CS 2750 Machine Learning
Lecture 11

SVMs for regression
Multilayer neural networks

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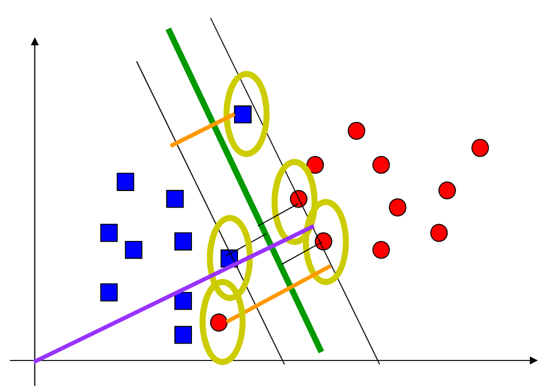
Linearly non-separable case

- Allow some flexibility on crossing the separating hyperplane



Linearly non-separable case

minimize $\|\mathbf{w}\|^2 / 2 + C\sum_{i=1}^{n} \xi_i$

$$\mathbf{w}^T \mathbf{x}_i + w_0 \geq 1 - \xi_i \quad \textbf{for} \quad y_i = +1$$

$$\mathbf{w}^T \mathbf{x}_i + w_0 \leq -1 + \xi_i \quad \textbf{for} \quad y_i = -1$$

$$\xi_i \geq 0$$

- Rewrite $\xi_i = \max\left[0, \quad 1 - y_i(\mathbf{w}^T \mathbf{x}_i + w_0)\right]$ in $\|\mathbf{w}\|^2 / 2 + C\sum_{i=1}^{n} \xi_i$

$$\|\mathbf{w}\|^2 / 2 + C\sum_{i=1}^{n} \max\left[0, \quad 1 - y_i(\mathbf{w}^T \mathbf{x}_i + w_0)\right]$$

Regularization penalty

Hinge loss

Support vector machines

- **The decision boundary:**

$$\hat{\mathbf{w}}^T \mathbf{x} + w_0 = \sum_{i \in SV} \hat{\alpha}_i y_i (\mathbf{x}_i^T \mathbf{x}) + w_0 = 0$$

- **The decision:**

$$\hat{y} = \text{sign}\left[\sum_{i \in SV} \hat{\alpha}_i y_i (\mathbf{x}_i^T \mathbf{x}) + w_0\right]$$

- **(!!):**
- Decision on a new $\mathbf{x}$ requires to compute the inner product between the examples $(\mathbf{x}_i^T \mathbf{x})$
- Similarly, the optimization depends on $(\mathbf{x}_i^T \mathbf{x}_j)$

$$J(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

Nonlinear case

- The linear case requires to compute $(\mathbf{x}_i^T \mathbf{x})$
- The non-linear case can be handled by using a set of features. Essentially we map input vectors to (larger) feature vectors

$$\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$$

- It is possible to use SVM formalism on feature vectors

$$\boldsymbol{\varphi}(\mathbf{x})^T \boldsymbol{\varphi}(\mathbf{x}')$$

- **Kernel function**

$$K(\mathbf{x}, \mathbf{x}') = \boldsymbol{\varphi}(\mathbf{x})^T \boldsymbol{\varphi}(\mathbf{x}')$$

- **Crucial idea:** If we choose the kernel function wisely we can compute linear separation in the feature space implicitly such that we keep working in the original input space !!!!

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Kernel function example

- Assume $\mathbf{x} = [x_1, x_2]^T$ and a feature mapping that maps the input into a quadratic feature set

$$\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x}) = [x_1^2, x_2^2, \sqrt{2}x_1 x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1]^T$$

- Kernel function for the feature space:

$$\begin{aligned} K(\mathbf{x}', \mathbf{x}) &= \boldsymbol{\varphi}(\mathbf{x}')^T \boldsymbol{\varphi}(\mathbf{x}) \\ &= x_1^2 x_1'^2 + x_2^2 x_2'^2 + 2x_1 x_2 x'_1 x'_2 + 2x_1 x'_1 + 2x_2 x'_2 + 1 \\ &= (x_1 x'_1 + x_2 x'_2 + 1)^2 \\ &= (1 + (\mathbf{x}^T \mathbf{x}'))^2 \end{aligned}$$

