

Advanced Machine Learning from Theory to Practice

Lecture 10

Introduction to Neural Networks

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Fall 2015

1 Introduction

2 Supervised Learning

3 (Deep) Neural Networks

4 Perceptron

5 Multilayer Perceptron

6 Backprop Algorithm

Spam detection (Text classification)



- Data: email collection
- Input: email
- Output : Spam or No Spam

Introduction

Motivation

Face Detection



- Data: Annotated database of images
- Input : Sub window in the image
- Output : Presence or no of a face...

Introduction

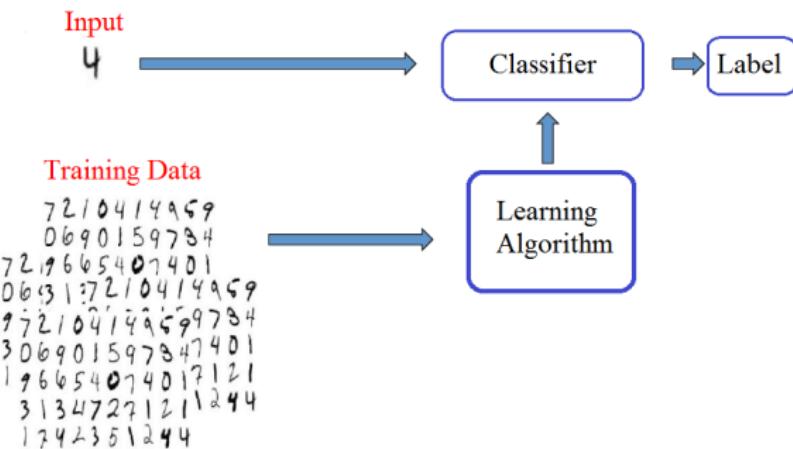
Motivation

Number Recognition

0	0	0	0	0
1	1	1	1	1
2	2	2	2	2
3	3	3	3	3
4	4	4	4	4
5	5	5	5	5
6	6	6	6	6
7	7	7	7	7
8	8	8	8	8
9	9	9	9	9

- Data: Annotated database of images (each image is represented by a vector of $28 \times 28 = 784$ pixel intensities)
- Input: Image
- Output: Corresponding number

Introduction 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.

1 Introduction

2 Supervised Learning

3 (Deep) Neural Networks

4 Perceptron

5 Multilayer Perceptron

6 Backprop Algorithm

Supervised Learning

Outline

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- 2 Supervised Learning
- 3 (Deep) Neural Networks
- 4 Perceptron
- 5 Multilayer Perceptron
- 6 Backprop Algorithm

Supervised Learning

Supervised Learning

Supervised Learning Framework

- Input measurement $\mathbf{X} = (X^{(1)}, X^{(2)}, \dots, X^{(d)}) \in \mathcal{X}$
- Output measurement $Y \in \mathcal{Y}$.
- $(\mathbf{X}, Y) \sim \mathbf{P}$ with \mathbf{P} unknown.
- **Training data** : $\mathcal{D}_n = \{(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)\}$ (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 $\mathcal{F} = \{f : \mathcal{X} \rightarrow \mathcal{Y} \text{ measurable}\}$

Goal

- Construct a **good** classifier \hat{f} from the training data.
- Need to specify the meaning of **good**.
- Formally, classification and regression are the same problem!

Supervised Learning

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:

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

- Examples:
 - Prediction loss: $\mathbb{E} [\ell(Y, f(\mathbf{X}))] = \mathbb{P} \{ Y \neq f(\mathbf{X}) \}$
 - Quadratic loss: $\mathbb{E} [\ell(Y, f(\mathbf{X}))] = \mathbb{E} [|Y - f(\mathbf{X})|^2]$
- **Beware:** As \hat{f} depends on \mathcal{D}_n , $\mathcal{R}(\hat{f})$ is a random variable!

Supervised Learning

Supervised Learning

Experience, Task and Performance measure

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

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

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

Supervised Learning

Best Solution

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

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

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} !

Supervised Learning

Goal

Machine Learning

- Learn a rule to construct a classifier $\hat{f} \in \mathcal{F}$ from the training data \mathcal{D}_n s.t. the risk $\mathcal{R}(\hat{f})$ 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

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

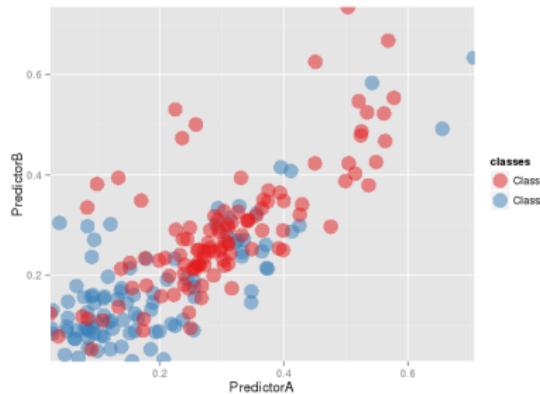
- Examples:
 - Linear regression
 - Linear discrimination with
$$\mathcal{S} = \{\mathbf{x} \mapsto \operatorname{sign}\{\beta^T \mathbf{x} + \beta_0\} / \beta \in \mathbb{R}^d, \beta_0 \in \mathbb{R}\}$$

Supervised Learning

Example: TwoClass Dataset

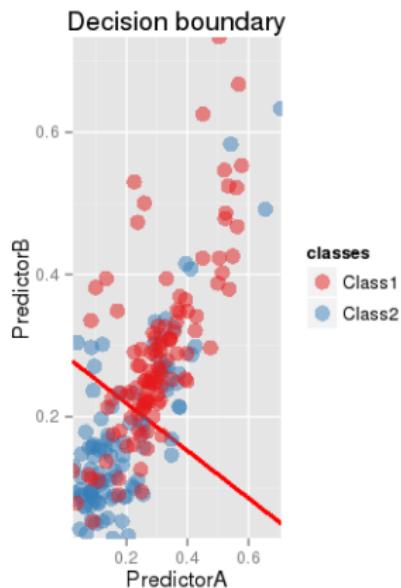
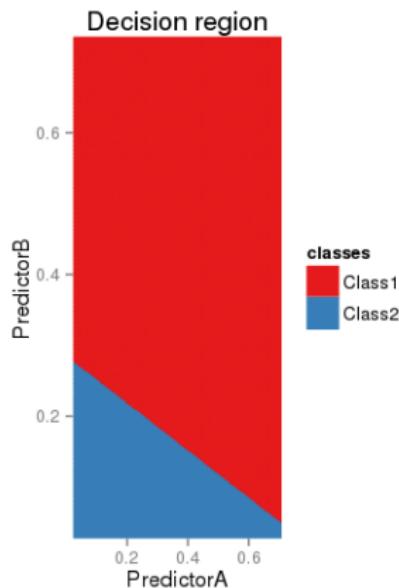
Synthetic Dataset

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



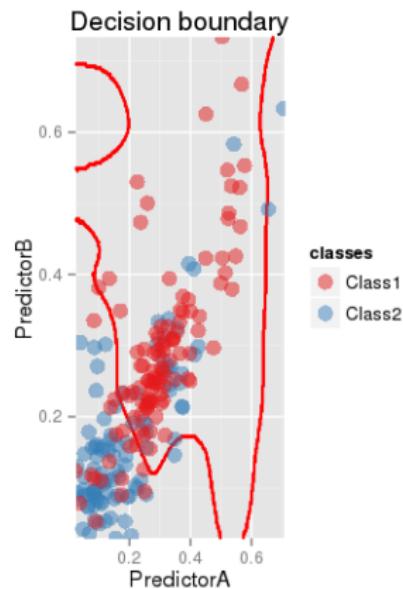
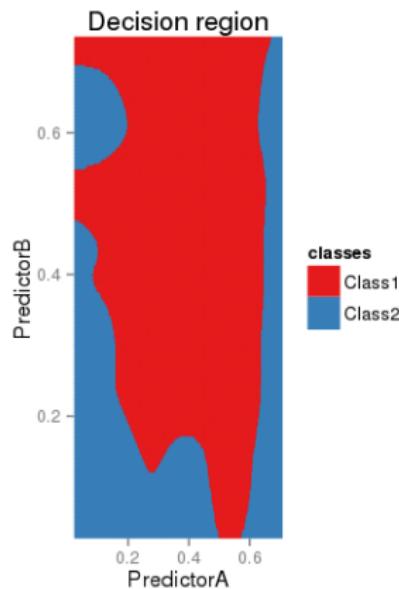
Supervised Learning

Example: Linear Discrimination



Supervised Learning

Example: More complex model

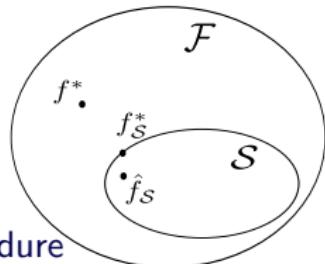


Supervised Learning

Bias-Variance Dilemma

- General setting:

- $\mathcal{F} = \{\text{measurable functions } \mathcal{X} \rightarrow \mathcal{Y}\}$
- Best solution: $f^* = \operatorname{argmin}_{f \in \mathcal{F}} \mathcal{R}(f)$
- Class $\mathcal{S} \subset \mathcal{F}$ of functions
- Ideal target in \mathcal{S} : $f_S^* = \operatorname{argmin}_{f \in \mathcal{S}} \mathcal{R}(f)$
- Estimate in \mathcal{S} : \hat{f}_S obtained with some procedure



Approximation error and estimation error (Bias/Variance)

$$\mathcal{R}(\hat{f}_S) - \mathcal{R}(f^*) = \underbrace{\mathcal{R}(f_S^*) - \mathcal{R}(f^*)}_{\text{Approximation error}} + \underbrace{\mathcal{R}(\hat{f}_S) - \mathcal{R}(f_S^*)}_{\text{Estimation error}}$$

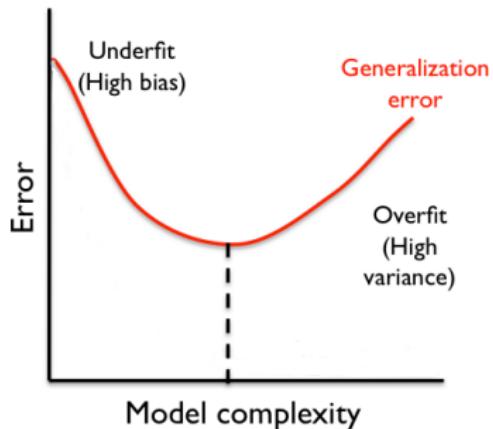
- Approx. error can be large if the model \mathcal{S} is not suitable.
- Estimation error can be large if the model is complex.

