CSCI 467, Introduction to Machine Learning

University of Southern California

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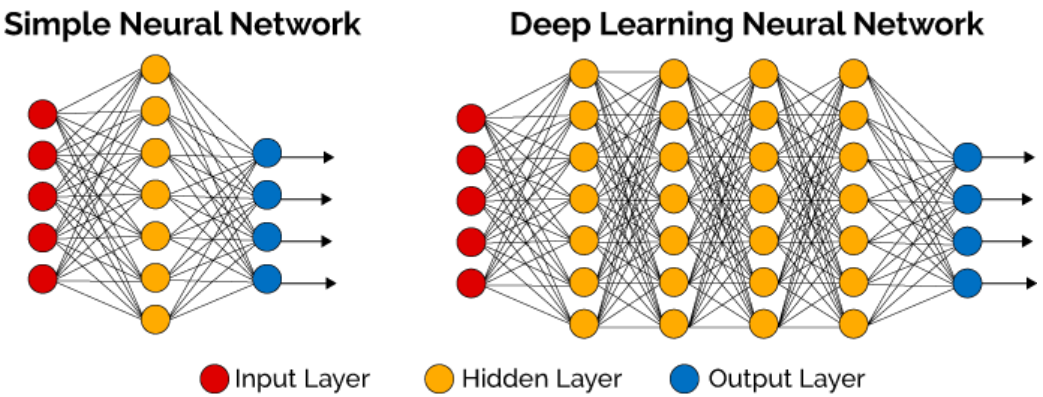
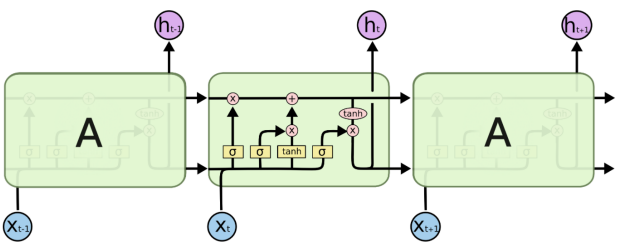
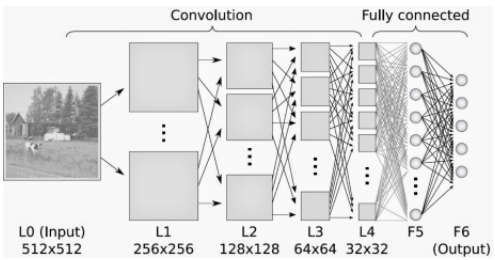
Lesson 10
Neural Networks and Deep Learning







Introductory Remark

In this lecture, we use matrix and vector notations. Matrices and vectors are shown by bold letters.

Vectors of functions are shown with bold letters (e.g. $\mathbf{f}$), and unless otherwise stated, act on vectors elementwise.

Perceptron

Perceptron is an algorithm for binary classification that uses a linear prediction function:

$$f(\mathbf{x}) = \begin{cases} 1, & \boldsymbol{\beta}^T\mathbf{x} + \beta_0 \geq 0 \\ -1, & \boldsymbol{\beta}^T\mathbf{x} + \beta_0 < 0 \end{cases}$$

This is called a *step function*, which reads:

- the output is 1 if "$\boldsymbol{\beta}^T\mathbf{x} + \beta_0 \geq 0$" is true, and the output is -1 if instead "$\boldsymbol{\beta}^T\mathbf{x} + \beta_0 < 0$" is true

Perceptron

Perceptron is an algorithm for binary classification that uses a linear prediction function:

$$f(\mathbf{x}) = \begin{cases} 1, & \boldsymbol{\beta}^T\mathbf{x} + \beta_0 \geq 0 \\ -1, & \boldsymbol{\beta}^T\mathbf{x} + \beta_0 < 0 \end{cases}$$

By convention, the two classes are +1 or -1.

Perceptron

Perceptron is an algorithm for binary classification that uses a linear prediction function:

$$f(\mathbf{x}) = \begin{cases} 1, & \boldsymbol{\beta}^T\mathbf{x} + \beta_0 \geq 0 \\ -1, & \boldsymbol{\beta}^T\mathbf{x} + \beta_0 < 0 \end{cases}$$

- Often these parameters are called **weights**.
- $\boldsymbol{\beta}=(\beta_1, \beta_2, \ldots, \beta_p)$

Perceptron

Perceptron is an algorithm for binary classification that uses a linear prediction function:

$$f(\mathbf{x}) = \begin{cases} 1, \boldsymbol{\beta}^T\mathbf{x} + \beta_0 \geq 0 \\ -1, \boldsymbol{\beta}^T\mathbf{x} + \beta_0 < 0 \end{cases}$$

By convention, ties are broken in favor of the positive class.

- If "$\boldsymbol{\beta}^T\mathbf{x} + \beta_0$ " is exactly 0, output +1 instead of -1.

Perceptron

The **β** parameters are unknown. This is what we have to learn.

$$f(\mathbf{x}) = \begin{cases} 1, & \boldsymbol{\beta}^T\mathbf{x} + \beta_0 \geq 0 \\ -1, & \boldsymbol{\beta}^T\mathbf{x} + \beta_0 < 0 \end{cases}$$

In the same way that linear regression learns the slope parameters to best fit the data points, perceptron learns the parameters to best separate the instances.

Learning the Weights

The perceptron algorithm learns the weights by:

1. Initialize all weights **β** to 0 or randomly.
2. Iterate through the training data. For each training instance, classify the instance.
    a) If the prediction (the output of the classifier) was correct, don't do anything. (It means the classifier is working, so leave it alone!)
    b) If the prediction was wrong, modify the weights by using the **update rule**.
3. Repeat step 2 some number of times (more on this later).

Learning the Weights

What does an **update rule** do?

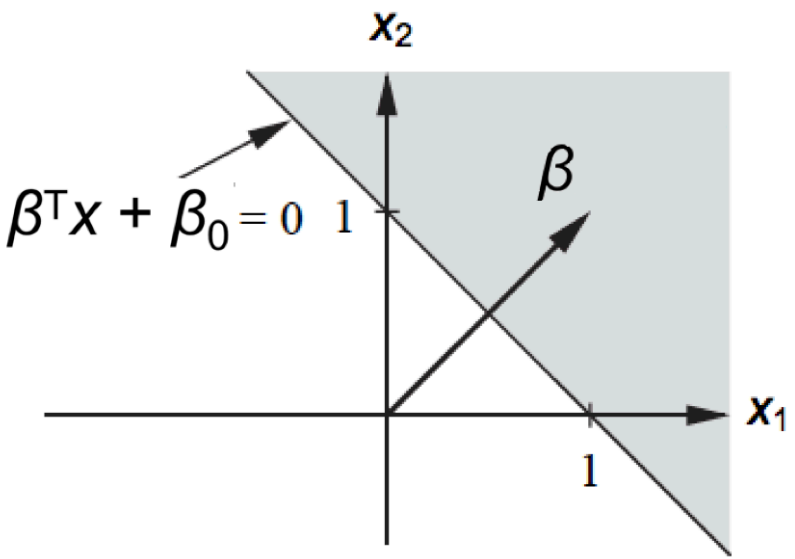
- If the classifier predicted an instance was negative but it should have been positive…

Currently: $\boldsymbol{\beta}^T\mathbf{x} + \beta_0 < 0$ Want: $\boldsymbol{\beta}^T\mathbf{x} + \beta_0 \geq 0$

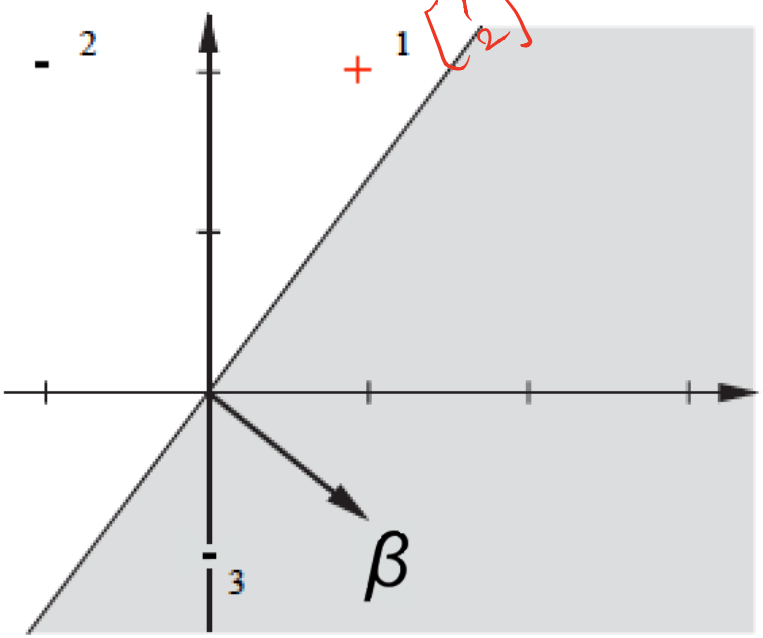
  - Adjust the weights $\boldsymbol{\beta}$ so that this function value moves toward positive
- If the classifier predicted positive but it should have been negative, shift the weights so that the value moves toward negative.

Structure of A Perceptron: Example

$$\beta_1 = 1 \quad \beta_2 = 1 \quad \beta_0 = -1$$

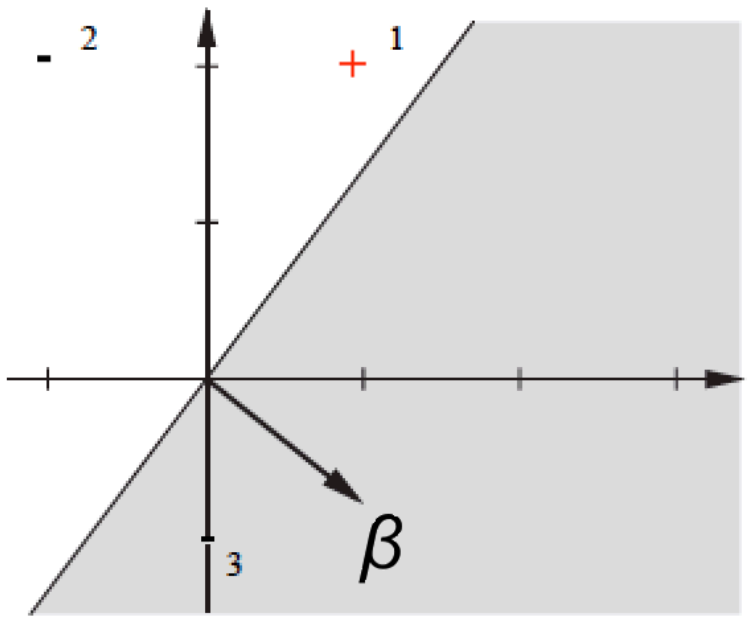


Learning the Weights



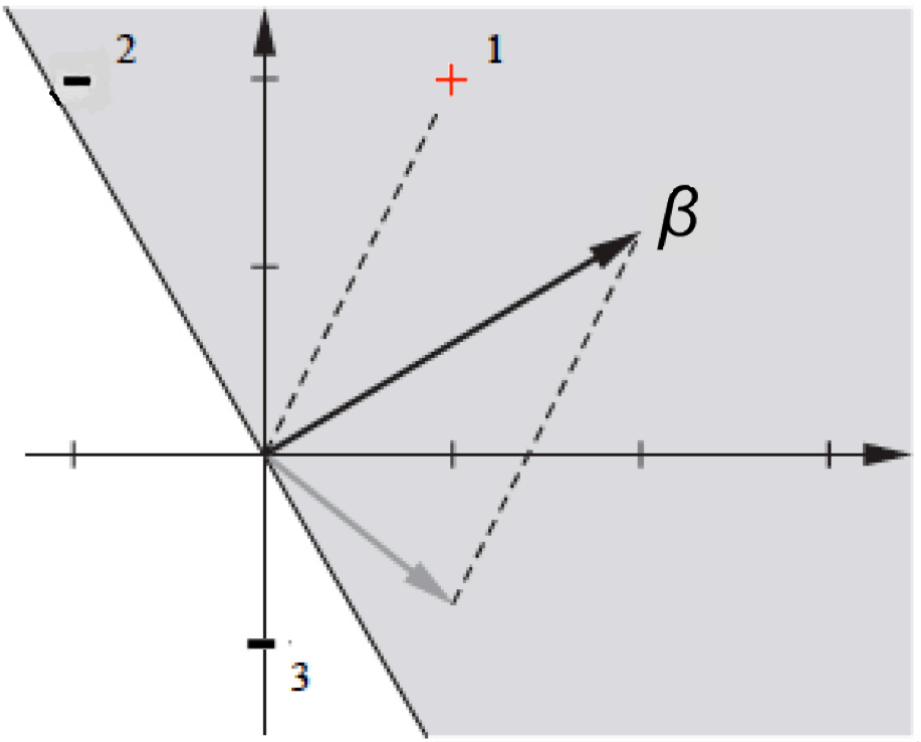
+ and - classes
Random initial weight:
$\boldsymbol{\beta}^T=[1, -0.8]$;
For now, assume that $\beta_0=0$ all the time.

Learning the Weights



The Perceptron classifies **x**(1) as - incorrectly, so the weights have to be changed.

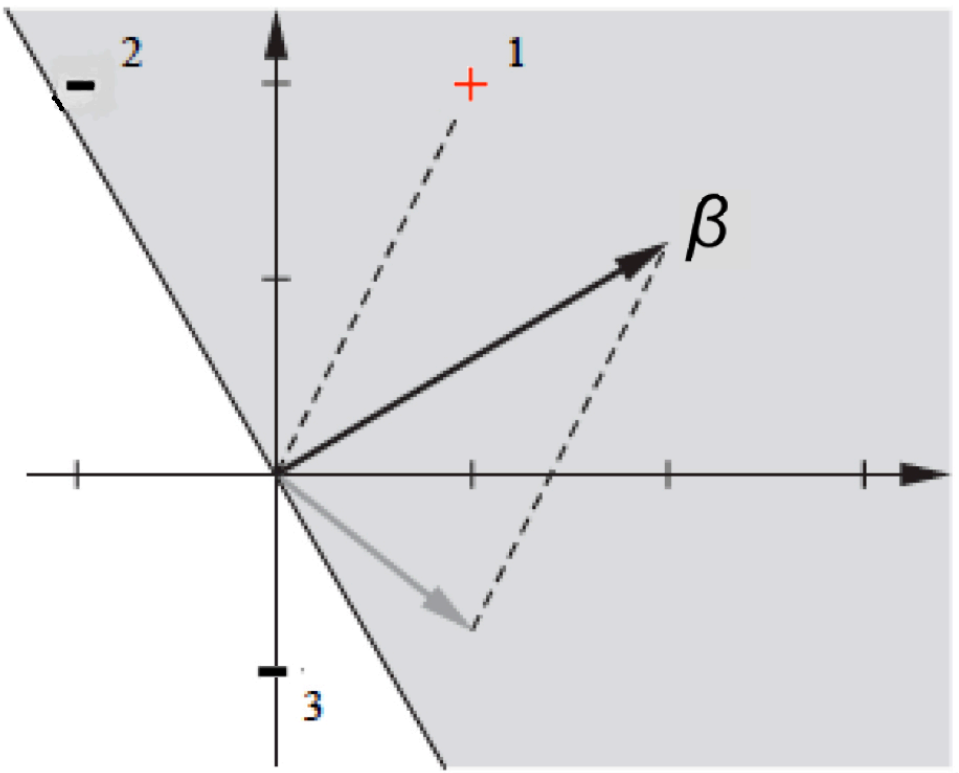
Learning the Weights



The weight vector has to move towards the misclassified vector.

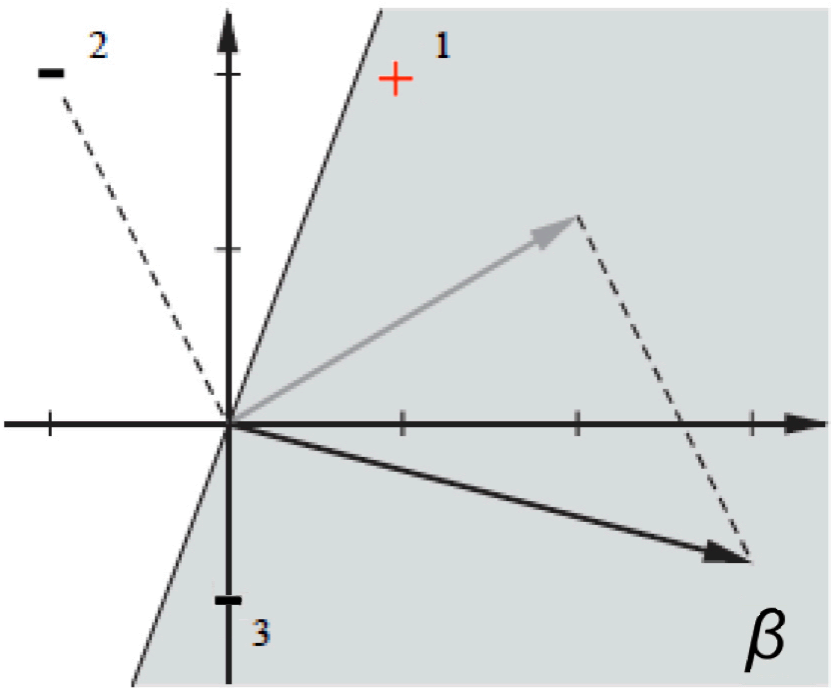
$\boldsymbol{\beta}^{new} = \boldsymbol{\beta}^{old} + \mathbf{x}(1)$

Learning the Weights



The Perceptron misclassifies **x**(2) as +.