- The computation of the linear separation in the higher dimensional space is performed implicitly in the original input space

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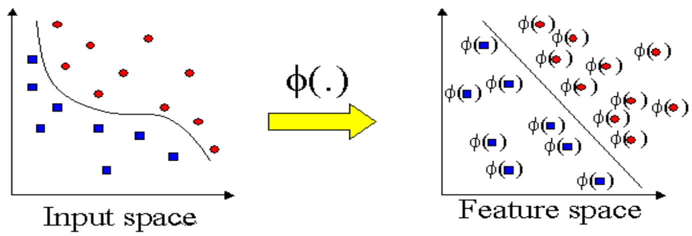
Nonlinear extension



Kernel trick

- Replace the inner product with a kernel
- A well chosen kernel leads to an efficient computation

Kernel functions

- **Linear kernel**

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}'$$

- **Polynomial kernel**

$$K(\mathbf{x}, \mathbf{x}') = \left[1 + \mathbf{x}^T \mathbf{x}'\right]^k$$

- **Radial basis kernel**

$$K(\mathbf{x}, \mathbf{x}') = \exp\left[-\frac{1}{2}\left\|\mathbf{x} - \mathbf{x}'\right\|^2\right]$$

Kernels

- **Kernels define** a **similarity measure** :
  - define a distance in between two objects
- **Design criteria:** we want kernels to be
  - **valid** – Satisfy **Mercer condition** of positive semi-definiteness
  - **good** – embody the "true similarity" between objects
  - **appropriate** – generalize well
  - **efficient** – the computation of K(x,x') is feasible
    - NP-hard problems abound with graphs

Kernels

- Research have proposed kernels for comparison of variety of objects:
  - Strings
  - Trees
  - Graphs
- **Cool thing:**
  - SVM algorithm can be now applied to classify a variety of objects

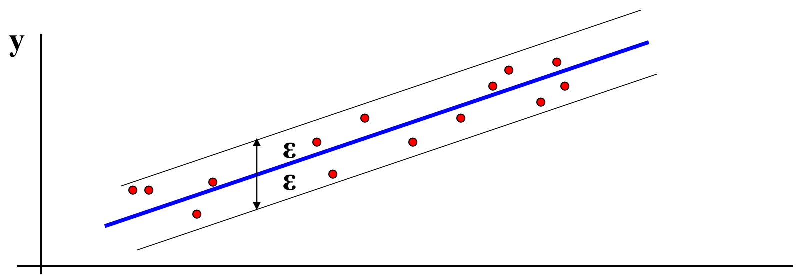
Support vector machine for regression

Regression = find a function that fits the data.

- A data point may be wrong due to the noise

Idea: Error from points which are close **should count as a valid noise**

- Line should be influenced by the real data not the noise.



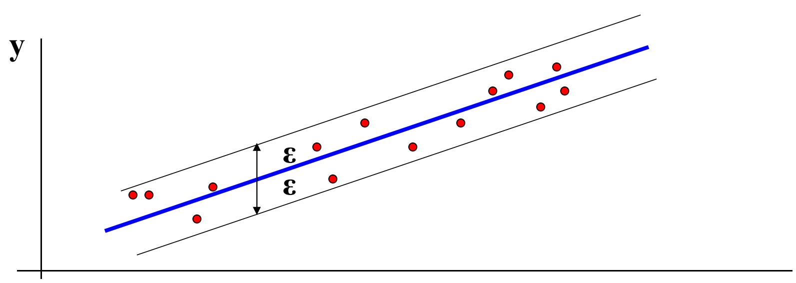
Linear model

- **Training data:**

$$\{(x_1, y_1), \ldots, (x_l, y_l)\}, \quad x \in R^n, y \in R$$

- Our goal is to find a function f(x) that has at most ε deviation from the actually obtained target for all the training data.

