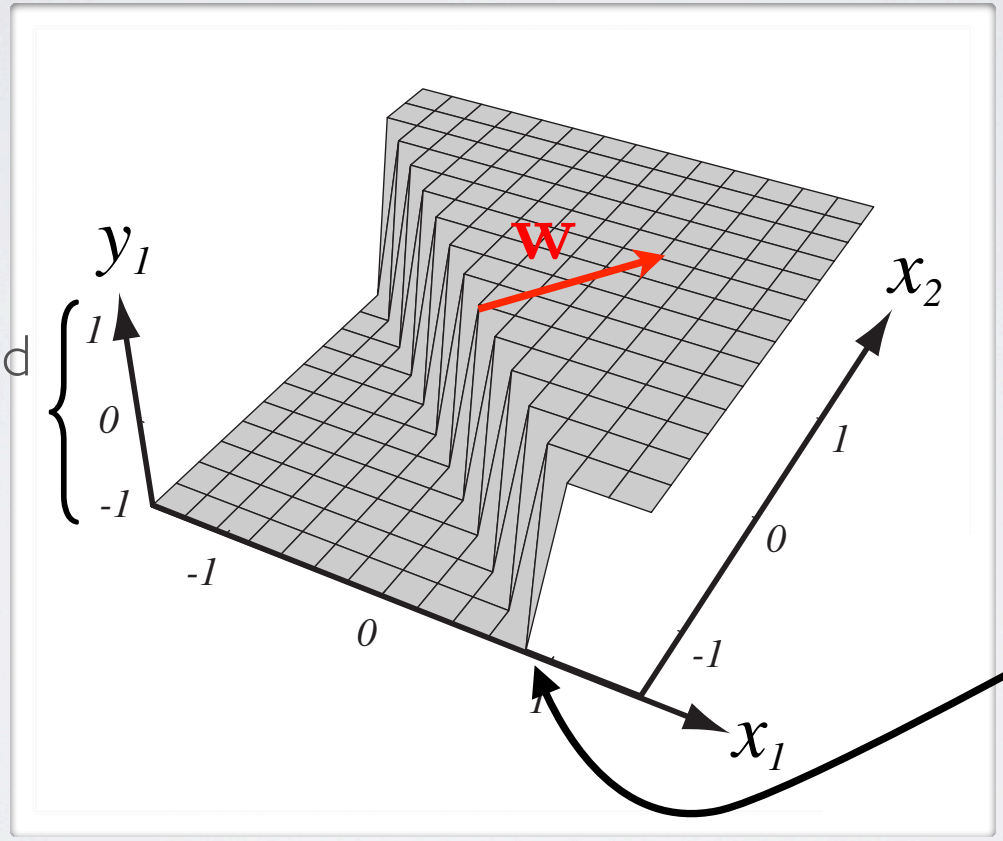


- $\mathbf{w}$ are the connection weights
- b is the neuron bias
- $g(\cdot)$ is called the activation function

ARTIFICIAL NEURON

Topics: connection weights, bias, activation function

range determined by $g(\cdot)$



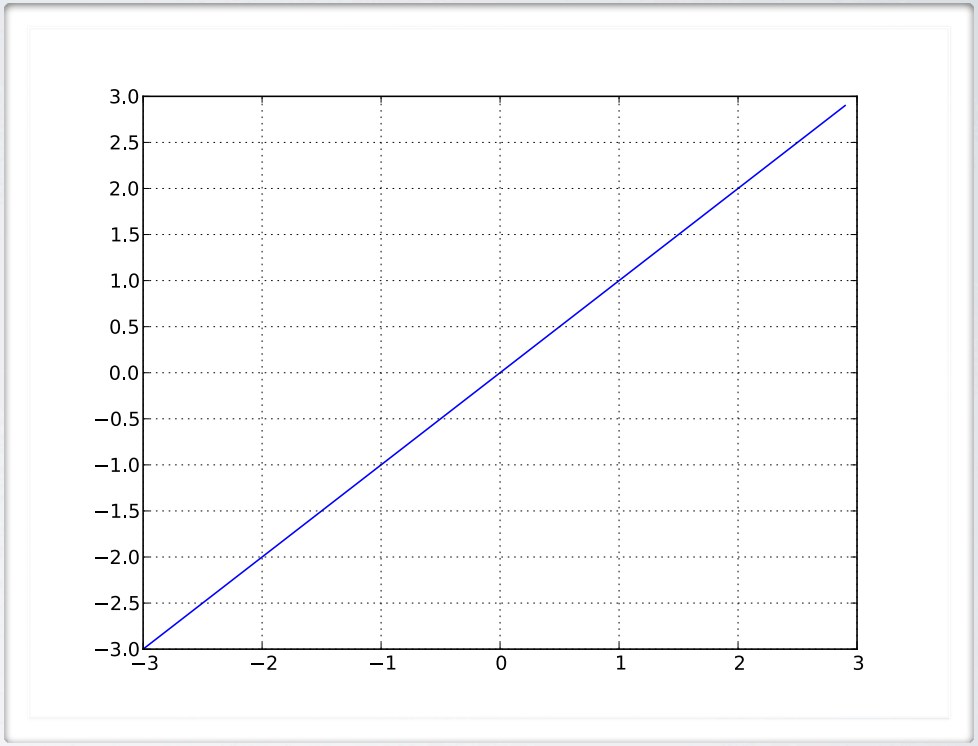
bias b only changes the position of the riff

(from Pascal Vincent's slides)

ARTIFICIAL NEURON

Topics: linear activation function

- Performs no input squashing
- Not very interesting...

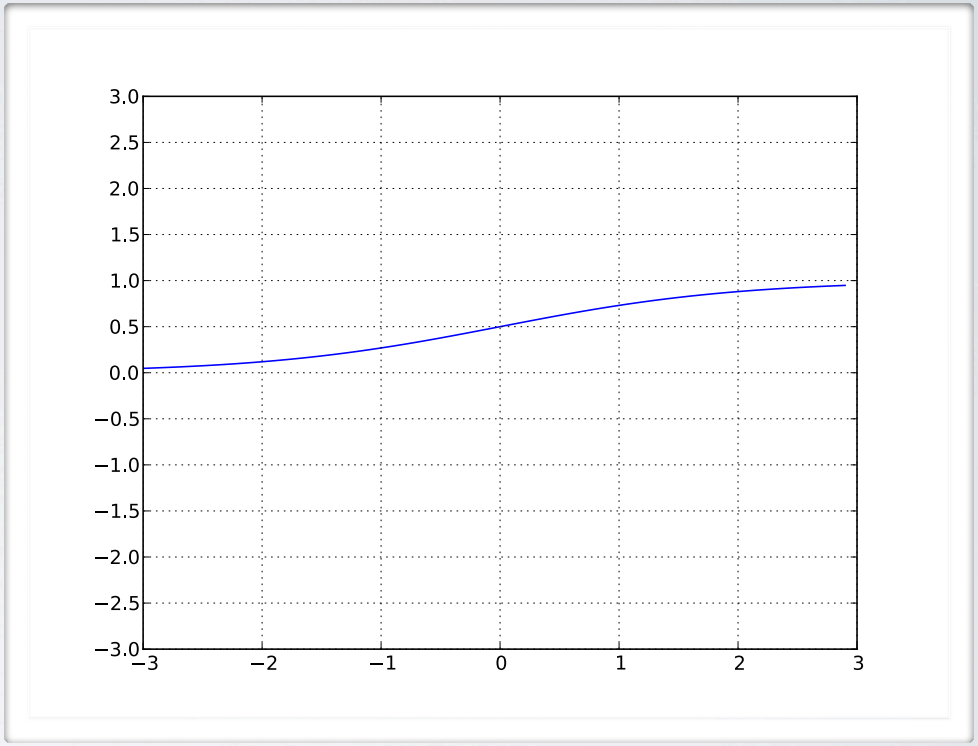


$$g(a) = a$$

ARTIFICIAL NEURON

Topics: sigmoid activation function

- Squashes the neuron's input between 0 and 1
- Always positive
- Bounded
- Strictly increasing



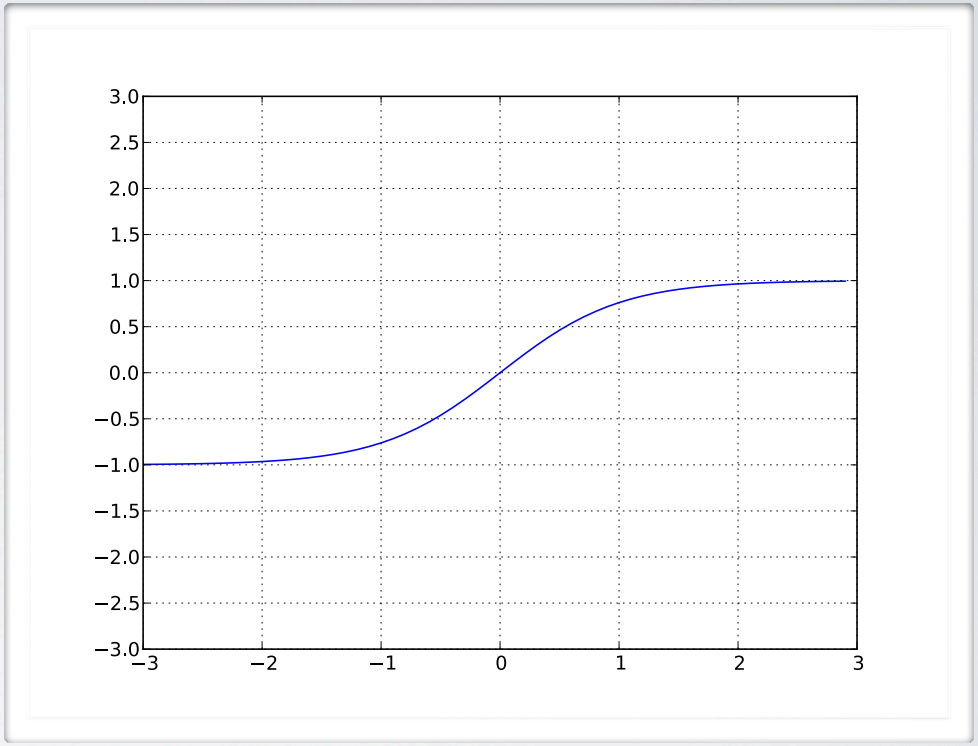
why we prefer sigmoid ?

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

ARTIFICIAL NEURON

Topics: hyperbolic tangent ("tanh") activation function

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

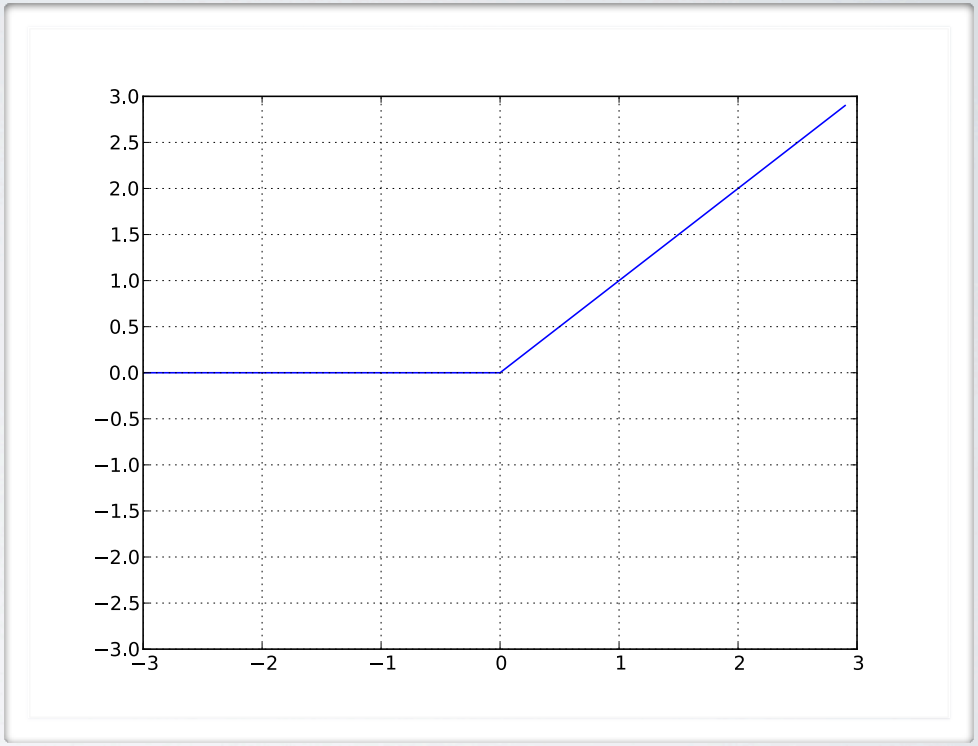


$$g(a) = \tanh(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} = \frac{\exp(2a) - 1}{\exp(2a) + 1}$$

ARTIFICIAL NEURON

Topics: rectified linear activation function

- Bounded below by 0 (always positive)
- Not upper bounded
- Strictly increasing
- Tends to give neurons with sparse activities



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

Activation and Loss

- Prediction by $f(\mathbf{X}) = \phi(\langle w, \mathbf{X} \rangle)$ (or its sign).

