CS 2750 Machine Learning
Lecture 13

Multilayer neural networks

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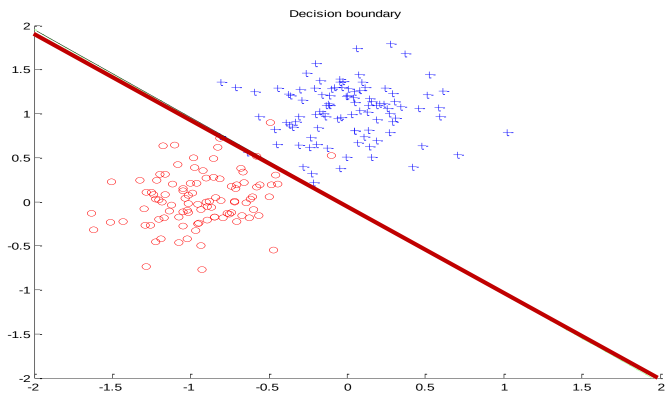
Classification with the linear model

The majority of the models covered so far are linear

Example: 2 classes (blue and red points)



Modeling nonlinearities

- **Feature (basis) functions** to model **nonlinearities**

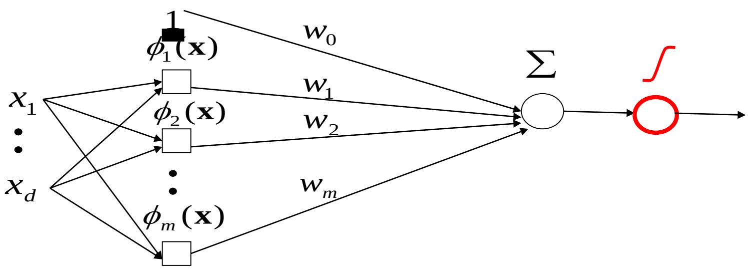
Linear regression

$$f(\mathbf{x}) = w_0 + \sum_{j=1}^{m} w_j \phi_j(\mathbf{x})$$

Logistic regression

$$f(\mathbf{x}) = g(w_0 + \sum_{j=1}^{m} w_j \phi_j(\mathbf{x}))$$

$\phi_j(\mathbf{x})$ - an arbitrary function of $\mathbf{x}$



Modeling nonlinearities

Feature (basis) functions model **nonlinearities**

Linear regression

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Logistic regression

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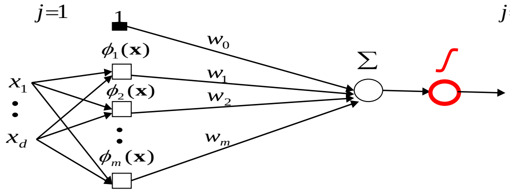


Advantage:

- The same problem as learning of the weights of linear units

Limitations/problems:

- How to define the right set of basis functions
- Many basis functions → many weights to learn

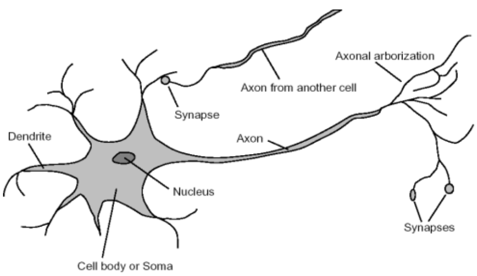
Modeling nonlinearities

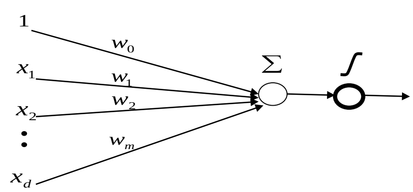
Support vector machines model nonlinearities via:
- **feature expansion**
- **Folded in efficient kernels**

Advantage:
- The learning problem is similar to the problem of learning weights of a linear model
- Efficient kernels reduce the computational complexity
- **Problem:**
- How to define the right the kernels

Multi-layered neural networks

- An alternative way to model **nonlinearities for regression /classification problems**
- **Idea:** Cascade several simple nonlinear models (e.g. logistic units) **to approximate nonlinear functions** for regression /classification. Learn/adapt these simple models.
- **Motivation:** neuron connections



