More Supervised Learning

Week 10

Perceptron
Deep Learning

Perceptron

Motivation & Algorithm Multi-layer Perceptron Back-propagation

Recap of Previous Lectures ...

- Linear/Logistic Regression
- K Nearest Neighbor
- Support Vector Machines
- Decision Trees

Random Forest

This Lecture is about ...

Motivation to Neural Networks

Perceptron

Multi-layer Perceptron (MLP)

Connections to Deep Learning

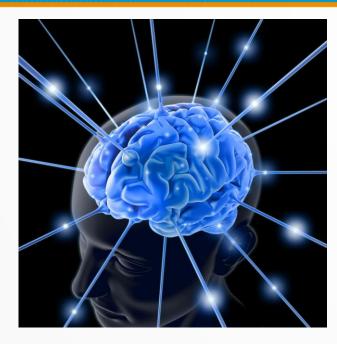
What is different about Neural Networks?

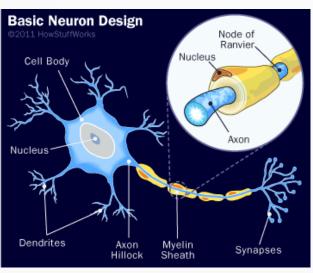
 Linear models may not be sufficient when the underlying functions/decision boundaries are extremely nonlinear.

• Support vector machines can construct nonlinear functions but use fixed feature transformations, which depends on the kernel function.

• Neural Networks allow the feature transformations to be learnt from data.

Historical Motivation





- Our brain has networks of inter-connected neurons and has highly-parallel architecture.
- ANN (artificial neural networks) are motivated by biological neural systems.
- Two groups of ANN researchers:
 - 1. Group that uses ANN to study/model the brain
 - Group that uses the brain as the motivation to design ANN as an effective learning machine, which might not be the true model of the brain.
- We would follow the second group's approach.

What is a Neural Network?

• A typical neural network (machine) has an input layer.

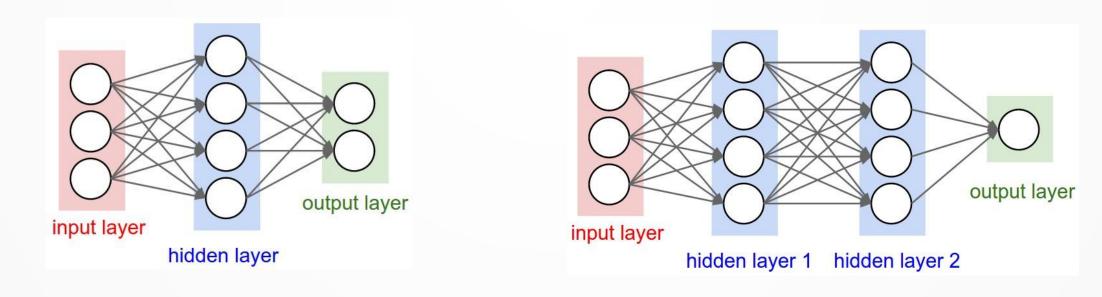
It has one or many hidden layers.

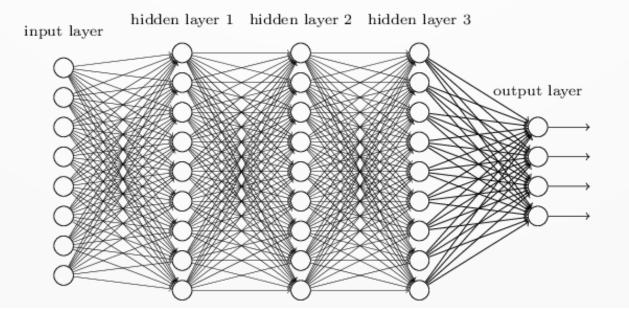
• It has combiners (sum functions).

It has nonlinear activation functions.

• It has an output layer.

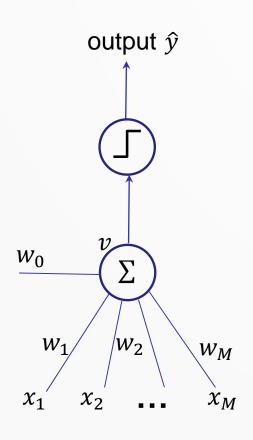
Some Examples of ANN





Perceptron

- Perceptron is a simple neural network used for binary classification.
- It has only one layer with single node.



- □ Given: input vector $\mathbf{x} = (x_1, x_2, ..., x_M)$ of M dimensions and weight vector $\mathbf{w} = (w_0, w_1, ..., w_M)$
- □ The perceptron produces output: $\hat{y} = \text{sign}[v(x, w)]$ where v(x, w) is the linear combiner:

$$v(\mathbf{x}, \mathbf{w}) = \sum_{i=1}^{M} w_i \ x_i + w_0$$

Better notation, let $x_0 = 1$ and $x = (x_0, x_1, ..., x_M)$ then $v(x, w) = w^T x = x^T w$ and $\hat{y}(x, w) = \text{sign}[w^T x]$

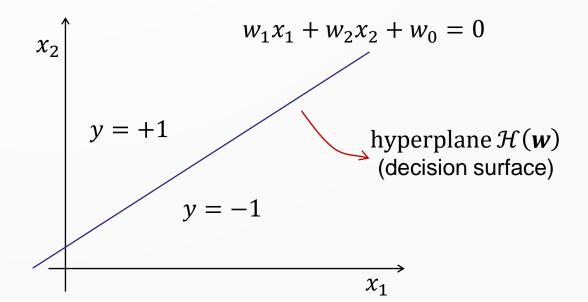
What Perceptron is doing

- Given weight **w**, the perceptron linearly divides input space into two regions:
 - All x's such that $\hat{y}(x, w) = 1$, or $v(x, w) \ge 0$
 - All x's such that $\hat{y}(x, w) = -1$, or v(x, w) < 0
- This corresponds to the two sides of the hyperplane defined by the equation:

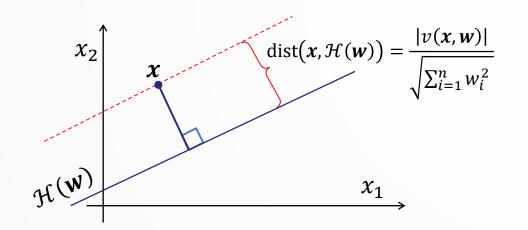
$$v(x, w) = \sum_{i=1}^{\infty} w_i x_i + w_0 = 0$$

• Note that |v(x, w)| is proportional to the distance from x to the hyperplane.