Activation function ϕ

- Hard threshold (non smooth)
- Sigmoid (logistic), tanh (smooth)
- Rectified Linear Unit (almost smooth, sparsification effect)

- Prediction error between Y and $f(\mathbf{X})$ measure with a loss...

Loss ℓ

- Error count (non smooth)
- Probabilistic approach: log-likelihood
- Optimization approach: convex relaxation, squared loss...

Gradient Descent Algorithm

- Empirical risk minimization:

$$\underset{w}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i, \phi(\langle w, \mathbf{X}_i \rangle))$$

- If ℓ and ϕ are almost differentiable (or convex):

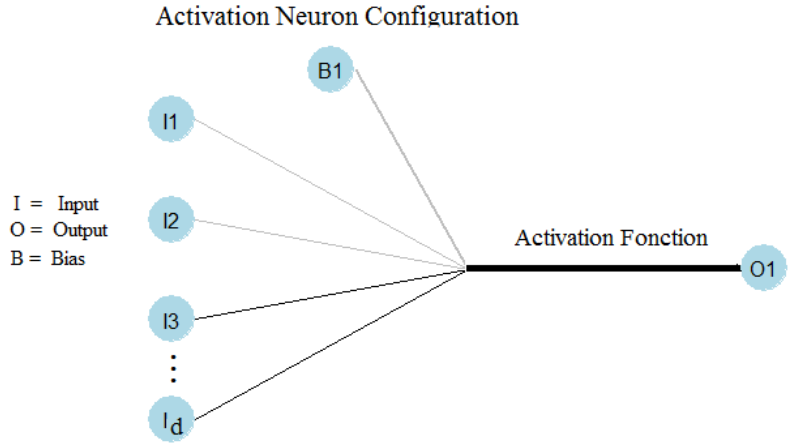
$$\nabla_i(w) = \frac{\partial \ell(Y_i, \phi(\langle w, \mathbf{X}_i \rangle))}{dw} = \mathbf{X}_i \phi'(\langle w, \mathbf{X}_i \rangle) \frac{\partial \ell}{df}(Y_i, \phi(\langle w, \mathbf{X}_i \rangle))$$

(Stochastic) Gradient descent rule:

$$w_{t+1} = w_t - h_y \frac{1}{|I_t|} \sum_{i \in I_i} \nabla_i(w_t)$$

- No convergence result except in the convex case...

Logistic Perceptron



Artificial neuron

- Structure:
  - Mix inputs with a weighted sum,
  - Apply a (non linear) activation function to this sum,
  - Eventually threshold the result to make a decision.
- Weights learned by minimizing a loss function.

Logistic unit

- Structure:
  - Mix inputs with a weighted sum,
  - Apply the logistic function $\sigma(t) = e^t/(1+e^t)$,
  - Threshold at $1/2$ to make a decision!
- Logistic weights learned by minimizing the -log-likelihood.

Outline

1 Supervised Learning

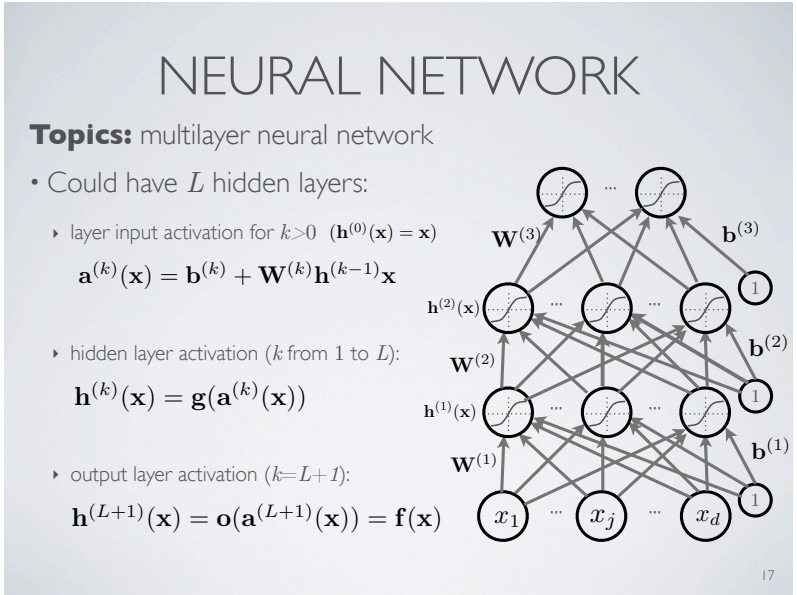
2 (Deep) Neural Networks

3 Perceptron

4 Multilayer Perceptron

5 Backprop Algorithm

Multilayer Perceptron



MLP (Rumelhart, McClelland, Hinton - 1986)

- Multilayer Perceptron: cascade of layers of artifical neuron units.
- Backprop algorithm to optimize it!

- Construction of a function by composing simple units.
- MLP corresponds to a specific direct acyclic graph structure.

Universal Approximation Theorem

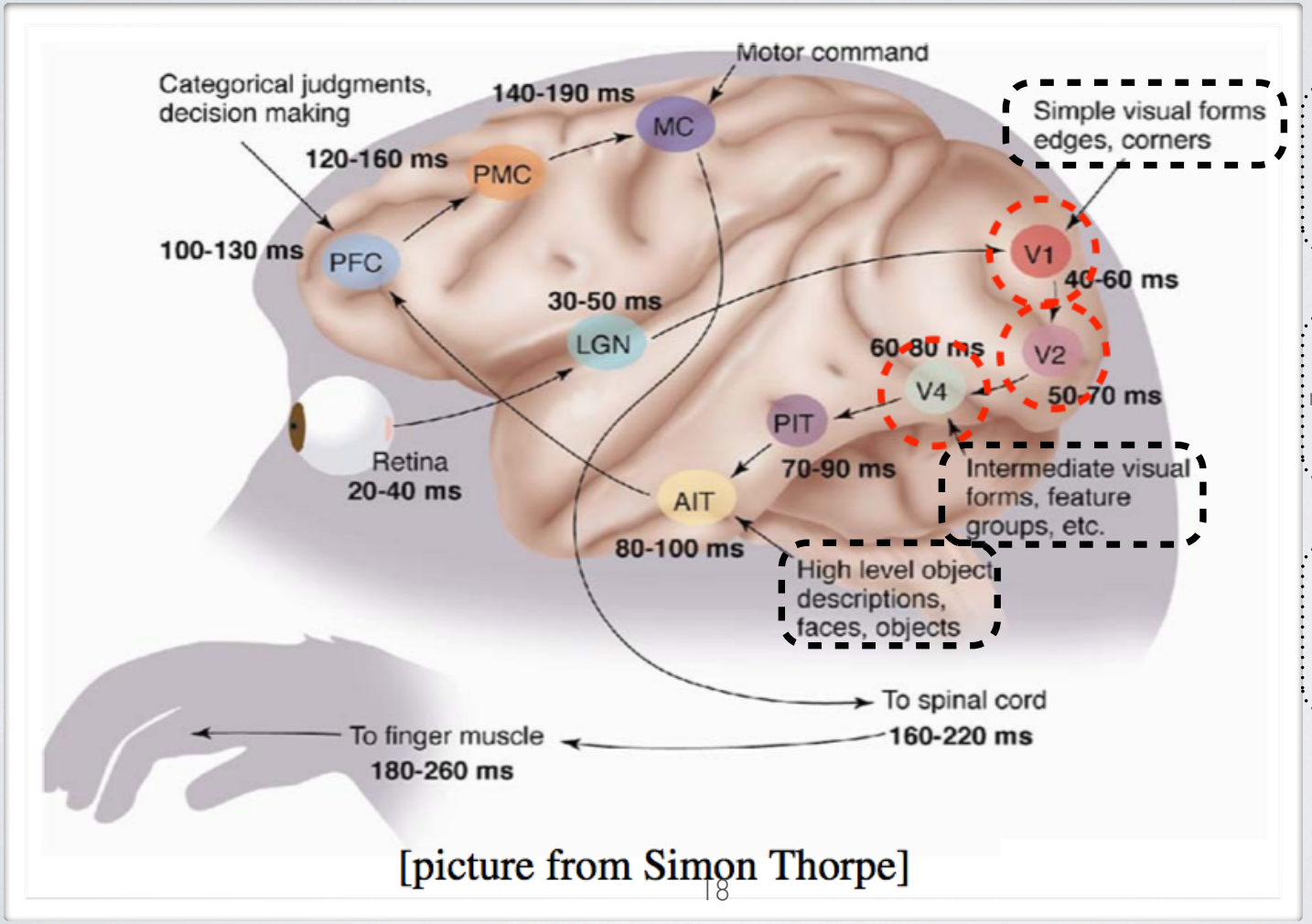
Universal Approximation Theorem (Hornik, 1991)

- A single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units

- Valid for most activations functions.
- A single hidden layer is sufficient but more may be more efficient.
- No bound on the number of required units... (Asymptotic flavour)

NEURAL NETWORK

Topics: parallel with the visual cortex



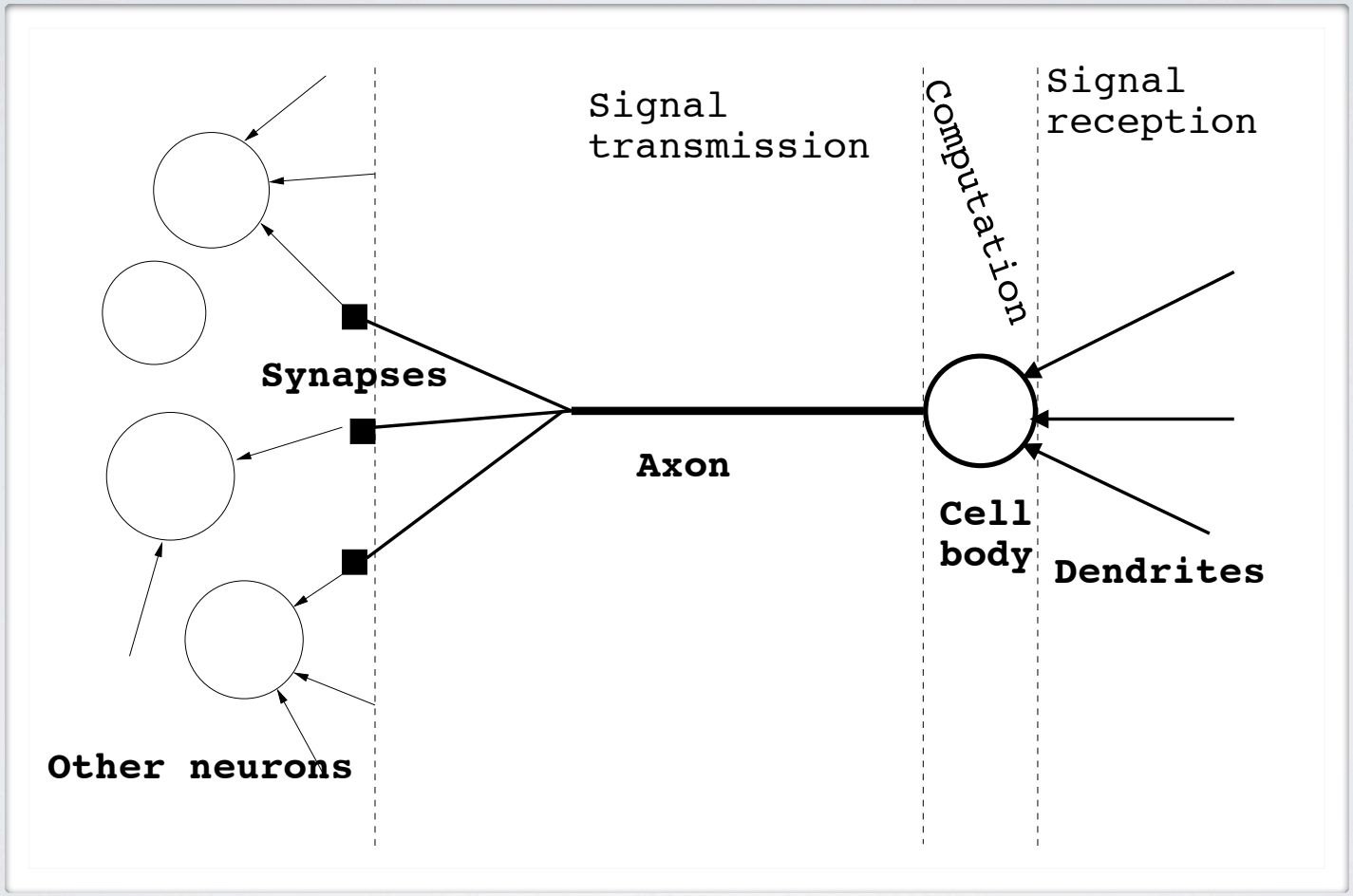
BIOLOGICAL NEURONS

Topics: synapse, axon, dendrite

- We estimate around 10^{10} and 10^{11} the number of neurons in the human brain:
  - they receive information from other neurons through their dendrites
  - the "process" the information in their cell body (soma)
  - they send information through a "cable" called an axon
  - the point of connection between the axon branches and other neurons' dendrites are called synapses

BIOLOGICAL NEURONS

Topics: synapse, axon, dendrite



(from Hyvärinen, Hurri and Hoyer's book)