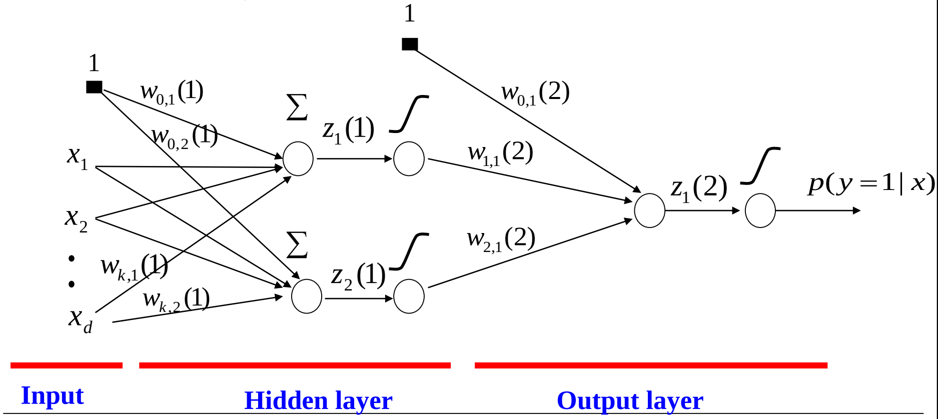


Multilayer neural network

Also called a **multilayer perceptron (MLP)**

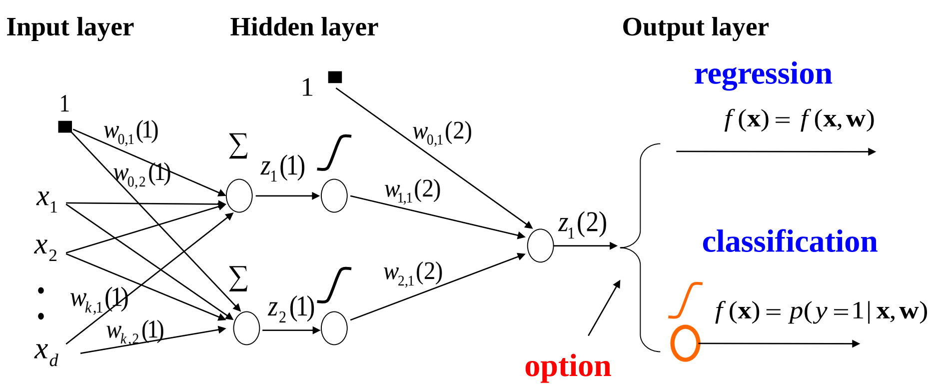
Cascades multiple **non-linear (e.g. logistic regression)** units

Example: (2 layer) classifier with non-linear decision boundaries



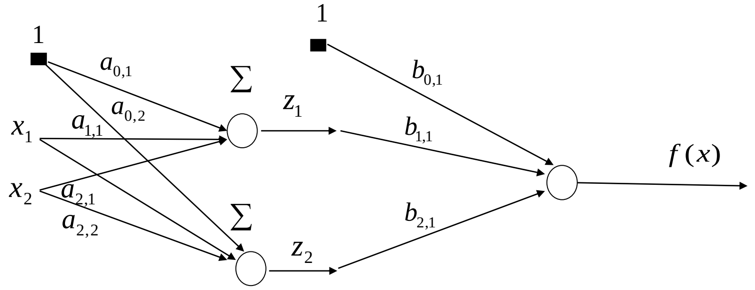
Multilayer neural network

- Models **non-linearity through nonlinear switching units**
- Can be applied to both **regression and binary classification problems**



Why we need nonlinearities? Why not multiple linear units

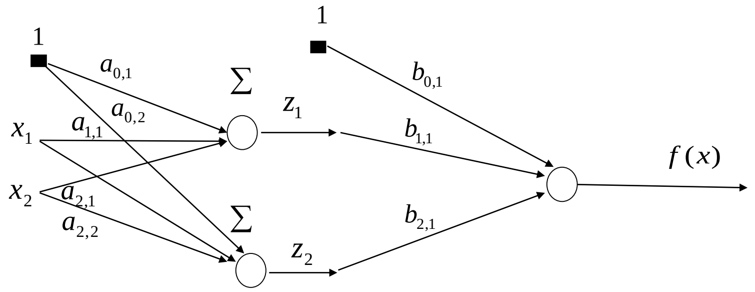
Cascading of multiple linear units is equivalent to one linear unit



$$f(\mathbf{x}) = b_{0,1} + b_{1,1}z_1 + b_{2,1}z_2$$

Why we need nonlinearities? Why not multiple linear units

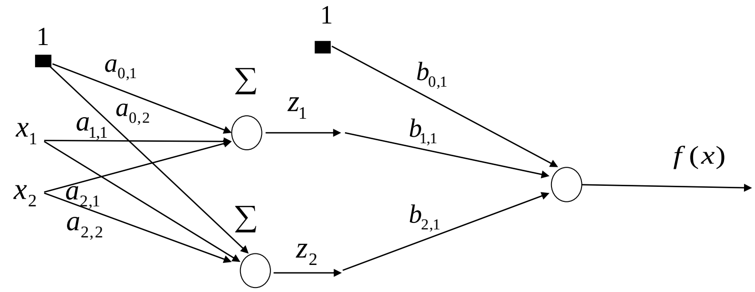
Cascading of multiple linear units is equivalent to one linear unit



$$f(\mathbf{x}) = b_{0,1} + b_{1,1}z_1 + b_{2,1}z_2$$
$$= b_{0,1} + b_{1,1}(a_{0,1} + a_{1,1}x_1 + a_{2,1}x_2) + b_{2,1}(a_{0,2} + a_{2,1}x_1 + a_{2,2}x_2)$$