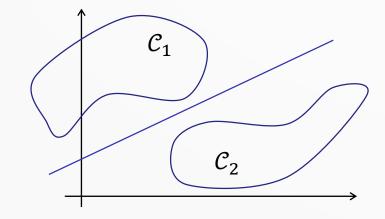
$$\operatorname{dist}(x, \mathcal{H}(w)) = \frac{\left|\sum_{i=1}^{M} w_i x_i + w_0\right|}{\sqrt{\sum_{i=1}^{M} w_i^2}}$$
$$= \frac{|v(x, w)|}{\sqrt{\sum_{i=1}^{M} w_i^2}}$$



What Perceptron is doing



- Thus the sign of v(x, w) indicates on which side of hyperplane $\mathcal{H}(w)$ is x.
- While the magnitude |v(x, w)| indicates how far away x is from $\mathcal{H}(w)$.

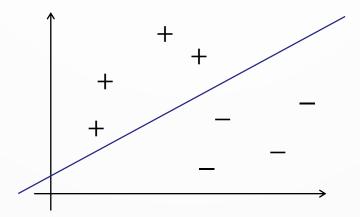


Linearly separable

□ Two sets C_1 and C_2 are called linearly separable if there exists a hyperplane $\mathcal{H}(\mathbf{w})$ that separates them.

Training (or Learning) Perceptron

• Find the weight vector w so that the perceptron correctly classify 2 classes, given sample training data



• Training data $D=\{(x_t,y_t)\},\,t=1,...,n$ where $x_t=(x_{t1},...,x_{tM})$ is the input vector at time t $y_t=\pm 1$ is the desired output

Learning Perceptron

Perceptron Learning Algorithm

- 1. Initialize w = 0
- 2. Retrieve next input x_t and desired output y_t

Compute actual output $\hat{y}_t = \text{sign}[x_t \cdot w]$

Compute output error $e_t = y_t - \hat{y}_t$

Update weight, for all *i*:

$$w_i \leftarrow w_i + \Delta w_i$$
 with $\Delta w_i = \eta e_t x_{ti}$

where $0 < \eta \le 1$ is learning rate

3. Repeat from step 2 until convergence

$$\mathbf{x}_{t} = (x_{t1}, \dots, x_{tM})$$

Remark: no update if $\hat{y}_t = y_t$, e.g., the current weight \boldsymbol{w} already correctly classify current sample $\boldsymbol{x}(t)$

Learning Perceptron

Example:

Current weight $\mathbf{w} = (-1, 2, 1)$

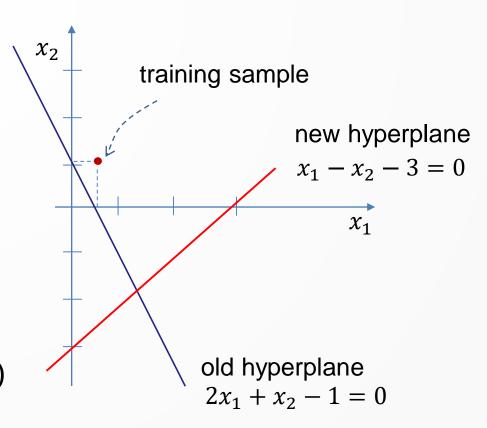
Current training sample $x = (\frac{1}{2}, 1), y = -1$

$$v(x, w) = 2 \times \frac{1}{2} + 1 \times 1 - 1 = 1$$

$$\hat{y}(x, w) = \text{sign}(1) = 1$$

$$e = y - \hat{y} = -2$$

New $w_i = w_i - 2\eta x_i = w_i - 2x_i$ (let $\eta = 1$) $w_0 = -1 - 2 x_0 = -3$ $w_1 = 2 - 2x_1 = 1$ $w_2 = 1 - 2x_2 = -1$



Learning Perceptron

Effect of the update rule

$$w' \leftarrow w + \eta e x = w + \eta (y - \hat{y}) x$$

• Inspect how w' classify x:

$$v' = \mathbf{w}' \cdot \mathbf{x} = [\mathbf{w} + \eta(y - \hat{y})\mathbf{x}] \cdot \mathbf{x}$$
$$= \mathbf{w} \cdot \mathbf{x} + \eta(y - \hat{y})\mathbf{x}^{2}$$
$$= v + \eta(y - \hat{y})\mathbf{x}^{2}$$

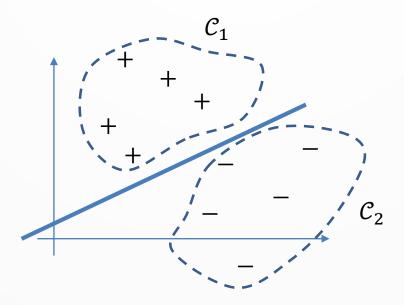
- Thus, when $\hat{y}=-1$ but y=1, i.e., v<0 and we want v>0 and indeed v'>v (why?)
- When $\hat{y} = 1$ but y = -1, i.e. $v \ge 0$ but we want v < 0, and indeed v' < v

The update rule creates new w' that is better than w in classifying x.

That's what we want!