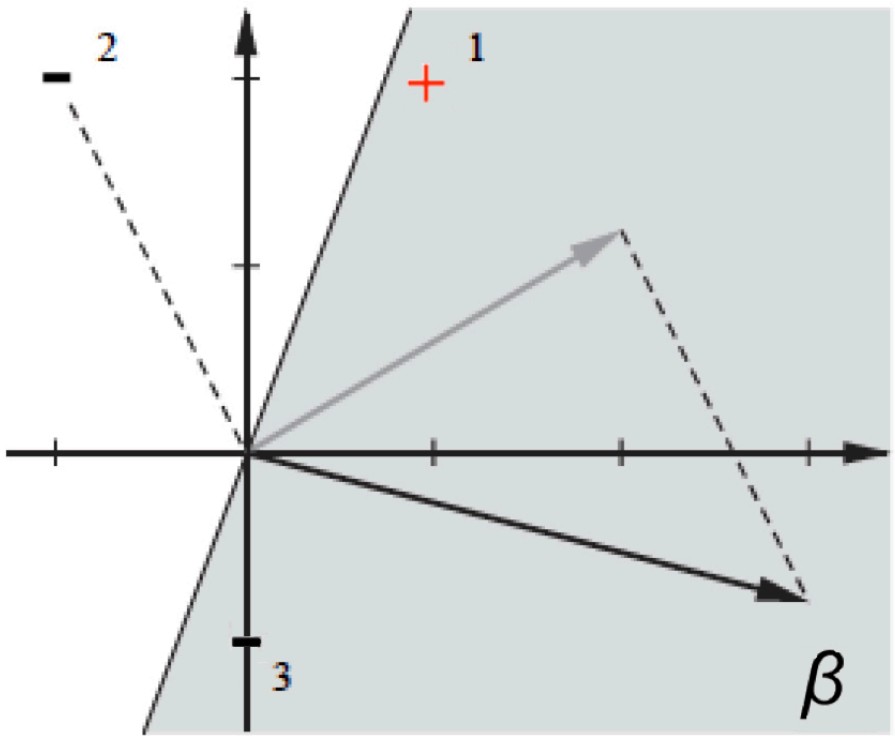
Learning the Weights



The weight vector has to move away from the misclassified vector.

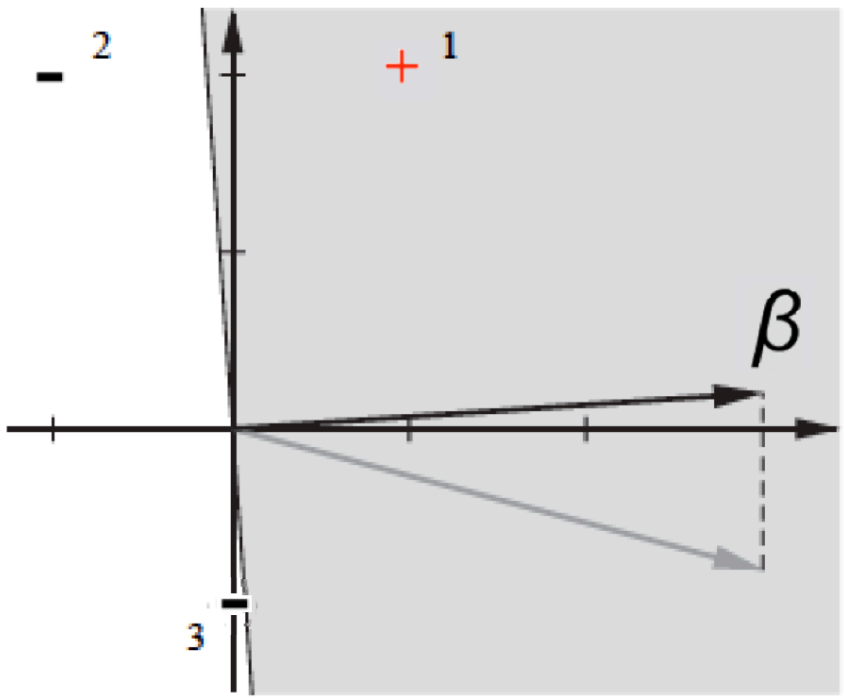
$\boldsymbol{\beta}^{new} = \boldsymbol{\beta}^{old} - \mathbf{x}(2)$

Learning the Weights



The Perceptron misclassifies **x**(3) as +.

Learning the Weights



The weight vector has to move away from $x^{(3)}$.

$\boldsymbol{\beta}^{new} = \boldsymbol{\beta}^{old} - \mathbf{x}^{(3)}$

Learning the Weights

The perceptron update rule:

$$\boldsymbol{\beta}(i+1) = \boldsymbol{\beta}(i) + 0.5[y(i)-f(\mathbf{x}(i))]\,\mathbf{x}(i)$$

desired class

class predicted by perceptron

Learning the Weights

The perceptron update rule:

$\boldsymbol{\beta}(i+1) = \boldsymbol{\beta}(i) + 0.5[y(i)-f(\mathbf{x}(i))]\,\mathbf{x}(i)$

If $y(i) = f(\mathbf{x}(i))$. i.e., if Perceptron correctly classifies the instance $x(i)$, the weights will not be updated.

Learning the Weights

The perceptron update rule:

$\boldsymbol{\beta}(i+1) = \boldsymbol{\beta}(i) + 0.5[y(i) - f(\mathbf{x}(i))]\,\mathbf{x}(i)$

If $y(i) = 1$ and $f(\mathbf{x}(i)) = -1$, then $.5[y(i) - f(\mathbf{x}(i))] = 1$, so the weights will move towards $x(i)$ to make $\boldsymbol{\beta}^T\mathbf{x}(i) + \beta_0$ more positive and $\mathbf{x}(i)$ is more likely to be classified correctly.

Learning the Weights

The perceptron update rule:

$\boldsymbol{\beta}(i+1) = \boldsymbol{\beta}(i) + 0.5[y(i)-f(\mathbf{x}(i))]\,\mathbf{x}(i)$

If $y(i) = -1$ and $f(\mathbf{x}(i))=+1$, then $.5[y(i)-f(\mathbf{x}(i))]=-1$, so the weights will move away from $x(i)$ to make $\boldsymbol{\beta}^T\mathbf{x}(i) + \beta_0$ more negative and $\mathbf{x}(i)$ is more likely to be classified correctly.

Learning the Weights

The perceptron update rule:
$\boldsymbol{\beta}(i+1) = \boldsymbol{\beta}(i) + 0.5e(i)\,\mathbf{x}(i)$

where $e(i) = y(i) - f(\mathbf{x}(i))$ is the *error* of the model in classifying $\mathbf{x}(i)$.

Learning the Weights

For the bias term we have:
$\beta_0(i+1)_= \beta_0(i)+.5[e(i)]$

This means if $e(i) = y(i)-f(\mathbf{x}(i))$ is positive, increase the bias term and if it is negative, decrease it, i.e.:

Move the decision boundary up or down to correct the classifier

Remark

So far, we have used **β** for showing the parameters of the decision hyperplane, which is a common notation for regression.

Using **w** is way more common for showing weights in neural networks. Let's switch to **w**.

The parameter β_0 is often called a bias, and is more commonly shown as b.

$\underline{w}^T \underline{x} + b$

$\underline{\beta}^T \underline{x} + \beta_0$

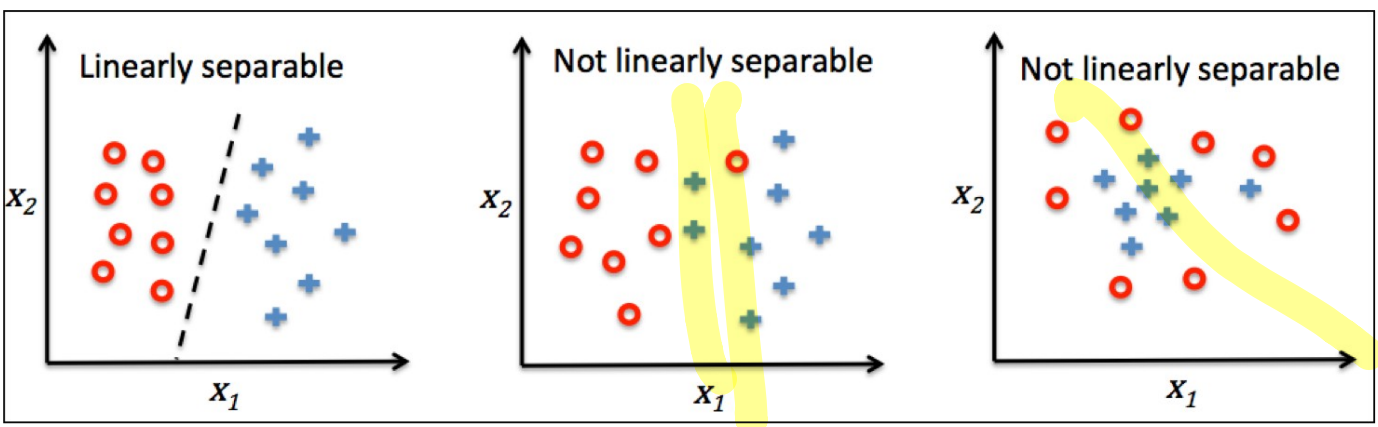
Perceptron vs. SVC

Note that Perceptron and SVC are both linear classifiers. However, SVC's optimization needs all data to yield a classifier, so it is a *batch* algorithm.

On the other hand, perceptron *adapts* its weights online, based on the data points that are presented to it. Thus it is an *online* algorithm.

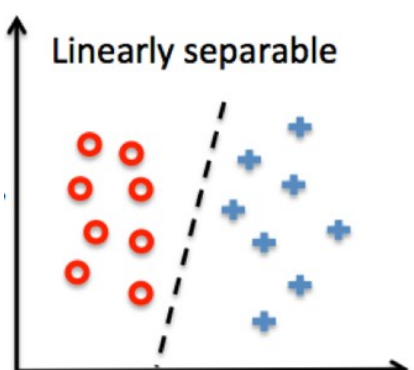
Linear Separability

RECALL: The training instances are **linearly separable** if there exists a hyperplane that will separate the two classes.



Linear Separability

If the training instances are linearly separable, the perceptron algorithm will eventually find weights **W** such that the classifier gets everything correct.



Linear Separability

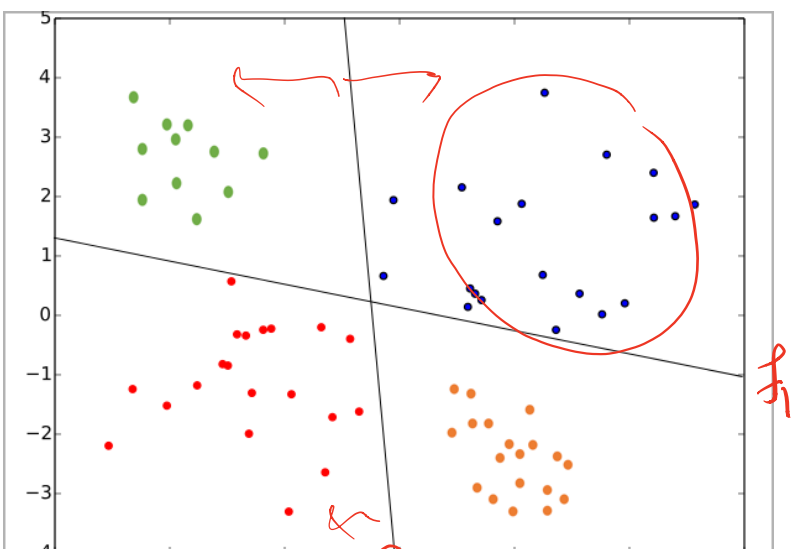
If the training instances are not linearly separable, the classifier will always get some predictions wrong.

- You need to implement some type of **stopping criteria** for when the algorithm will stop making updates, or it will run forever.
- Usually this is specified by running the algorithm for a maximum number of **iterations** or **epochs**.

4/15/20

Multi-class Perceptron: Architecture

Using S hyperplanes, one can partition the space $\mathbf{R}^p$ to 2^S regions. Each region can represent a class. For $p = 2$ and $S = 2$:



$f_1(x)$ ω_1

$f_2(x)$ ω_2

$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ C_1

$\begin{bmatrix} 1 \\ -1 \end{bmatrix}$ C_2

$\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ C_3

$\begin{bmatrix} -1 \\ -1 \end{bmatrix}$ C_4

Multi-class Perceptron

The weights associated with each hyperplane can be represented as the columns of a *weight matrix* **W***:*

$\mathbf{W} = [\mathbf{w}_1|\mathbf{w}_2|\ldots|\mathbf{w}_S]$

The biases can be augmented in a vector **b**:
$\mathbf{b} = [b_1\, b_2 \ldots b_S]^T$

Multi-class Perceptron: Learning Rule

The weights can be updated for multiclass perceptron. Assume that $\mathbf{e}(i)$ *is the vector of errors at epoch i*

$$\mathbf{W}(i+1) = \mathbf{W}(i) + 0.5\mathbf{x}(i)\mathbf{e}^T(i)$$

As well as the biases

$$\mathbf{b}^T(i+1) = \mathbf{b}^T(i) + 0.5\mathbf{e}^T(i)$$

$$[\underline{w}_1(i+1) \quad \underline{w}_2(i+1) \cdots \underline{w}_s(i+1)]$$

$$= [\underline{w}_1(i) \quad \underline{w}_2(i) \cdots \underline{w}_s(i)]$$

$$+ .5\,\underline{x}(i)[e_1(i) \quad e_2(i) \cdots e_s(i)]$$

$$\underline{e}(i) = \begin{bmatrix} e_1(i) \\ \vdots \\ e_s(i) \end{bmatrix}$$

$e_j(i)$: the error of the j^{th} hyperplane at epoch i

The desired bit

$$e_j(i) = y_j - f_j(\underline{x}(i))$$

You can see that this implements the Perceptron learning rule for each hyperplane

$$\underline{w}_j(i+1) = \underline{w}_j(i) + .5\,\underline{x}(i)e_j(i)$$

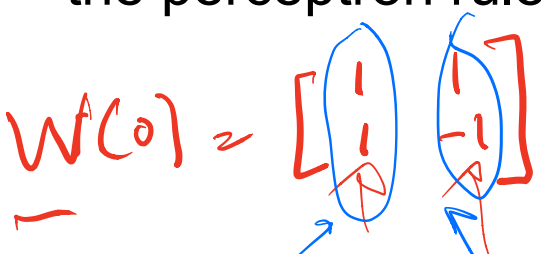
$$b_j(i+1) = b_j(i) + .5\,e_j(i)$$

Multi-class Perceptron: Learning Rule

Example: Assume that biases are kept zero and

$\mathbf{w}_1(0) = [1\ 1]^T$
$\mathbf{w}_2(0) = [1\ -1]^T$

Assume that $\mathbf{x} = [1\ 0]^T$ is in a class encodes as $C_1 = [1\ -1]^T$ and $\mathbf{x}' = [0\ -1]^T$ is in a class encoded as $C_0 = [-1\ -1]^T$. Update the weights according to the perceptron rule.



$$\underline{W}(1) = \underline{W}(0) + .5\,\underline{x}(1)\,\underline{e}^T(1)$$

$$\underline{W}^T(0)\underline{x}(1) = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}^T \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$f(W(0)x(1)) = \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\text{desired} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$e(1) = \begin{bmatrix} 1 \\ -1 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ -2 \end{bmatrix}$$

$$W(1) = W(0) + .5 \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & -2 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} + .5 \begin{bmatrix} 0 & -2 \\ 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix}$$

As an exercise, do the same, but separately for $\underline{w}_1$ and $\underline{w}_2$

Learning Rate

Let's make a modification to the update rule:

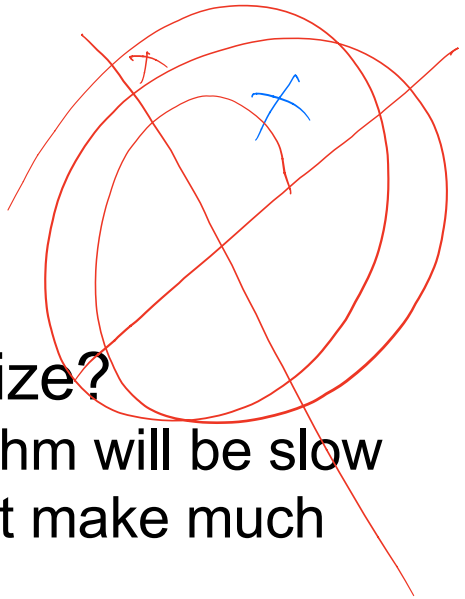
$$\mathbf{W}(i+1) = \mathbf{W}(i) + \alpha \mathbf{x}(i)\mathbf{e}^T(i)$$

$$\mathbf{b}^T(i+1) = \mathbf{b}^T(i) + \alpha \mathbf{e}^T(i)$$

where α is called the **learning rate** or **step size**.