Why we need nonlinearities? Why not multiple linear units

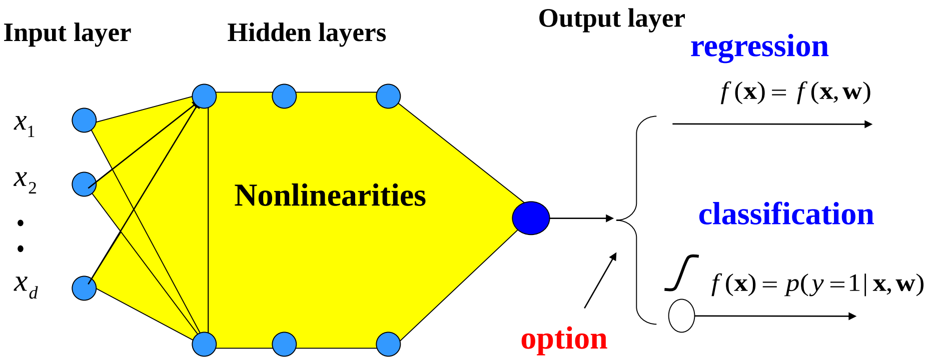
Cascading of multiple linear units is equivalent to one linear unit



$$
\begin{aligned}
f(\mathbf{x}) &= b_{0,1} + b_{1,1} z_1 + b_{2,1} z_2 \\
&= b_{0,1} + b_{1,1}(a_{0,1} + a_{1,1} x_1 + a_{2,1} x_2) + b_{2,1}(a_{0,2} + a_{2,1} x_1 + a_{2,2} x_2) \\
&= b_{0,1} + b_{1,1} a_{0,1} + b_{1,1} a_{1,1} x_1 + b_{1,1} a_{2,1} x_2 + b_{2,1} a_{0,2} + b_{2,1} a_{2,1} x_1 + b_{2,1} a_{2,2} x_2 \\
&= b_{0,1} + b_{1,1} a_{0,1} + b_{2,1} a_{0,2} + (b_{1,1} a_{1,1} + b_{2,1} a_{2,1}) x_1 + (b_{1,1} a_{2,1} + b_{2,1} a_{2,2}) x_2 \\
&= c + d_1 x_1 + d_2 x_2
\end{aligned}
$$

Multilayer neural network

- **Non-linearities are modeled using multiple hidden nonlinear units (organized in layers)**
- The output layer determines whether it is a **regression or a binary classification problem**

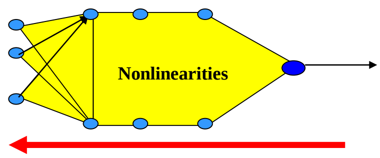


Learning with MLP

- How to learn the parameters of the neural network?
- **Gradient descent algorithm**
  - Weight updates based on the error: $J(D, \mathbf{w})$

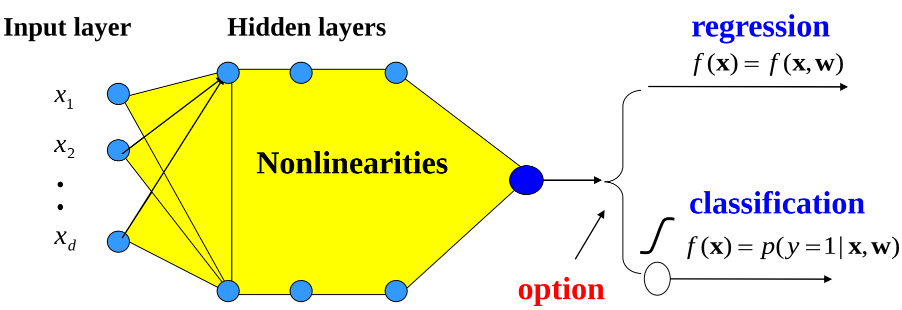
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} J(D, \mathbf{w})$$

- We need to **compute gradients for weights in all units**
- **Can be computed in one backward sweep through the net !!!**



- The process is called **back-propagation**

Backpropagation: error function

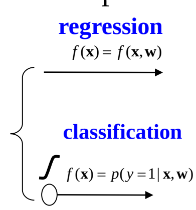


- **Error function**: $J(D, \mathbf{w})$ (online) error where D is a data point
  - **Regression**

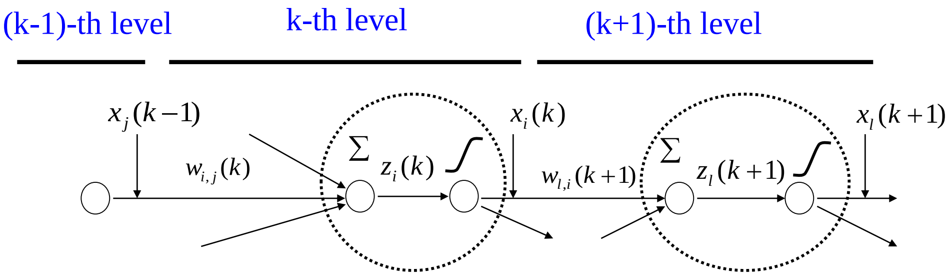
$$J(D, \mathbf{w}) = (y_u - f(\mathbf{x}_u))^2$$