BIOLOGICAL NEURONS

Topics: action potential, firing rate

- An action potential is an electrical impulse that travels through the axon:
  - this is how neurons communicate
  - it generates a "spike" in the electric potential (voltage) of the axon
  - an action potential is generated at neuron only if it receives enough (over some threshold) of the "right" pattern of spikes from other neurons

- Neurons can generate several such spikes every seconds:
  - the frequency of the spikes, called firing rate, is what characterizes the activity of a neuron
    - neurons are always firing a little bit, (spontaneous firing rate), but they will fire more, given the right stimulus

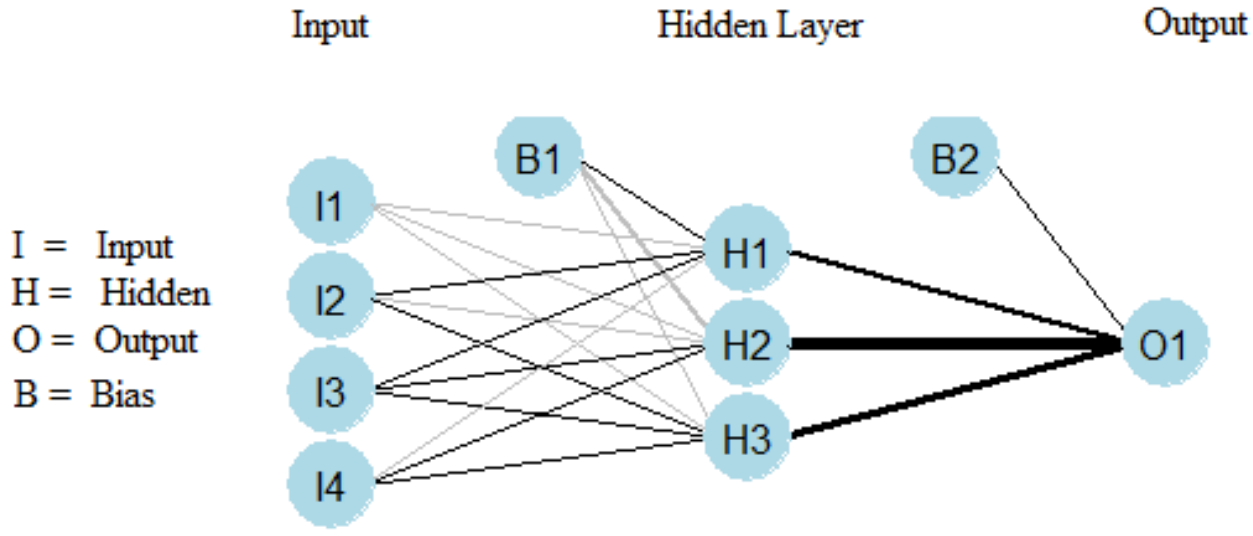
BIOLOGICAL NEURONS

Topics: action potential, firing rate

- Firing rates of different input neurons combine to influence the firing rate of other neurons:
  - depending on the dendrite and axon, a neuron can either work to increase (excite) or descrease (inhibit) the firing rate of another neuron

- This is what artificial neurons approximate:
  - the activation corresponds to a "sort of" firing rate
  - the weights between neurons model whether neurons excite or inhibit each other
  - the activation function and bias model the thresholded behavior of action potentials

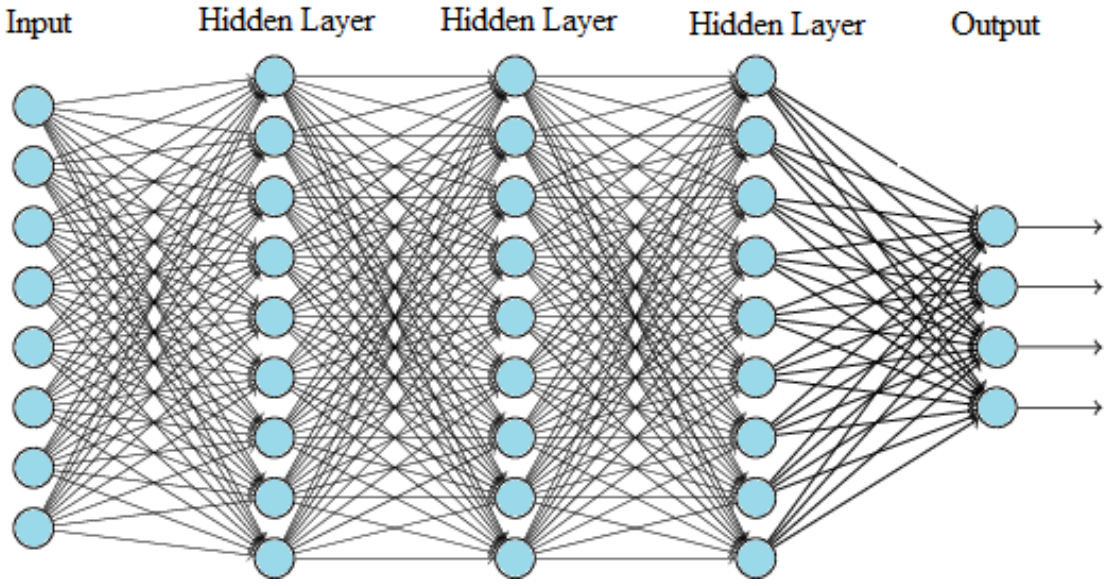
Network Architecture



Design

- Number of layers
- Connectivity
- Tricks: convolution (weight sharing), pooling...

Network Architecture



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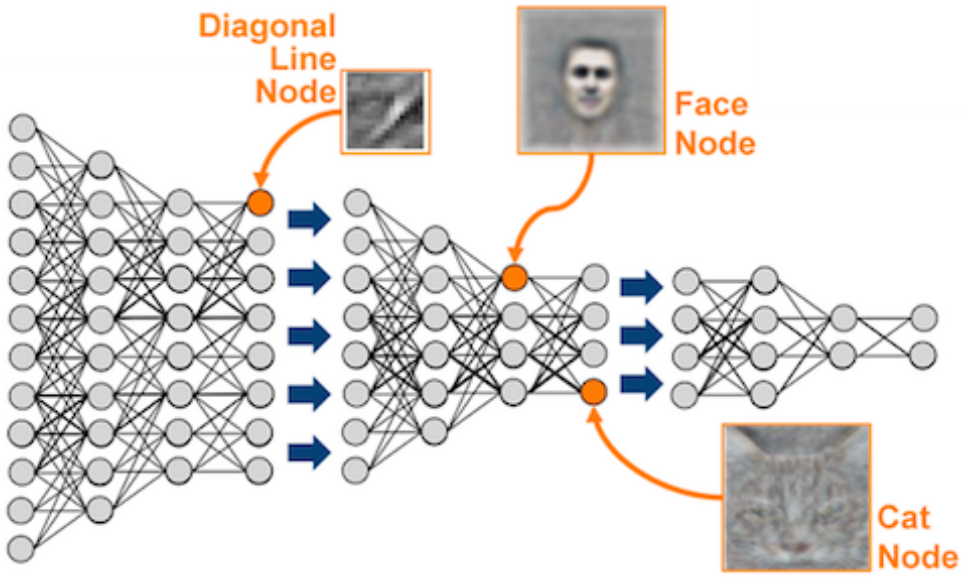

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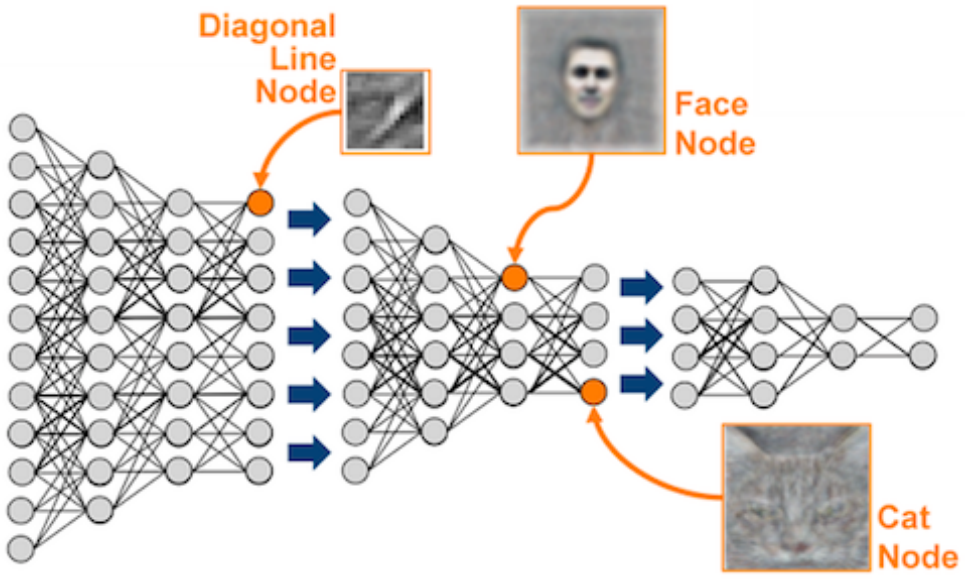
Network Architecture



Design

- Number of layers
- Connectivity
- Tricks: convolution (weight sharing), pooling...

Softmax Output

- Generalization of the logistic ouput for multiclass.

A probabilistic approach

- At the outer nodes, computes an *activation* a_i for all classes.
- Use a *joint* **softmax** activation function:

$$o_i = \frac{e^{a_i}}{\sum_{i'=1}^{K} e^{a_{i'}}}$$

- Amounts to model the probability of each class by a conditional multinomial logistic model on the output of the last hidden layer.

- Perfectly fit for ML approach.
- **Rk:** Slight overparameterization...

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)

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

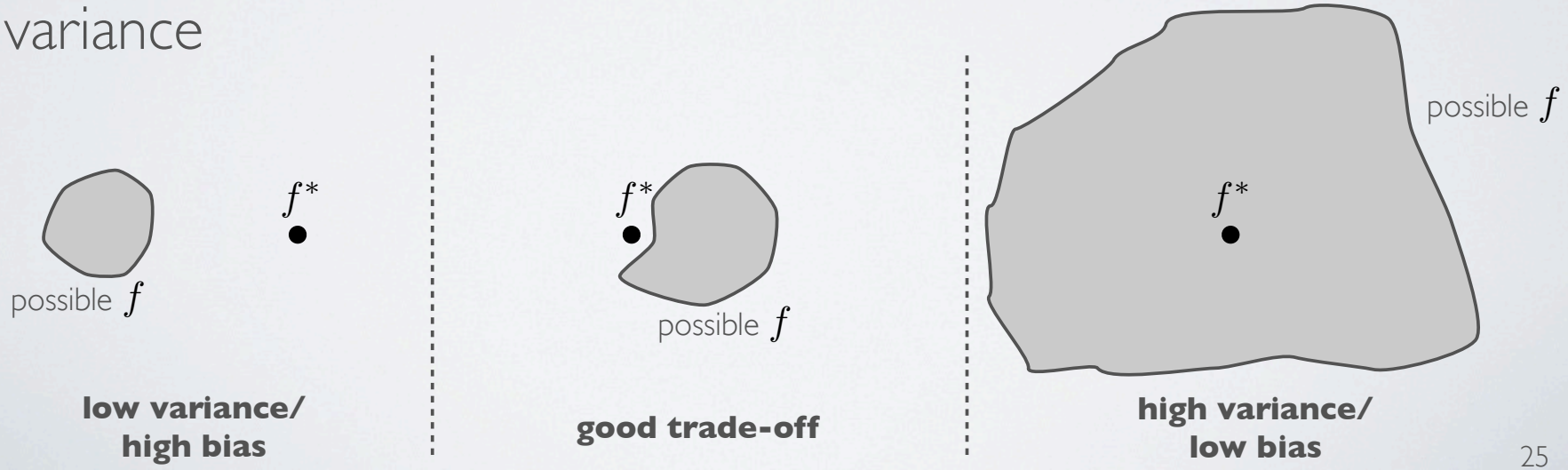
$$\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j |W_{i,j}^{(k)}|$$

- 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

MACHINE LEARNING

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 bias and the variance



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Backprop Algorithm

A Clever Gradient Descent Implementation

- Popularized by Rumelhart, McClelland, Hinton in 1986.
- Can be traced back to Werbos in 1974.
- Nothing but the use of chain rule derivation with a touch of dynamic programing.

- Key ingredient to make the Neural Networks work!
- Still at the core of Deep Learning algorithm.