- When you update w_j to be more positive or negative, this controls the size of the change you make (or, how large a "step" you take).
- If $\alpha = 0.5$ (a common value), then this is the same update rule from the earlier slide.

Learning Rate

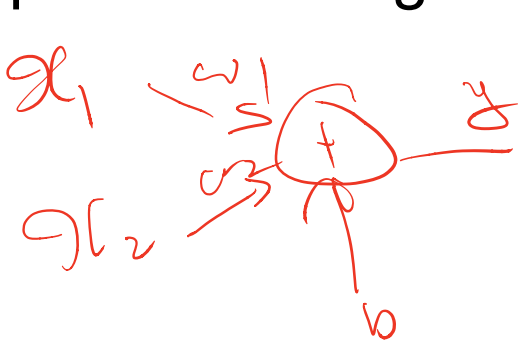


How to choose the step size?

- If α is too small, the algorithm will be slow because the updates won't make much progress.
- If α is too large, the algorithm will be slow because the updates will "overshoot" and may cause previously correct classifications to become incorrect.
- One choice: in first iterations choose a large learning rate and then reduce it $\alpha(i) = \alpha_0/(i+c)$

A Little Bit of History

- McCulloch and Pitts in 1943 contended that neurons with a binary threshold activation function can implement logical functions.
- In 1949, Hebb observed a working principle in neurons that inspired the invention of Perceptron Learning Rule.



$y = x_1 \vee x_2$

$y = x_1 \wedge x_2$

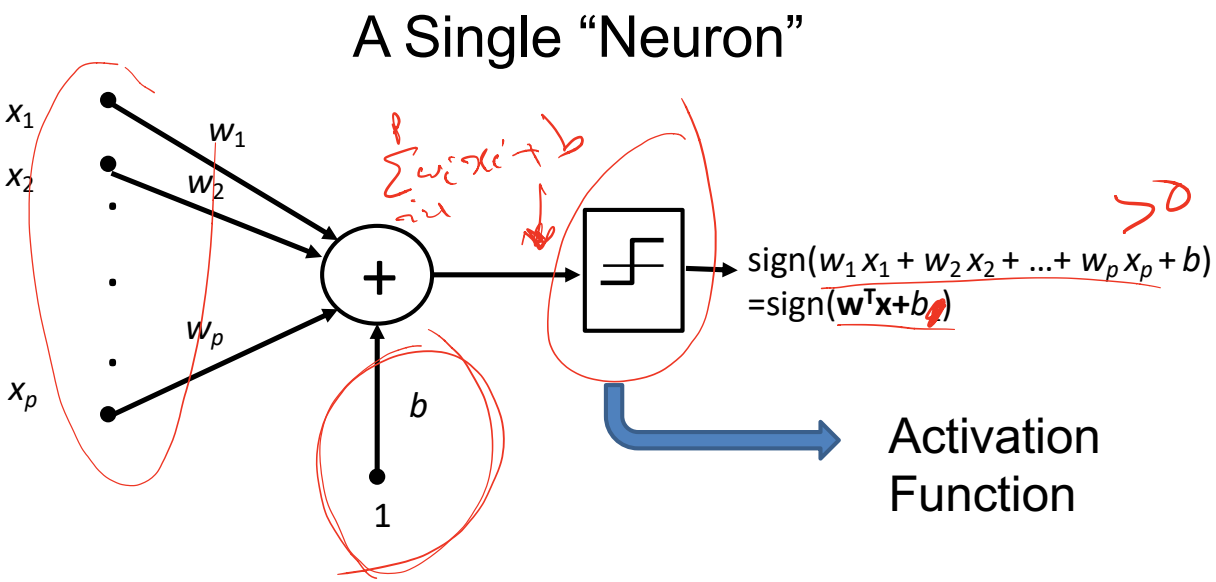
A Little Bit of History

- Hebb observed that, when two neurons fire together, the connection between the neurons is strengthened
- He concluded that this is one of the fundamental operations necessary for learning and memory.

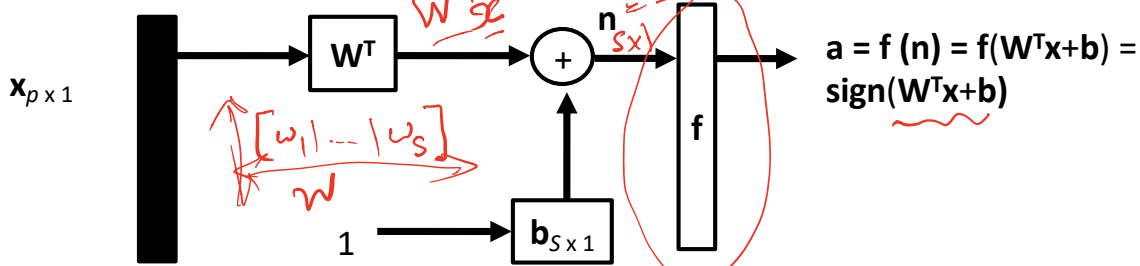
A Little Bit of History

•Rosenblatt, using the McCulloch-Pitts neuron and the findings of Hebb, went on to develop the first Perceptron Learning Rule.
•Perceptron could learn in the Hebbian sense through the weighting of inputs
•Perceptron was instrumental in the later formation of neural networks.

Perceptron as A Neural Architecture



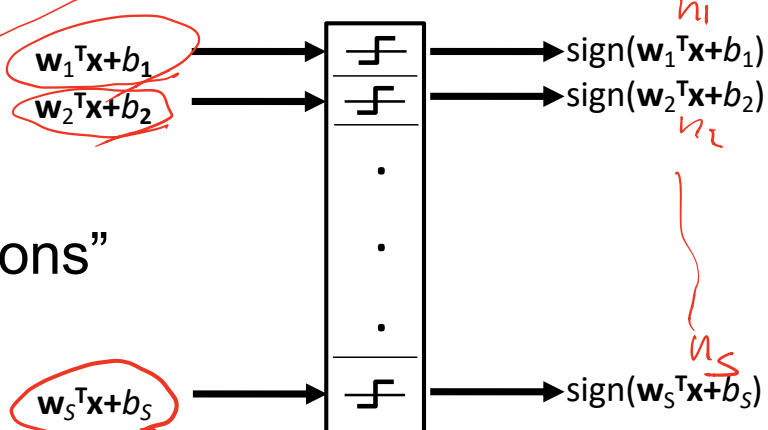
Perceptron as A Neural Architecture



Dimensions:

$W_{p \times S}$

$W^T{}_{S \times p}$



Multiple "Neurons"

Adaptation in Neural Systems

- The Perceptron Learning Rule acts like a simple neural system: it *adapts* its weights based on the *error* that is a result of *mismatch* between its output and the desired output
- This general process is the basis of supervised learning with a large class of *neural networks*.

Caveat: Linear Separability

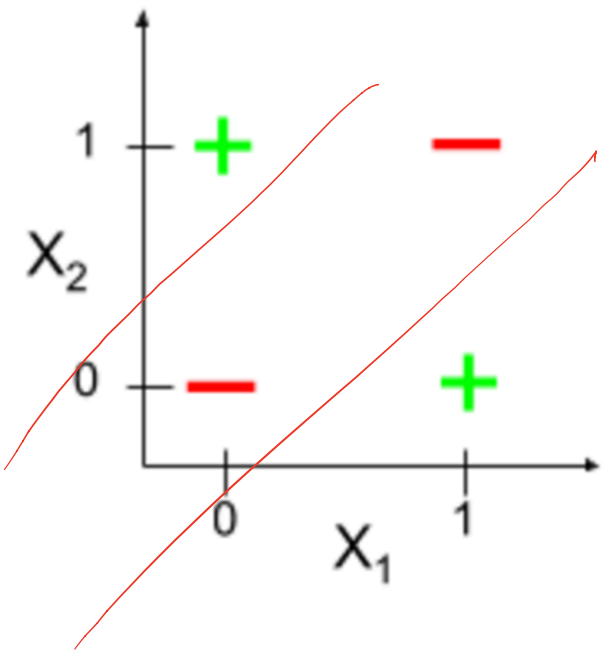
- If the training set is not separable, the Perceptron rule never converges.
- Naturally, it may have a large classification error.

Solution?

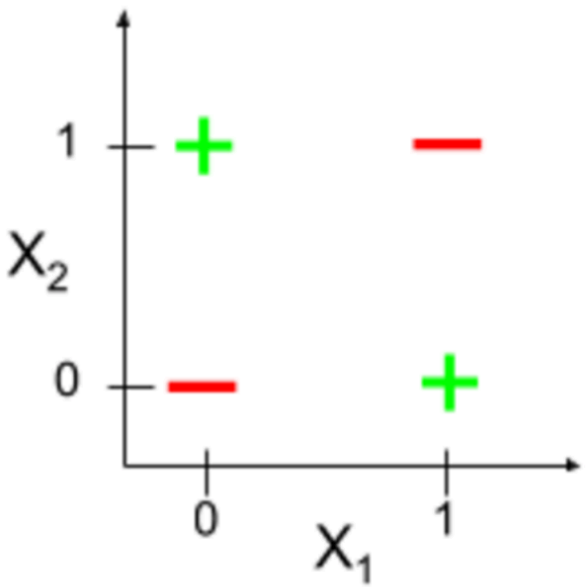
- The general solution is to represent the data in a *feature space* where they are linearly separable.
- One idea is two use *layers* of perceptrons and adjust their weights to learn the feature representations

more layers to learn feature expansions!

Example: XOR Problem

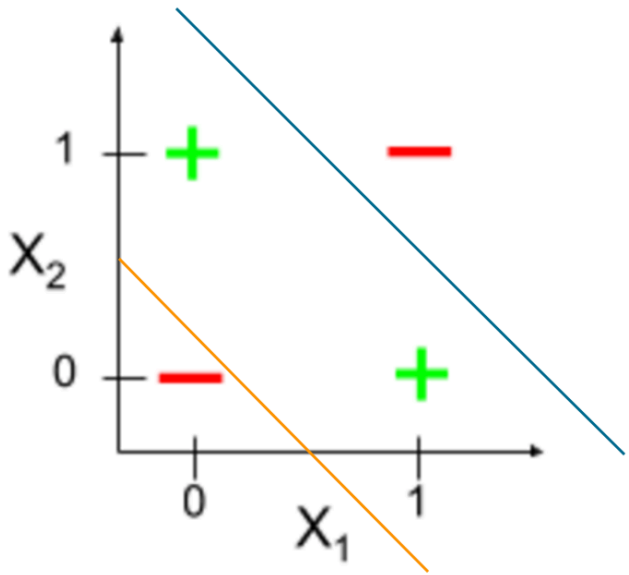


Example: XOR Problem

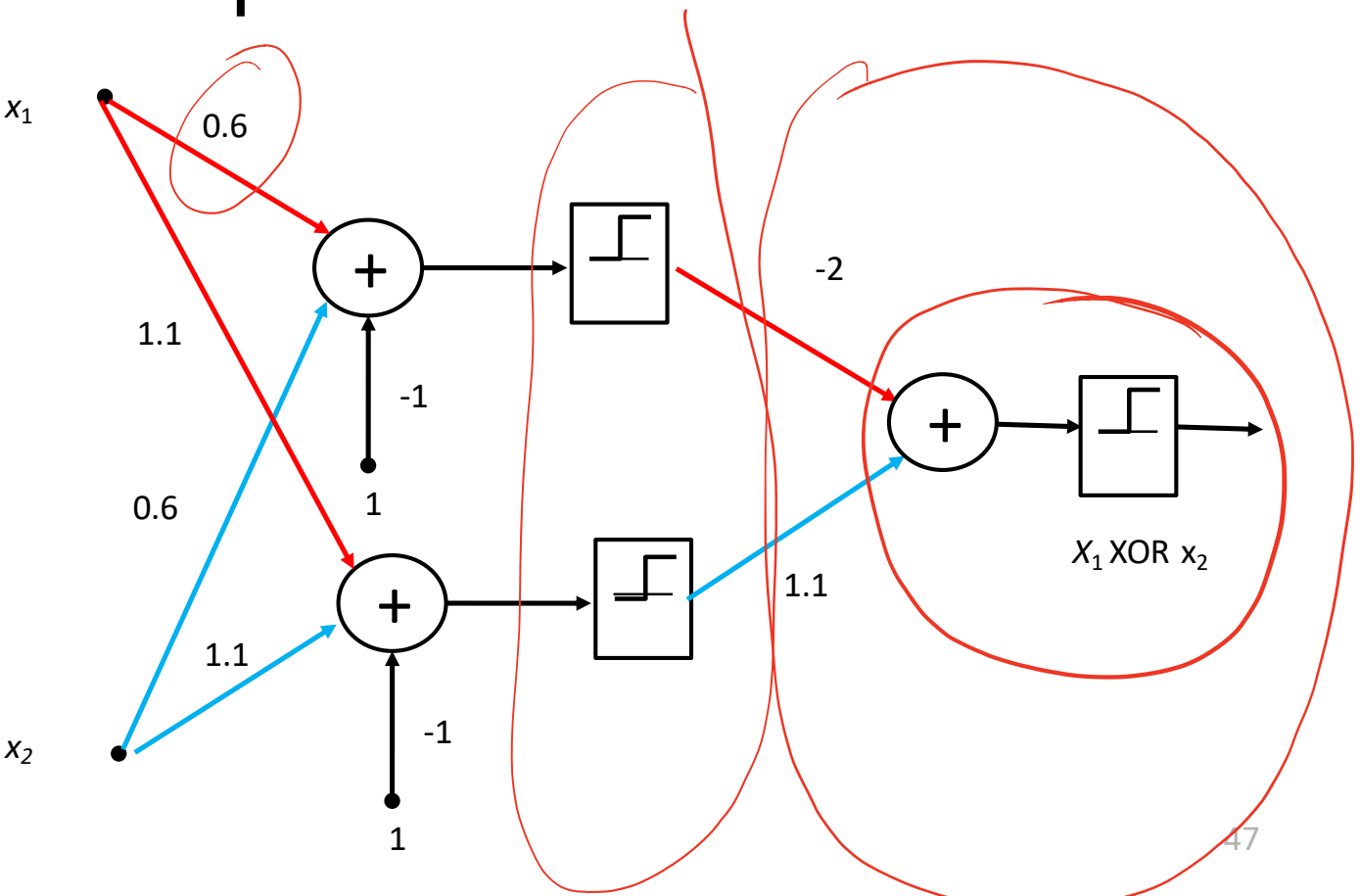


Inputs		Outputs
X_1	X_2	Y
0	0	0
0	1	1
1	0	1
1	1	0

Example: XOR Problem



Example: XOR Problem



Caveat

- Finding the weights is ad-hoc and becomes complicated when implementing complex functions with multiple inputs.
- A principled way of representing and training multiple layers of Perceptrons is needed.