Agnostic approach

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

Supervised Learning

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 \iff avoid overfitting and underfitting

Supervised Learning

Statistical and Optimization Point of View Framework

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

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

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

Problems

- How to choose 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

(Deep) Neural Networks

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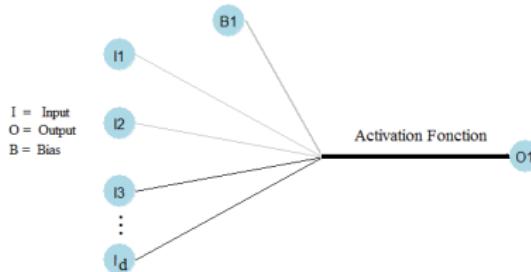
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(Deep) Neural Networks

Artificial Neuron and Logistic Regression

Activation Neuron Configuration



Artificial neuron

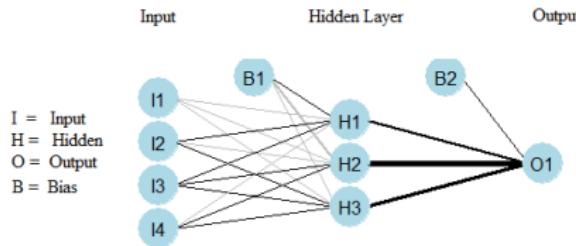
- Structure:
 - Mix inputs with a weighted sum,
 - Apply a (non linear) activation function to this sum,
 - Eventually threshold the result to make a decision.
- Weights learned by minimizing a loss function.

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.

(Deep) Neural Networks

Neural network



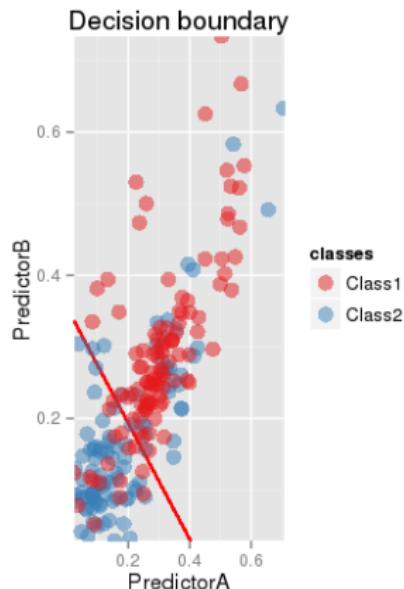
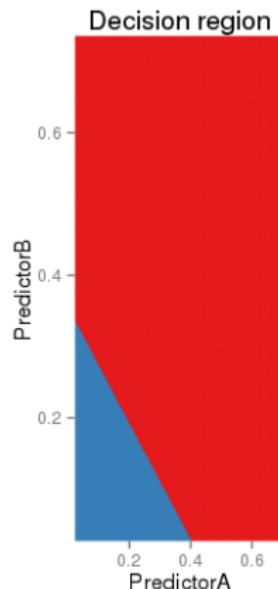
Neural network structure

- 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 (Back propagation)
- Non convex and thus may be trapped in local minima.

(Deep) Neural Networks

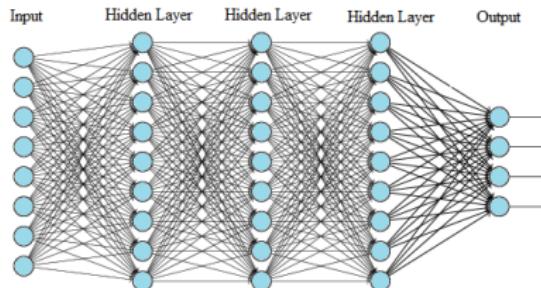
Neural network

Neural Network



(Deep) Neural Networks

Deep Neural Network



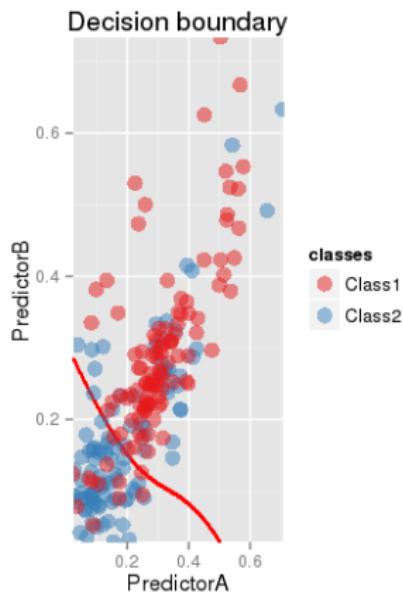
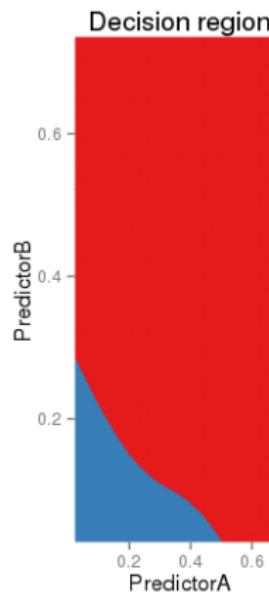
Deep Neural Network structure

- Deep cascade of layers!
- No conceptual novelty optimization becomes a crucial issue.
- Clever initialization, clever stochastic optimization, clever use of GPU...
- Very impressive results!

(Deep) Neural Networks

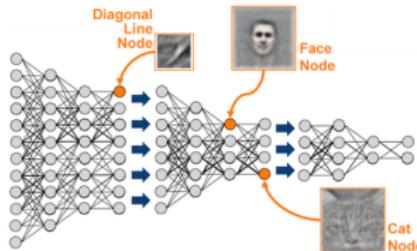
Deep Neural Network

H2O NN



(Deep) Neural Networks

Deep Learning



Family of Machine Learning algorithm combining:

- a (deep) multilayered structure,
- a clever (often unsupervised) initialization,
- a clever stochastic fine tuning optimization.
- Examples: Deep Neural Network, Deep (Restricted) Boltzman Machine, Stacked Encoder...
- Appears to be very efficient but lack of theoretical fundation!

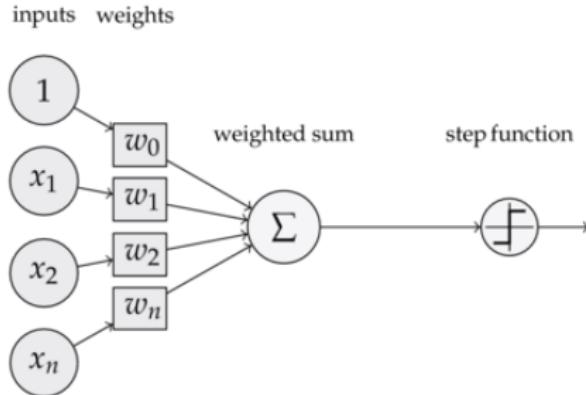
Perceptron

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Perceptron

Perceptron

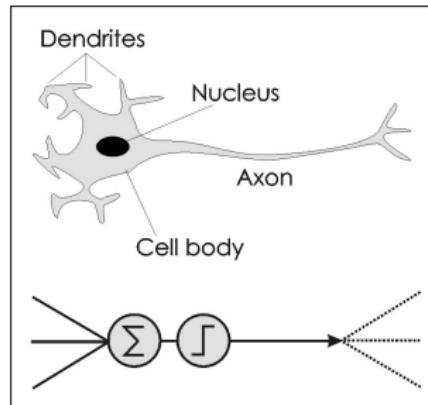


Perceptron (Rosenblatt 1957)

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

Perceptron

Perceptron

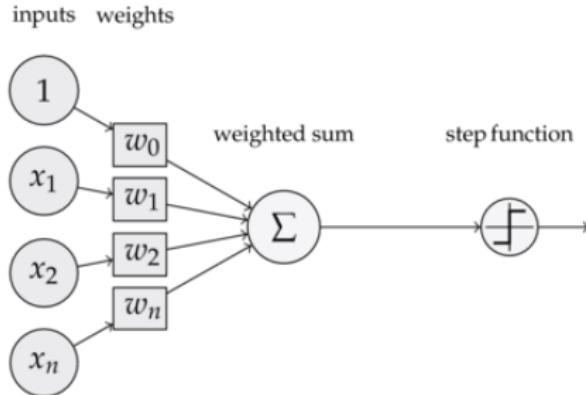


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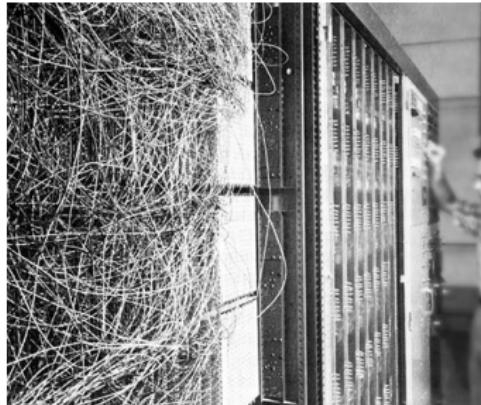


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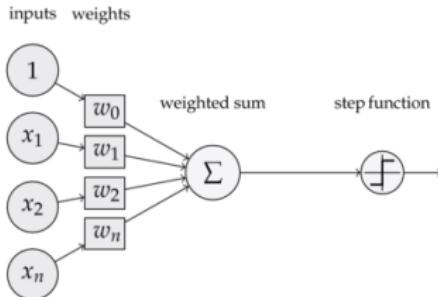


Perceptron (Rosenblatt 1957)

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

Perceptron

The Perceptron Algorithm



- Key contribution: first (iterative) learning algorithm!