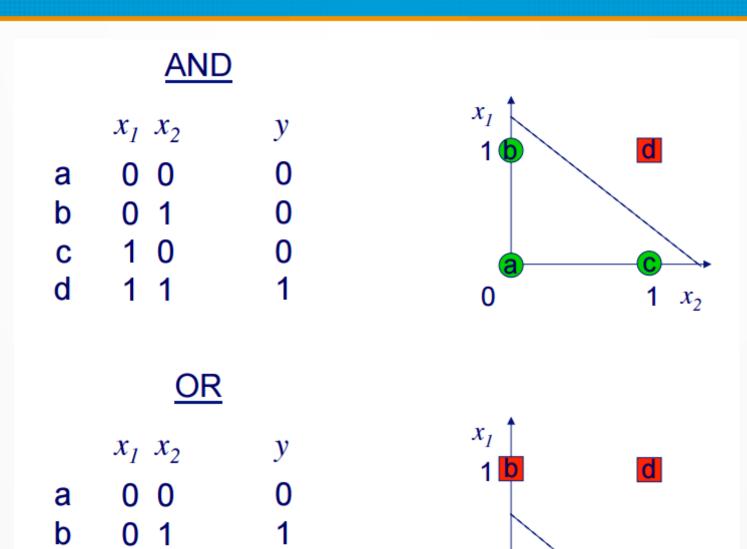
Perceptron Convergence Theorem

• If training instances are drawn from two linearly separate sets C_1 and C_2 , then the perceptron learning rule will converge after finite iterations.



• However, no guarantee for convergence if C_1 and C_2 are not linearly separable!

Some Linearly Separable Problems

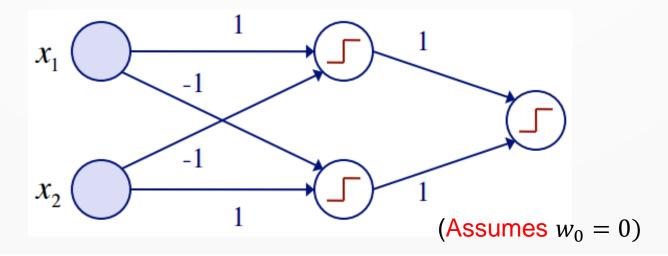


XOR Problem

Perceptron can not deal with problems such as XOR!

а	$x_1 \ x_2$	у О	x_1 1	đ
b	0 1	1		
С	1 0	1	а	
d	1 1	0	0	$\overline{1}$ x_2

A multilayer Perceptron (MLP) can represent XOR problem



Learning Perceptron in Python

sklearn.linear_model.Perceptron

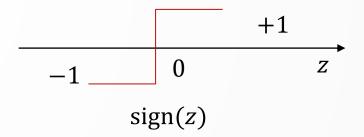
class sklearn.linear_model. Perceptron (penalty=None, alpha=0.0001, fit_intercept=True, n_iter=5, shuffle=True, verbose=0, eta0=1.0, n_jobs=1, random_state=0, class_weight=None, warm_start=False) [source]

Methods

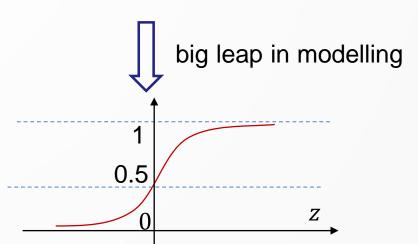
decision_function (X)	Predict confidence scores for samples.			
densify()	Convert coefficient matrix to dense array format.			
<pre>fit (X, y[, coef_init, intercept_init,])</pre>	Fit linear model with Stochastic Gradient Descent.			
<pre>fit_transform(X[, y])</pre>	Fit to data, then transform it.			
<pre>get_params ([deep])</pre>	Get parameters for this estimator.			
${\tt partial_fit} \ (X, y[, classes, sample_weight])$	Fit linear model with Stochastic Gradient Descent.			
predict(X)	Predict class labels for samples in X.			
score (X, y[, sample_weight])	Returns the mean accuracy on the given test data and labels.			
set_params (*args, **kwargs)				
sparsify()	Convert coefficient matrix to sparse format.			
transform (*args, **kwargs)	DEPRECATED: Support to use estimators as feature selectors will be removed in version 0.19.			

Multi-layer Feed-forward NN

 Perceptron is quite weak in what it can represent.



• For complex, non-linear decision surfaces, we need multi-layer network.



- Choice of node in multi-layer network
 - Perceptron: discontinuity
 - Answer: sigmoid function!

• Sigmoid node: like a perceptron, but with the sigmoid function $\sigma(z) = (1 + e^{-z})^{-1}$ instead of the sign function, i.e., $y = \sigma(\mathbf{w}^T \mathbf{x})$.

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$\frac{d\sigma(z)}{dz} = \sigma(z)(1 - \sigma(z))$$

Multi-layer Perceptron

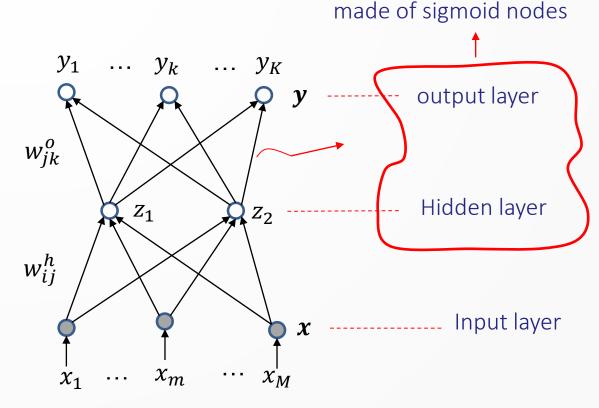
- A feedforward neural network is an ANN wherein connections between units do not form a cycle.
- Multi-layer feed-forward NN is also known as Multi-layer Perceptron (MLP).
- The term "MLP" is really a misnomer.
 - Why? Because the model comprises multiple layers of logistic regression like models (with continuous nonlinearities) rather than multiple Perceptrons (with discontinuous nonlinearities).
- Although a misnomer, we will continue using MLP term.