$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \langle \mathbf{w}, \mathbf{x} \rangle + b$$



Linear model

Linear function:

$$f(\mathbf{x}) = \mathbf{w}^{T}\mathbf{x} + b = \langle \mathbf{w}, \mathbf{x} \rangle + b$$

We want a function that is:

- **flat:** means that one seeks small **w**
- all data points are within its ε neighborhood

The problem can be formulated as a **convex optimization problem:**

$$\text{minimize} \quad \frac{1}{2}\|w\|^2$$

$$\text{subject to} \quad \begin{cases} y_i - \langle w_i, x_i \rangle - b \le \varepsilon \\ \langle w_i, x_i \rangle + b - y_i \le \varepsilon \end{cases}$$

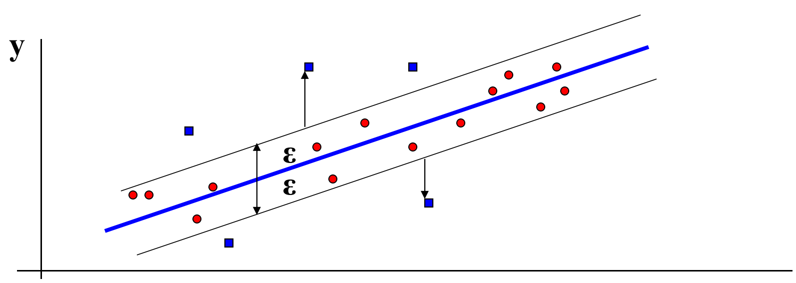
All data points are assumed to be in the ε neighborhood

Linear model

- **Real data: not all data points always fall into the** ε neighborhood

$$f(\mathbf{x}) = \mathbf{w}^{T}\mathbf{x} + b = \langle \mathbf{w}, \mathbf{x} \rangle + b$$

- **Idea:** penalize points that fall outside the ε neighborhood



Linear model

Linear function:

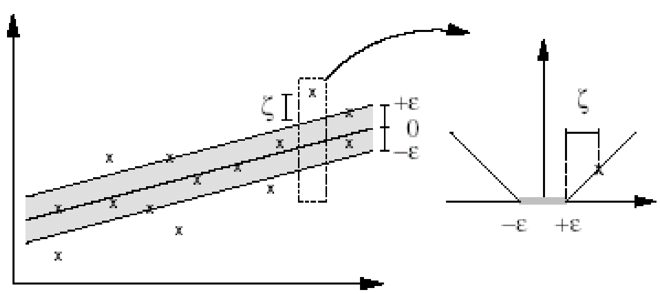
$$f(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + b = \langle \mathbf{w}, \mathbf{x} \rangle + b$$

Idea: penalize points that fall outside the ε neighborhood

$$\text{minimize} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{l}(\xi_i + \xi_i^*)$$

$$\text{subject to} \quad \begin{cases} \mathrm{y}_{\mathrm{i}} - \langle w_i, x_i \rangle - b \le \varepsilon + \xi_i \\ \langle w_i, x_i \rangle + b - \mathrm{y}_{\mathrm{i}} \le \varepsilon + \xi_i^* \\ \xi_i, \xi_i^* \ge 0 \end{cases}$$

Linear model



$$|\xi|_{\varepsilon} = \begin{cases} 0 & \text{for } |\xi| \le \varepsilon \\ |\xi| - \varepsilon & \text{otherwise} \end{cases}$$

ε-intensive loss function

Optimization

Lagrangian that solves the optimization problem

$$L = \frac{1}{2}\langle w, w\rangle + C\sum_{i=1}^{l}(\xi_i + \xi_i^*)$$
$$- \sum_{i=1}^{l} a_i(\varepsilon - \xi_i - y_i + \langle w, x_i\rangle + b) - \sum_{i=1}^{l} a_i^*(\varepsilon + \xi_i^* + y_i - \langle w, x_i\rangle - b)$$
$$- \sum_{i=1}^{l}(\eta_i \xi_i + \eta_i^* \xi_i^*)$$