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

LOSS FUNCTION

Topics: loss function for classification

- Neural network estimates $f(\mathbf{x})_c = p(y = c|\mathbf{x})$
  - we could maximize the probabilities of $y^{(t)}$ given $\mathbf{x}^{(t)}$ in the training set

- To frame as minimization, we minimize the negative log-likelihood

natural log (ln)

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

  - we take the log to simplify for numerical stability and math simplicity
  - sometimes referred to as cross-entropy

LOSS FUNCTION

Topics: loss gradient at output

- Partial derivative:

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

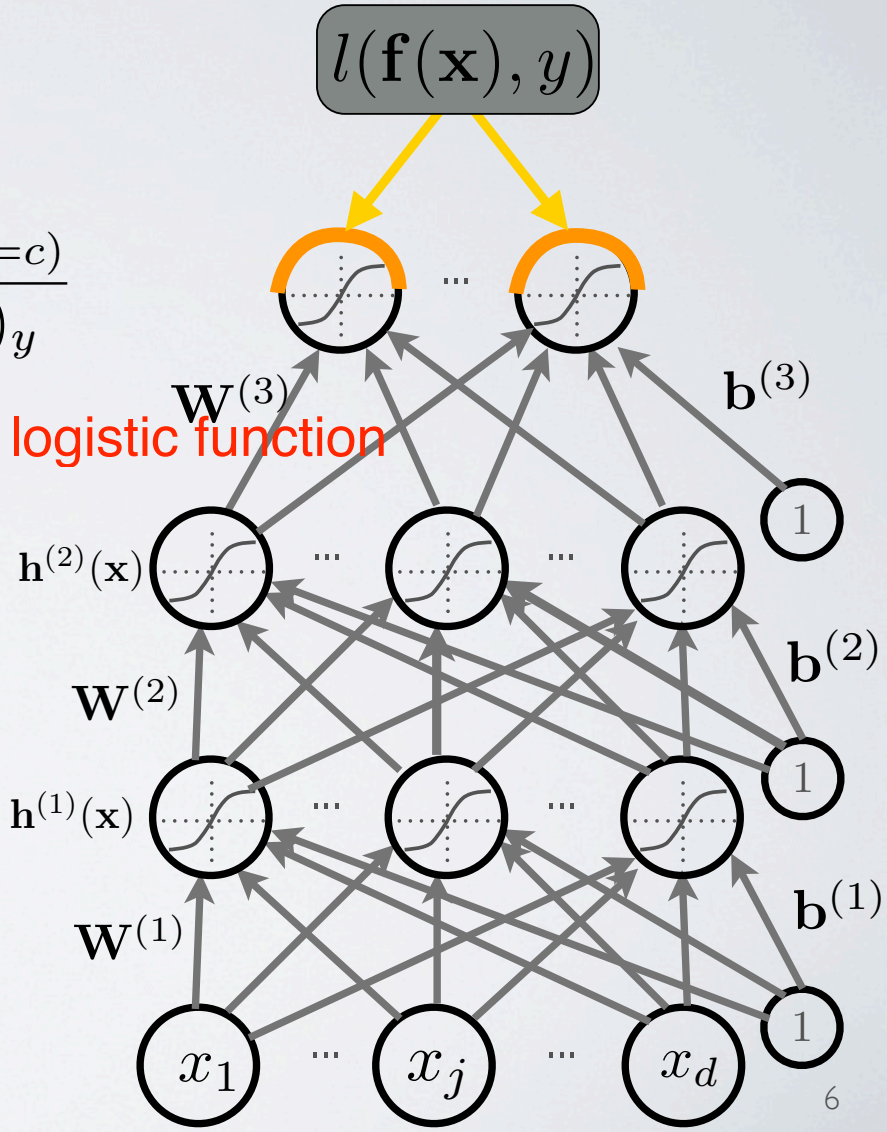
f here is softmax, or logistic function

- 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

Topics: loss gradient at output (before activation)

- Partial derivative:

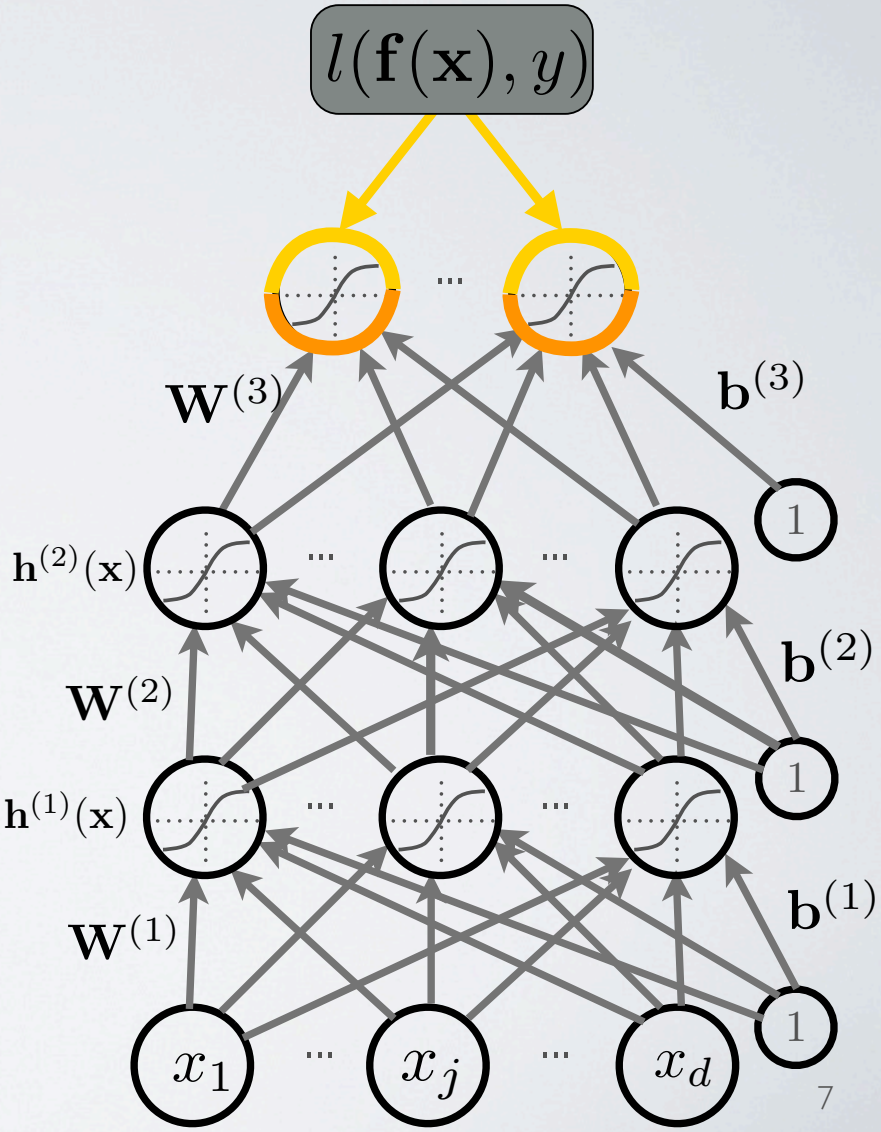
$$\frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} - \log f(\mathbf{x})_y$$

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

- Gradient:

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

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



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

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

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

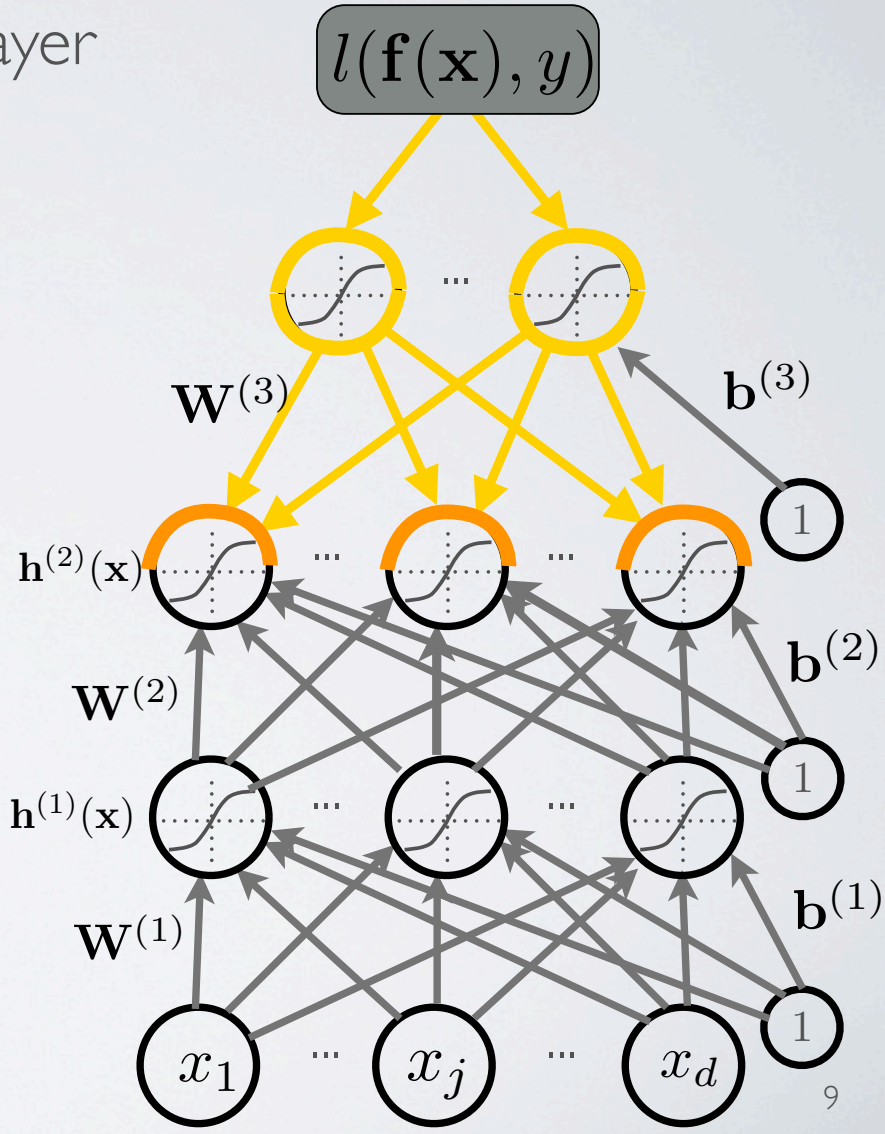
$$
\begin{aligned}
& \frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} - \log f(\mathbf{x})_y \\
= \quad & \frac{-1}{f(\mathbf{x})_y} \frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} f(\mathbf{x})_y \\
= \quad & \frac{-1}{f(\mathbf{x})_y} \frac{\partial}{\partial a^{(L+1)}(\mathbf{x})_c} \text{softmax}(\mathbf{a}^{(L+1)}(\mathbf{x}))_y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

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

LOSS FUNCTION

Topics: loss gradient at hidden layer

- ... this is getting complicated!!



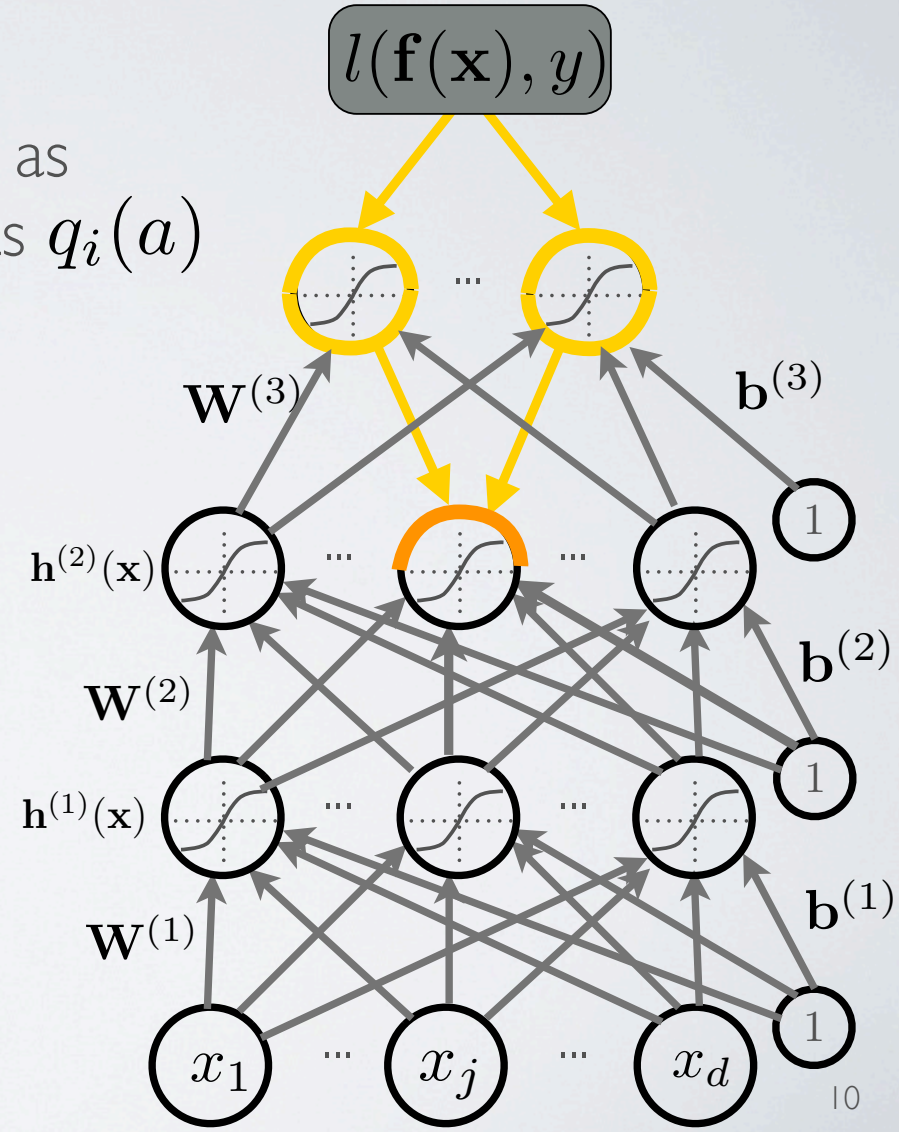
LOSS FUNCTION

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 input of units in the layer above
  - $p(a)$ is the loss function