Multi-Layer Perceptron (MLP)

- MLP consists of multiple layers of Perceptrons
- Each layer may have a different number of neurons
- Different types of activation functions can be used, not just the sign (threshold) function

Multi-Layer Perceptron (MLP)

- MLPs can essentially be represented as nested functions:

$$\mathbf{g}(\mathbf{x}) = \mathbf{g}^{(M)}(\mathbf{g}^{(M-1)}(\ldots(\mathbf{g}^{(3)}(\mathbf{g}^{(2)}(\mathbf{g}^{(1)}(\mathbf{x}))))\ldots))$$

- For example, a three layer perceptron can be represented as:
- $\mathbf{g}(\mathbf{x}) = \mathbf{g}^{(3)}(\mathbf{g}^{(2)}(\mathbf{g}^{(1)}(\mathbf{x})))$

Multi-Layer Perceptron (MLP)

- Each $\mathbf{g}^{(i)}$ is a layer of neurons with its weight matrix $\mathbf{W}^{(i)}$ and bias vector $\mathbf{b}^{(i)}$ and activation function $\mathbf{f}^{(i)}$

Multi-Layer Perceptron (MLP)

- This means the output of the i^{th} layer, $\mathbf{a}^{(i)}$ is:

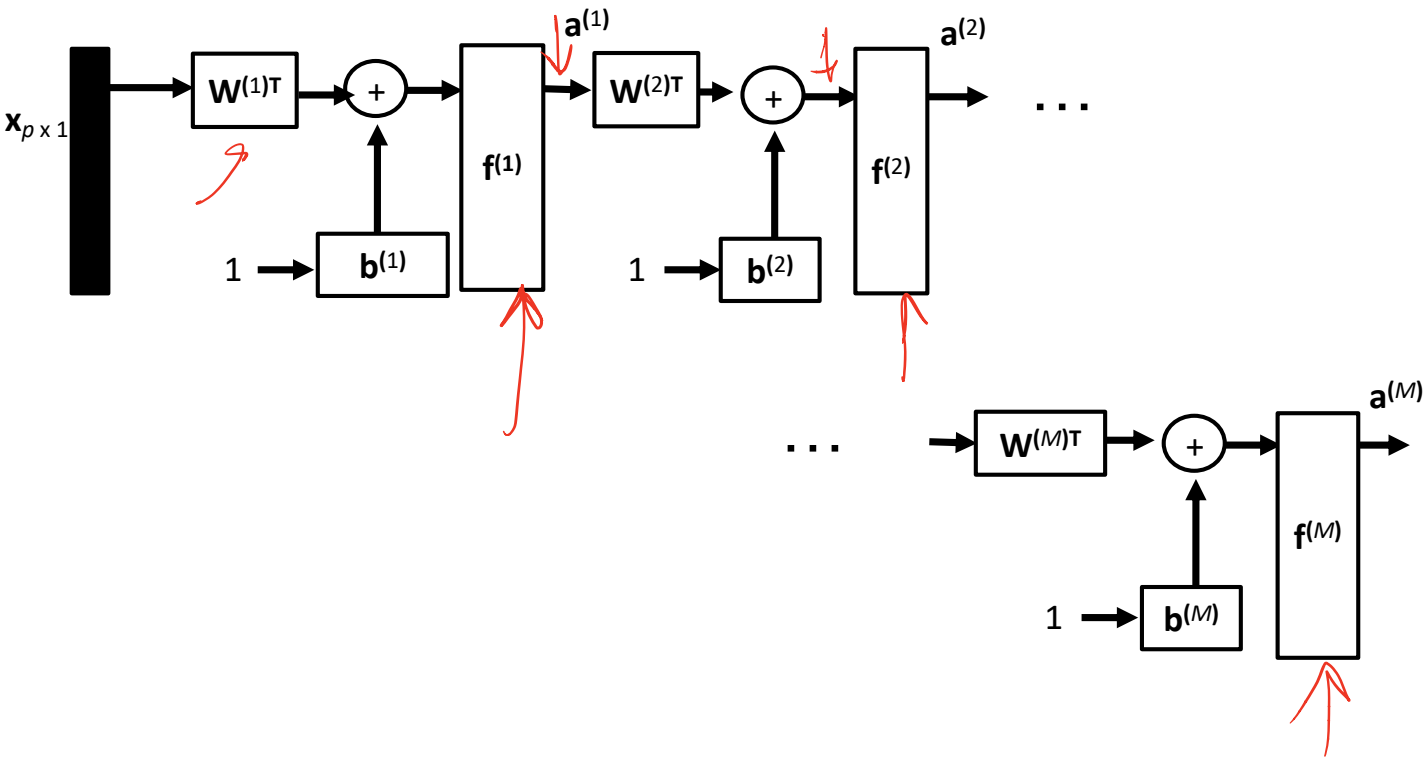
$$\mathbf{a}^{(i)} = \mathbf{f}^{(i)}(\mathbf{W}^{(i)\,T}\mathbf{a}^{(i-1)} + \mathbf{b}^{(i)}) = \mathbf{g}^{(i)}(\mathbf{a}^{(i-1)})$$

The output of the i-th layer

element-wise

output of layer $i-1$

Multi-Layer Perceptron (MLP)



Multi-Layer Perceptron (MLP)

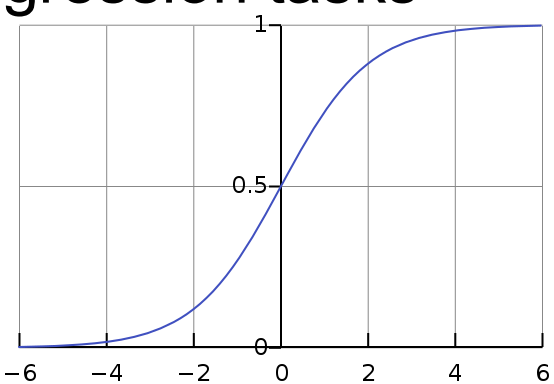
- MLPs are also called Feedforward Neural Networks
- Especially when the number of layers is large (e.g. M >10), they are called Deep Feedforward Neural Networks

Multi-Layer Perceptron (MLP)

•Weights in each layer can be learned so that the MLP is used for either classification or regression tasks.

Types of Activation Functions Used

- Traditionally, sigmoid functions were commonly used for both classification and regression tasks

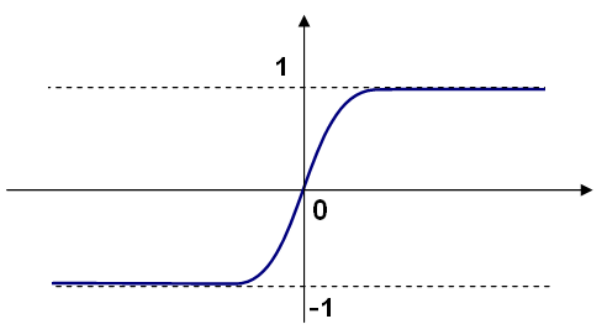


$$f(x) = \frac{1}{1 + e^{-x}}$$

$$= \frac{e^{x}}{e^{x} + 1}$$

Types of Activation Functions Used

•Traditionally, tanh sigmoid functions were commonly used for both classification and regression tasks

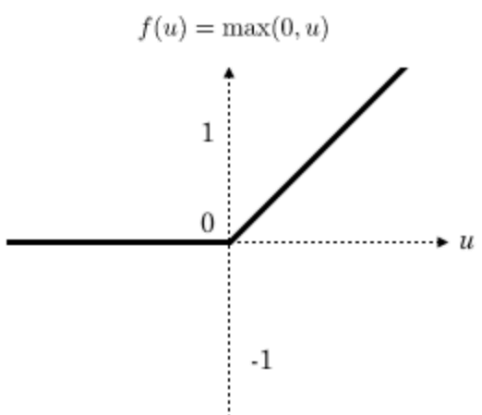


$$f(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$$

$$= \frac{e^{2x} - 1}{e^{2x} + 1}$$

Types of Activation Functions Used

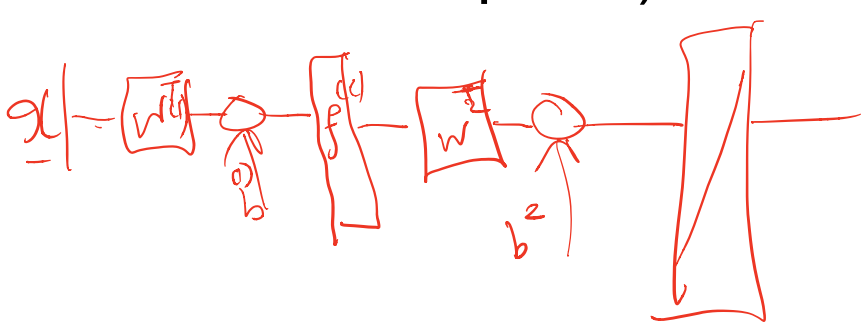
- In more modern practices for training deep neural networks, the Rectified Linear Unit (ReLu) is commonly used



MLPs are Powerful Tools for Regression

Cybenko 95

- It can be proven mathematically that any *smooth* function can be approximated with any precision using an MLP with only two layers:
  - A *hidden layer* of smooth nonlinear functions (e.g. sigmoids)
  - An *output layer* of smooth functions (even linear functions are adequate!)



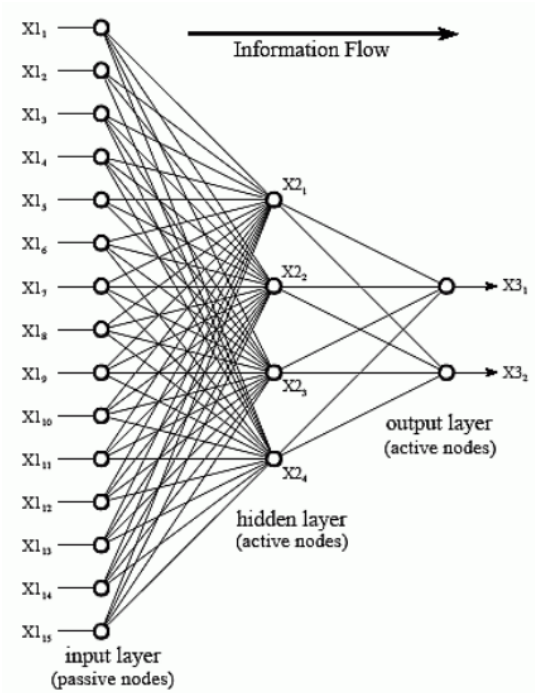
- This means that MLPs are *universal approximators!*

MLPs are Powerful Tools for Classification

- MLPs can be used for classification usually with at least:
  - A *hidden layer* of smooth nonlinear functions (e.g. sigmoids)
  - An *output layer* of linear functions followed by threshold functions.
  - Classes are usually encoded using
    - Binary encoding
    - One hot encoding
  - Therefore, desired outputs are vectors representing each class

Architectural Considerations

- Choice of depth (number of layers) of network
- Choice of width (number of neurons) of each layer



Architectural Considerations

- Deeper networks have
  - Far fewer units in each layer
  - Often generalize well to the test set
- They are often more difficult to train
  - Ideal network architecture must be found via experimentation guided by validation set error

4/20/20

There is No Free Lunch!

There is no universal procedure for examining a training set of specific examples and choosing a function that will generalize to points not in training set.

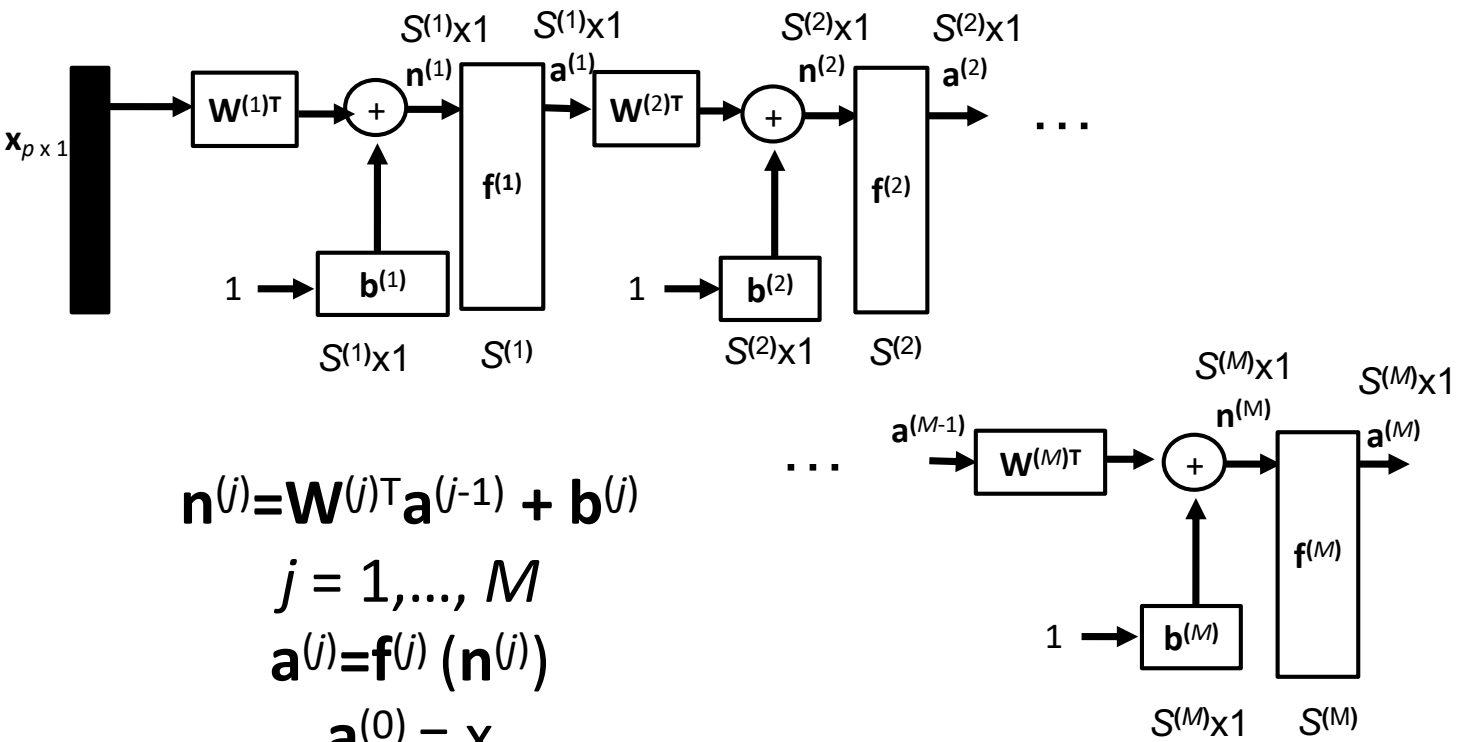
How to Train MLPs

- MLPs are trained using optimization algorithms.
- Optimization algorithms need calculation of Gradients to be numerically solved

How to Train MLPs

- *Backpropagation* (of errors) is a brilliant yet simple method to calculate gradients used to adjust the weights in MLPs to learn regression and classification tasks
- It was proposed by Rumelhart, Hinton, and Williams in 80's
- Still used in modern practices

Multi-Layer Perceptron (MLP)



$$\mathbf{n}^{(j)} = \mathbf{W}^{(j)T}\mathbf{a}^{(j-1)} + \mathbf{b}^{(j)}$$

$$j = 1, \ldots, M$$

$$\mathbf{a}^{(j)} = \mathbf{f}^{(j)}\left(\mathbf{n}^{(j)}\right)$$

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

Training Formulation for MLP

- Training Set
- {**x**(1), **y**(1)} , {**x**(2), **y**(2)} ,… , {**x**(N), **y**(N)}
- We would like to minimize some objective function *J* by finding "suitable" weight matrices for each layer.

Training Formulation for MLP

- A suitable objective function J is expected sum of square errors

$$J = E\left\{\sum_{i=1}^{S^M} e_i^2\right\} = E\left\{\sum_{i=1}^{S^M} (y_i - a_i^M)^2\right\}$$

$$= E\{\mathbf{e}^T\mathbf{e}\}$$

Training formulation for MLP

$$J = E\{\mathbf{e}^T\mathbf{e}\} \approx \frac{1}{N}\sum_{k=1}^{N}\mathbf{e}(k)^T\mathbf{e}(k)$$

$$\mathbf{e}(k) = \mathbf{y}(k) - \mathbf{a} = \mathbf{y}(k) - \mathbf{a}^{(M)}$$

$$= \mathbf{y}(k) - \mathbf{g}^{(M)}(\mathbf{g}^{(M-1)}(\ldots(\mathbf{g}^{(3)}(\mathbf{g}^{(2)}(\mathbf{g}^{(1)}(\mathbf{x}(k)))))\ldots))$$

Training formulation for MLP

$$J = E\{\mathbf{e}^T\mathbf{e}\} \approx \frac{1}{N}\sum_{k=1}^{N}\mathbf{e}(k)^T\mathbf{e}(k)$$

- We don't know *J* at each moment that some pair **x**(*k*) and **y**(*k*) becomes available.

Training formulation for MLP

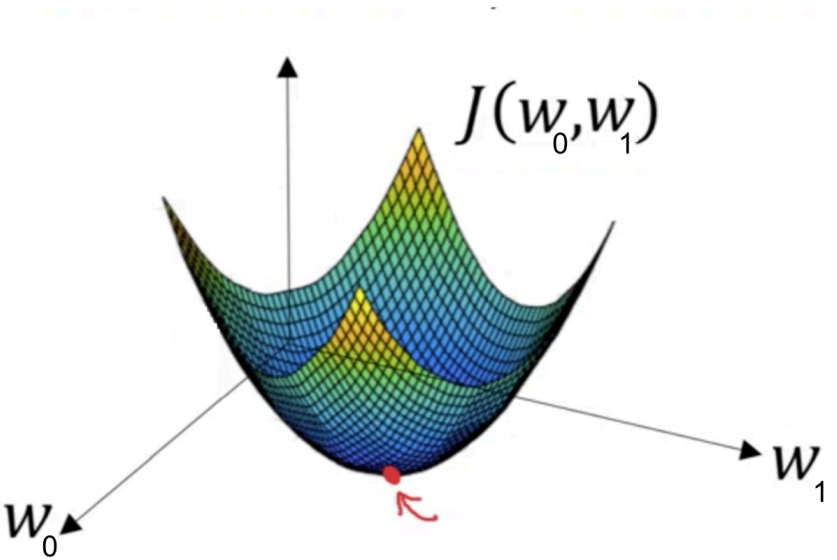
$$J = E\{\mathbf{e}^T\mathbf{e}\} \approx \frac{1}{N}\sum_{k=1}^{N}\mathbf{e}(k)^T\mathbf{e}(k)$$

- We approximate *J* based on the error of the network with respect to the pair **x**(*k*) and **y**(*k*), i. e. $J \approx \mathbf{e}(k)^{\mathsf{T}}\mathbf{e}(k)$
- Alternatively, one can use a "mini-batch" of *L* pairs. For simplicity, we use only one pair.