Structure of Multi-layer Perceptron

Consider a two-layer network: input layer, hidden layer and output layer

Remarks:

- Output now is a <u>vector</u>
- Two kinds of weights:
 - input → hidden
 - hidden → output
- w_{ij}^h : from i^{th} input $\rightarrow j^{th}$ hidden
- w_{jk}^o : from j^{th} hidden $\rightarrow k^{th}$ output
- Input layer does no computation, only to relay input vector.
- Can have more than one hidden layers.
- Doesn't have to be fully connected.

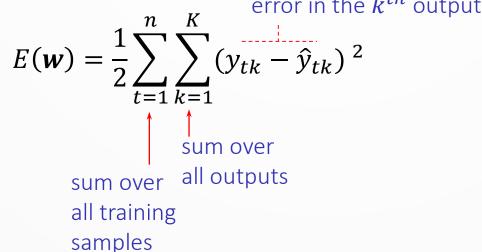


MLP Formulation

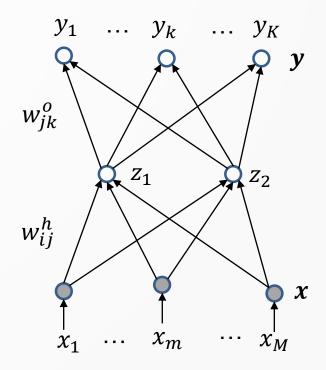
• Given input x_t and desired output y_t , t = 1, ..., n, find the network weights w such that

$$\widehat{\boldsymbol{y}}_t \approx \boldsymbol{y}_t, \forall t$$

• Stating above as an optimization problem: find w to minimize the error function w error in the k^{th} output



- We will use gradient-descent for minimization.
- E(w) is not convex, but a complex function with possibly many local minima.
- We will use an algorithm called Backpropagation.



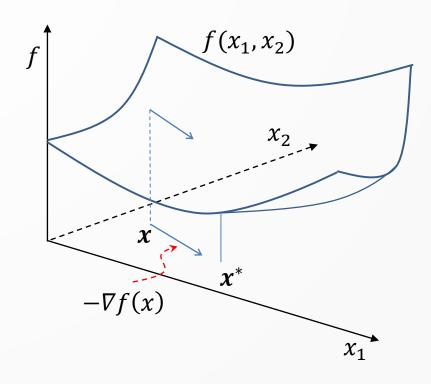
Detour: Gradient-based Optimization

□ At a point $\mathbf{x} = (x_1, x_2)$, the gradient vector of the function $f(\mathbf{x})$ w.r.t \mathbf{x} is

$$\nabla f(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}\right)$$

 $\neg \nabla f(x)$ represents the direction that produces steepest increase in f.

□ Similarly $-\nabla f(x)$ is the direction of steepest decrease in f



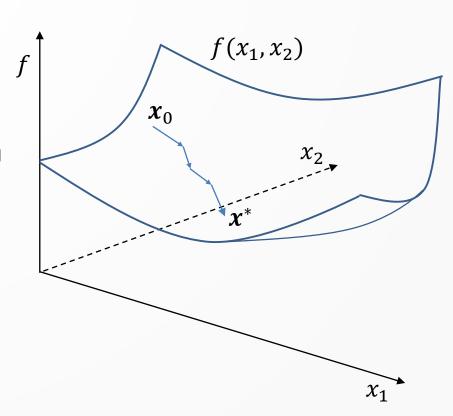
Detour: Gradient-Descent

- To minimize a functional f(x), use gradient-descent:
 - Initialize random x_0
 - Slide down the surface of *f* in the direction of steepest decrease:

$$x_{t+1} = x_t - \underbrace{\eta}_{\text{learning rate}} \times \nabla f(x_t)$$

• Similarly, to maximize f(x), use gradient-ascent.

$$\boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \boldsymbol{\eta} \times \nabla f(\boldsymbol{x}_t)$$



Detour: Stochastic Gradient Descent (SGD)

• Instead of minimizing E(w), SGD minimizes the instantaneous approximation of E(w) using only t-th instance, i.e.,

$$E_t(\mathbf{w}) = \frac{1}{2} \sum_{k=1}^{K} (y_{tk} - \hat{y}_{tk})^2$$

• Update rule (where t denotes the current training sample) is

$$w_i \leftarrow w_i - \eta \frac{\partial E_t(\mathbf{w})}{\partial w_i}$$

• SGD is cheap to perform and guaranteed to reach a local minimum in a stochastic sense.

Training MLP: Backpropagation

- It is in fact a stochastic gradient-descent rule!
- Minimizing instantaneous approximation for current training sample (x_t, y_t)

$$E_t(\mathbf{w}) = \frac{1}{2} \sum_{k=1}^{K} (\hat{y}_k - y_k)^2$$

- Gradient-descent rule: $w_{jk}^o \leftarrow w_{jk}^o \eta \frac{\partial E_t(w)}{\partial w_{jk}^o}$
- Let \bar{y}_k be the (unsigmoided) argument value at output node \hat{y}_k , i.e., $\hat{y}_k = \sigma(\bar{y}_k)$, we have:

$$\frac{\partial E_t}{\partial w_{jk}^o} = \frac{\partial E_t}{\partial \bar{y}_k} \times \frac{\partial \bar{y}_k}{\partial w_{jk}^o} \longrightarrow = z_j \quad \text{since } \bar{y}_k = \sum w_{jk}^0 z_j$$

$$\downarrow \qquad \qquad (1 - \hat{y}_k) \hat{y}_k$$

$$\frac{\partial E_t}{\partial \bar{y}_k} = \frac{\partial E_t}{\partial \hat{y}_k} \times \frac{\partial \hat{y}_k}{\partial \bar{y}_k} \longrightarrow -(y_k - \hat{y}_k)$$

$$-\delta_k^o = -(y_k - \hat{y}_k)(1 - \hat{y}_k) \hat{y}_k$$

• This gradient rule implies: $w_{jk}^o \leftarrow w_{jk}^o + \eta \delta_k^o z_j$