LOSS FUNCTION

Topics: loss gradient at hidden layers

- Partial derivative:

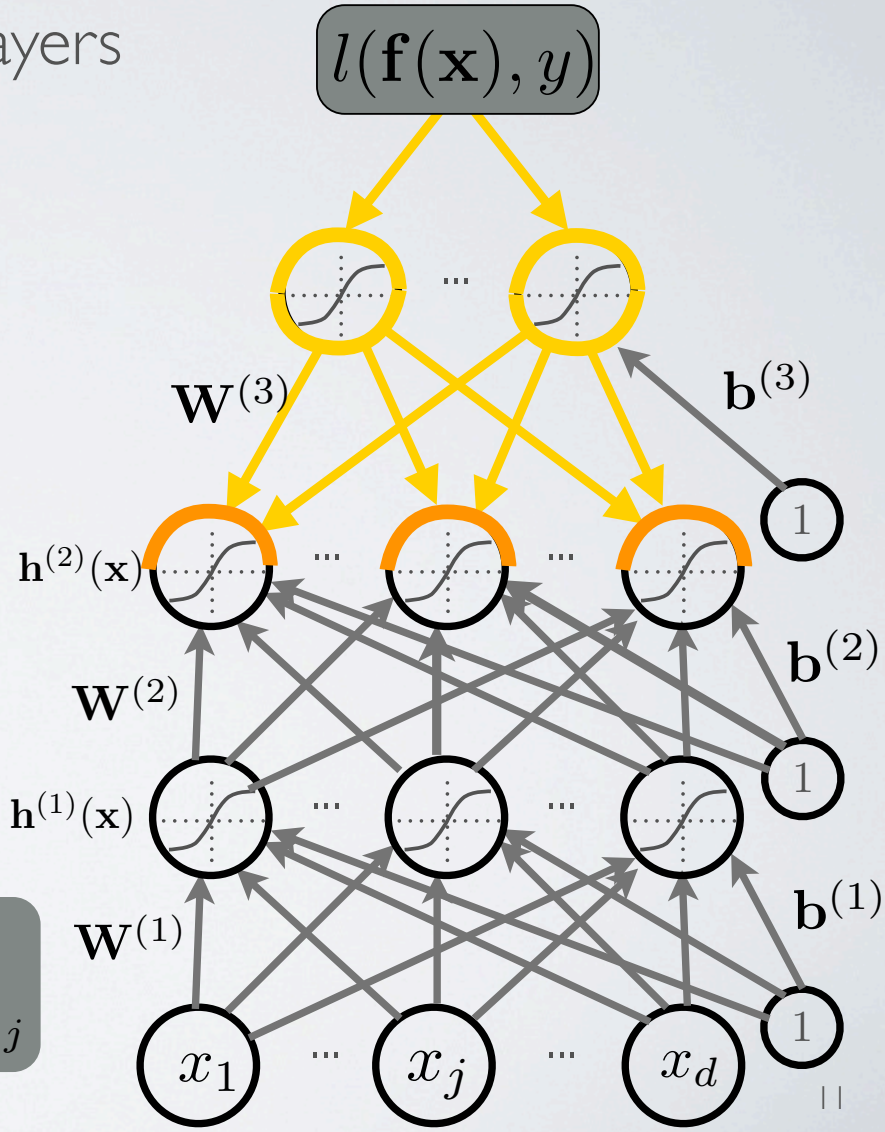
$$\frac{\partial}{\partial h^{(k)}(\mathbf{x})_j} - \log f(\mathbf{x})_y$$

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

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

REMINDER

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



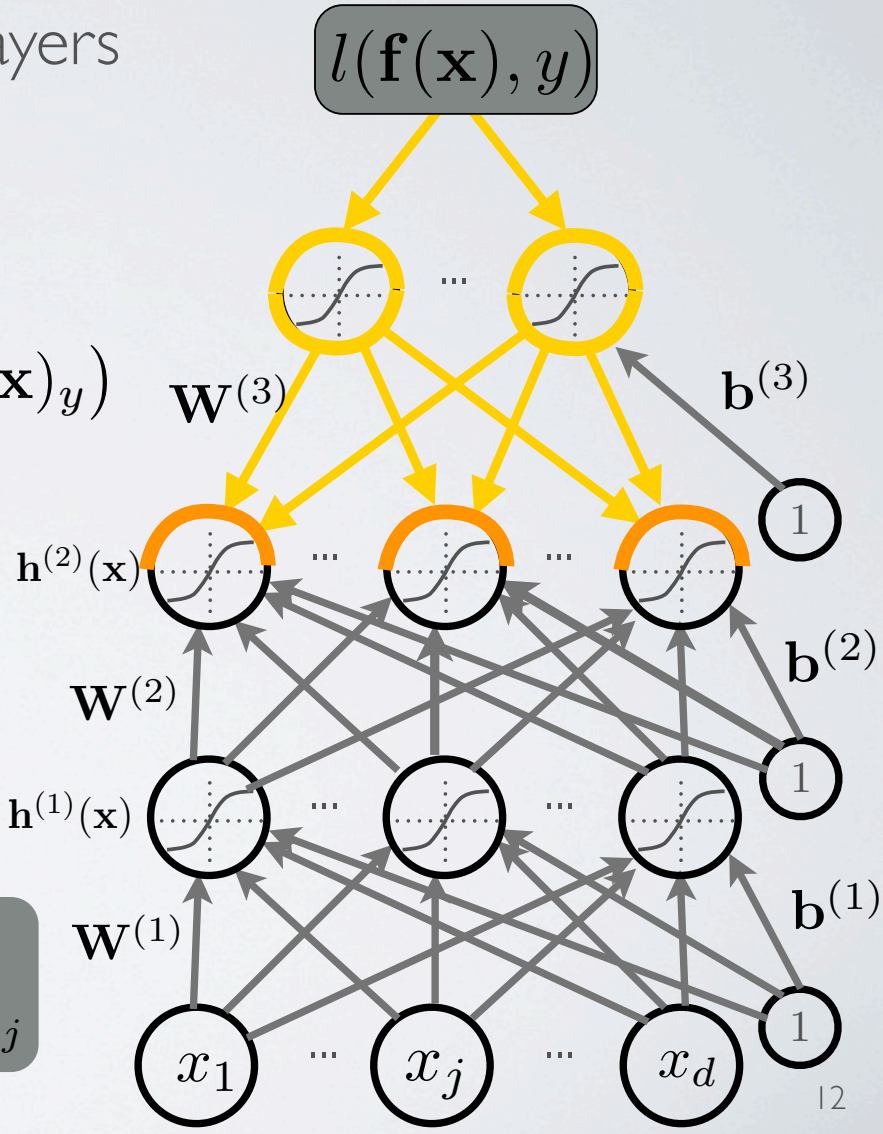
LOSS FUNCTION

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

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

LOSS FUNCTION

Topics: loss gradient at hidden layers (before activation)

- Partial derivative:

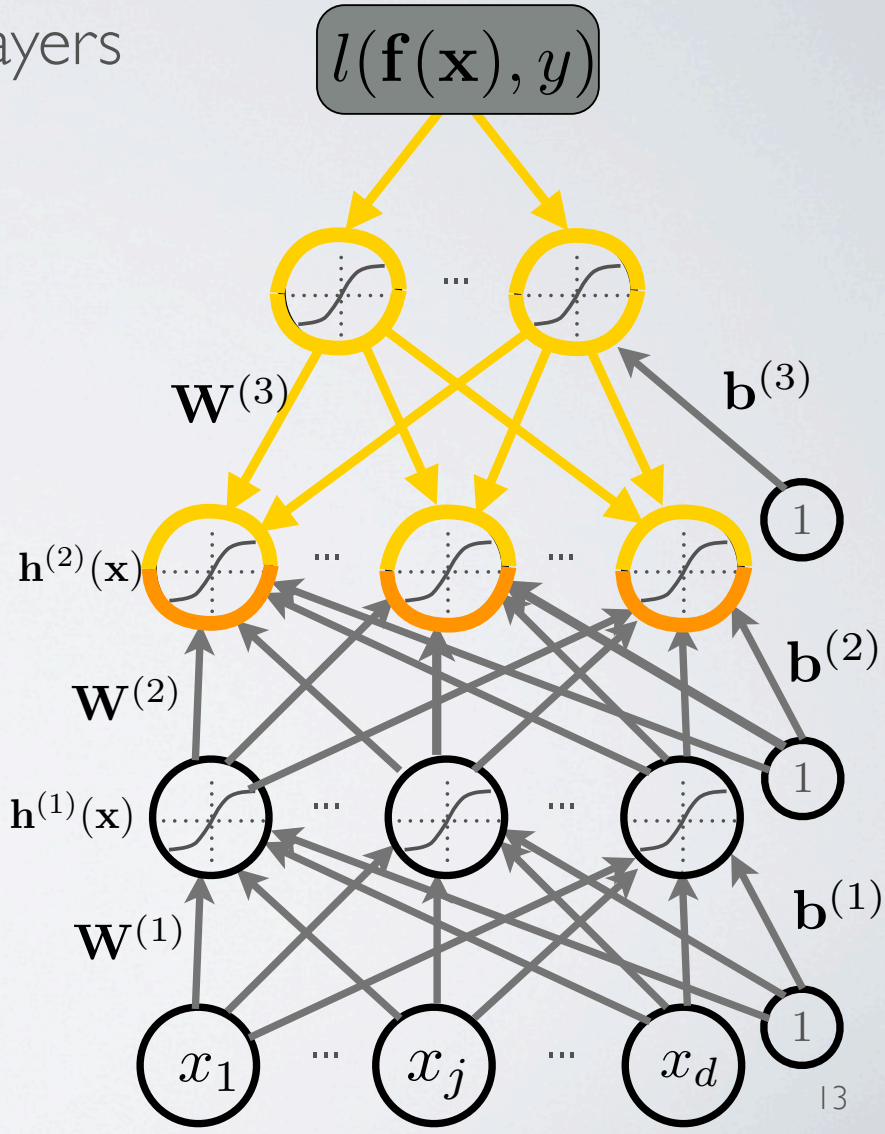
$$\frac{\partial}{\partial a^{(k)}(\mathbf{x})_j} - \log f(\mathbf{x})_y$$

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

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

REMINDER

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



LOSS FUNCTION

Topics: loss gradient at hidden layers (before activation)

- Gradient:

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

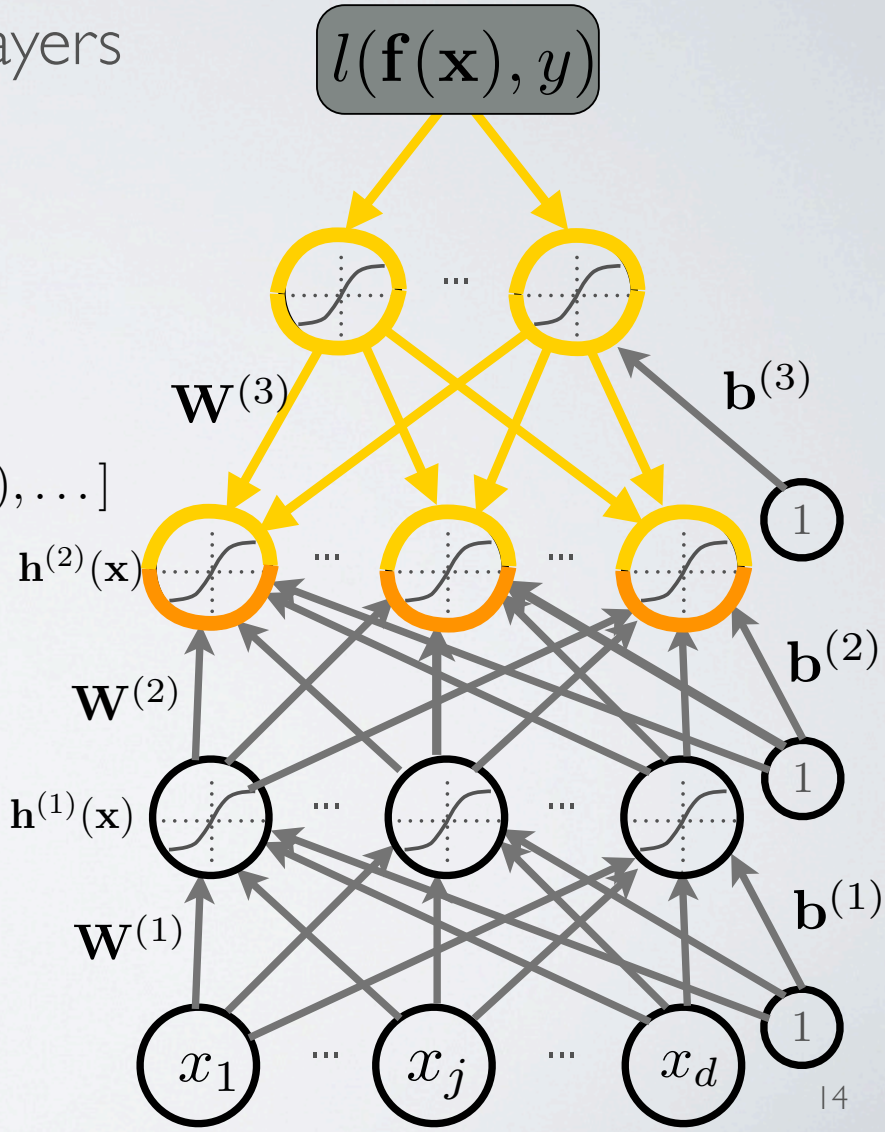
$$= \left(\nabla_{\mathbf{h}^{(k)}(\mathbf{x})} - \log f(\mathbf{x})_y\right)^\top \nabla_{\mathbf{a}^{(k)}(\mathbf{x})} \mathbf{h}^{(k)}(\mathbf{x})$$