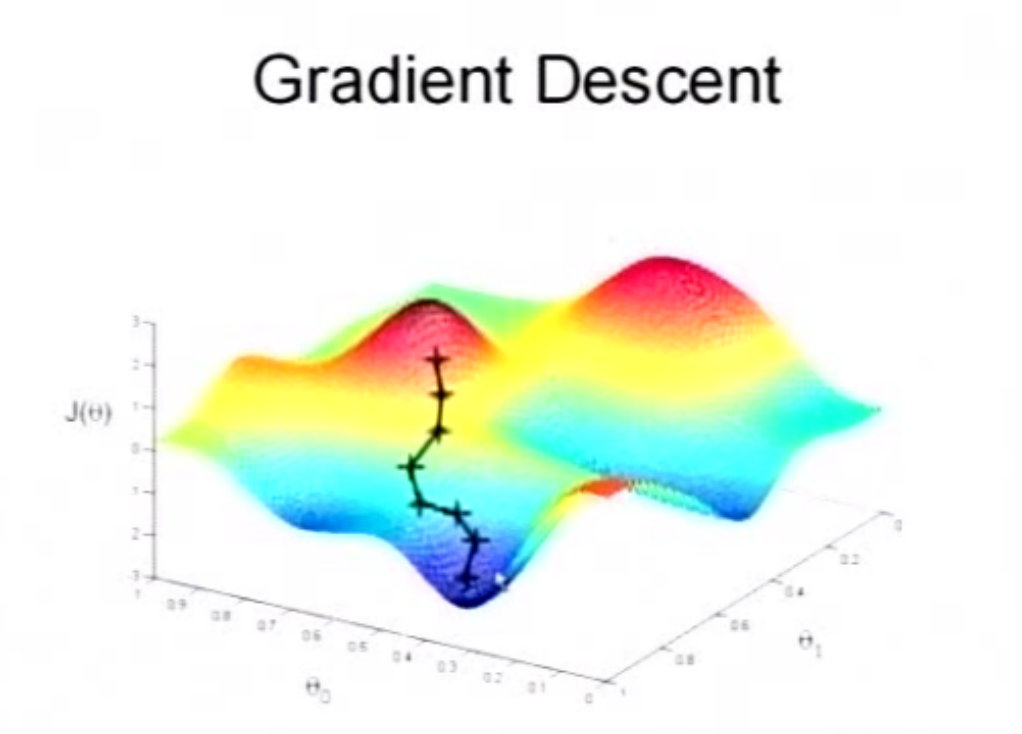
Approximate Gradient Descent

- $w_{ij}^{m}(k+1) = w_{ij}^{m}(k) - \alpha \partial J / \partial w_{ij}^{m}$
- $b_{i}^{m}(k+1) = b_{i}^{m}(k) - \alpha \partial J / \partial b_{i}^{m}$

Gradient Descent Formulation



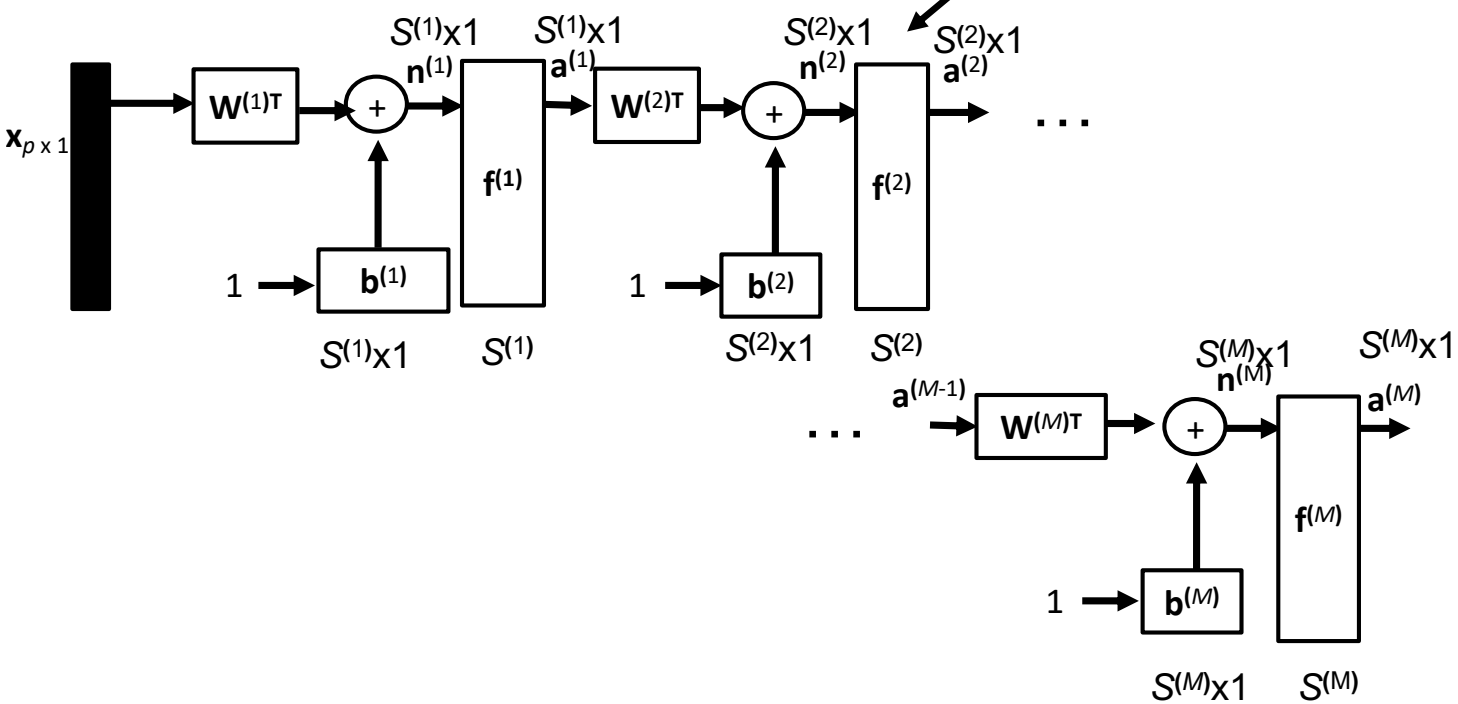
Gradient Descent Formulation



Forward Propagation

- $\mathbf{a}^{(0)} = \mathbf{x}(k)$
- $\mathbf{a}^{(m+1)} = \mathbf{f}^{(m+1)}(\mathbf{W}^{(m+1)\mathrm{T}}\mathbf{a}^{(m)} + \mathbf{b}^{(m+1)})$
- $m = 0, 1, 2, \ldots, M-1$
- $\mathbf{a}^{(M)} = \mathbf{a}$

Elementwise operation



Back Propagation

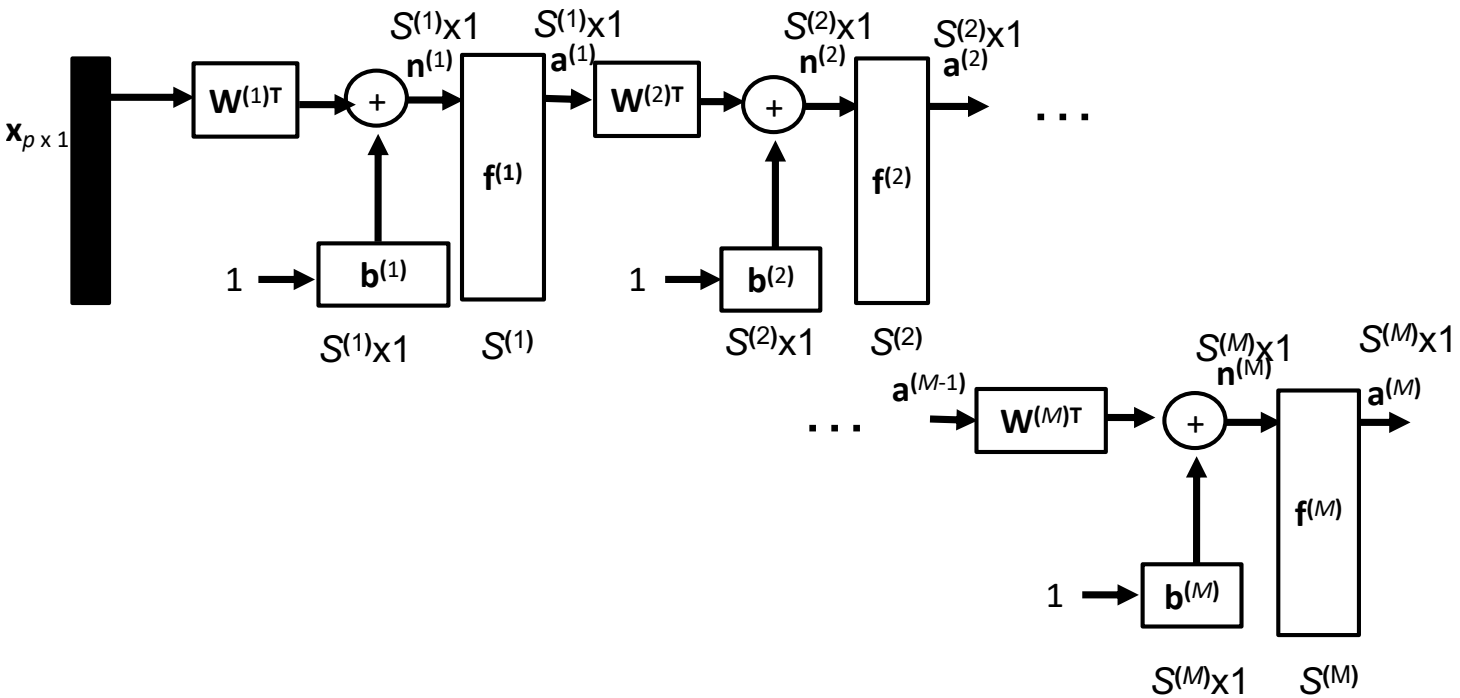
- Define $\mathbf{F}'^{(m)}(\mathbf{n}^{(m)})$ as:

$$\begin{bmatrix} \dot{f}^m(n_1^m) & 0 & \dots & 0 \\ 0 & \dot{f}^m(n_2^m) & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \dot{f}^m(n_{S^m}^m) \end{bmatrix}$$

$$\dot{f}^m(n_j^m) = \frac{\partial f^m(n_j^m)}{\partial n_j^m}$$

Back Propagation

- $\mathbf{s}^{(M)} = -2\mathbf{F}'^{(M)}(\mathbf{n}^{(M)})(\mathbf{y}-\mathbf{a})$
- $\mathbf{s}^{(m)} = \mathbf{F}'^{(m)}(\mathbf{n}^{(m)})\mathbf{W}^{(m+1)}\mathbf{s}^{(m+1)}$
- $m = M-1,\ldots,2,1$
- $\mathbf{a}^{(M)} = \mathbf{a}$



Back Propagation

- The sensitivities are computed by starting at the last layer, and then propagating backwards through the network to the first layer.

$$\mathbf{s}^{M} \rightarrow \mathbf{s}^{M-1} \rightarrow \ldots \rightarrow \mathbf{s}^{2} \rightarrow \mathbf{s}^{1}$$

Back Propagation

- For an objective function other than $J = \mathbf{e}^T\mathbf{e}$, the term $-2(\mathbf{y}-\mathbf{a})$ in sensitivity calculation
  $\mathbf{s}^{(M)} = -2\mathbf{F}'^{(M)}(\mathbf{n}^{(M)})(\mathbf{y}-\mathbf{a})$
  will be replaced with $\nabla_{\mathbf{a}} J$

Weight Update

- $\mathbf{W}^{(m)}(k+1) = \mathbf{W}^{(m)}(k) - \alpha \mathbf{a}^{(m-1)} \mathbf{s}^{(m)T}$
- $\mathbf{b}^{(m)T}(k+1) = \mathbf{b}^{(m)T}(k) - \alpha \mathbf{s}^{(m)T}$
- Compare these equations with the Perceptron update rule.

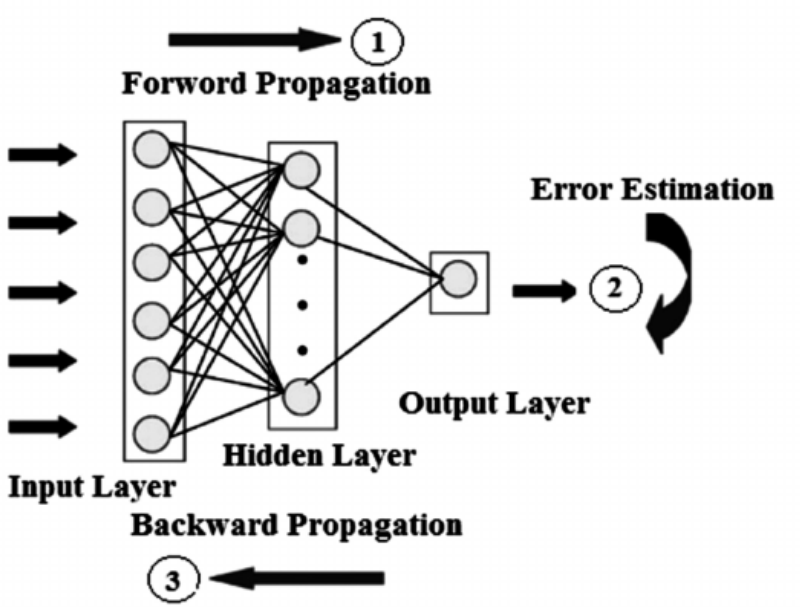
Weight Update

- $\mathbf{W}^{(m)}(k+1) = \mathbf{W}^{(m)}(k) - \alpha \mathbf{a}^{(m-1)} \mathbf{s}^{(m)T}$
- $\mathbf{b}^{(m)T}(k+1) = \mathbf{b}^{(m)T}(k) - \alpha \mathbf{s}^{(m)T}$
- We present each (randomly selected) training sample (or batch of samples) and use the forward and backward paths to calculate sensitivities and update the weights.
- This is called an iteration.

Weight Update

- $\mathbf{W}^{(m)}(k+1) = \mathbf{W}^{(m)}(k) - \alpha \mathbf{a}^{(m-1)} \mathbf{s}^{(m)T}$
- $\mathbf{b}^{(m)T}(k+1) = \mathbf{b}^{(m)T}(k) - \alpha \mathbf{s}^{(m)T}$
- Each time we finish presenting the whole training set to the network, we complete an epoch.
- An epoch includes multiple iterations.
- Training the network requires multiple epochs.

Backpropagation Schema



Regularization Methods

- In general, any method to prevent overfitting or help the optimization is considered regularization.
- One can add L1 and L2 regularizers to the objective function in backpropagation.
- However, empirical regularization is also very popular for Neural Networks.