Training MLP: Backpropagation

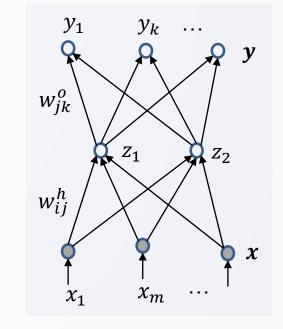
Similarly for input → hidden weights

$$E_t(\mathbf{w}) = \frac{1}{2} \sum_{k=1}^{K} (\hat{y}_k - y_k)^2$$
 $z_j = \sigma(\bar{z}_j) \text{ where } \bar{z}_j = \sum_{i=1}^{M} x_i w_{ij}^h$

$$w_{ij}^h \leftarrow w_{ij}^h - \eta \frac{\partial E_t(\mathbf{w})}{\partial w_{ij}^h}$$

$$\frac{\partial E_t(\mathbf{w})}{\partial w_{ij}^h} = \frac{\partial E_t}{\partial \bar{z}_j} \times \frac{\partial \bar{z}_j}{\partial w_{ij}^h} \times \frac{\partial z_j}{\partial z_j} = z_j (1 - z_j)$$

$$\frac{\partial E_t}{\partial \bar{z}_j} = \frac{\partial E_t}{\partial z_j} \times \frac{\partial z_j}{\partial \bar{z}_j}$$
chain rule
$$= w_{ik}^0 \text{ sin}$$



Gradient descent update

$$w_{ij}^h \leftarrow w_{ij}^h + \eta \delta_j^h x_i$$

$$\sum_{k=1}^{K} \frac{\partial E_t}{\partial \bar{y}_k} \times \frac{\partial \bar{y}_k}{\partial z_j}$$

$$= w_{jk}^0 \text{ since } \bar{y}_k = \sum w_{jk}^0 z_j$$

$$\frac{\partial E_t}{\partial \bar{z}_j} = -\delta_j^h = -z_j (1 - z_j) \sum_{k=1}^{K} w_{jk}^o \delta_k^o$$

$$-\delta_k^o$$

Backpropagation (SGD)

Algorithm

```
Input: training data
Initialize weights // use small random numbers, between -0.5 and 0.5
Until stopping criteria is met do
      For each training sample do
          // propagate input forward
          Compute values of hidden nodes z and output nodes \hat{y}
          // propagate error backward
          Compute output error term: \delta_k^o = \hat{y}_k (1 - \hat{y}_k)(y_k - \hat{y}_k)
          Compute hidden error term: \delta_i^h = z_i (1 - z_i) \sum_{k=1}^K w_{ik}^o \delta_k^o
          Update weights:
                Hidden \rightarrow output: w_{ik}^o \leftarrow w_{ik}^o + \eta \delta_k^o h_j
                Input \rightarrow hidden: w_{ij}^h \leftarrow w_{ij}^h + \eta \delta_i^h x_i
Output: trained weights
```

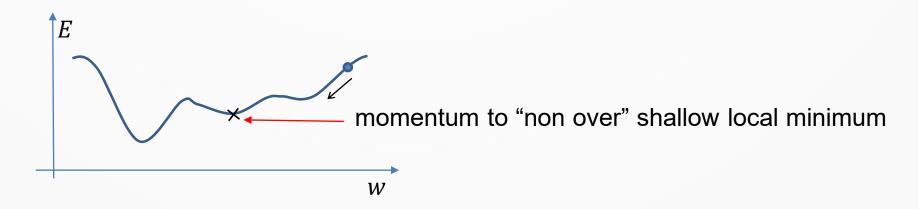
Issues with Backpropagation

Local minima.

- Possible fixes:
 - Add a momentum term in the update rule, e.g.,

$$w_{jk}^o \leftarrow w_{jk}^o + \eta \delta_k^o z_j + \alpha \Delta^{t-1} w_{jk}^o$$
 momentum constant >0

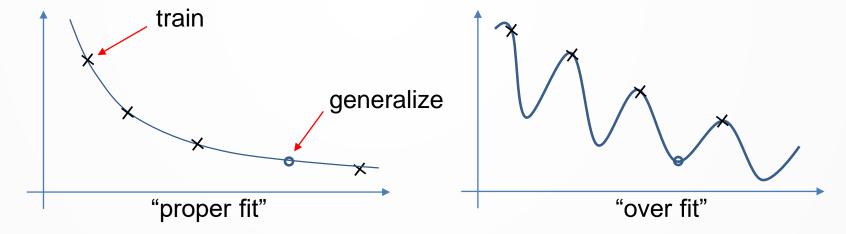
last amount of update of w_{jk}^o • Can prevent getting stuck in shallow local minimum



 Multiple restarts and choose final network with best performance.

Issues with Backpropagation

Overfitting



- The tendency of the network to "memorize" all training samples, leading to poor generalization
- Usually happens with network of too many hidden nodes and overtrained.
- Possible fixes:
 - Use cross validation, e.g., stop training when validation error starts to grow.
 - Weight decaying: minimize also the magnitude of weights, keeping weights small (since the sigmoid function is almost linear near 0, if weights are small, decision surfaces are less non-linear and smoother)
 - Keep small number of hidden nodes!