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

element-wise product

REMINDER

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



LOSS FUNCTION

Topics: loss gradient of parameters

- Partial derivative (weights):

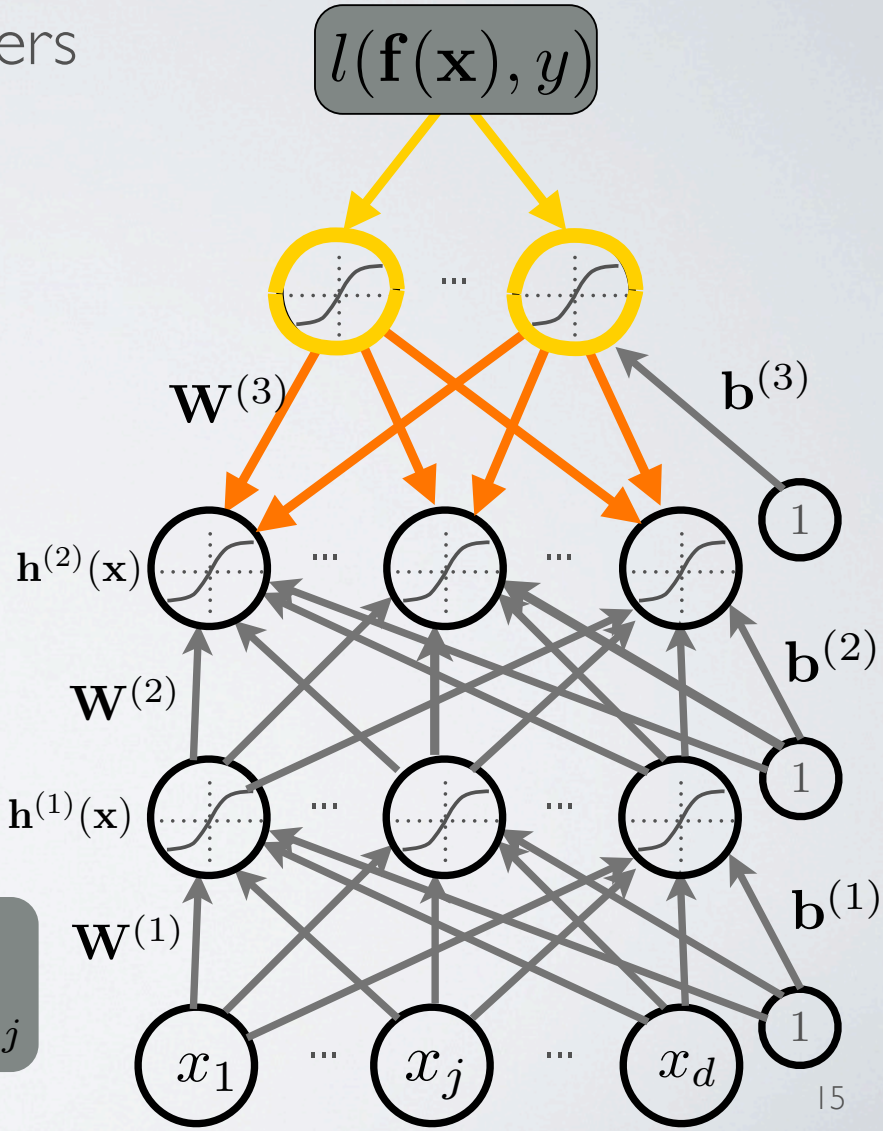
$$\frac{\partial}{\partial W_{i,j}^{(k)}} - \log f(\mathbf{x})_y$$

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

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

REMINDER

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

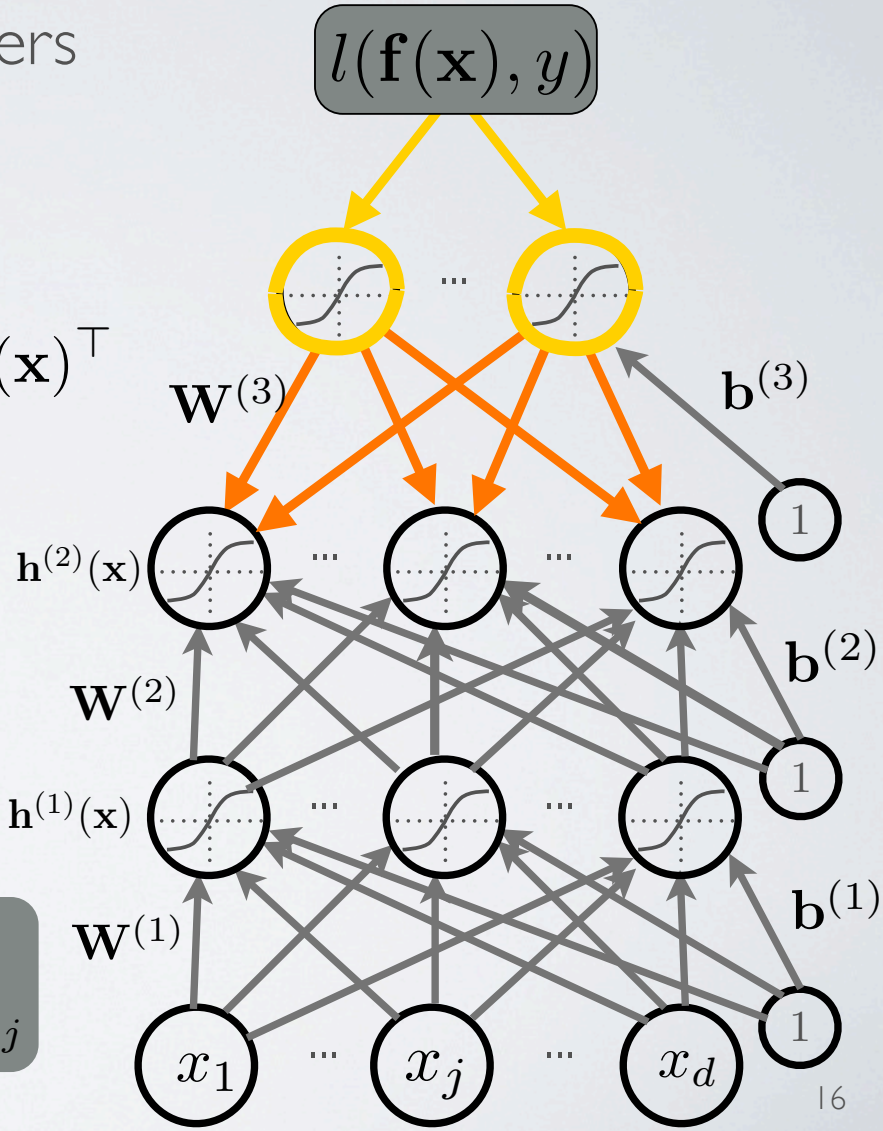


LOSS FUNCTION

Topics: loss gradient of parameters

- Gradient (weights):

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



REMINDER

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

LOSS FUNCTION

Topics: loss gradient of parameters

- Partial derivative (biases):

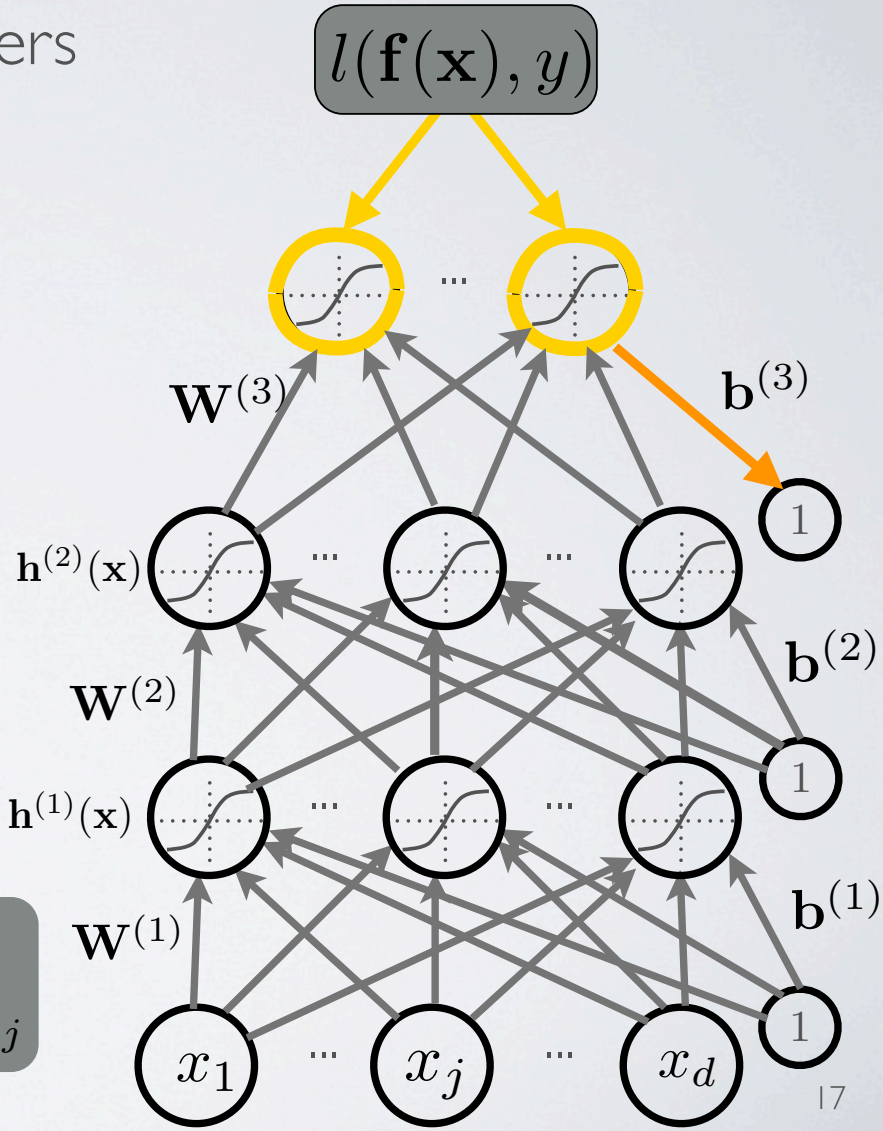
$$\frac{\partial}{\partial b_i^{(k)}} - \log f(\mathbf{x})_y$$

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

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

REMINDER

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

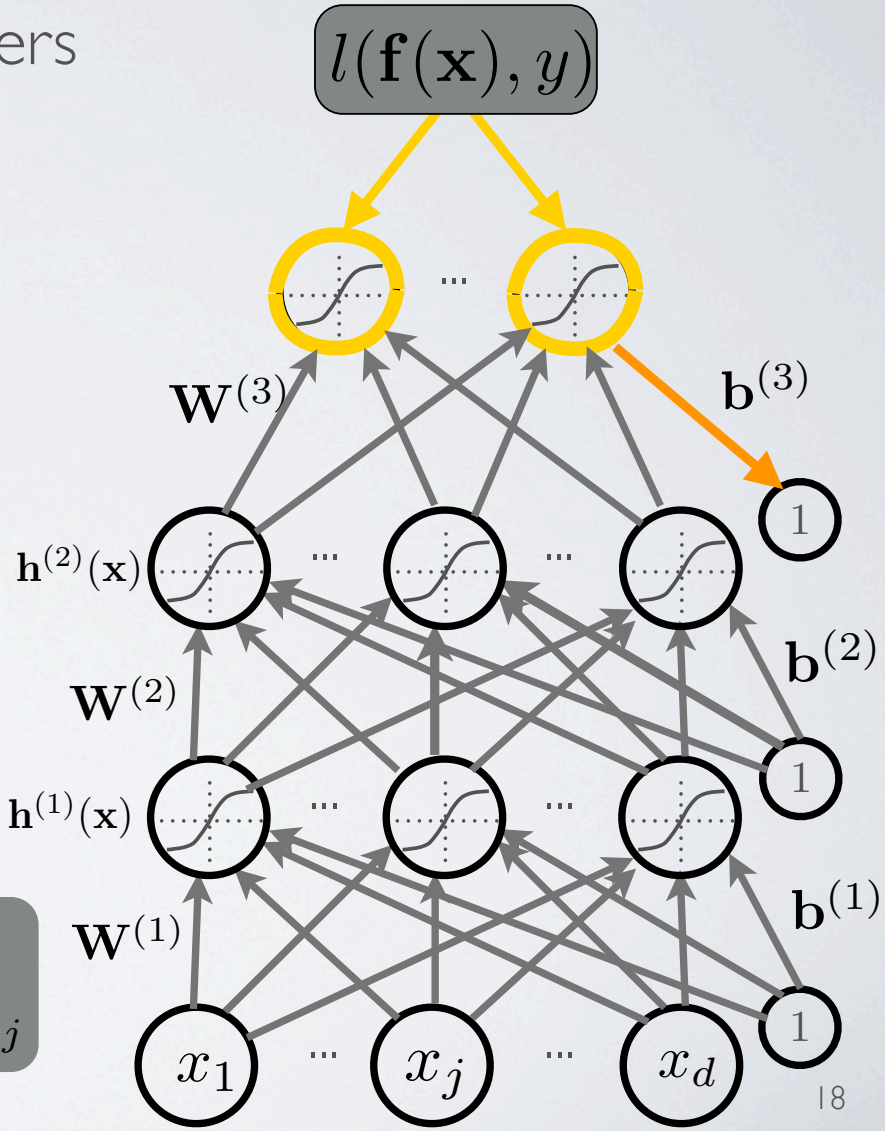


LOSS FUNCTION

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

- compute output gradient (before activation)