Subject to $a_i, a_i^*, \eta_i, \eta_i^* \geq 0$

Primal variables w, b, ξ_i, ξ_i^*

Optimization

Derivatives with respect to primal variables

$$\frac{\partial L}{\partial b} = \sum_{i=1}^{l}(a_i^* - a_i) = 0$$

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{l}(a_i^* - a_i)\mathbf{x}_i = \mathbf{0}$$

$$\frac{\partial L}{\partial \xi_i^{(*)}} = C - a_i^{(*)} - \eta_i^{(*)} = 0$$

$$\frac{\partial L}{\partial \xi_i} = C - a_i - \eta_i = 0$$

Optimization

$$L = \frac{1}{2}\langle w, w\rangle + \sum_{i=1}^{l} C\xi_i + \sum_{i=1}^{l} C\xi_i^*$$

$$- \sum_{i=1}^{l} a_i\varepsilon - \sum_{i=1}^{l} a_i\xi_i - \sum_{i=1}^{l} a_i y_i - \sum_{i=1}^{l} a_i\langle \omega, x_i\rangle + \sum_{i=1}^{l} a_i b$$

$$- \sum_{i=1}^{l} a_i^*\varepsilon - \sum_{i=1}^{l} a_i^*\xi_i^* - \sum_{i=1}^{l} a_i^* y_i + \sum_{i=1}^{l} a_i^*\langle \omega, x_i\rangle + \sum_{i=1}^{l} a_i^* b$$

$$- \sum_{i=1}^{l} \eta_i\xi_i - \sum_{i=1}^{l} \eta_i^*\xi_i^*$$

Optimization

$$L = \frac{1}{2}\langle w, w\rangle + \sum_{i=1}^{l} \xi_i \underbrace{(C - \eta_i - a_i)}_{=0\,(C-\eta_i - a_i = 0)} +$$

$$\sum_{i=1}^{l} \xi_i^* \underbrace{(C - \eta_i^* - a_i^*)}_{=0\,(C-\eta_i^{(*)} - a_i^{(*)} = 0)} - \sum_{i=1}^{l} (a_i + a_i^*)\varepsilon - \sum_{i=1}^{l} (a_i + a_i^*) y_i$$

$$- \sum_{i=1}^{l} \underbrace{(a_i - a_i^*)\langle \omega, x_i\rangle}_{=\langle w, w\rangle\,(\omega = \sum_{i=1}^{l}(a_i + a_i^*) x_i)} + \sum_{i=1}^{l} \underbrace{(a_i^* - a_i) b}_{=0\,(\sum_{i=1}^{l}(a_i^* - a_i) = 0)}$$

Optimization

$$L = -\frac{1}{2}\langle w, w\rangle - \sum_{i=1}^{l}(a_i + a_i^*)\varepsilon - \sum_{i=1}^{l}(a_i + a_i^*)y_i$$

Maximize the dual

$$L(a, a^*) = -\frac{1}{2}\sum_{i=1}^{l}(a_i - a_i^*)(a_j - a_j^*)\langle x_i, x_j\rangle$$
$$- \sum_{i=1}^{l}(a_i + a_i^*)\varepsilon - \sum_{i=1}^{l}(a_i + a_i^*)y_i$$

subject to $:\begin{cases}\sum_{i=1}^{l}(a_i - a_i^*) = 0 \\ a_i, a_i^* \in [0, C]\end{cases}$

SVM solution

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{l}(a_i^* - a_i)\mathbf{x}_i = \mathbf{0}$$

$$\mathbf{w} = \sum_{i=1}^{l}(a_i - a_i^*)\mathbf{x}_i$$

We can get:

$$f(\mathbf{x}) = \sum_{i=1}^{l}(a_i - a_i^*)\langle \mathbf{x_i}, \mathbf{x}\rangle + b$$

at the optimal solution the Lagrange multipliers are non-zero only **for points outside the ε band.**