Algorithm

- Start with $w = 0$.
- Repeat over all samples:
 - if $\langle w, \mathbf{X}_i \rangle < Y_i < 0$ 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)

Perceptron

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,

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

while

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

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

$$\langle w^*, w_0 \rangle + t\rho \leq \|w^*\| (\|w_0\|^2 + tC^2)$$

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

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

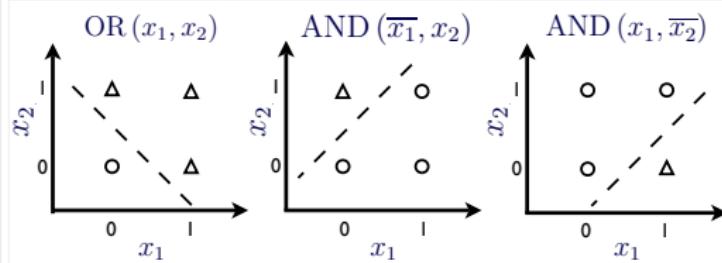
Perceptron

Perceptron Limitations

ARTIFICIAL NEURON

Topics: capacity of single neuron

- Can solve linearly separable problems



9

Limitations

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

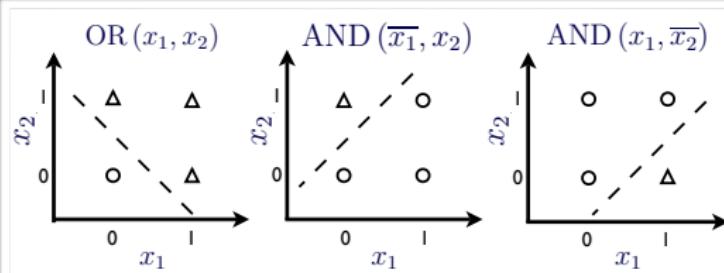
Perceptron

Perceptron Limitations

ARTIFICIAL NEURON

Topics: capacity of single neuron

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- Algorithm not robust to non linear separability!

Perceptron

Activation

- Prediction by $f(\mathbf{X}) = \varphi(\langle w, \mathbf{X} \rangle)$ (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:

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

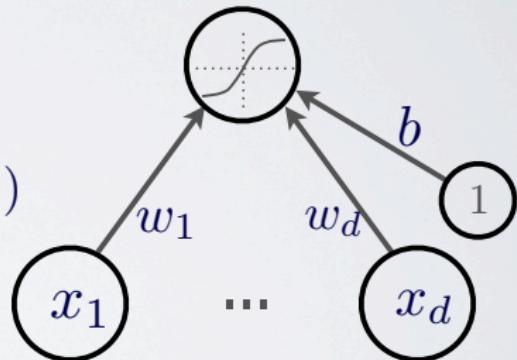
- Neuron (output) activation

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

- \mathbf{w} are the connection weights

- b is the neuron bias

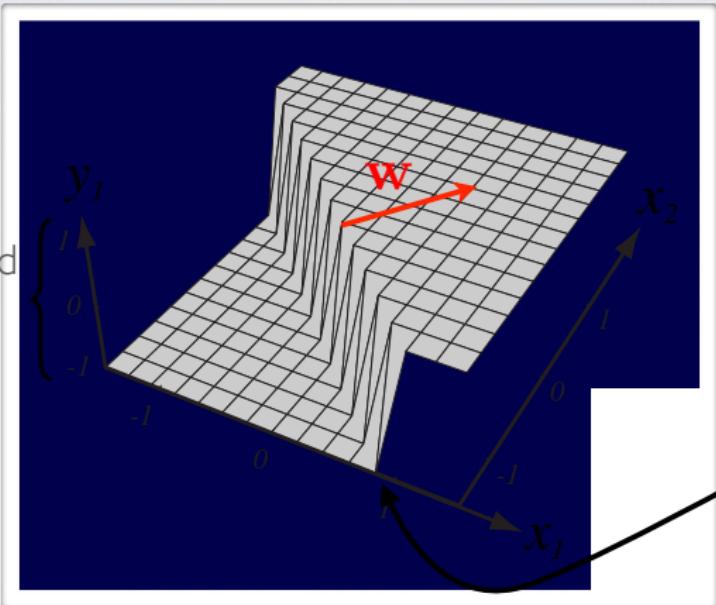
- $g(\cdot)$ is called the activation function



ARTIFICIAL NEURON

Topics: connection weights, bias, activation function

range determined
by $g(\cdot)$



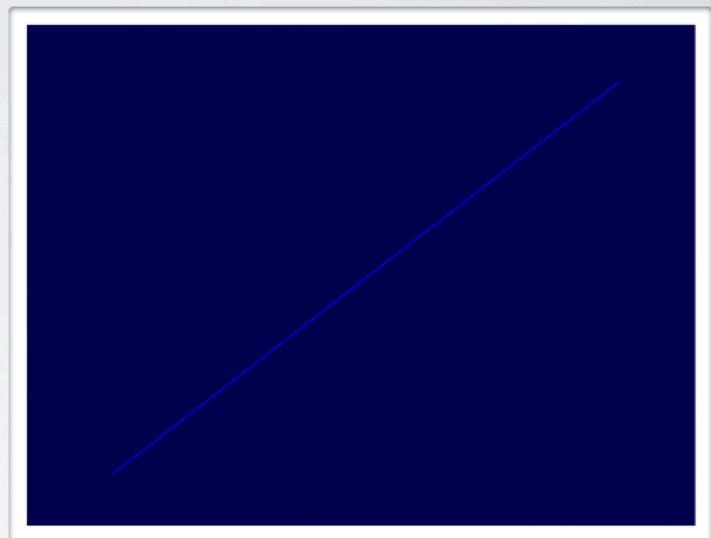
bias b only
changes the
position of
the rift

(from Pascal Vincent's slides)

ARTIFICIAL NEURON

Topics: linear activation function

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

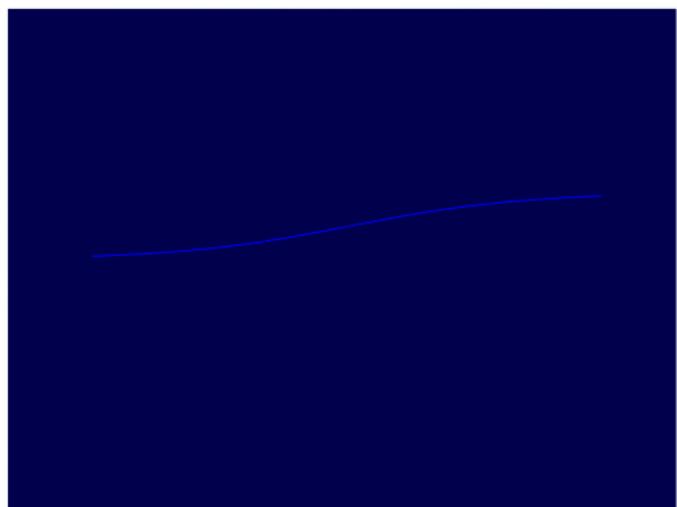


$$g(a) = a$$

ARTIFICIAL NEURON

Topics: sigmoid activation function

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

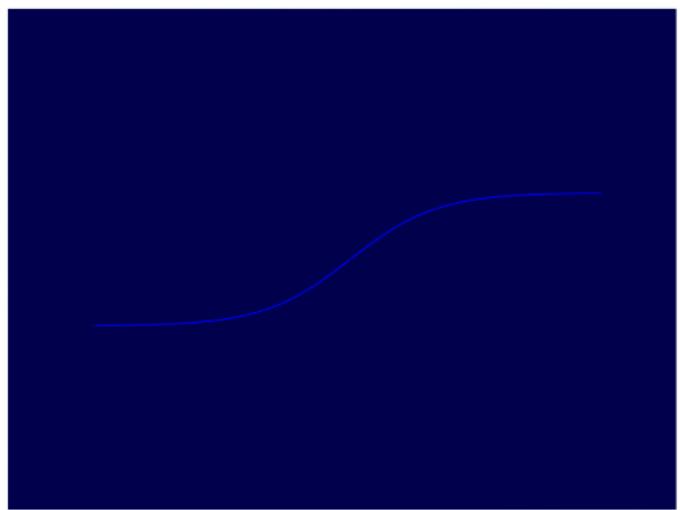


$$g(a) = \text{sigm}(a) = \frac{1}{1+\exp(-a)}$$

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

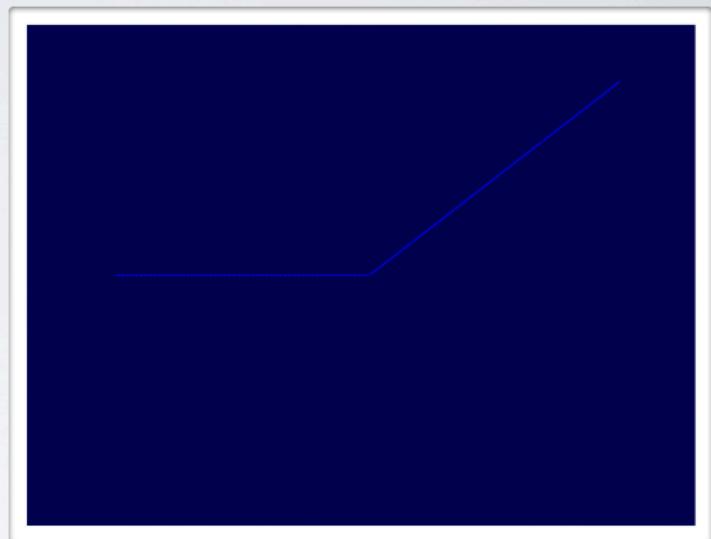


$$g(a) = \tanh(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} = \frac{\exp(2a) - 1}{\exp(2a) + 1}$$

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



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

Perceptron

Activation and Loss

- Prediction by $f(\mathbf{X}) = \varphi(\langle w, \mathbf{X} \rangle)$ (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...