  - **Classification**

$$J(D, \mathbf{w}) = -\log p(y_u \mid f(\mathbf{x}_u))$$



Backpropagation



$x_i(k)$ - output of the unit i on level k

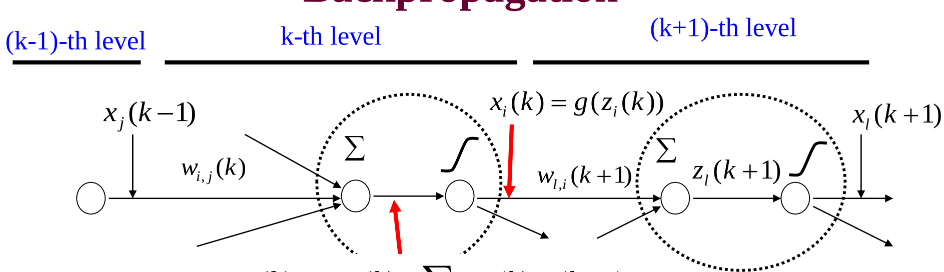
$x_i(k) = g(z_i(k))$

$z_i(k)$ - input to the sigmoid function on level k

$z_i(k) = w_{i,0}(k) + \sum_j w_{i,j}(k) x_j(k-1)$

$w_{i,j}(k)$ - weight between units j and i on levels (k-1) and k

Backpropagation



$z_i(k) = w_{i,0}(k) + \sum_j w_{i,j}(k) x_j(k-1)$

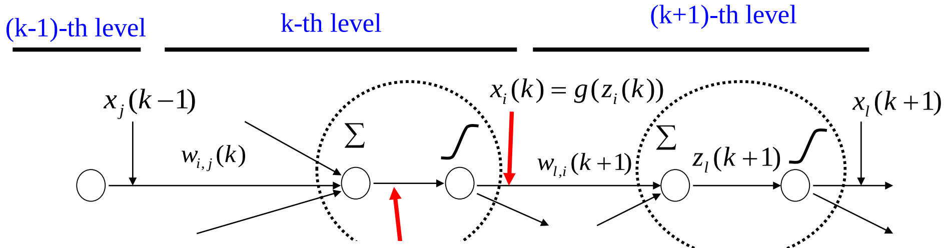
- **Gradient descent:** $w_{i,j}(k) \leftarrow w_{i,j}(k) - \alpha \frac{\partial}{\partial w_{i,j}(k)} J(D, \mathbf{w})$

$$\frac{\partial}{\partial w_{i,j}(k)} J(D,\mathbf{w}) = \frac{\partial J(D,\mathbf{w})}{\partial z_i(k)} \frac{\partial z_i(k)}{\partial w_{i,j}(k)} = \delta_i(k) x_j(k-1)$$

$$\delta_i(k) = \frac{\partial}{\partial z_i(k)} J(D,\mathbf{w}) \qquad x_j(k-1)$$

$$\boxed{\frac{\partial f(g(u))}{\partial u} = \frac{\partial f(g(u))}{\partial g(u)} \frac{\partial g(u)}{\partial u}}$$

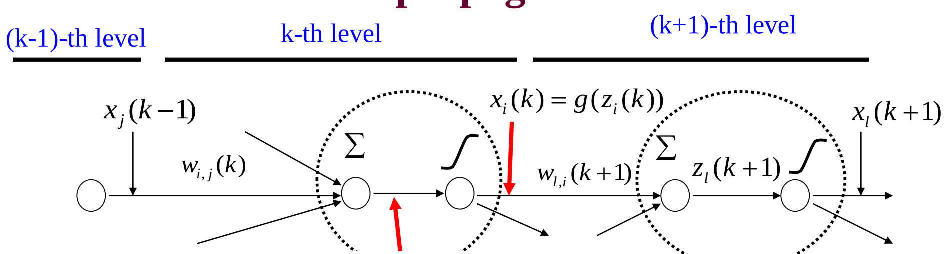
Backpropagation



$$z_i(k) = w_{i,0}(k) + \sum_j w_{i,j}(k) x_j(k-1)$$

- **Derivation:** $$\delta_i(k) = \frac{\partial}{\partial z_i(k)} J(D,\mathbf{w}) = \frac{\partial}{\partial x_i(k)} J(D,\mathbf{w}) * \frac{\partial x_i(k)}{\partial z_i(k)}$$