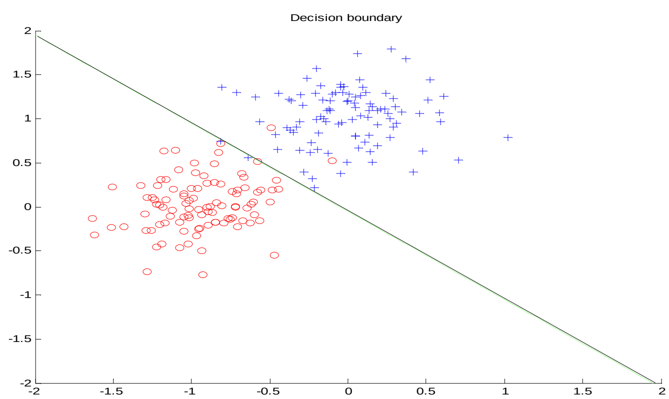
Multilayer neural networks

Or another way of modeling nonlinearities for regression and classification problems

Classification with the linear model.

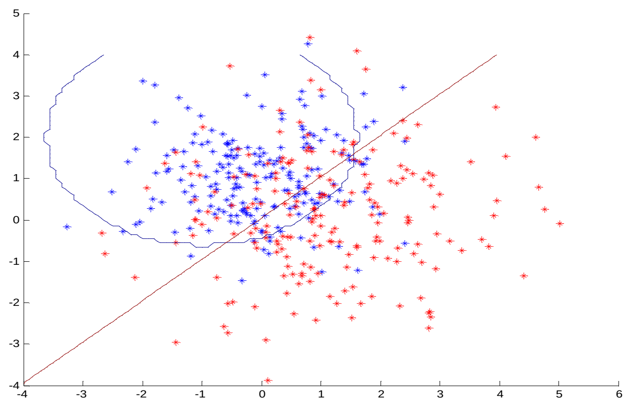
Logistic regression model defines a linear decision boundary

- Example: 2 classes (blue and red points)



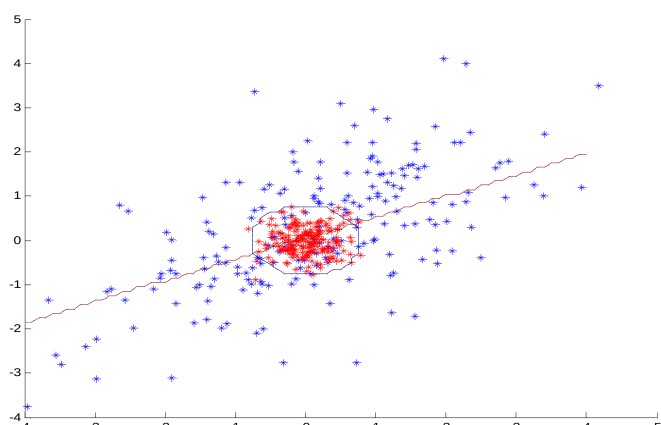
Linear decision boundary

- logistic regression model is not optimal, but not that bad



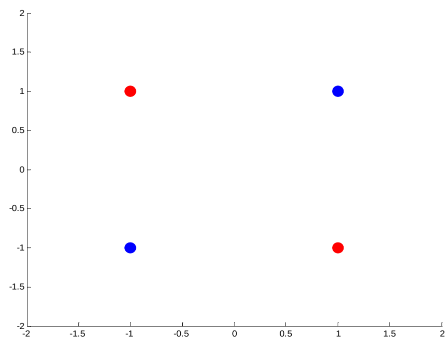
When logistic regression fails?

- Example in which the logistic regression model fails



Limitations of linear units.

- Logistic regression does not work for **parity functions**
  - no linear decision boundary exists