Perceptron

Gradient Descent Algorithm

- Empirical risk minimization:

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

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

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

(Stochastic) Gradient descent rule:

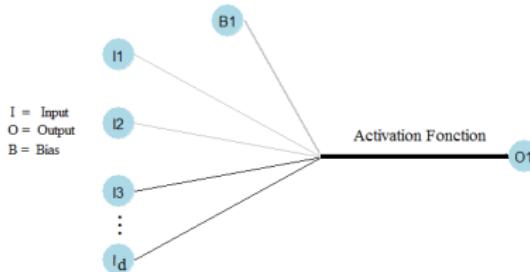
$$w_{t+1} = w_t - h_y \frac{1}{|I_t|} \sum_{i \in I_t} \nabla_i(w_t)$$

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

Perceptron

Logistic Perceptron

Activation Neuron Configuration



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,
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- Logistic weights learned by minimizing the -log-likelihood.

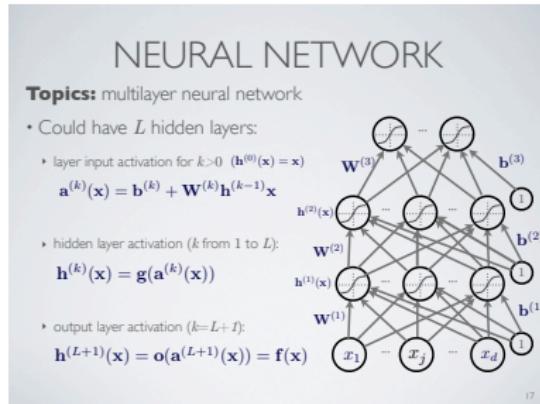
Multilayer Perceptron

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- 6 Backprop Algorithm

Multilayer Perceptron

Multilayer Perceptron



MLP (Rumelhart, McClelland, Hinton - 1986)

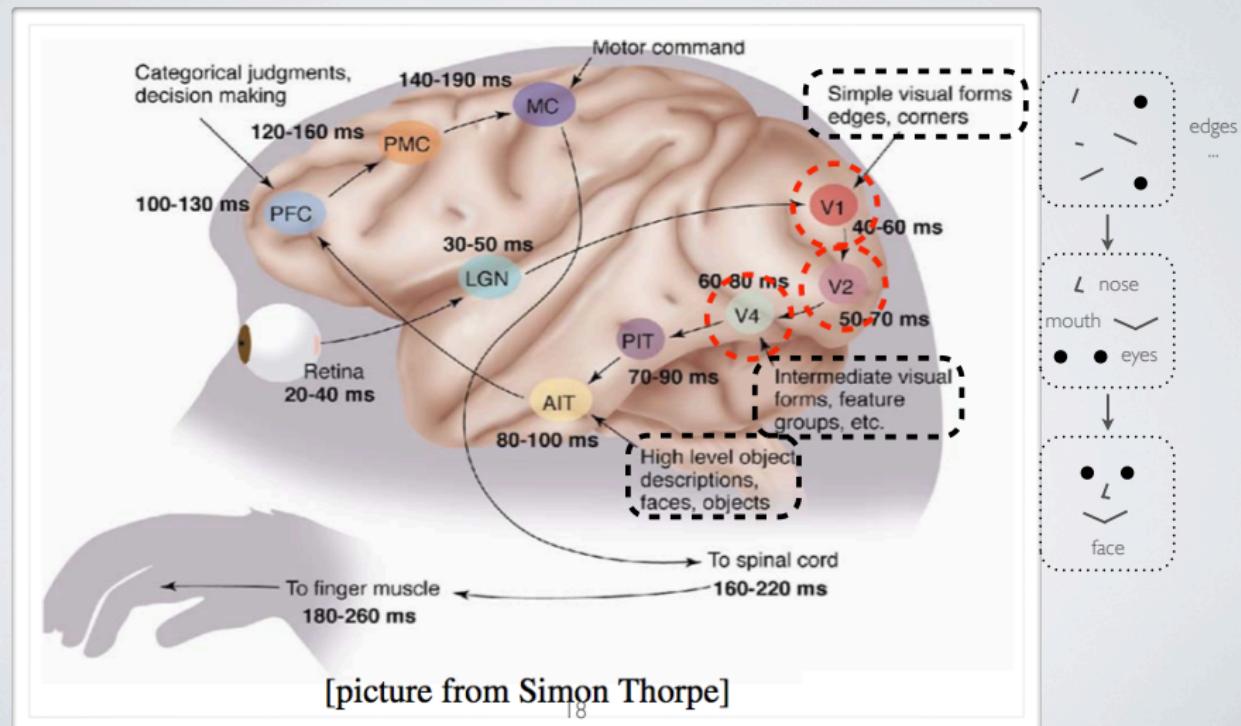
- Multilayer Perceptron: cascade of layers of artificial neuron units.
- Backprop algorithm to optimize it!
- Construction of a function by composing simple units.
- MLP corresponds to a specific direct acyclic graph structure.

Universal Approximation Theorem (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 activation functions.
- A single hidden layer is sufficient but more may be more efficient.
- No bounds on the number of required units... (Asymptotic flavour)

NEURAL NETWORK

Topics: parallel with the visual cortex



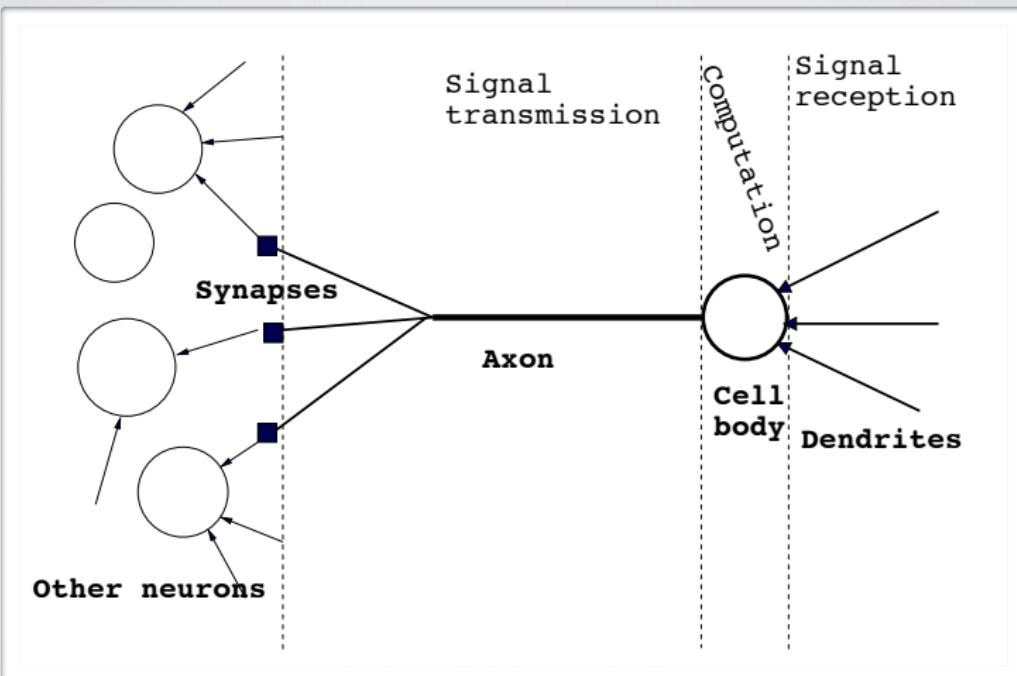
BIOLOGICAL NEURONS

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
 - they “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

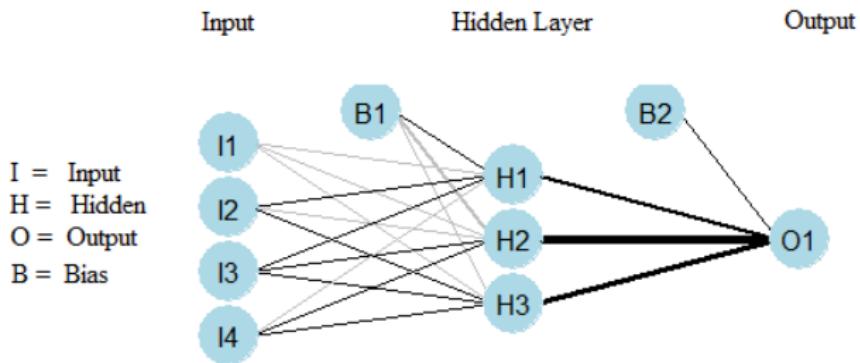
- An action potential is an electrical impulse that travels through the axon:
 - ▶ this is how neurons communicate
 - ▶ it generates a “spike” in the electric potential (voltage) of the axon
 - ▶ an action potential is generated at neuron only if it receives enough (over some threshold) of the “right”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

Multilayer Perceptron Network Architecture

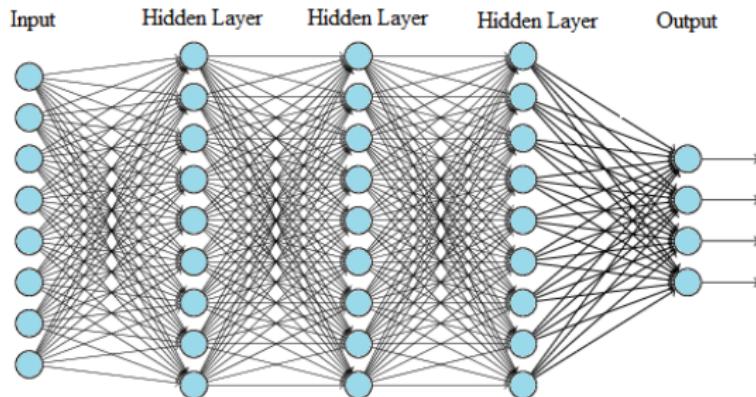


Design

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

Multilayer Perceptron

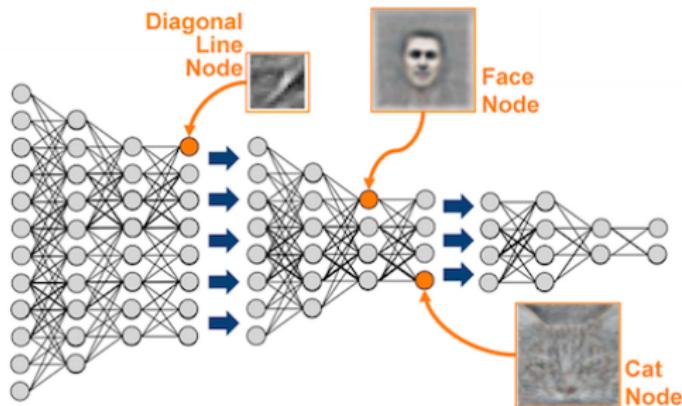
Network Architecture



Design

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

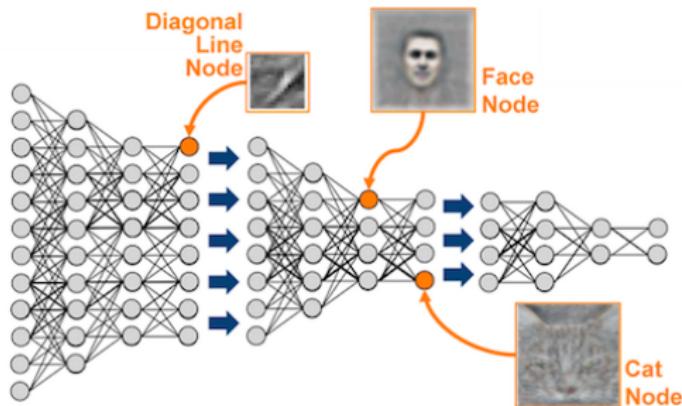
Multilayer Perceptron Network Architecture