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

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

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

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

  - compute gradient of hidden layer below

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

  - compute gradient of hidden layer below (before activation)

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

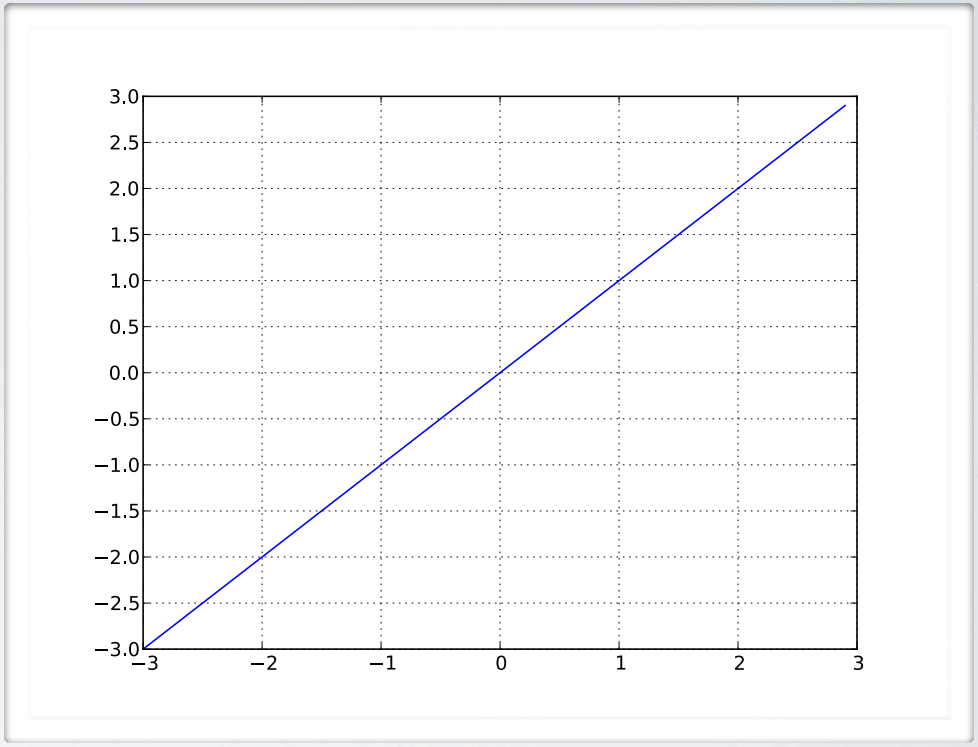
- This assumes a forward propagation has been made before

ACTIVATION FUNCTIONS

Topics: linear activation function gradient

- Partial derivative:

$$g'(a) = 1$$



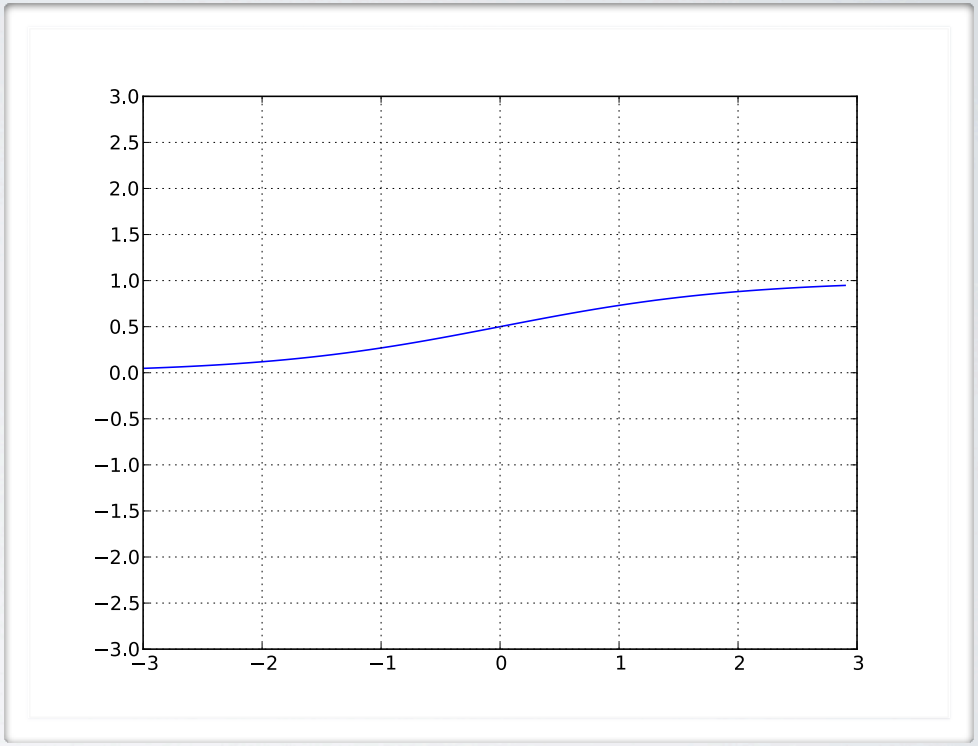
$$g(a) = a$$

ACTIVATION FUNCTIONS

Topics: sigmoid activation function gradient

- Partial derivative:

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



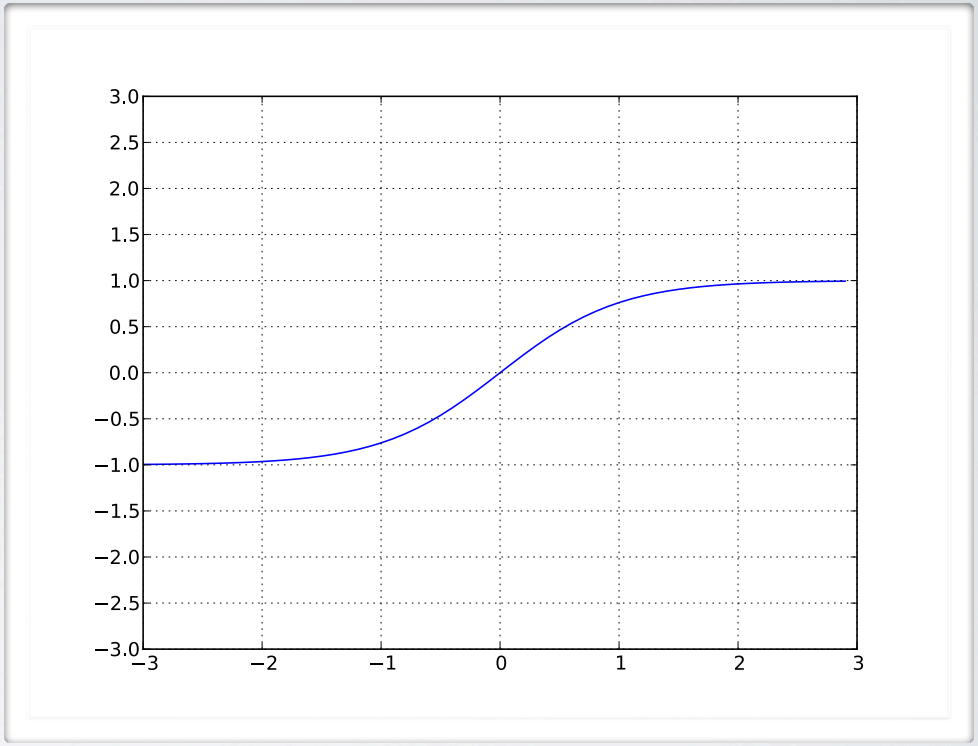
$$g(a) = \text{sigm}(a) = \frac{1}{1+\exp(-a)}$$

ACTIVATION FUNCTIONS

Topics: tanh activation function gradient

- Partial derivative:

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



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

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

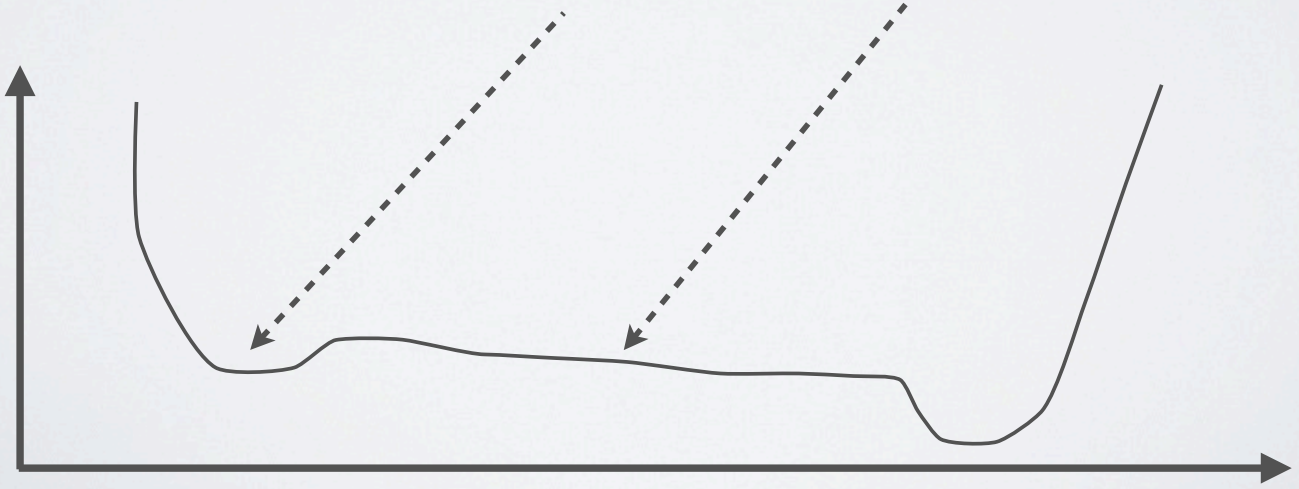
size of $\mathbf{h}^{(k)}(\mathbf{x})$

    - 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)

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



OPTIMIZATION

Topics: local optimum, global optimum, plateau

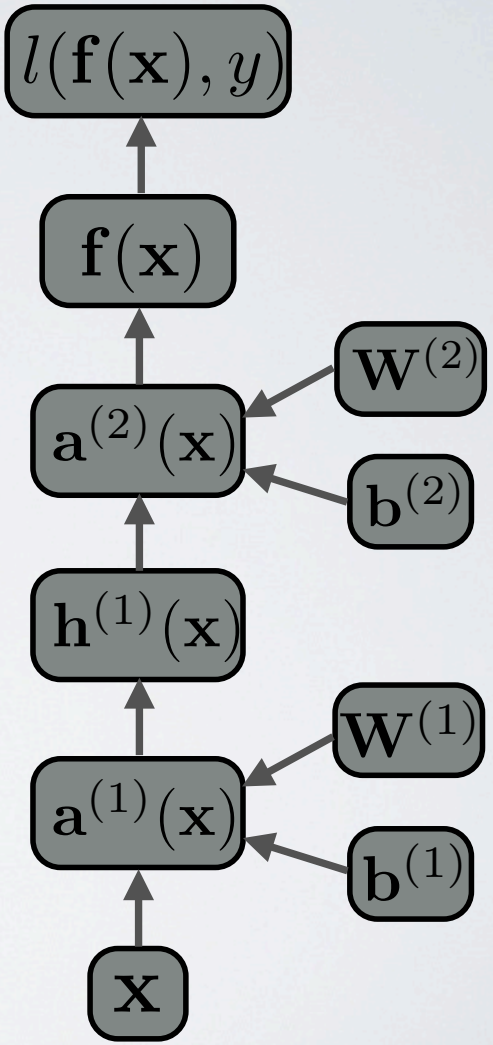
Neural network training demo

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

FLOW GRAPH

Topics: flow graph

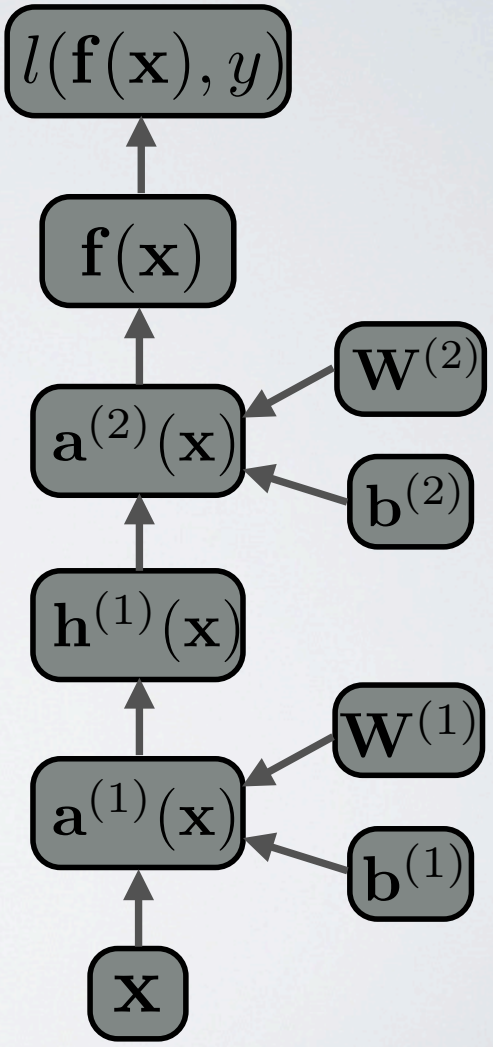
- Forward propagation can be representated as an acyclic flow graph
- It's a nice way of implementing forward propagation in a modular way
  - each box is an object with an fprop method, that outputs the value of the box given its children
  - calling the fprop method of each box in the right order yield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