Backpropagation



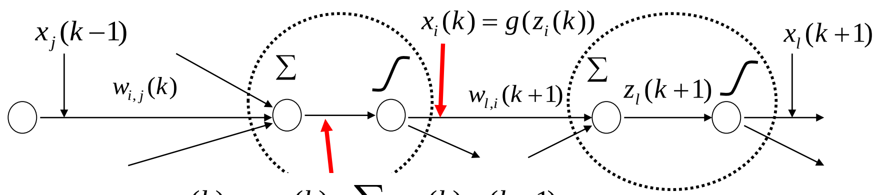
$$z_i(k) = w_{i,0}(k) + \sum_j w_{i,j}(k) x_j(k-1)$$

- **Derivation:** $$\delta_i(k) = \frac{\partial}{\partial z_i(k)} J(D,\mathbf{w}) = \boxed{\frac{\partial}{\partial x_i(k)} J(D,\mathbf{w})} * \boxed{\frac{\partial x_i(k)}{\partial z_i(k)}}$$

$$\boxed{\frac{\partial}{\partial x_i(k)} J(D,\mathbf{w})} = \sum_l \underbrace{\frac{\partial}{\partial z_l(k+1)} J(D,\mathbf{w})}_{\delta_l(k+1)} * \underbrace{\frac{\partial z_l(k+1)}{\partial x_i(k)}}_{w_{l,i}(k+1)}$$

Backpropagation

(k-1)-th level — k-th level — (k+1)-th level



$$z_i(k) = w_{i,0}(k) + \sum_j w_{i,j}(k) x_j(k-1)$$

- **Derivation:**

$$\delta_i(k) = \frac{\partial}{\partial z_i(k)} J(D,\mathbf{w}) = \boxed{\frac{\partial}{\partial x_i(k)} J(D,\mathbf{w})} * \boxed{\frac{\partial x_i(k)}{\partial z_i(k)}}$$

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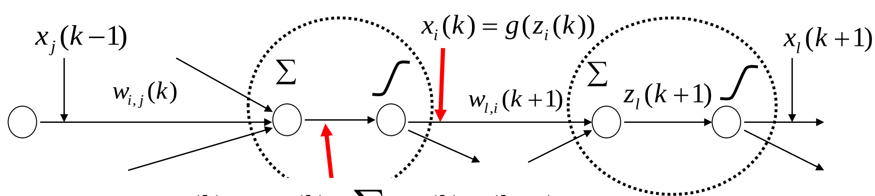
Backpropagation

(k-1)-th level — k-th level — (k+1)-th level



$$z_i(k) = w_{i,0}(k) + \sum_j w_{i,j}(k) x_j(k-1)$$

- **Derivation:**

$$\delta_i(k) = \frac{\partial}{\partial z_i(k)} J(D,\mathbf{w}) = \boxed{\frac{\partial}{\partial x_i(k)} J(D,\mathbf{w})} * \boxed{\frac{\partial x_i(k)}{\partial z_i(k)}}$$

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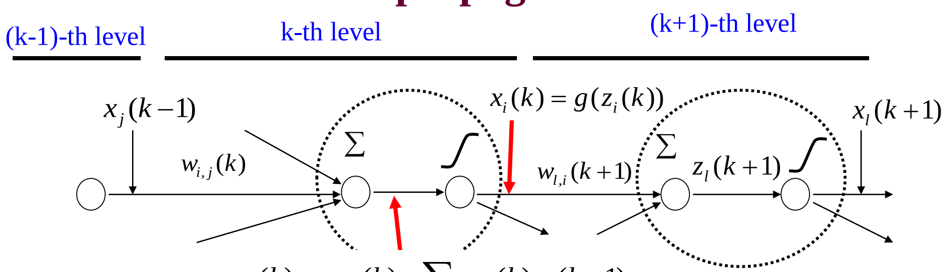
$$\delta_i(k) = \left[\sum_l \delta_l(k+1) w_{l,i}(k+1)\right] x_i(k)(1-x_i(k))$$

Backpropagation



$$z_i(k) = w_{i,0}(k) + \sum_j w_{i,j}(k) x_j(k-1)$$

- **Gradient:**

$$w_{i,j}(k) \leftarrow w_{i,j}(k) - \alpha\left[\delta_i(k) x_j(k-1)\right]$$

$$\delta_i(k) = \left[\sum_l \delta_l(k+1) w_{l,i}(k+1)\right] x_i(k)(1 - x_i(k))$$

- **Last unit** (is the same as for the regular linear units),

  E.g. for regression:

$$\delta_i(K) = -(y_u - f(\mathbf{x}_u, \mathbf{w}))$$

Backpropagation

Update weight $w_{i,j}(k)$ using data D $\quad D = \{< \mathbf{x}, y >\}$

$$w_{i,j}(k) \leftarrow w_{i,j}(k) - \alpha \frac{\partial}{\partial w_{i,j}(k)} J(D, \mathbf{w})$$