Design

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

Multilayer Perceptron Network Architecture



Design

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

Multilayer Perceptron

Softmax Output

- Generalization of the logistic output 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

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

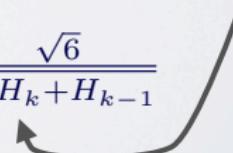
- $l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$ is a loss function
- $\Omega(\boldsymbol{\theta})$ is a regularizer (penalizes certain values of $\boldsymbol{\theta}$)
- Learning is cast as optimization
 - ideally, we'd optimize classification error, but it's not smooth
 - loss function is a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

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 $U[-b, b]$ where $b = \frac{\sqrt{6}}{\sqrt{H_k + H_{k-1}}}$
 - 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)

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



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

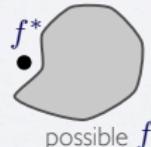
Topics: bias-variance trade-off

- 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



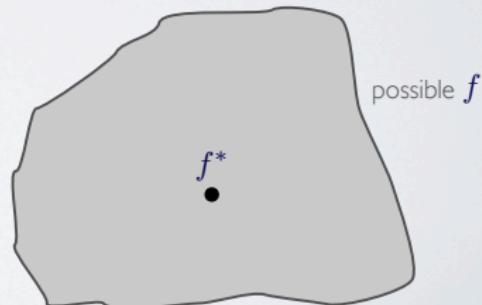
low variance/
high bias

f^*



good trade-off

f^*



high variance/
low bias

Backprop Algorithm

Outline

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

Backprop Algorithm

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 programming.
-
- 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 $\boldsymbol{\theta}$ ($\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \dots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$)

 - 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

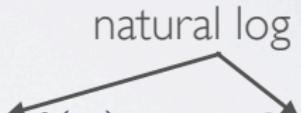
LOSS FUNCTION

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

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

natural log (\ln)



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

LOSS FUNCTION

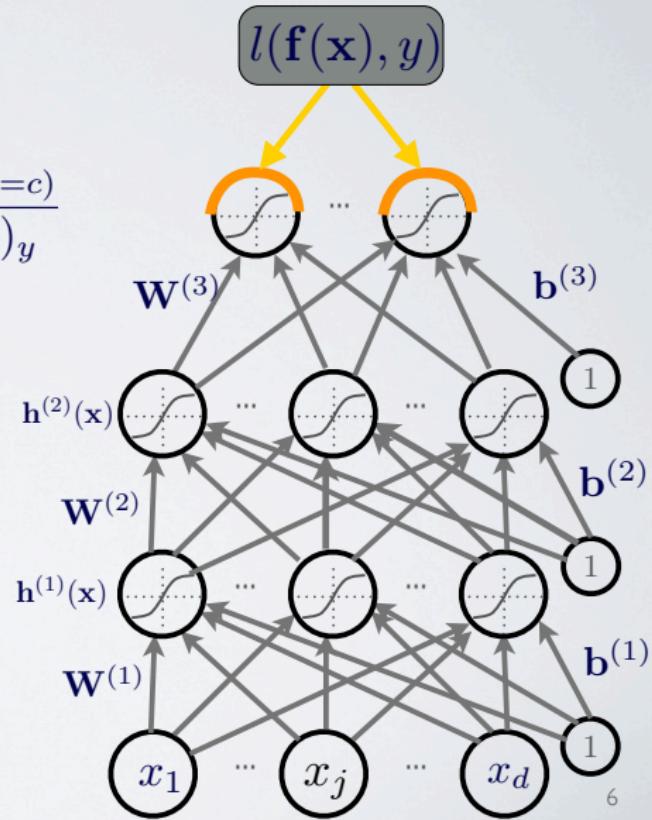
Topics: loss gradient at output

- Partial derivative:

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

- Gradient:

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



LOSS FUNCTION

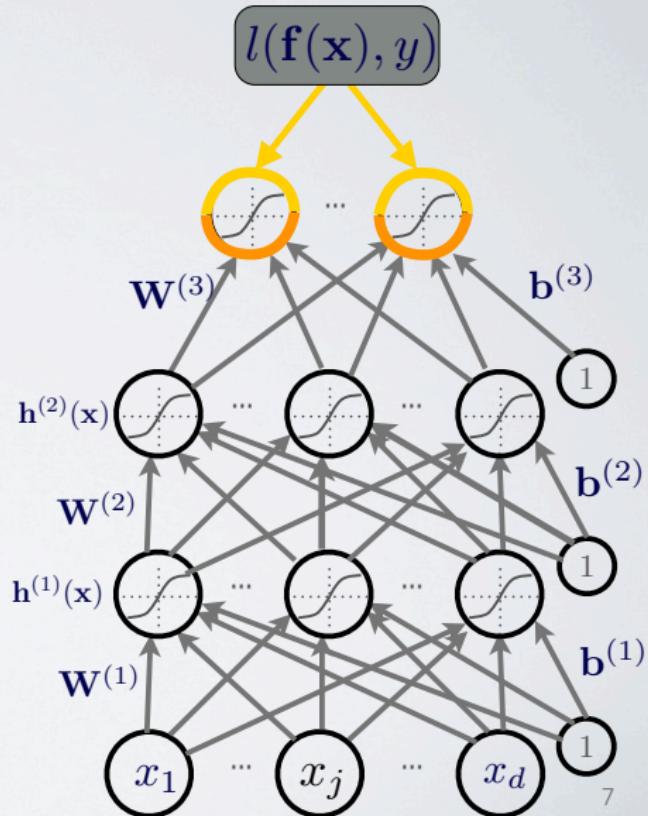
Topics: loss gradient at output
(before activation)

- Partial derivative:

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

- Gradient:

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



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

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

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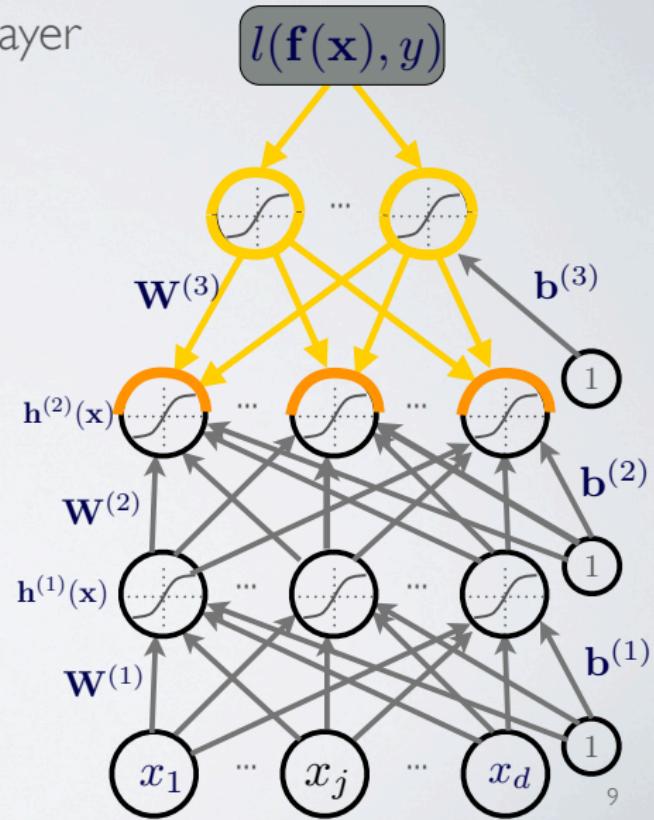
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= & -(1_{(y=c)} - f(\mathbf{x})_c)
\end{aligned}$$

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

LOSS FUNCTION

Topics: loss gradient at hidden layer

- ... this is getting complicated!!