Using MLP in Scikit Learn Python

sklearn.neural_network.MLPClassifier

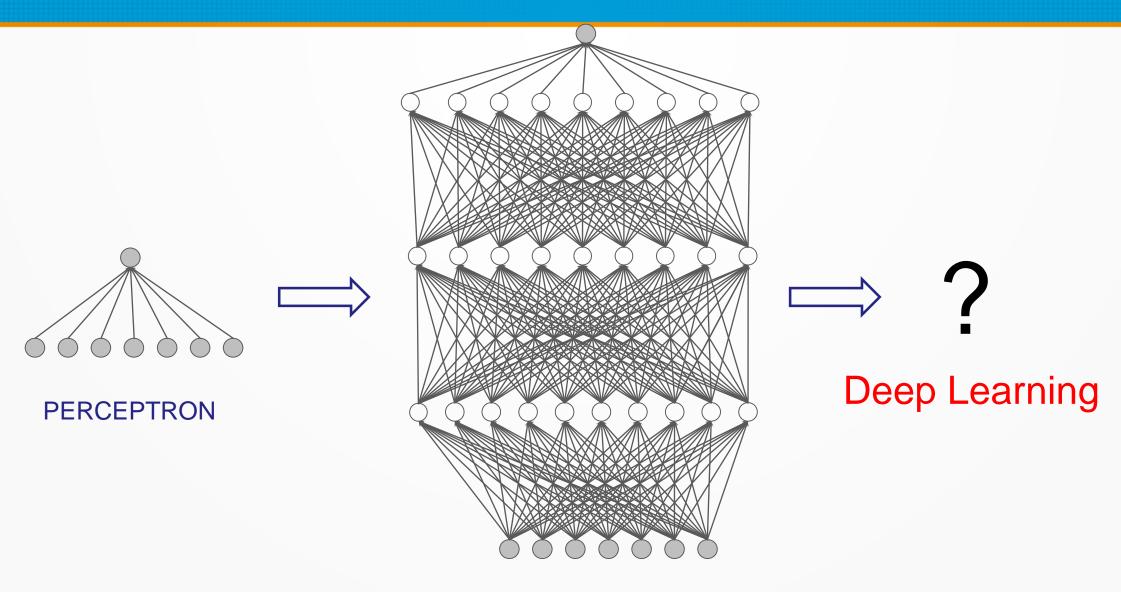
class sklearn.neural_network. MLPClassifier (hidden_layer_sizes=(100,), activation='relu', solver='adam', alpha=0.0001, batch_size='auto', learning_rate='constant', learning_rate_init=0.001, power_t=0.5, max_iter=200, shuffle=True, random_state=None, tol=0.0001, verbose=False, warm_start=False, momentum=0.9, nesterovs_momentum=True, early_stopping=False, validation_fraction=0.1, beta_1=0.9, beta_2=0.999, epsilon=1e-08)

Multi-layer Perceptron classifier.

Methods

fit (X, y)	Fit the model to data matrix X and target y.			
<pre>get_params ([deep])</pre>	Get parameters for this estimator.			
predict(X)	Predict using the multi-layer perceptron classifier			
<pre>predict_log_proba (X)</pre>	Return the log of probability estimates.			
<pre>predict_proba(X)</pre>	Probability estimates.			
score (X, y[, sample_weight])	Returns the mean accuracy on the given test data and labels.			
set_params (**params)	Set the parameters of this estimator.			

Where to go from here?



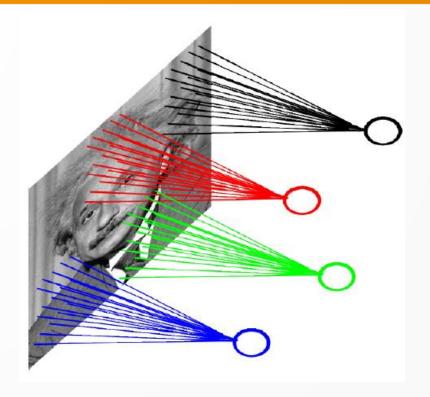
MULTILAYER PERCEPTRON (aka Feed Forward Neural Network)

Deep Learning

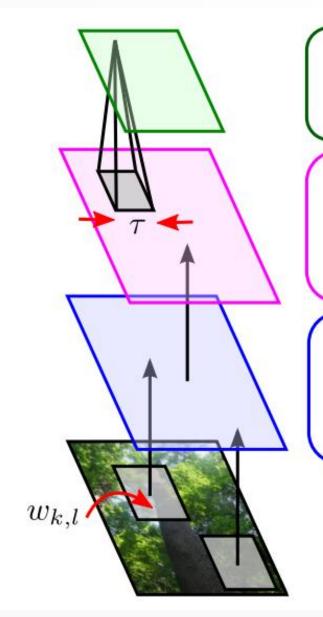
- ✓ Deep Learning methods are advanced neural networks.
- ✓ They have been successful in learning many real world tasks e.g. handwritten digit recognition, image recognition!
- ✓ Some of the common Deep Learning architectures are:
 - ✓ **Convolutional Networks** (Due to Le Cun *et al.*)
 - ✓ **Autoencoders** (Due to Yoshua Bengio *et al.*)
 - ✓ Deep Belief Networks (due to Geoff Hinton *et al.*)
 - ✓ Boltzmann Machines
 - ✓ Restricted Boltzmann Machines
 - ✓ Deep Boltzmann Machines
 - ✓ Deep Neural Networks

Convolutional Neural Networks

- Also called CNN or ConvNets.
- Motivation:
 - vision processing in our brain is fast
 - Also (Hubel & Wiesel, 62'):
 - Simple cells detect local features
 - Complex cells pool local features
- Translated in technical terms:
 - Sparse interactions: sparse weights within a smaller kernel (e.g., 3x3, 5x5) instead of the whole input. This helps reduce #params.
 - Parameter <u>sharing</u>: a kernel use the same set of weights while applying onto different location (sliding windows).
 - Translation invariance.