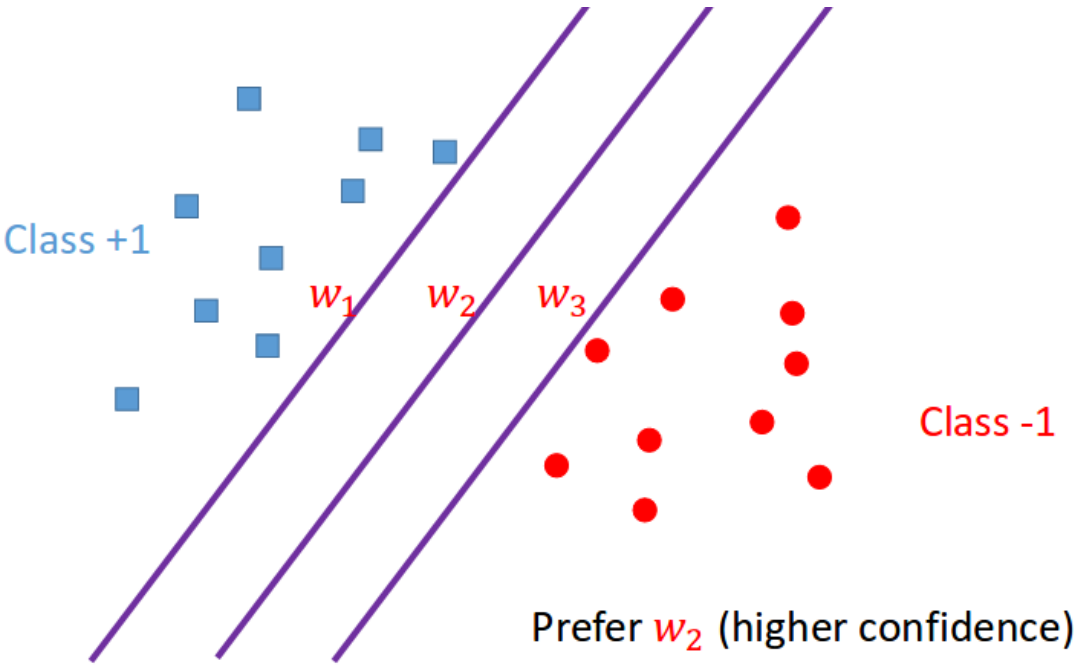
Regularization Methods

- One can show that L2 regularization is equivalent to *weight decay*
- $\mathbf{W}^{(m)}(k+1) = (1-\eta\alpha)\mathbf{W}^{(m+1)}(k) - \alpha\mathbf{a}^{(m-1)}\mathbf{s}^{(m)T}$
- $\mathbf{b}^{(m)T}(k+1) = (1-\eta\alpha)\mathbf{b}^{(m)T}(k) - \alpha\mathbf{s}^{(m)T}$
- *η is called the decay rate.*

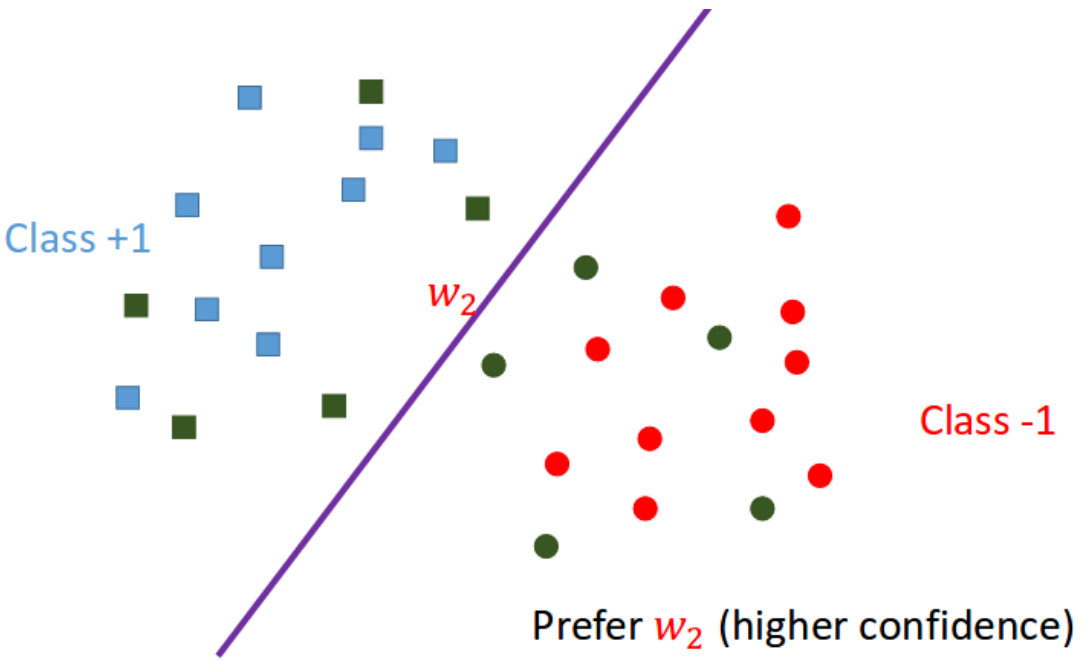
Regularization Methods

- Empirical regularization is also very popular for Neural Networks.

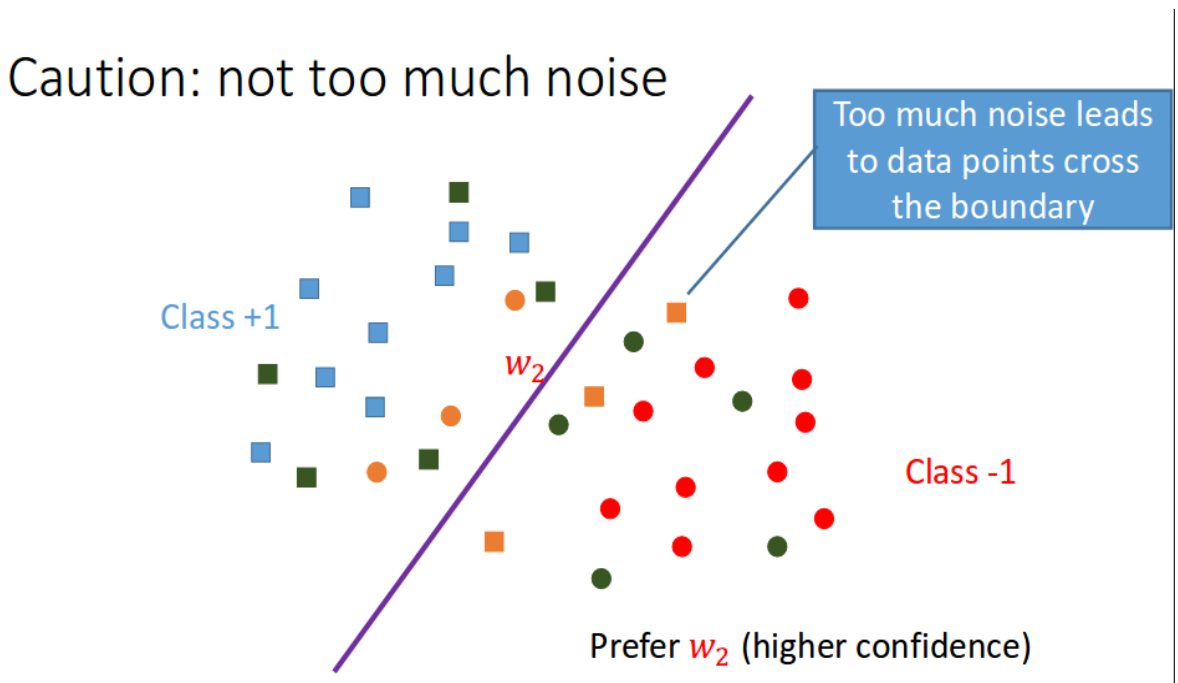
Adding Noise to The Input



Adding Noise to The Input



Drawback: Too much noise is harmful



Adding Noise to Weights

- Adding noise to the weights can be shown to be equivalent to adding a regularization term to the objective function\
- Noise has shown to have benefits when added to many learning algorithms.

Data Augmentation

- Adding noisy or transformed versions of training data to the training set

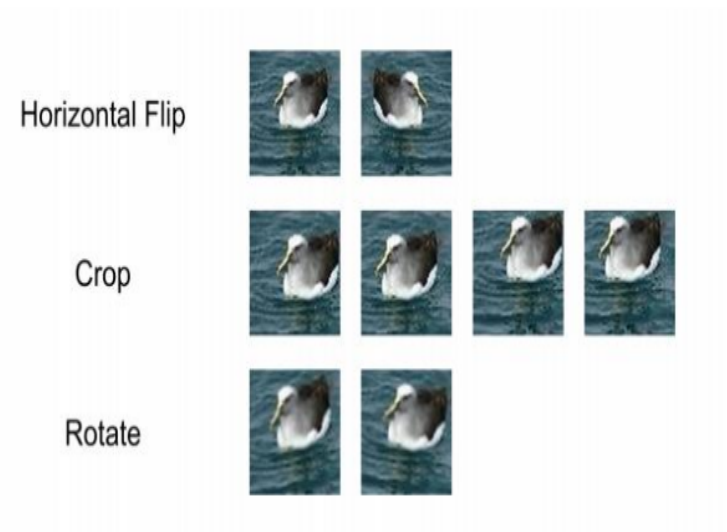


Figure from *Image Classification with Pyramid Representation and Rotated Data Augmentation on Torch 7*, by Keven Wang

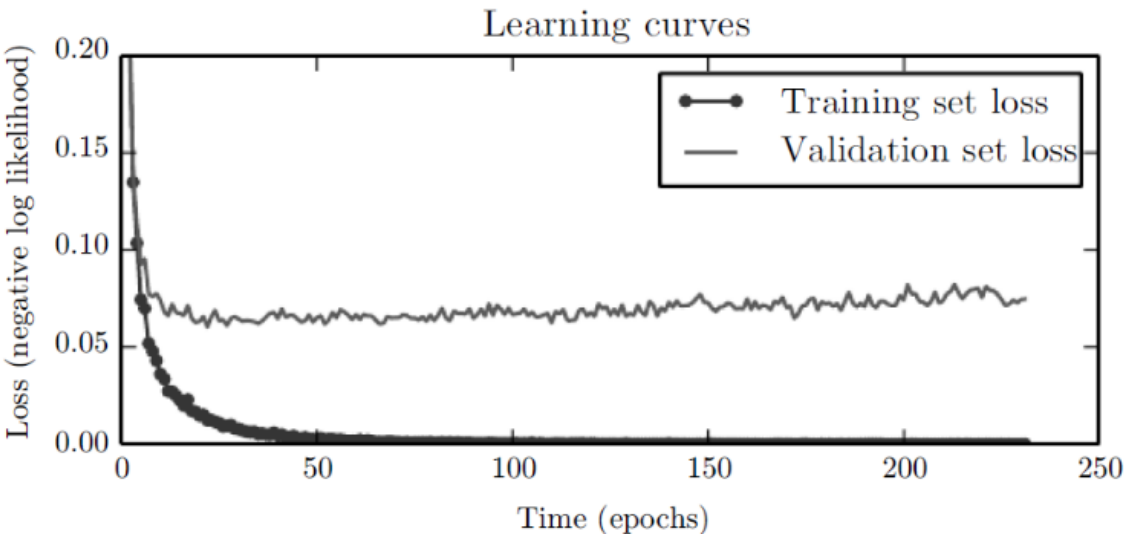
Be Careful!

- Be careful about the transformation applied:
- Example: classifying ‘b’ and ‘d’
- Example: classifying ‘6’ and ‘9’

Early Stopping

- Idea: don't train the network to have very small training error
- Prevent overfitting: use a validation set and validation error to decide when to stop the algorithm
- When the validation error starts increasing, overfitting is occurring.

Early Stopping



Another Version of Early Stopping

- When training, monitor validation error
- Every time validation error improved, store a copy of the weights
- When validation error not improved for some time, stop
- Return the copy of the weights stored

Early Stopping: Pros and Cons

- Advantage
  - Efficient: along with training; only store an extra copy of weights
  - Simple: no change to the model/algorithm
- Disadvantage:
  - Need validation data

Early Stopping: Pros and Cons

- How to remedy the disadvantage?
- After early stopping of the first run, train a second run and reuse validation data

Early Stopping: Pros and Cons

- How to reuse validation data?
  - 1.Start fresh, train with both training data and validation data up to the previous number of epochs
  - 2. Start from the weights in the first run, train with both training data and validation data until the training loss < the validation loss at the early stopping point

Dropout

- **Randomly** select weights to update
- More precisely, in each update step:
- Randomly sample a different binary mask to all the input and hidden units
- Multiple the mask bits with the units and do the update as usual
- Typical dropout probability: 0.2 for input and 0.5 for hidden units

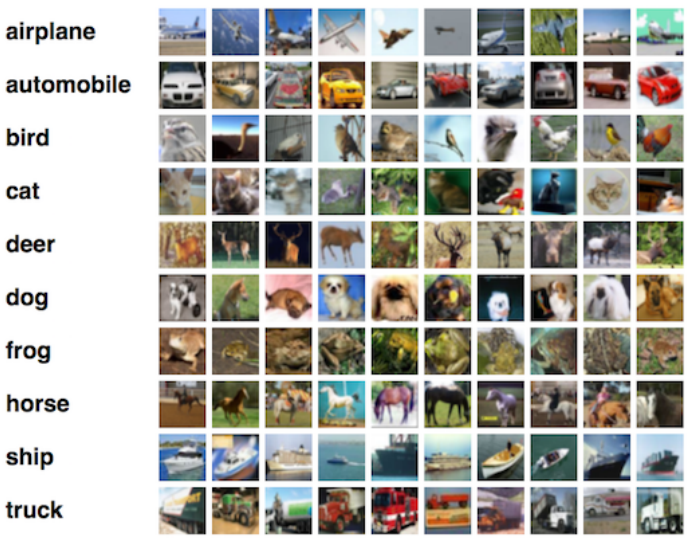
What regularizations are frequently used?

- L2 regularization
- Early stopping
- Dropout
- Data augmentation if the transformations known/easy to implement

The Challenge of Dealing with Images

MNIST: Handwritten digit recognition
CIFAR-10: 10 distinct classes – airplane, automobile, bird, cat, deer, dog, frog, horse, ship & truck)

MNIST



CIFAR-10

Image Classification and MLPs

- A two-layer MLP can achieve an accuracy of 98.2%, which can be quite easily improved.
- Fully connected MLPs will usually not be the model of choice for image-related tasks
- It is far more typical to make advantage of a convolutional neural network (CNN) for images.

Image Classification and MLPs: Weight Proliferation

- The number of parameters (weights) of MLPs fed with raw image data is very large for images
- CIFAR-10: 32×32×3 colored images

Image Classification and MLPs: Weight Proliferation

- If we treat each channel of each pixel as an independent input to an MLP, each neuron of the first hidden layer adds ~3000 new parameters to the model!
- The number of weights quickly becomes unmanageable as image sizes grow larger

Image Classification and MLPs: Weight Proliferation

- If we treat each channel of each pixel as an independent input to an MLP, each neuron of the first hidden layer adds 3072 new parameters to the model!
- The number of weights quickly becomes unmanageable as image sizes grow larger
- This is sometimes called weight proliferation

Image Classification and MLPs: Downsampling

- Common solution: *down-sampling* the images to have fewer weights
- Drawback: direct down-sampling = loosing valuable information
- Key concept: images carry more information than their vectorized versions
- Adjacent pixels carry some information about the image

Exploiting The Structure

- The information carried by adjacent pixels can be summarized.
- Summarization is performed by the so-called convolution operator.

1	1	1	0	0
0	1	1	1	0
0	0	1	1	1
0	0	1	1	0
0	1	1	0	0

A Simple “Image”

The Convolution Operator: Kernel/ Filter

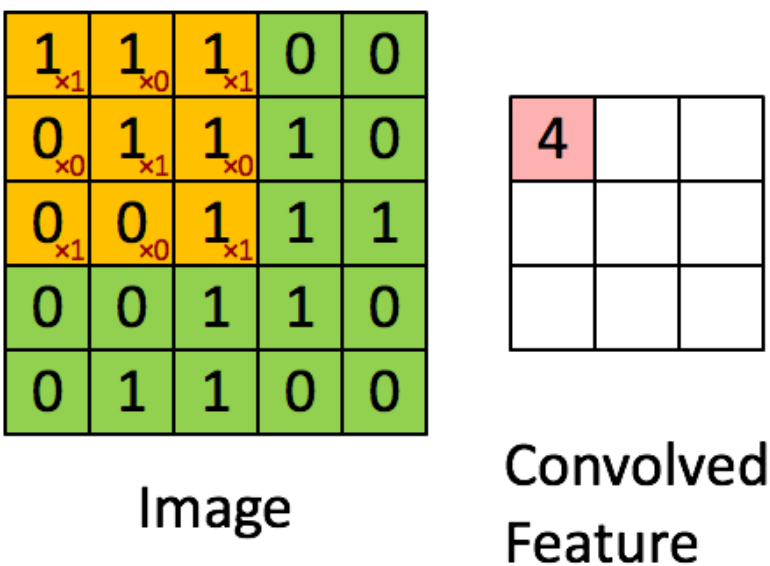
- The Kernel (or Filter) in the convolution operator is a small matrix which encodes a way of extracting an interesting feature of an image.

1	0	1
0	1	0
1	0	1

A Simple Kernel

The Convolution Operator

- The result is called a feature map, convolved feature, or activation map.



Different Kernels?

- It is evident that different Kernels will produce different Feature Maps for the same input image.
- Consider the following image:

Sharpen

0	0	0	0	0
0	0	-1	0	0
0	-1	5	-1	0
0	0	-1	0	0
0	0	0	0	0

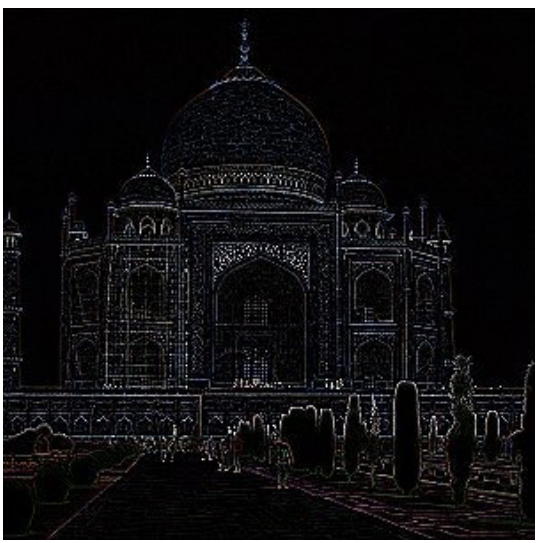
Blur

0	0	0	0	0
0	1	1	1	0
0	1	1	1	0
0	1	1	1	0
0	0	0	0	0

Edge enhance

	0	0	0	
	-1	1	0	
	0	0	0	

Edge detect



	0	1	0	
	1	-4	1	
	0	1	0	

Emboss

	-2	-1	0	
	-1	1	1	
	0	1	2	

The Convolution Operator: A More Practical Example

Which Kernel to Use?