FLOW GRAPH

Topics: automatic differentiation

- Each object also has a bprop method
  - it outputs the gradient of the loss given 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



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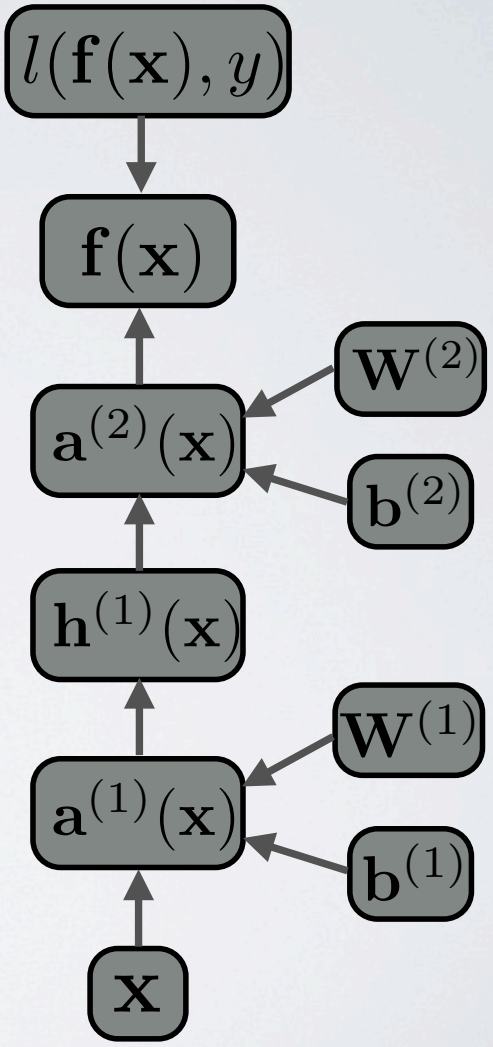

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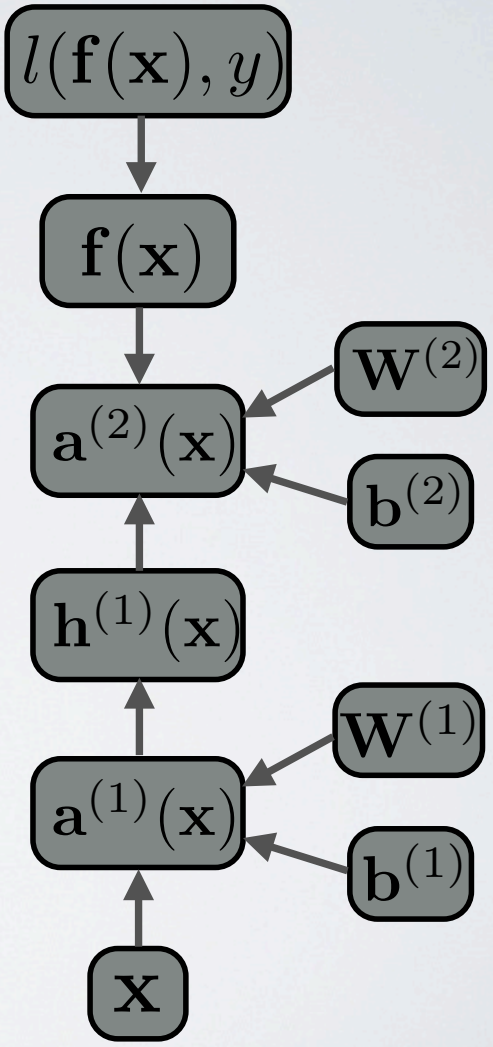

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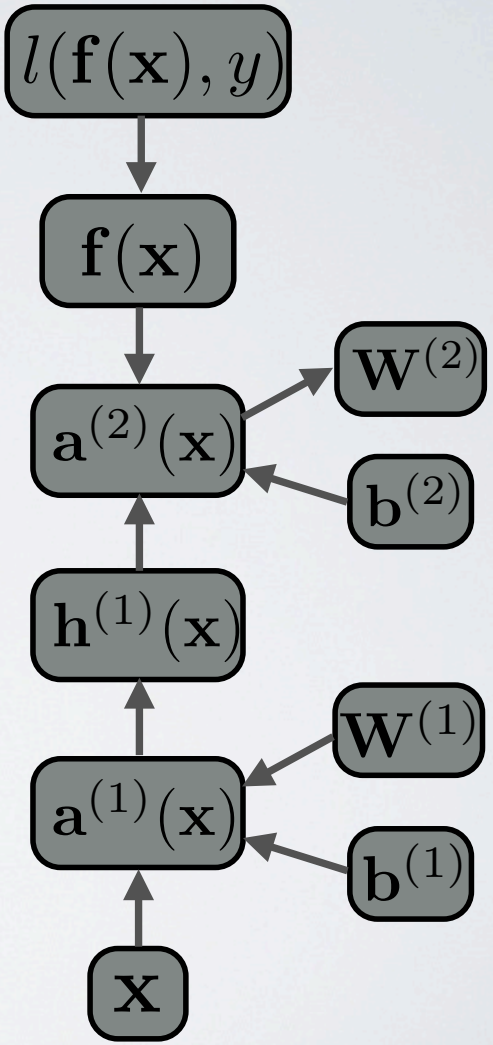

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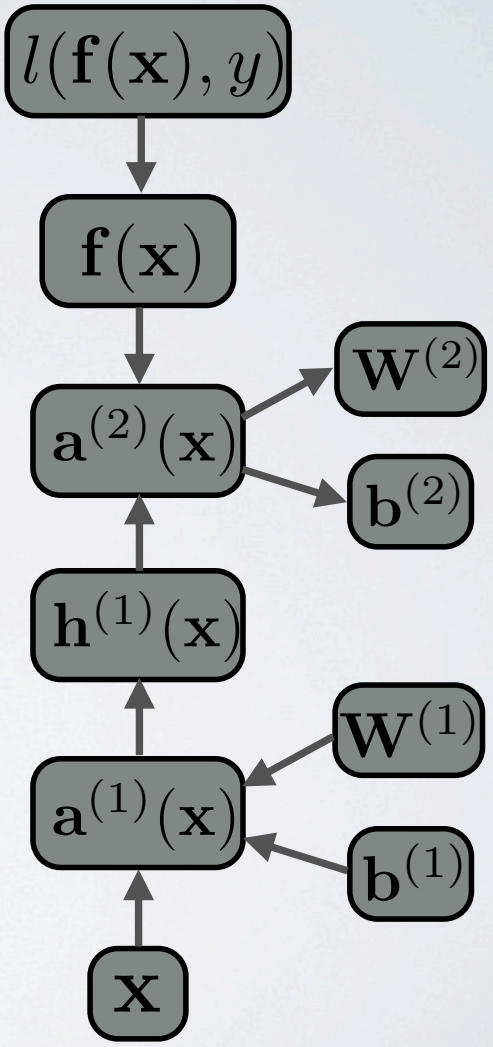

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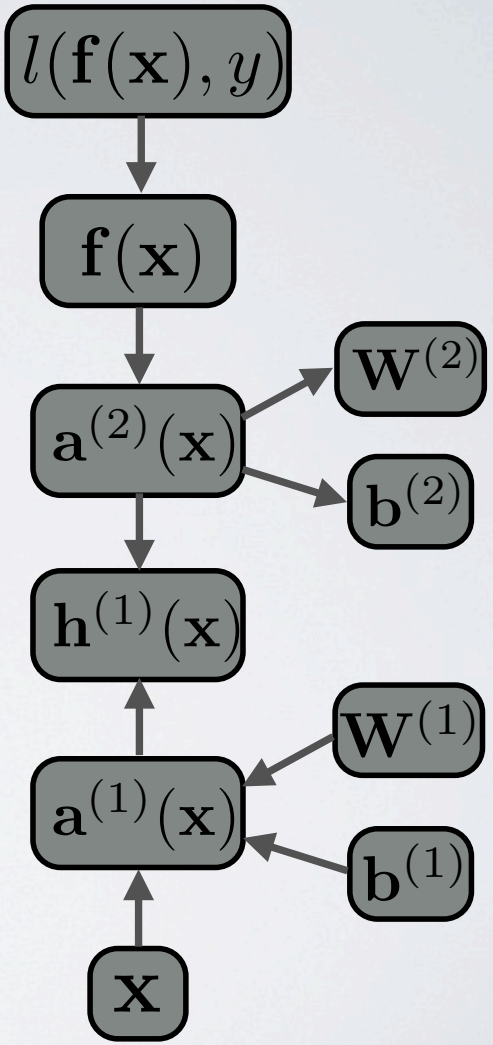

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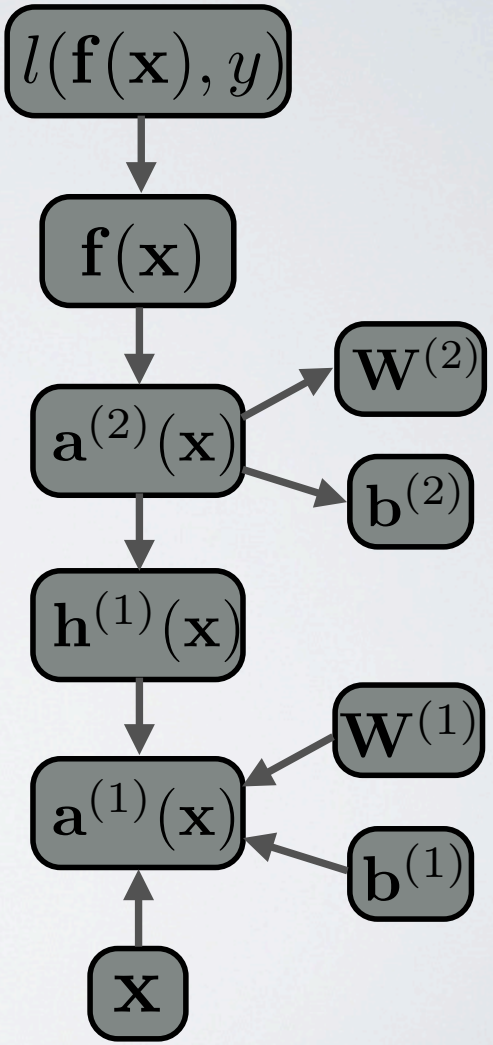

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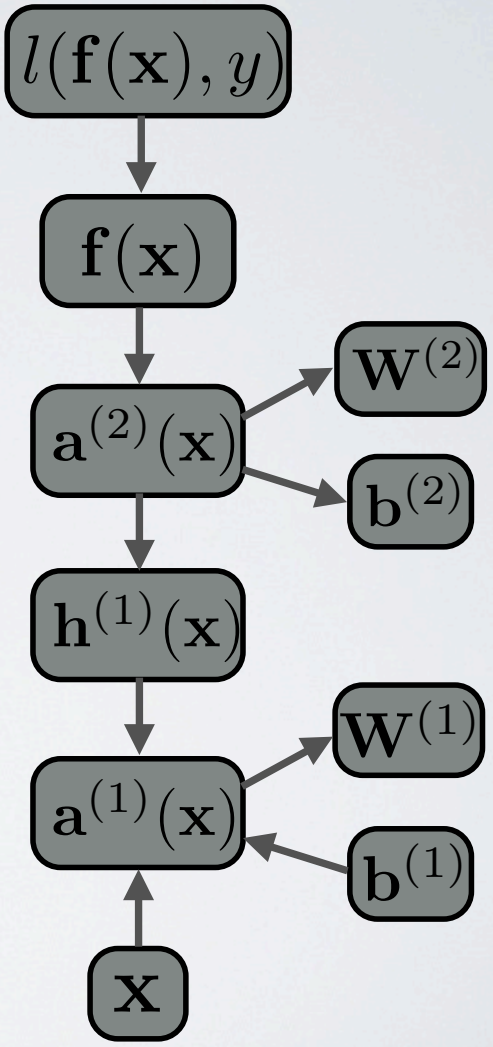

FLOW GRAPH

Topics: automatic differentiation

- Each object also has a bprop method
  - it outputs the gradient of the loss given 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