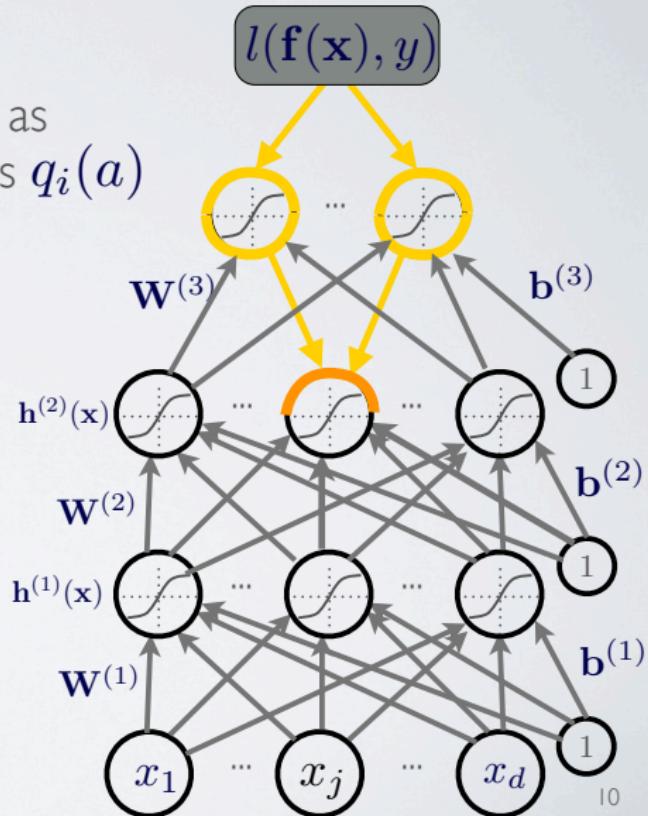
LOSS FUNCTION

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

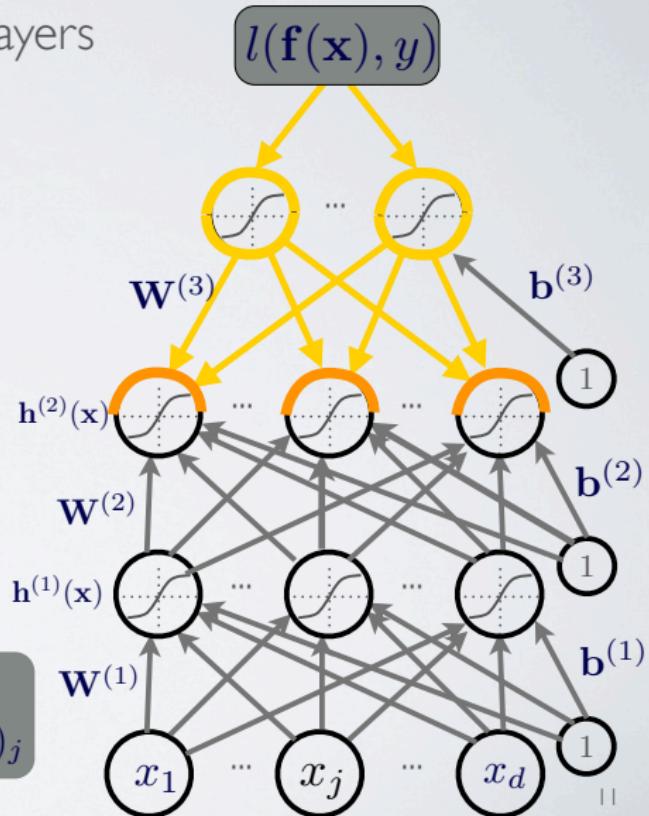
Topics: loss gradient at hidden layers

- Partial derivative:

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

REMINDER

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

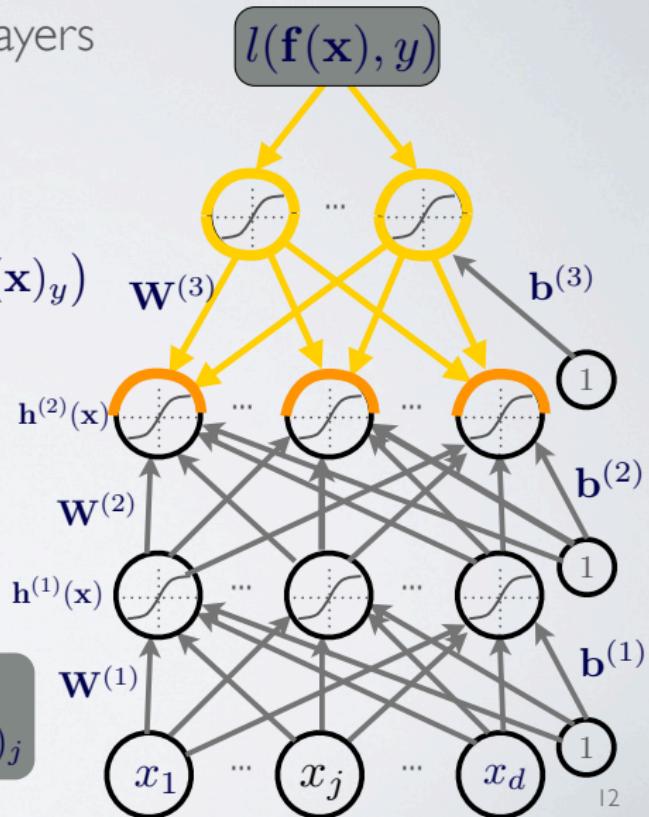


LOSS FUNCTION

Topics: loss gradient at hidden layers

- Gradient:

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



REMINDER

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

LOSS FUNCTION

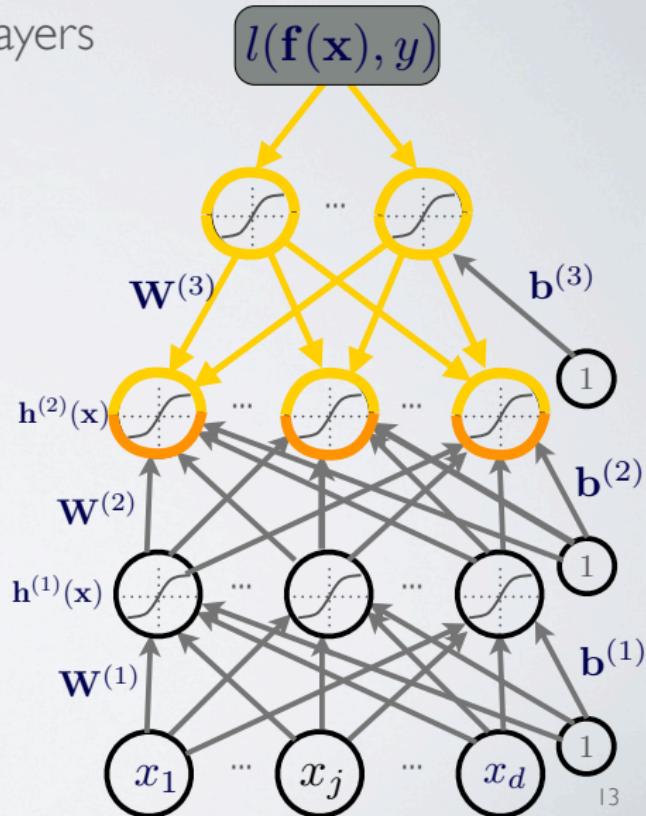
Topics: loss gradient at hidden layers
(before activation)

- Partial derivative:

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

REMINDER

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



LOSS FUNCTION

Topics: loss gradient at hidden layers
(before activation)

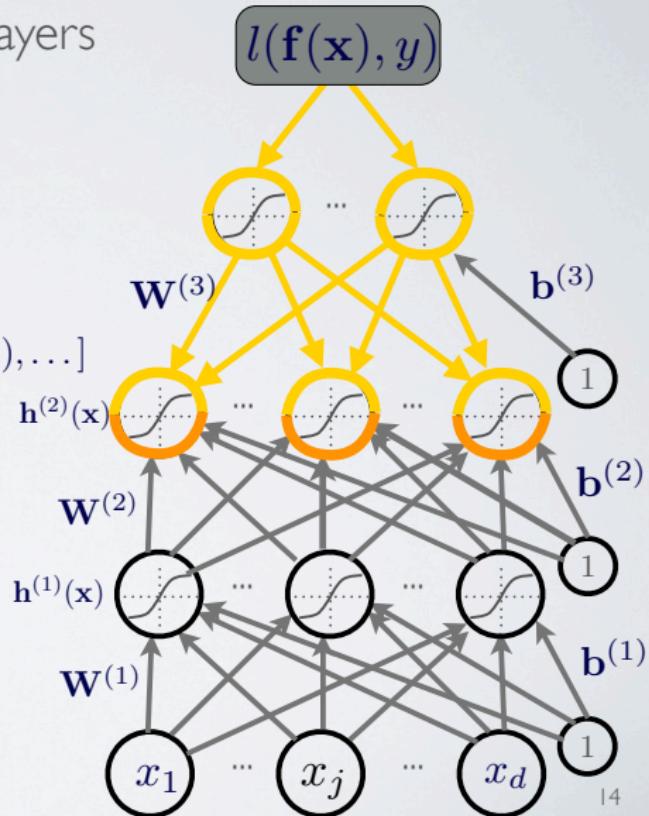
- Gradient:

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

↑
element-wise
product

REMINDER

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



LOSS FUNCTION

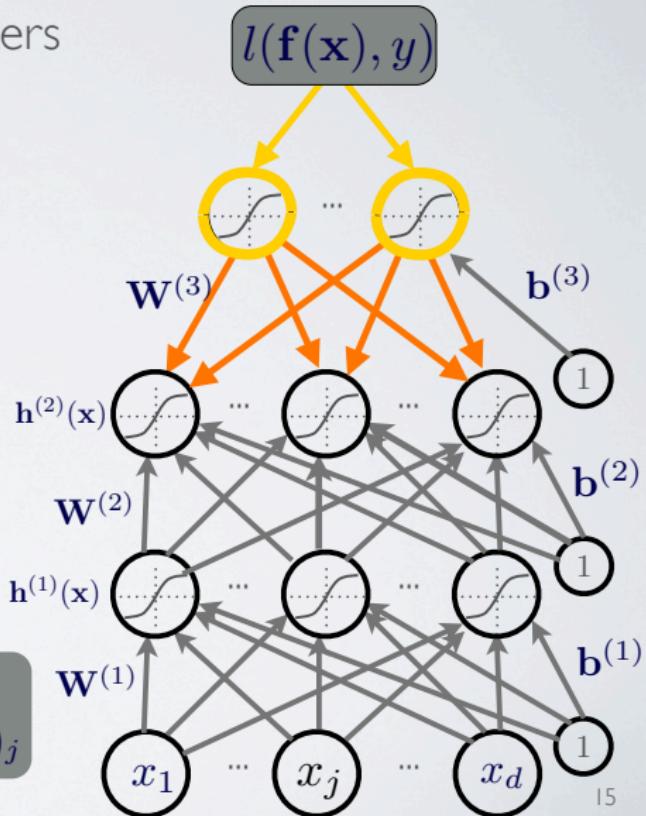
Topics: loss gradient of parameters

- Partial derivative (weights):