Solution: a model of a non-linear decision boundary

Extensions of simple linear units

- use **feature (basis) functions** to model **nonlinearities**

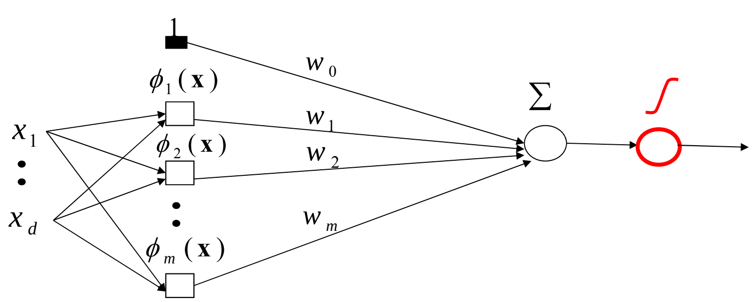
Linear regression

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

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 $\mathbf{x}$



Learning with extended linear units

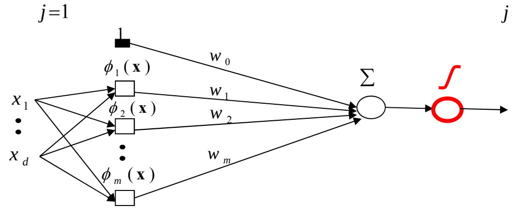
Feature (basis) functions model **nonlinearities**

Linear regression

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

Logistic regression

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



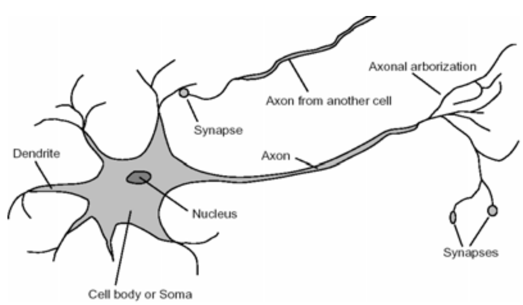
Important property:

- The same problem as learning of the weights for linear units , the input has changed– but the weights are linear in the new input

Problem: too many weights to learn

Multi-layered neural networks

- An alternative way to introduce **nonlinearities to regression/classification models**
- **Key idea: Cascade several simple neural models with logistic units.** Much like neuron connections.

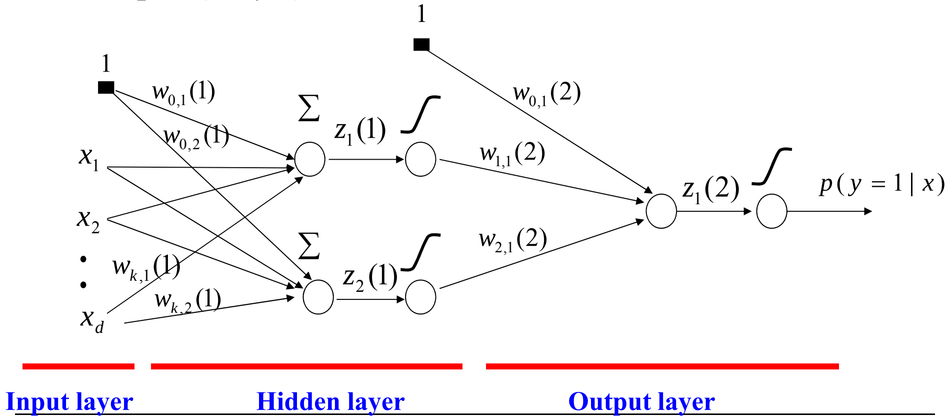


Multilayer neural network

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

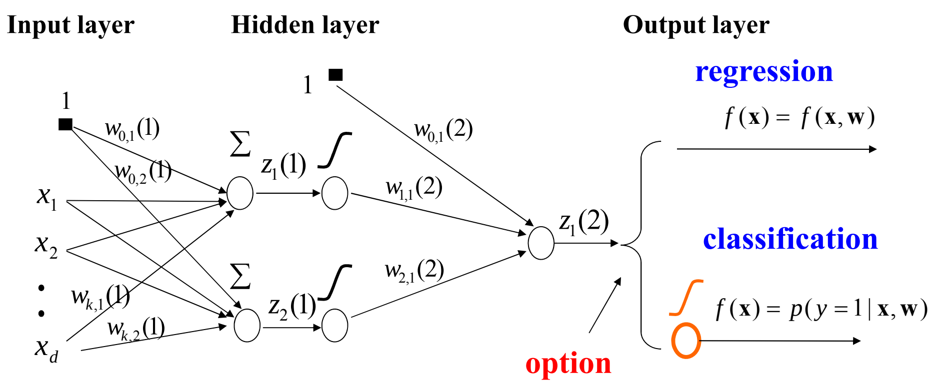
Cascades multiple logistic regression units