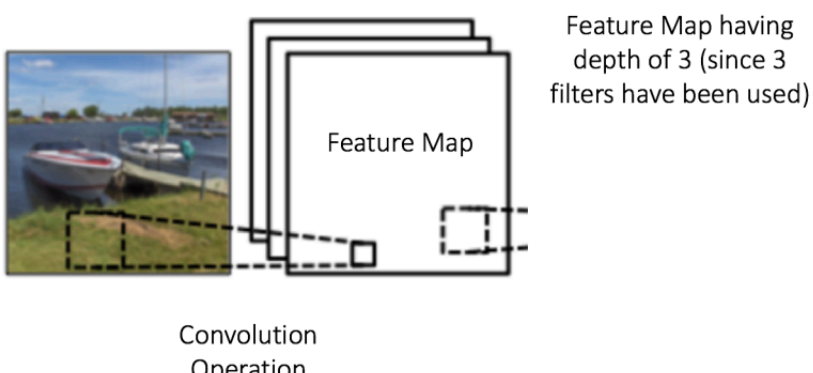
- Modern Machine Learning is about using machines to decide which features are the best
- A structure called a Convolutional Neural Network *learns* the values of these filters

Structure of a CNN

- The size of the Feature Map (Convolved Feature) is controlled by three parameters:
  - Depth
  - Stride
  - Zero-padding

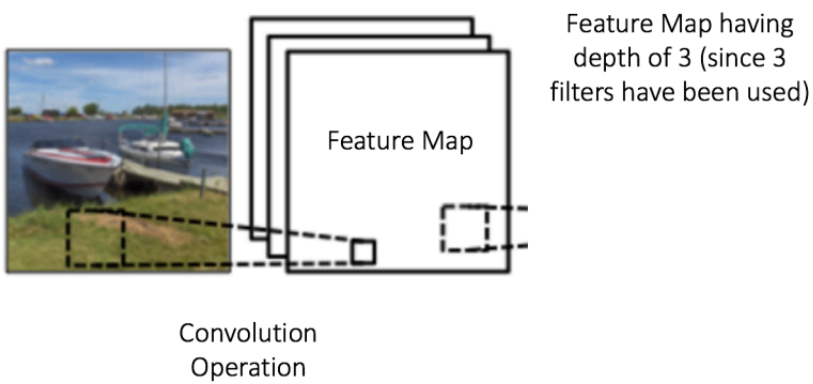
Structure of a CNN: Depth

- Depth is the number of filters used for convolution.
- In the following network, three distinct filters are used, thus three different feature maps



Structure of a CNN: Depth

- These three feature maps can be viewed as three stacked matrices, so, the “depth” of the feature map would be three.



Structure of a CNN: Stride

- Stride: the number of pixels by which we slide our filter matrix over the input matrix.
- Stride = 1: the filters move one pixel at a time.
- Stride = 2: the filters jump 2 pixels at a time .
- Larger stride yield smaller feature maps.

Structure of a CNN: Zero-Padding

- Sometimes, we pad the input matrix with zeros around the border to apply the filter to bordering elements of the input image matrix.

Structure of a CNN: Zero-Padding

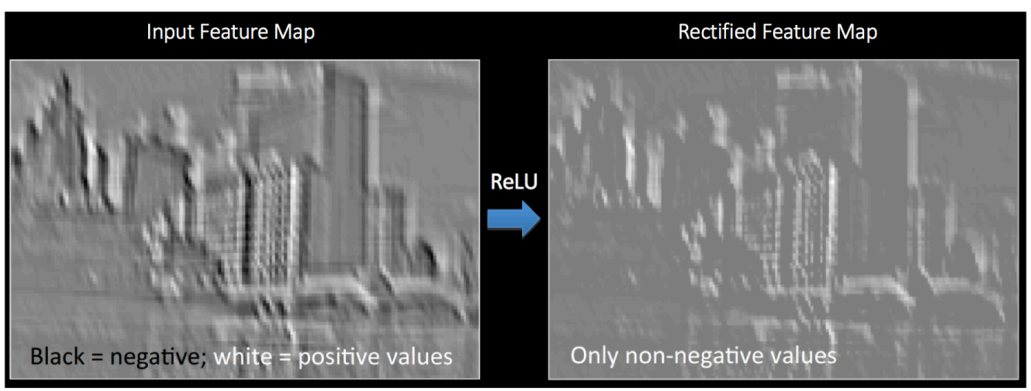
- Zero padding controls the size of the feature maps.
- Adding zero-padding: *wide convolution*
- Not using zero-padding : *narrow convolution*.

Introducing Nonlinearity

- ReLU is applied element-wise (per pixel) and replaces all negative pixel values in the feature map by zero.
- ReLU introduces nonlinearity in CNN to deal with inherent nonlinearity of classification problems

Introducing Nonlinearity

- ReLU is applied to feature maps yielding Rectified Feature Maps
- *Tanh* and *sigmoids* have also been used
- ReLU has shown better performance.



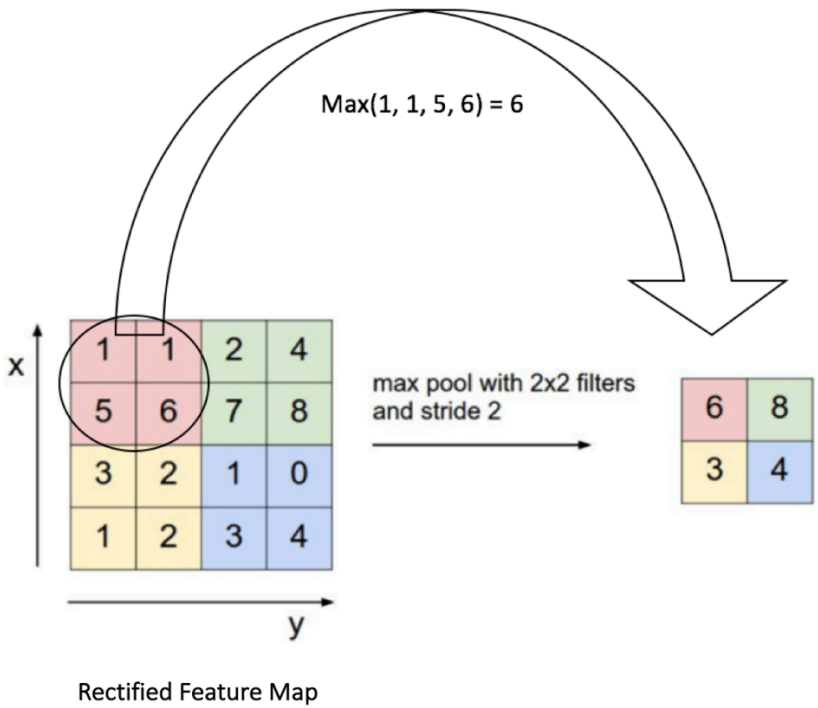
Pooling = Downsampling

- Spatial Pooling (also called subsampling or downsampling) reduces the dimensionality of each feature map but retains the most important information.
- Spatial Pooling can be of different types: Max, Average, Sum etc.

Pooling = Downsampling

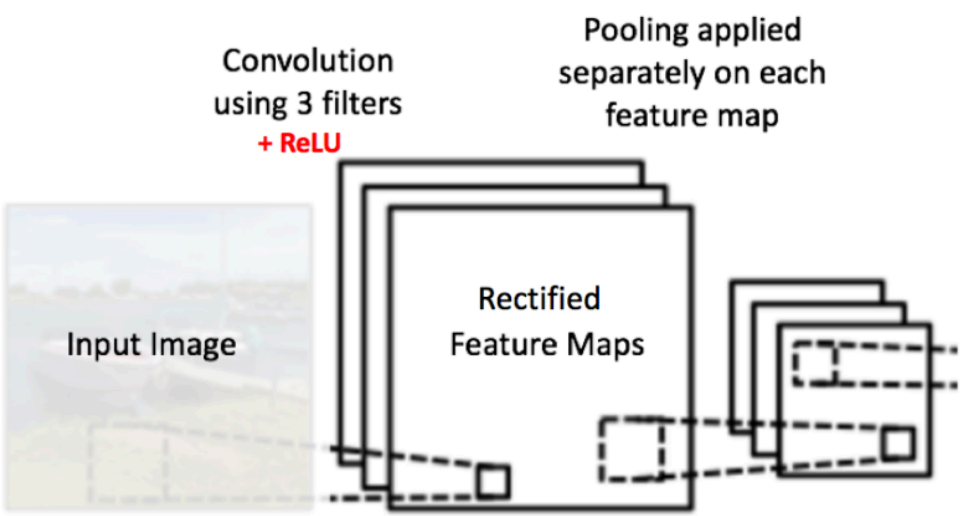
- Max Pooling: define a spatial neighborhood (e.g., a 2×2 window) and take the largest element within that window.
- Instead the largest element the average (Average Pooling) or sum of all elements could be taken.
- In practice, Max Pooling has been shown to work better.

Max Pooling Example



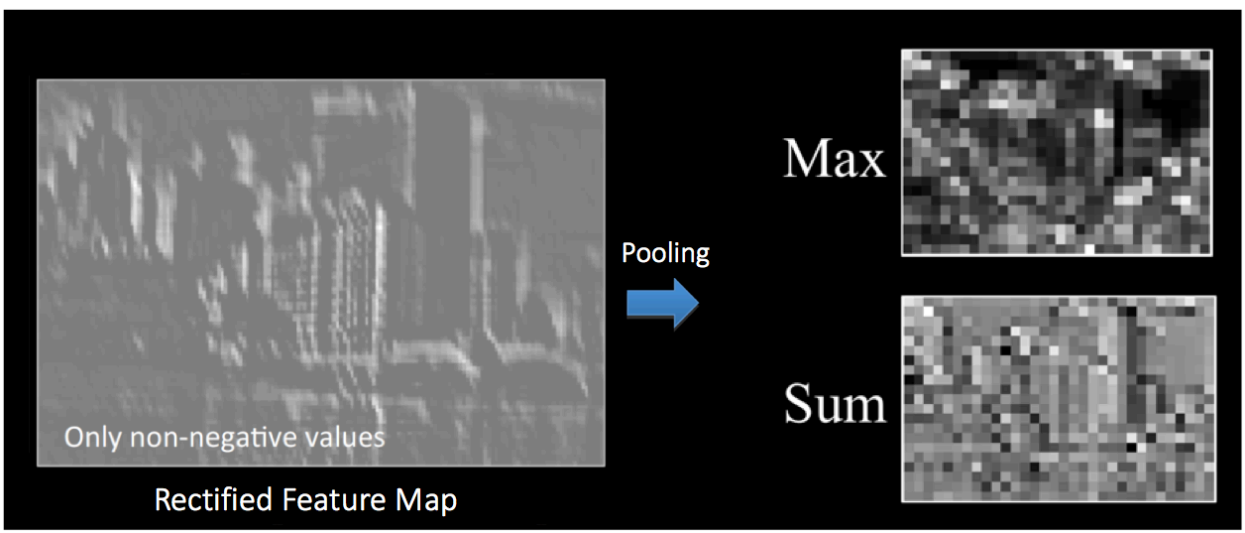
Max Pooling Strides

- Slide the 2 x 2 window by 2 cells (also called “stride”) and take the maximum value in each region to reduces the dimensionality of the feature map.



Max Pooling Strides

- Comparing Max Pooling and Sum Pooling on the Rectified Feature Map of The Buildings Image



Properties of Pooling

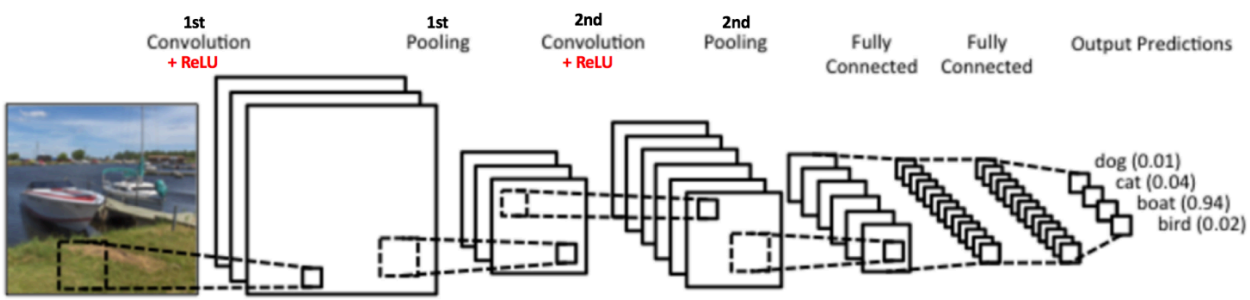
- Reduces the dimensions of the input
- Reduces the number of parameters and, therefore, controls overfitting
- Is invariant to **small** transformations, distortions and translations in the input image
  - A small distortion in input will not change the output of Pooling too much – since we take the maximum / average value in a local neighborhood

Properties of Pooling

- Yields an almost scale invariant representation of our image.
- This is very powerful since we can detect objects in an image no matter where they are located
- In essence, convolutions extract features from the image and pooling makes the features invariant to transformations

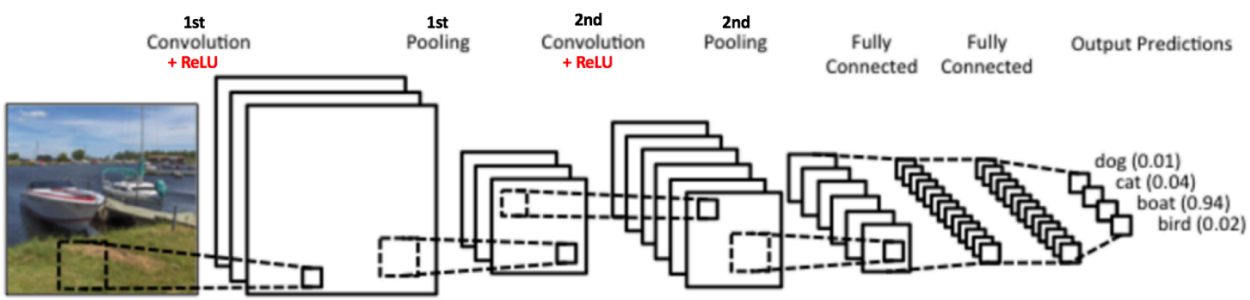
Convolution-ReLU-Pooling Repeated

- The convolution-ReLU-Pooling operation can be repeated many times in many convolutional "layers" with different depths and strides



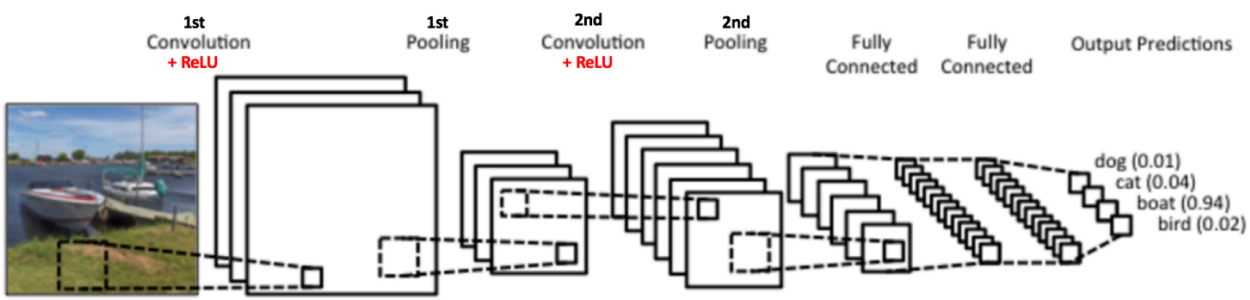
Fully Connected Layer

- Convolutional Layers play the role of feature extractors for a Deep Neural Network
- The output layer of the MLP must be softmax



Other Classification Techniques?