Let $\quad \delta_i(k) = \dfrac{\partial}{\partial z_i(k)} J(D, \mathbf{w})$

Then: $\quad \dfrac{\partial}{\partial w_{i,j}(k)} J(D, \mathbf{w}) = \dfrac{\partial J(D, \mathbf{w})}{\partial z_i(k)} \dfrac{\partial z_i(k)}{\partial w_{i,j}(k)} = \delta_i(k) x_j(k-1)$

S.t. $\delta_i(k)$ is computed from $x_i(k)$ and the next layer $\delta_l(k+1)$

$$\delta_i(k) = \left[\sum_l \delta_l(k+1) w_{l,i}(k+1)\right] x_i(k)(1 - x_i(k))$$

Last unit (is the same as for the regular linear units):

$$\delta_i(K) = -(y_u - f(\mathbf{x}_u, \mathbf{w}))$$

It is the same for the classification with the log-likelihood measure of fit and linear regression with least-squares error!!!

Learning with MLP

- **Online gradient descent algorithm**
  - Weight update:

$$w_{i,j}(k) \leftarrow w_{i,j}(k) - \alpha \frac{\partial}{\partial w_{i,j}(k)} J_{\text{online}}(D_u, \mathbf{w})$$

$$\frac{\partial}{\partial w_{i,j}(k)} J_{online}(D_u, \mathbf{w}) = \frac{\partial J_{online}(D_u, \mathbf{w})}{\partial z_i(k)} \frac{\partial z_i(k)}{\partial w_{i,j}(k)} = \delta_i(k) x_j(k-1)$$

$$\boxed{w_{i,j}(k) \leftarrow w_{i,j}(k) - \alpha \delta_i(k) x_j(k-1)}$$

$x_j(k-1)$ - j-th output of the (k-1) layer

$\delta_i(k)$ - derivative computed via backpropagation

α - a learning rate

Online gradient descent algorithm for MLP

Online-gradient-descent (D, *number of iterations*)

Initialize all weights $w_{i,j}(k)$

for i=1:1*: number of iterations*

do **select** a data point D_u=<$\mathbf{x}$,y> from D

set learning rate α

compute outputs $x_j(k)$ for each unit

compute derivatives $\delta_i(k)$ via **backpropagation**

update all weights (in parallel)

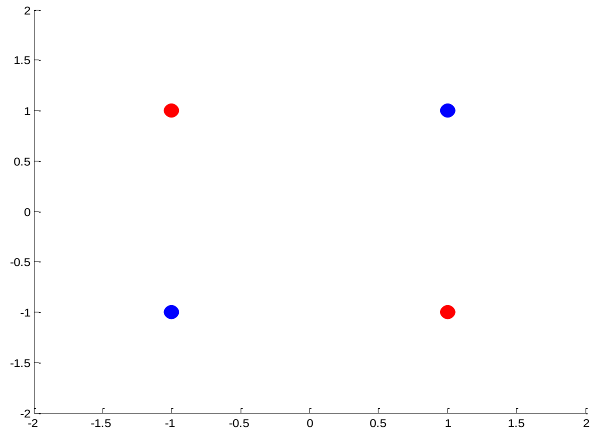
$$w_{i,j}(k) \leftarrow w_{i,j}(k) - \alpha \delta_i(k) x_j(k-1)$$

end for

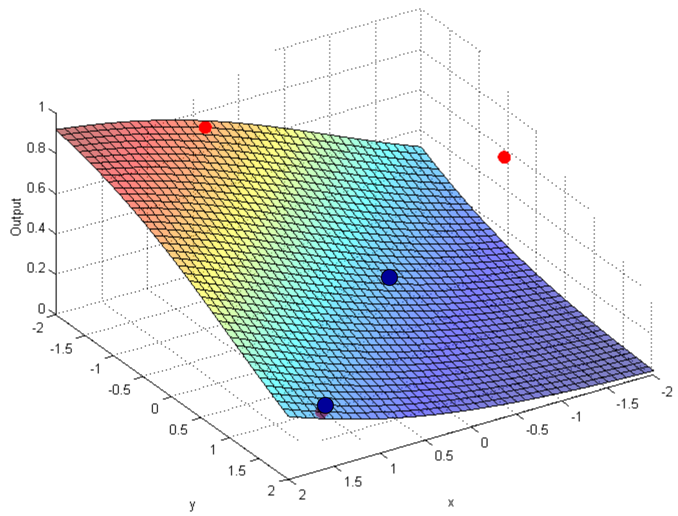
return weights $\mathbf{w}$

Xor Example.