Convolutional Neural Networks



$$x_{i,j} = \max_{|k| < \tau, |l| < \tau} y_{i-k,j-l}$$
 pooling mean or subsample also used stage

$$y_{i,j} = f(a_{i,j})$$
 e.g. $f(a) = [a]_+$ $f(a) = \operatorname{sigmoid}(a)$

non-linear stage

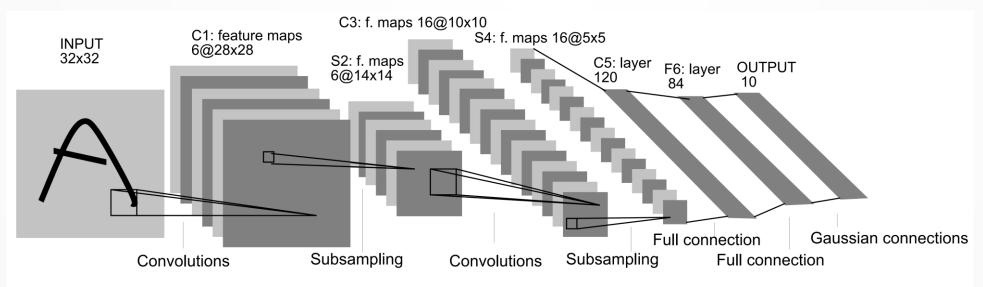
$$a_{i,j} = \sum_{k,l} w_{k,l} z_{i-k,j-l}$$
 only parameters