- Instead of MLP, other classifiers such as SVM can be used

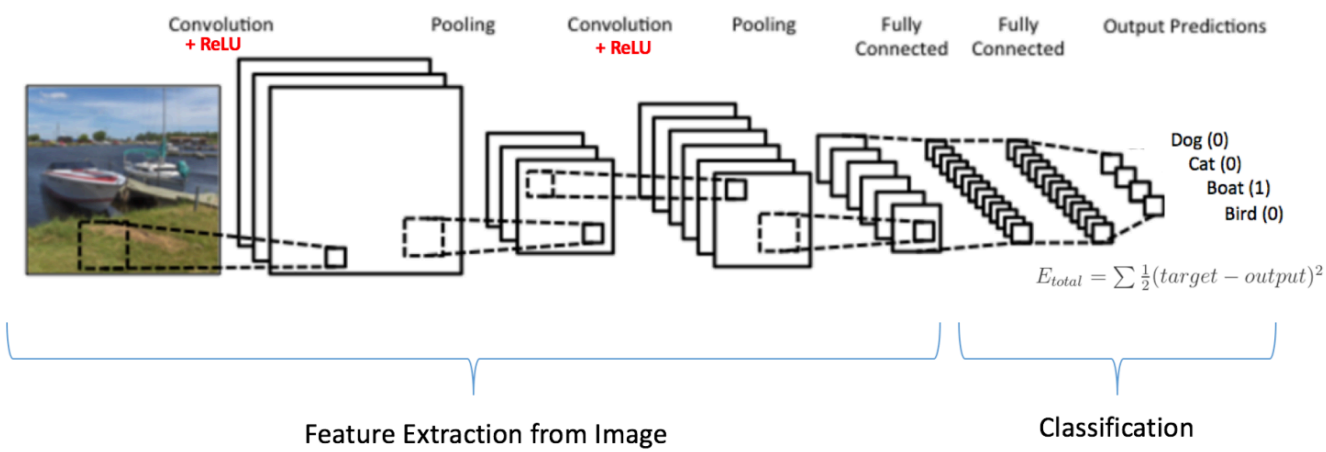


MLP: Even Better Feature Learning!

- Adding a fully-connected layer is also a (usually) cheap way of learning non-linear combinations of these features.
- Most of the features from convolutional and pooling layers may be good for the classification task, but combinations of those features might be even better

Putting It Altogether: Train Using Backpropagation

- Input Image = Boat
- Target Vector = [0, 0, 1, 0]



Putting It Altogether: Train Using Backpropagation

- Initialize weights and filters randomly and repeat the following steps for the training set many times
- Pass each image through the network (forward pass) and read the output
- Calculate the total error
  - **Total Error = $\sum$ (target probability – output probability) ^{2}**
- Target Vector = [0, 0, 1, 0]
- Output Vector =[0.2, 0.4, 0.3, 0.1]
- Error =0.7

Putting It Altogether: Train Using Backpropagation

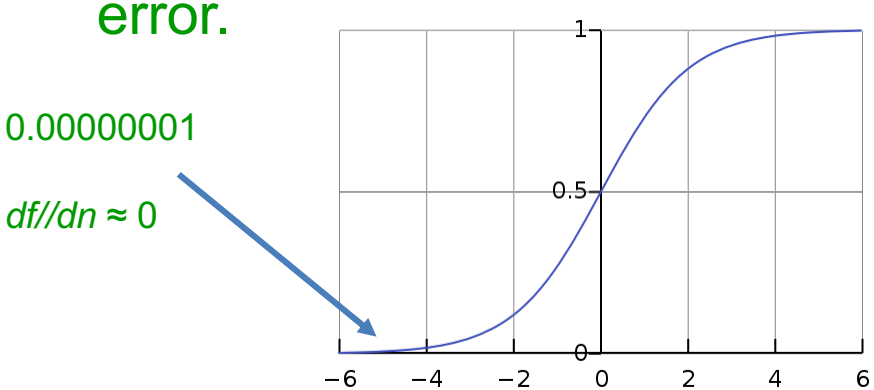
- Use Backpropagation to calculate the *gradients* of the error with respect to all weights in the network and use *gradient descent* to update all filter values / weights and to minimize the output error.
  - The weights are adjusted in proportion to their contribution to the total error.

Putting It Altogether: Train Using Backpropagation

- Number of filters, filter sizes, architecture of the network etc are fixed and do not change during training process
- Only the values of the filter matrix and connection weights are updated.

Problems with squared error

- The squared error measure has some drawbacks:
  - If the desired output is 1 and the actual output is 0.00000001 there is almost no gradient for a sigmoid unit to fix up the error.



Problems with squared error

- The squared error measure has some drawbacks:
  - If we are trying to assign probabilities to mutually exclusive class labels, we know that the outputs should sum to 1, but we are depriving the network of this knowledge.

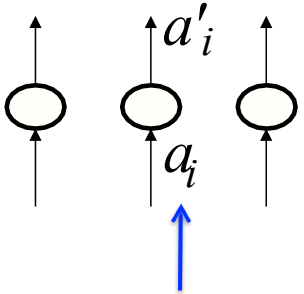
Problems with squared error

- Is there a different cost function that works better?
  - Yes: Force the outputs to represent a probability distribution across discrete alternatives.

Softmax

The output units in a softmax group use a non-local non-linearity:

$$a_i' = \frac{e^{a_i}}{\sum_{j \in group} e^{a_j}}$$

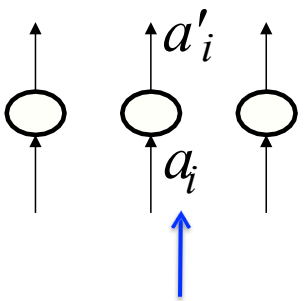


softmax group

$$\frac{\partial a_i'}{\partial a_i} = a_i'(1 - a_i')$$

this is called the "logit"

Relationship with Logistic Regression?



softmax group

this is called the "logit"

$$a'_i = \frac{e^{a_i}}{\sum_{j \in group} e^{a_j}}$$

$$\frac{\partial a'_i}{\partial a_i} = a'_i(1 - a'_i)$$

In logistic regression, logits are *linear functions* of the features. In neural networks, they are features learned by multiple layers of the network!

Relationship with Logistic Regression?

In fact,

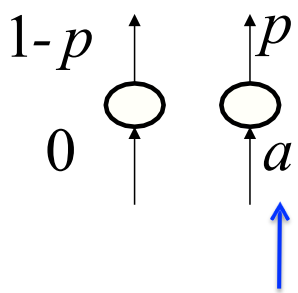
$a = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p$

$= \beta^T \mathbf{x}(j) + \beta_0$

and

1

are the logits for two classes, where $\mathbf{x}(j)$ is the j^{th} data point whose label is $z(j) \in \{0,1\}$.



Relationship with Logistic Regression?

Consequently, for the positive class:

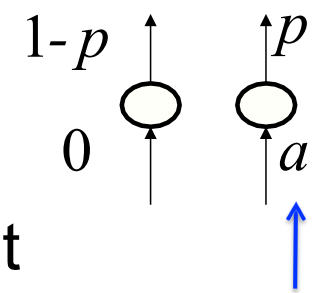
$p=e^a/(e^0+e^a)=e^a/(1+e^a)$

And obviously the output for the negative class is:

$1-p=1/(1+e^a)$

The log-likelihood loss for this single data point **x**(*j*) is:

$-z(j)\log p-(1-z(j))\log(1-p)$

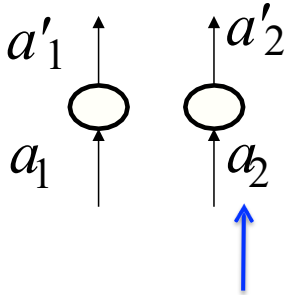


Relationship with Logistic Regression?

The log-likelihood loss for this single data point **x**(*i*) is:

$-z(j)\log p-(1-z(j))\log(1-p)$

If we rename the desired outputs 1-*z*(*j*) and *z*(*j*) to y_1 and y_2, and the probability outputs of softmax as 1-p=a'_1 and p=a'_2, the negative log-likelihood becomes the cross-entropy function:

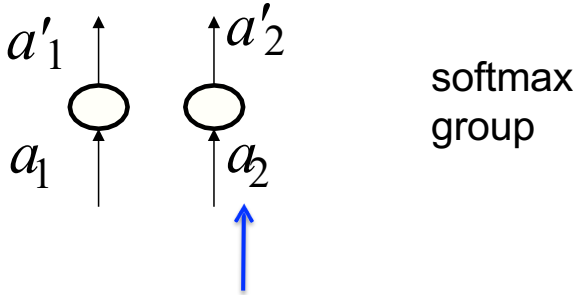


softmax group

Linear Function of Features

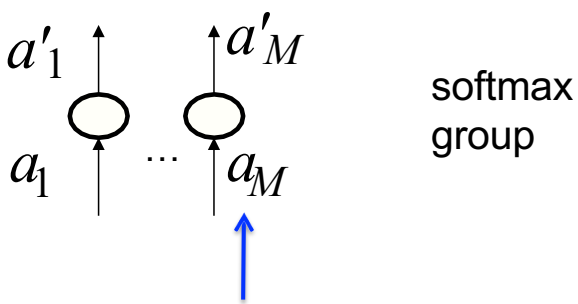
Relationship with Logistic Regression?

If we rename the desired outputs 1-$z(j)$ and $z(j)$ to y_1 and y_2, and the probability outputs of softmax as 1-p=a'_1 and p=a'_2, the negative log-likelihood becomes the cross entropy function:



Relationship with Logistic Regression?

In this case, we only have two neurons representing two classes. If we have more than two classes, we have *M* neurons, and the cross-entropy loss for one data point is:



Cross-entropy: the right cost function to use with softmax

- This cost function is the right cost function.

$$J' = -\sum_{i=1}^{M} y_i \log a'_i$$

$$\frac{\partial J'}{\partial a_i} = \sum_j \frac{\partial J'}{\partial a'_j} \frac{\partial a'_j}{\partial a_i}$$

$$= (a'_i - y_i)$$

Cross-entropy: the right cost function to use with softmax

- J'_2 has a very big gradient when the target value is 1 and the output is almost zero.

$$J' = -\sum_i y_i \log a'_i$$

$$\frac{\partial J'}{\partial a_i} = \sum_j \frac{\partial J'}{\partial a'_j} \frac{\partial a'_j}{\partial a_i}$$

$$= (a'_i - y_i)$$

Cross-entropy: the right cost function to use with softmax

- This basically makes FFNNs with a softmax output layer a nonlinear version of logistic regression, where logits are highly nonlinear functions of the input that are learned from data.

$$J' = -\sum_i y_i \log a'_i$$

$$\frac{\partial J'}{\partial a_i} = \sum_j \frac{\partial J'}{\partial a'_j} \frac{\partial a'_j}{\partial a_i}$$

$$= (a'_i - y_i)$$

Sigmoids in hidden layers

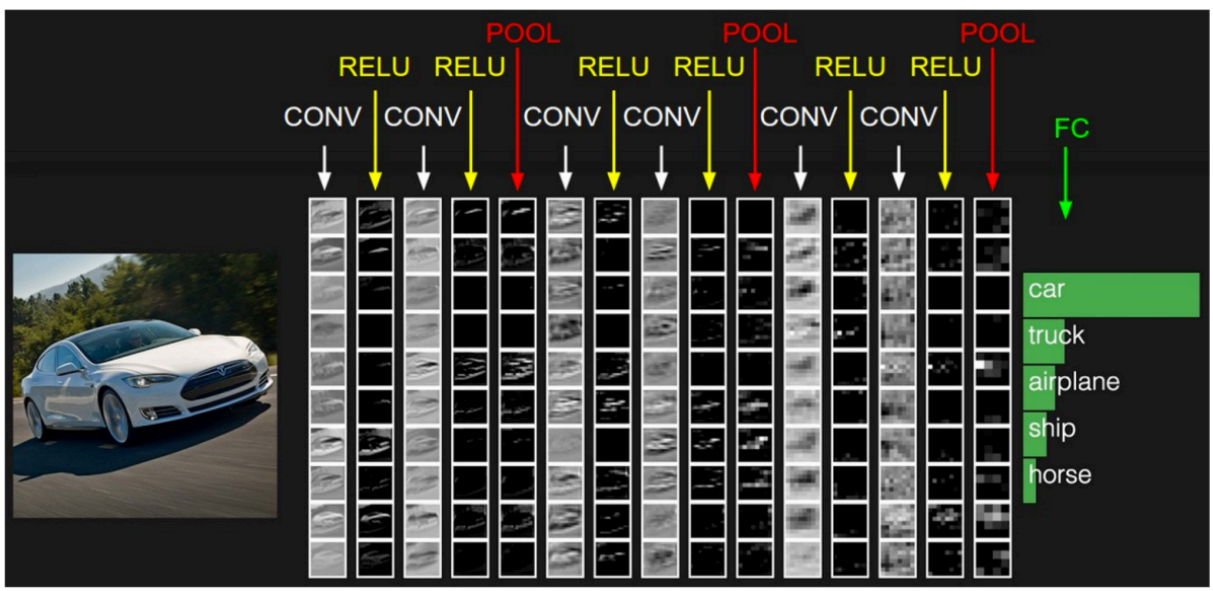
- Using cross entropy and softmax remedies the problem of sigmoids in the output layer being in their saturation region.
- In hidden layers, this cannot be done and sigmoids may cause problems, especially if there are many hidden layers.
- To solve this problem, ReLUs are used way more often than sigmoids in hidden layers in modern Deep Learning.

Note!

- Some of the best performing CNNs have tens of Convolution and Pooling layers
- Not necessary to have a Pooling layer after every Convolutional Layer.

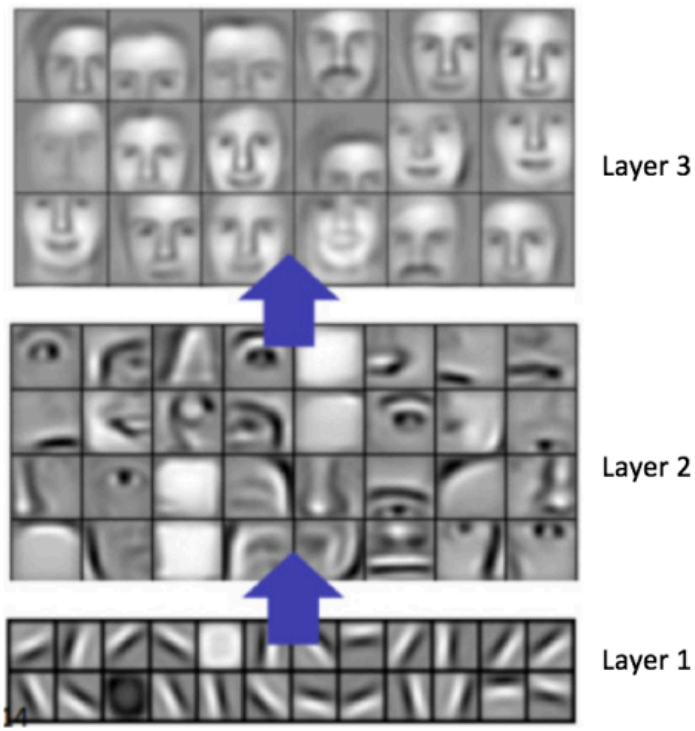
Note!

- Multiple Convolution + ReLU operations in succession before having a Pooling operation:



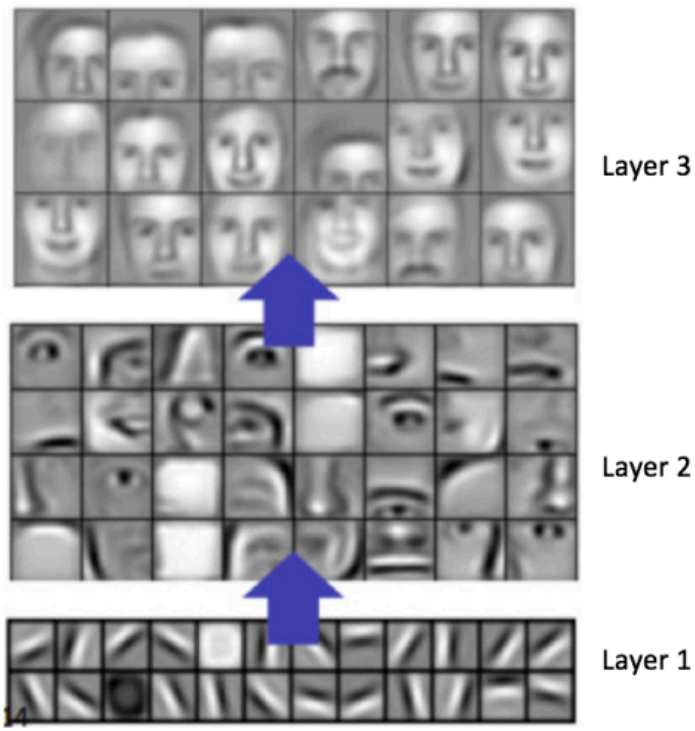
Visualizing CNNs

- Learning High-Level Features

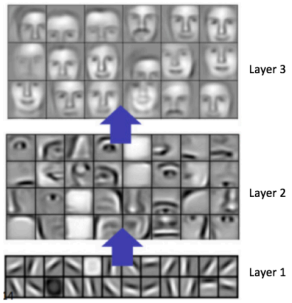


Visualizing CNNs: Example

- Learning High-Level Features

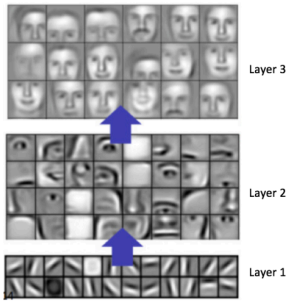


Visualizing CNNs: Example



- Detect edges from raw pixels in the first layer
- Uses the edges to detect simple shapes in the second layer,
- Use these shapes to deter higher-level features, such as facial shapes, in higher layers

Visualizing CNNs: Example



- This is only an example: real life convolution filters may detect objects that have no meaning to humans.