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

REMINDER

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

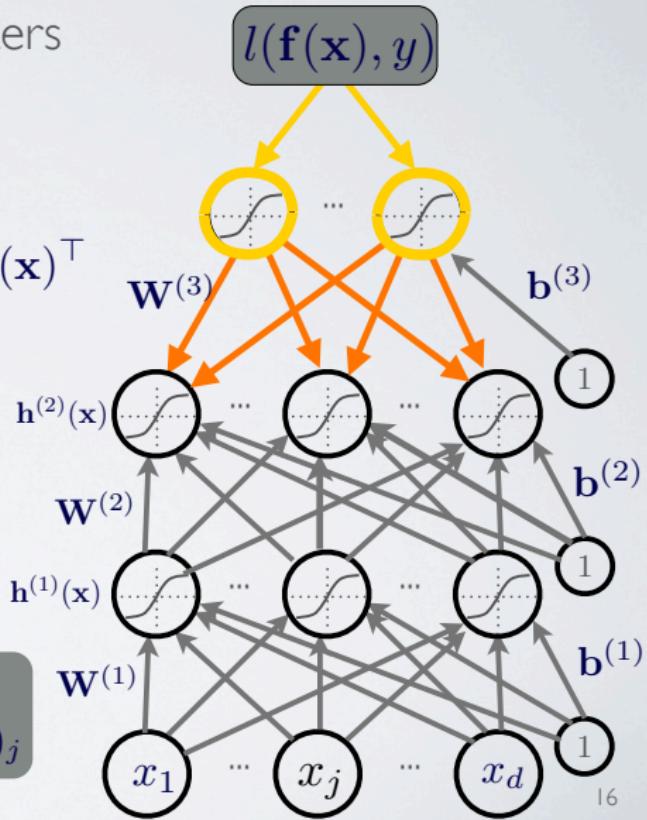


LOSS FUNCTION

Topics: loss gradient of parameters

- Gradient (weights):

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



REMINDER

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

LOSS FUNCTION

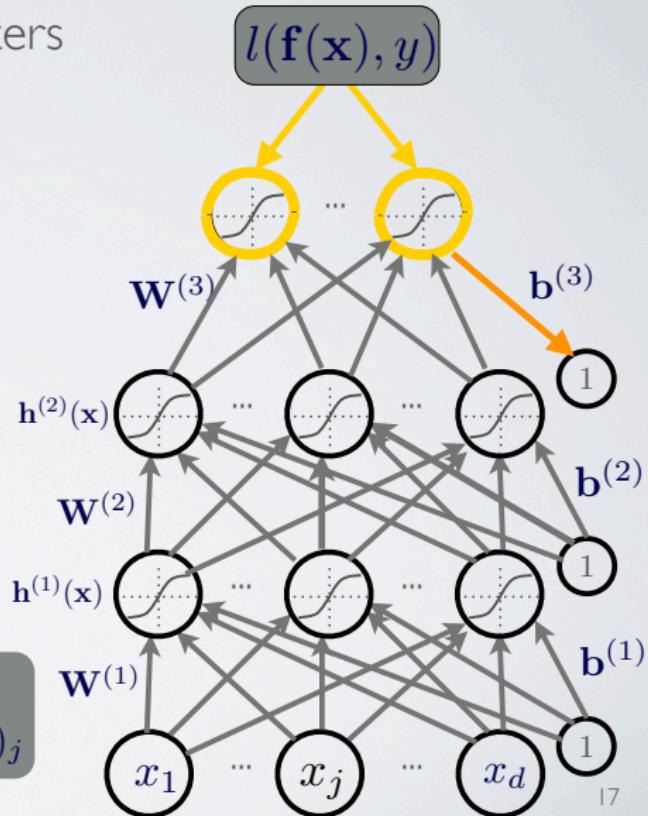
Topics: loss gradient of parameters

- Partial derivative (biases):

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

REMINDER

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

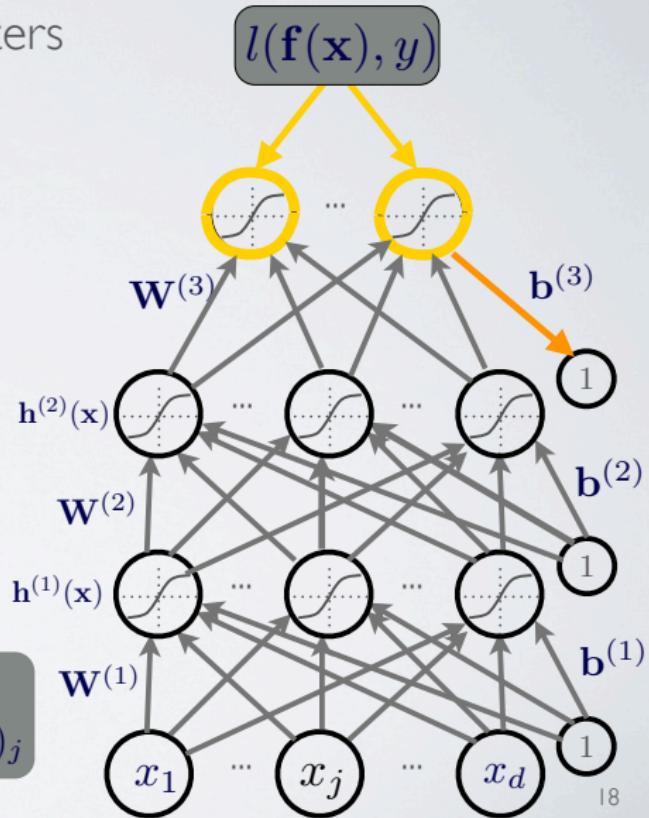


LOSS FUNCTION

Topics: loss gradient of parameters

- Gradient (biases):

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



REMINDER

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

BACKPROPAGATION

Topics: backpropagation algorithm

- 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

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

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

- compute gradient of hidden layer below

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

- compute gradient of hidden layer below (before activation)

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

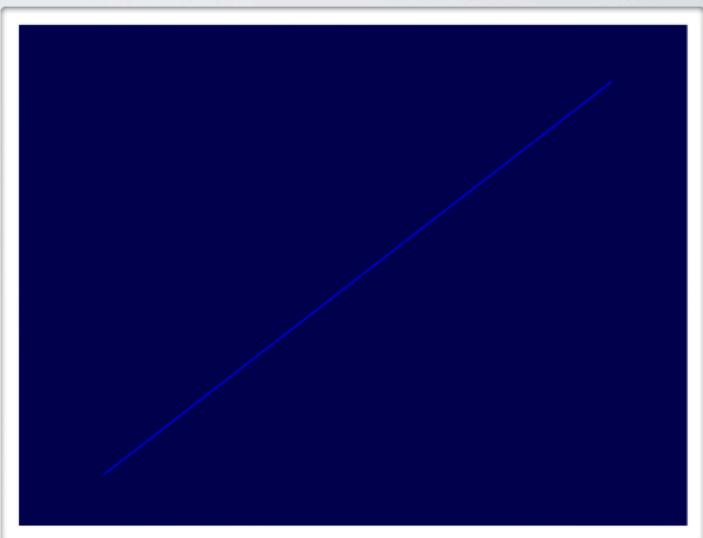
- This assumes a forward propagation has been made before

ACTIVATION FUNCTIONS

Topics: linear activation function gradient

- Partial derivative:

$$g'(a) = 1$$



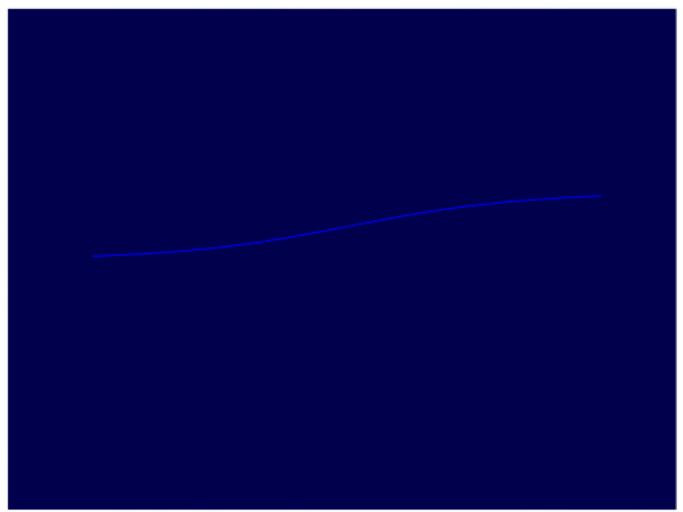
$$g(a) = a$$

ACTIVATION FUNCTIONS

Topics: sigmoid activation function gradient

- Partial derivative:

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



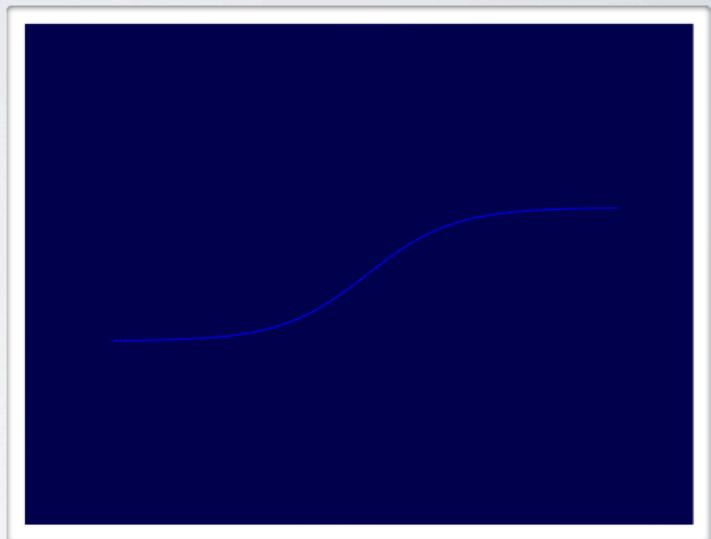
$$g(a) = \text{sigm}(a) = \frac{1}{1+\exp(-a)}$$

ACTIVATION FUNCTIONS

Topics: tanh activation function gradient

- Partial derivative:

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



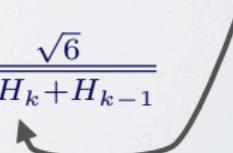
$$g(a) = \tanh(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} = \frac{\exp(2a) - 1}{\exp(2a) + 1}$$

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 $U[-b, b]$ where $b = \frac{\sqrt{6}}{\sqrt{H_k + H_{k-1}}}$
 - 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)

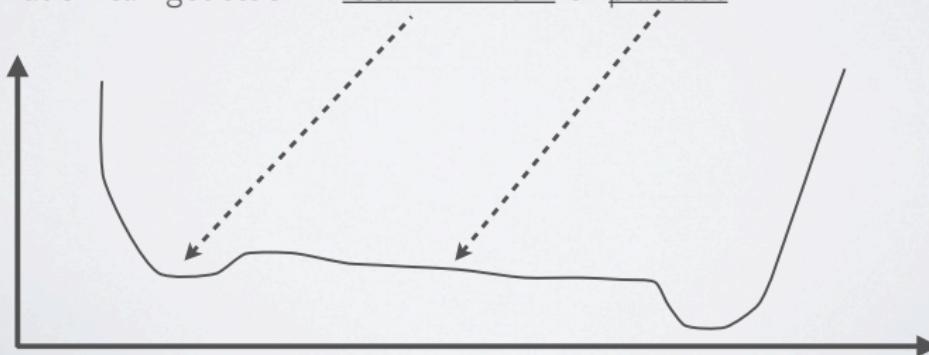
size of $\mathbf{h}^{(k)}(\mathbf{x})$



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

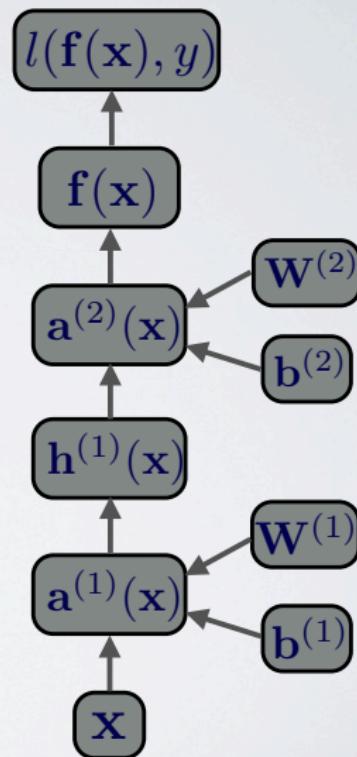
Neural network training demo

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

FLOW GRAPH

Topics: flow graph

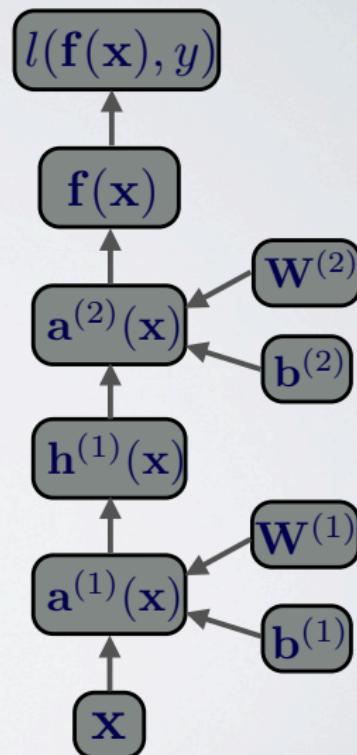
- Forward propagation can be represented as an acyclic flow graph
- It's a nice way of implementing forward propagation in a modular way
 - each box is an object with an fprop method, that outputs the value of the box given its children
 - calling the fprop method of each box in the right order yield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



FLOW GRAPH

Topics: automatic differentiation

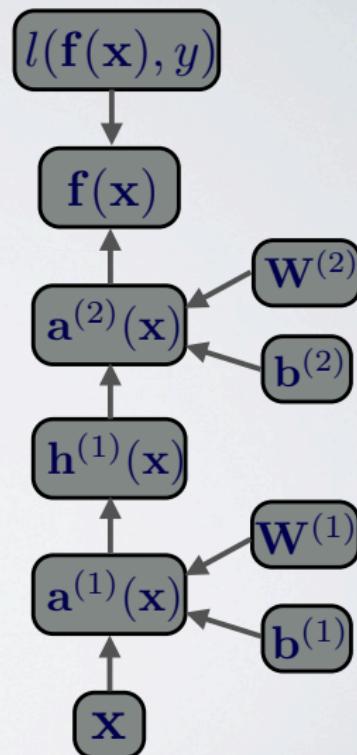
- Each object also has a bprop method
 - it outputs the gradient of the loss given each children
 - fprop depends on the fprop of a box's children, while bprop depends the bprop of a box's parents
- By calling bprop in the reverse order, we get backpropagation
 - only need to reach the parameters



FLOW GRAPH

Topics: automatic differentiation

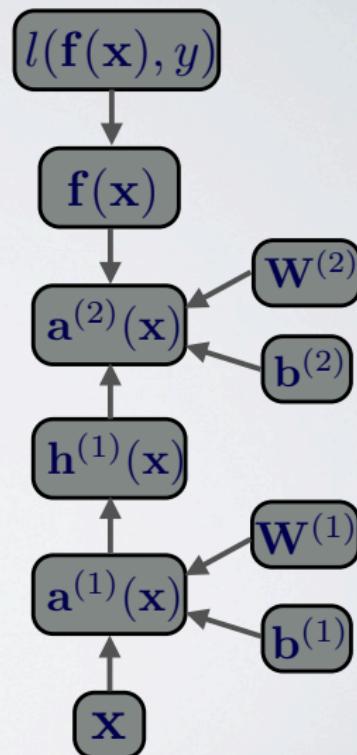
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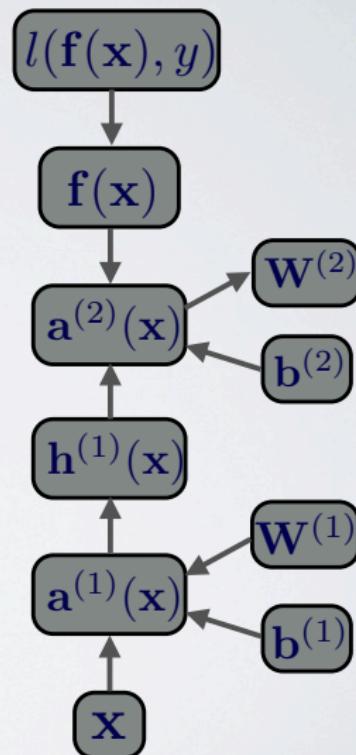
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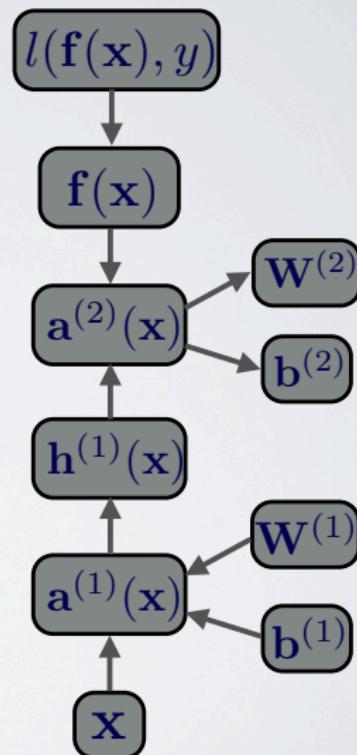
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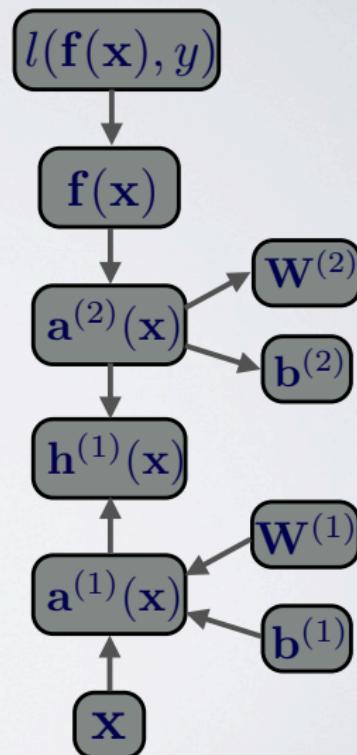
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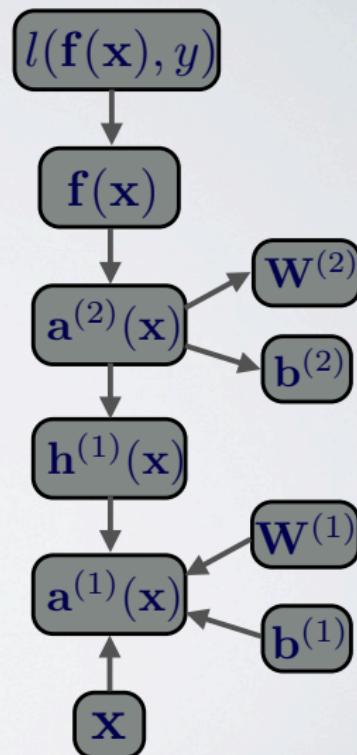
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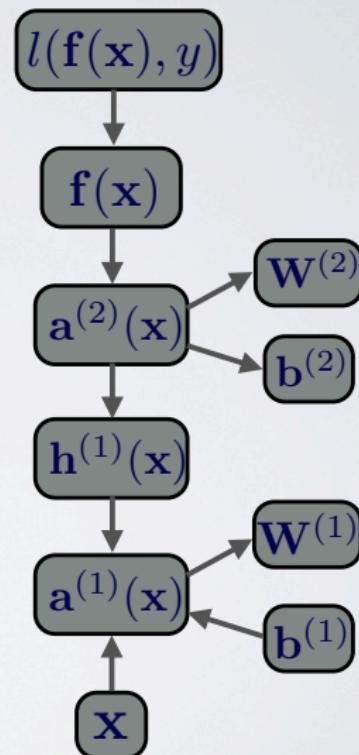
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