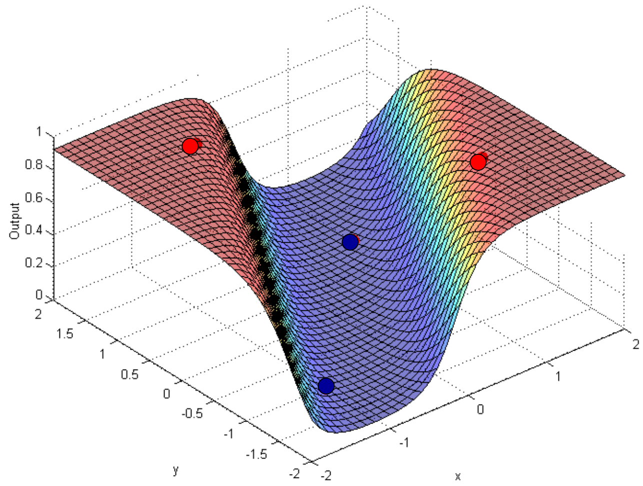
- linear decision boundary does not exist



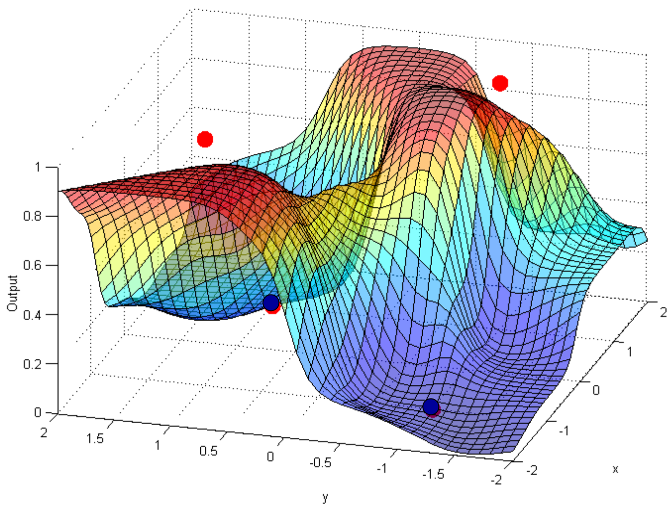
Xor example. Linear unit



Xor example.
Neural network with 2 hidden units



Xor example.
Neural network with 10 hidden units



Neural networks

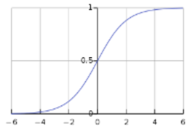
Activation (transfer) functions

- **Determine how inputs are transformed to output**

Possible choices of nonlinear transfer functions:

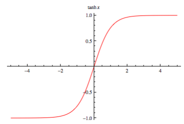
- **Logistic function**

$$f(z) = \frac{1}{1+e^{-z}} \qquad f(z)' = f(z)(1-f(z))$$



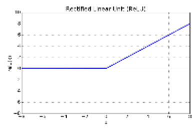
- **Hyperbolic tangent**

$$f(z) = \tanh(z) = \frac{2}{1+e^{-2z}} - 1 \qquad f(z)' = 1 - f(z)^2$$



- **Rectified linear function (Relu)**

$$f(z) = \begin{cases} 0 & z < 0 \\ z & z \geq 0 \end{cases}$$



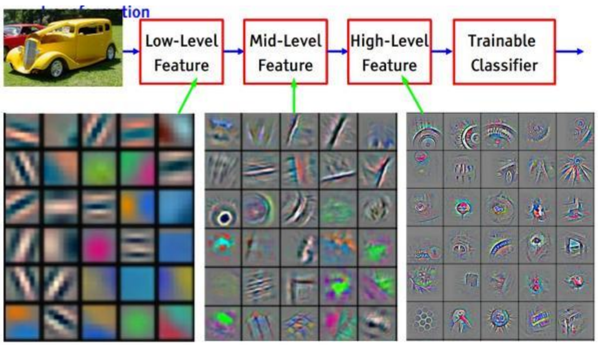
Limitation of standard NNs

Standard NN:

- **do not scale well to high dimensional data (e.g. images)**
  - 100x100 image + 100 hidden units = 1 million parameters.
  - Overfitting;
  - Tremendous requirements of computation and storage.
- **Sensitive to small translation of inputs**
  - Images: objects can have size, slant or position variations
  - Speech: varying speed, pitch or intonation.
- **Ignores the topology of the input**
  - i.e. the input variables can be presented in any order without affecting the outcome of training.
  - However, images or speech have a strong local structure
    - E.g. pixels nearby are highly correlated.

Deep learning

- **Deep learning.** Machine learning algorithms based on learning multiple levels of representation / abstraction. More than one layer of non-linear feature transformation.

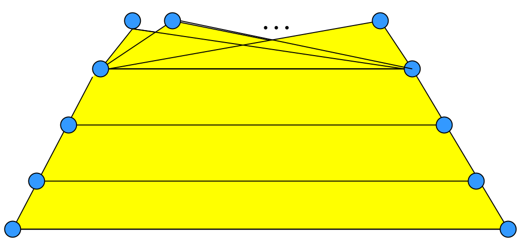


Deep neural networks

Early efforts

- **Optical character recognition** – digits 20x20
  - Automatic sorting of mails
  - 5 layer network with multiple output functions and somewhat restricted topology

10 outputs (0,1,…9)