convolutional stage

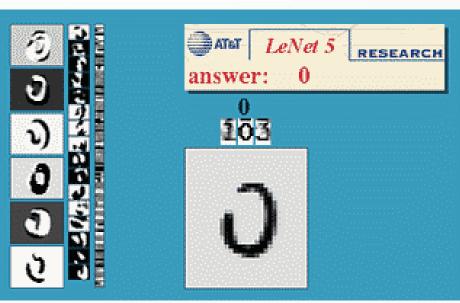
 $z_{i,j}$

input image

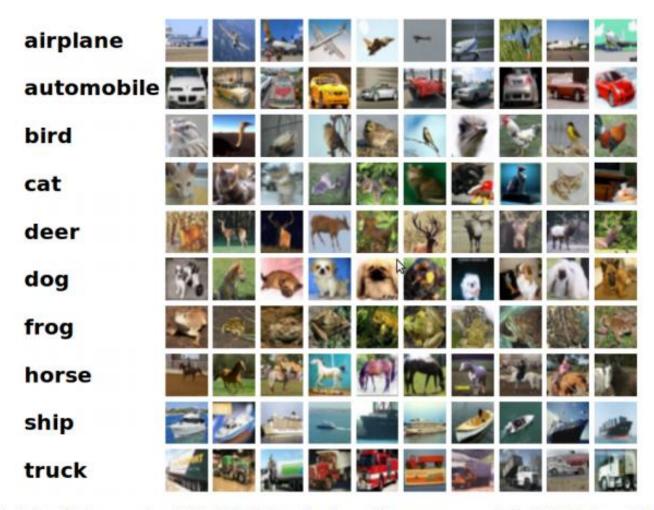
LeNet5



src: http://yann.lecun.com/

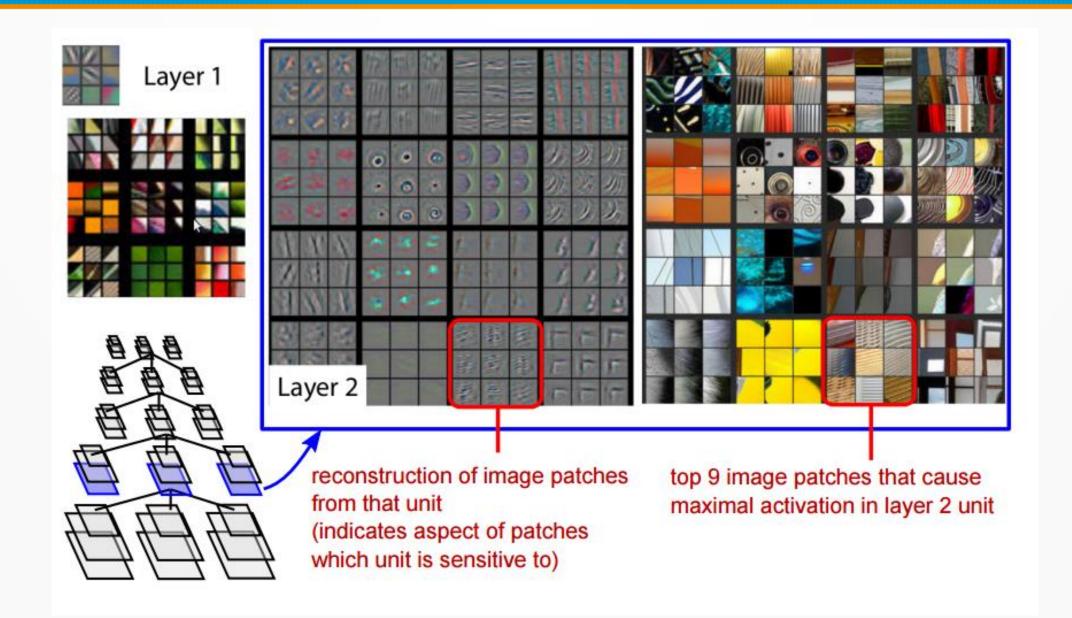


Application of CNN

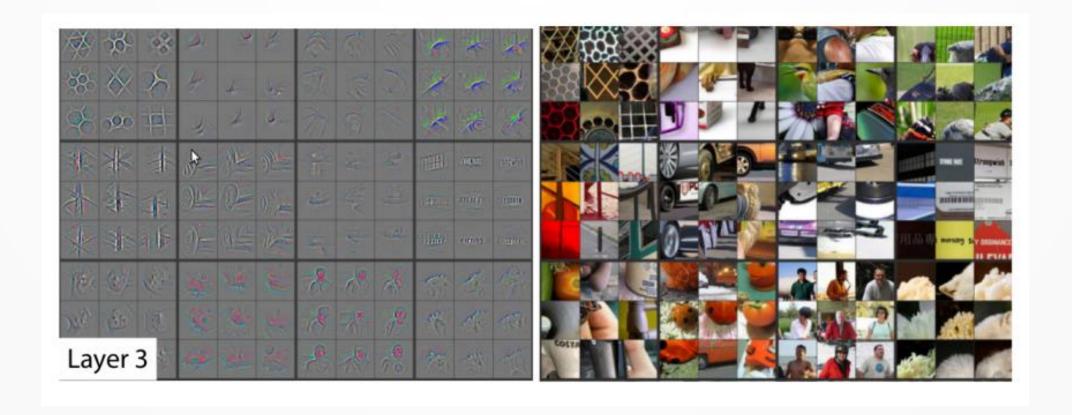


CIFAR 10 dataset: 50,000 training images, 10,000 test images http://cs.stanford.edu/people/karpathy/convnetjs/demo/cifar10.html

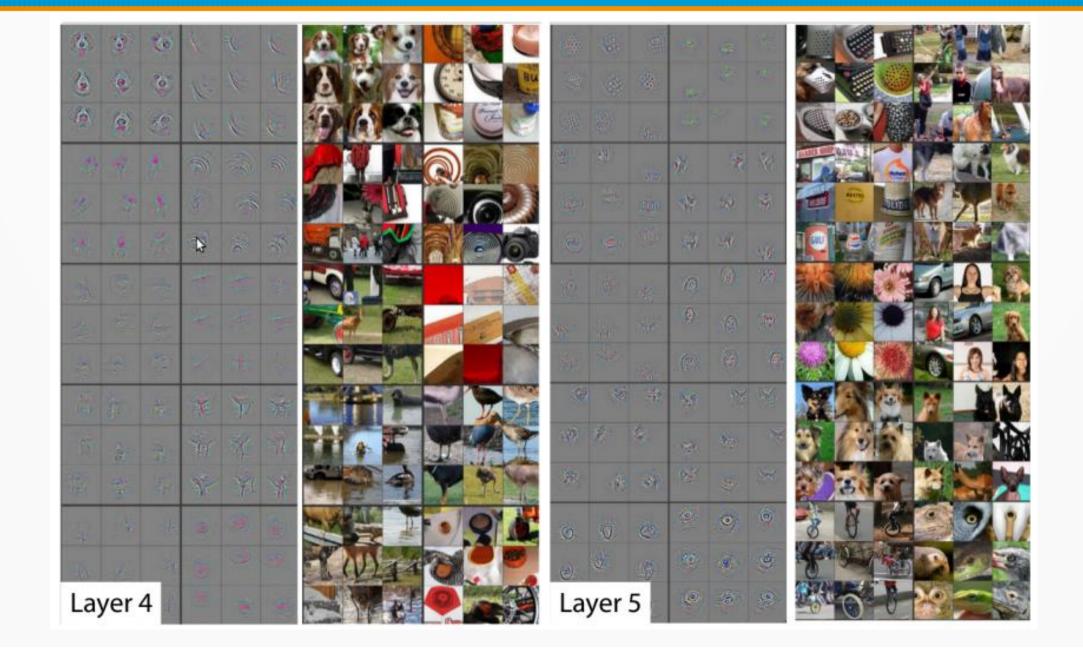
Peeping into CNN's Brain



Peeping into CNN's Brain



Peeping into CNN's Brain



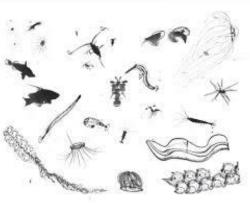
ConvNets won all recent Computer Vision Challenges

Galaxy



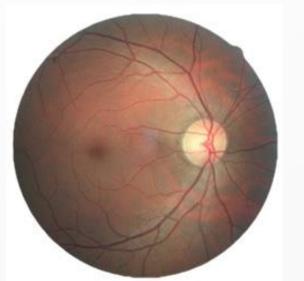
Plankton

121 classes



- Retina (high-res images)
 - Diabetes recognition from retina image





Read here:

http://benanne.github.i o/2014/04/05/galaxyzoo.html

http://benanne.github.i o/2015/03/17/plankton .html

So what helped Deep Learning?

- Larger models with new training techniques:
 - Dropout, Maxout, Maxnorm, ReLU,...
- Large ImageNet dataset [Fei-Fei et al. 2012]
 - 1.2 million training samples
 - 1000 categories
- Fast graphical processing units (GPU)
 - Capable of 1 trillion operations per second

















Resources

Books

- Deep learning textbook (Goodfellow et. al., 2016):
 http://www.deeplearningbook.org/
- Deep learning: an overview (Jurgen, 2015):
 http://people.idsia.ch/~juergen/deep-learning-overview.html
- Deep learning (Michael Nielsen, 2016):
 http://neuralnetworksanddeeplearning.com/
- A statistical view of deep learning (Shakir Mohamed, 2015)

Resources

Courses/Tutorials

- Hinton Coursera: https://www.coursera.org/course/neuralnets
- Hugo Youtube channel: https://www.youtube.com/user/hugolarochelle
- Colah's blog (http://colah.github.io/): very nice visualizations for easier and better understanding.
- Karpathy's blog (http://karpathy.github.io/): deep learning in web browsers.

Resources

Tools

- Tensorflow (Google)
 - Keras
- Theano (Montreal Bengio et. al.)
 - Lasange, Keras
- Caffe (Berkeley)
- Torch (Facebook)
- Deep Scalable Sparse Tensor Network Engine (DSSTNE) (Amazon)
- MatConvNet (Oxford, MATLAB)

Thank You.