20x20 = 400 inputs

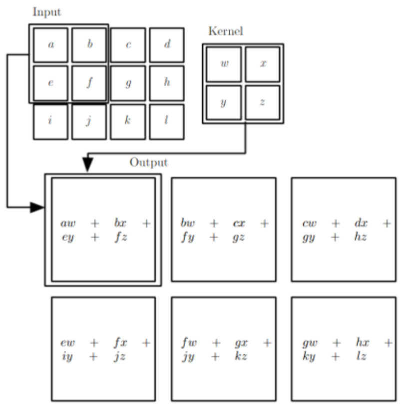
layer	Neurons	Weights
5	10	3000
4	300	1200
3	1200	50000
2	784	3136
1	3136	78400

Convolutional NN

Take advantage of the local structure of the data (image, speech)

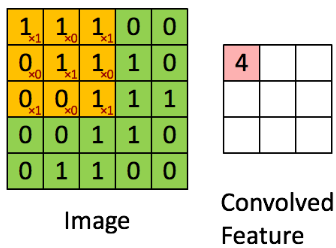
Convolution in Machine Learning

- the **input** array
  - e.g. image pixels.
- a **filter or kernel**
  - a smaller (local) matrix of parameters
- Output: a **feature map**
  - Filter applied to the image



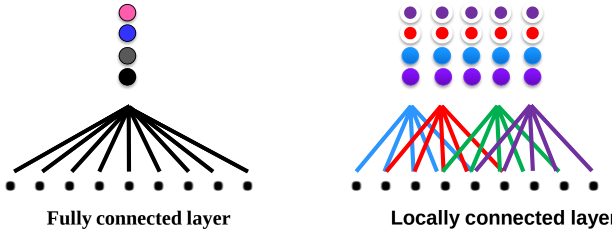
Feature Extraction using Convolution

- The statistics of one part of the image are the same as any other part.
- Meaning that different parts of an image can share the same feature parameters (**kernel**).
- Use this kernel to **convolve** a set of features.
- This is called one feature mapping.



Feature Extraction using Convolution

4 features on full data (image) **4 features on the local data**



9 weights per hidden unit
9 x 4 = 36 weights

5 weights per hidden unit
5 x 4 = 20 weights

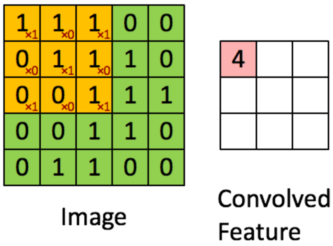
Increased #input, #hidden unit, but fewer weights

Pooling (Subsampling, Down-sampling)

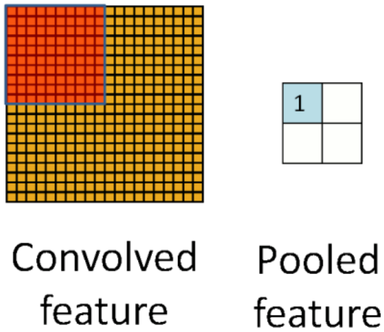
- **Assumption:** Features useful in one region are likely to be useful for other regions.
- To describe a large image, statistics can be **aggregated.**
- For example, one can calculate mean or max of a particular feature over a region.
  - Called **mean pooling**, **max pooling** respectively.
- These summary statistics are much lower in dimension.
- Also can improve results (less-overfitting).

Convolution and Pooling

Convolution

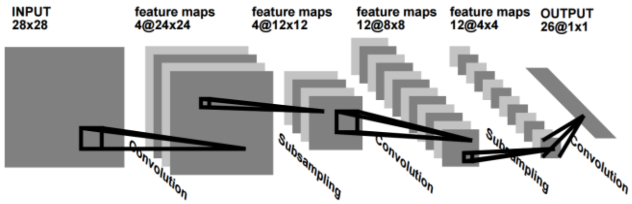


Pooling



Convolutional NN

- CNN = (≥ 1) convolution layer(s) + standard NN
- **One convolution layer is:**
  - Convolution operation + activation function + pooling
- You can view the convolution layer(s) as a feature extractor.
  - Input: raw image pixels, raw time series
  - Output: summarized features.



CNN vs. NN

- NN is sensitive to local distortions of unstructured data.
  - NN can theoretically be trained to be invariant to these distortions, probably resulting in multiple units with identical weights.
  - But such a training task requires a large number of training instances.
- CNN with pooling can be invariant to small translations:
  - Shifts (automatically)
  - Rotation (with extra mechanism)

Object Recognition Task

- ImageNet Data (2009 - 2016)

ImageNet 2012

Data

- Size:
  - Number of images
    - 1.2 million training images
    - 50K validation images
    - 150K testing images
  - Variable image size

- Supervised task
  - Labeled using Amazon's Mechanical Turk
- Categories:
  - 1000 categories (objects)
    - Approximately 1000 in each categor
- RGB pictures

Goal

Provide a probability for different categories that an image can belong to

Object Recognition

- **ImageNet**
  - Achieves state-of-the-art on many object recognition tasks.