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



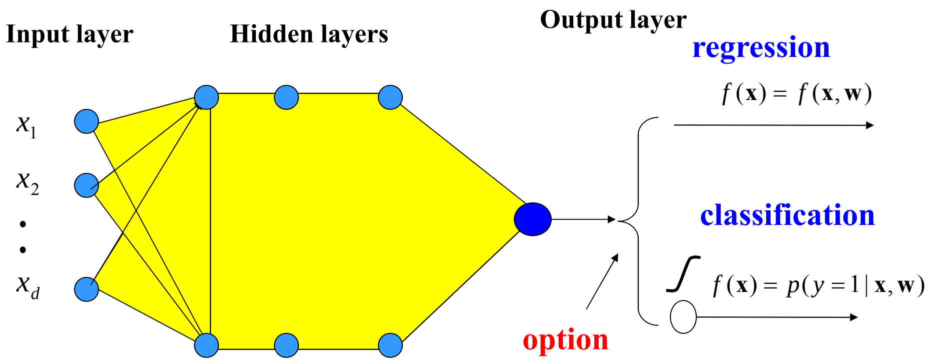
Multilayer neural network

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



Multilayer neural network

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

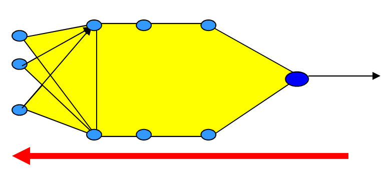


Learning with MLP

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

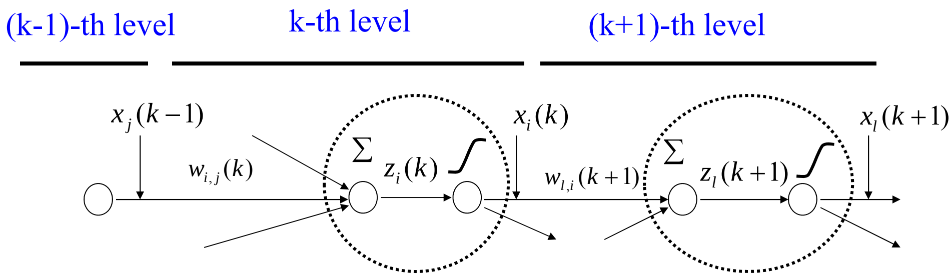
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} J(D, \mathbf{w})$$

- 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



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

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

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

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

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

Backpropagation

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

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

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

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

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):

$$\delta_i(K) = -\sum_{u=1}^{n} (y_u - f(\mathbf{x}_u, \mathbf{w}))$$

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

Learning with MLP

- **Gradient descent algorithm**
  - Weight update:

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

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

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

$x_j(k-1)$ - j-th output of the (k-1) layer
$\delta_i(k)$ - derivative computed via back-propagation
α - a learning rate

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

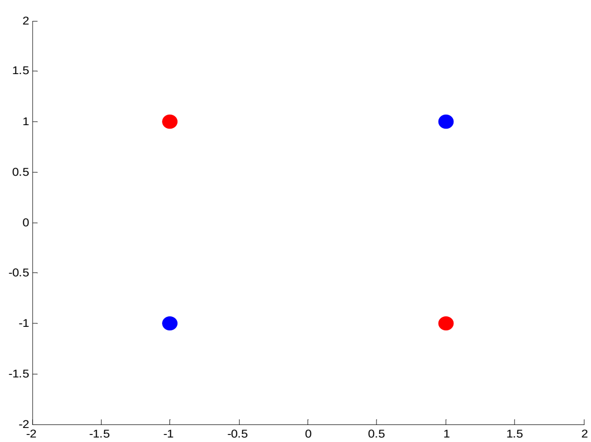
Online-gradient-descent (*D, number of iterations*)
Initialize all weights $w_{i,j}(k)$
for i=1:1: *number of iterations*
do **select** a data point D_u=<**x**,*y*> from *D*
set learning rate α
compute outputs $x_j(k)$ for each unit
compute derivatives $\delta_i(k)$ via **backpropagation**
update all weights (in parallel)

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

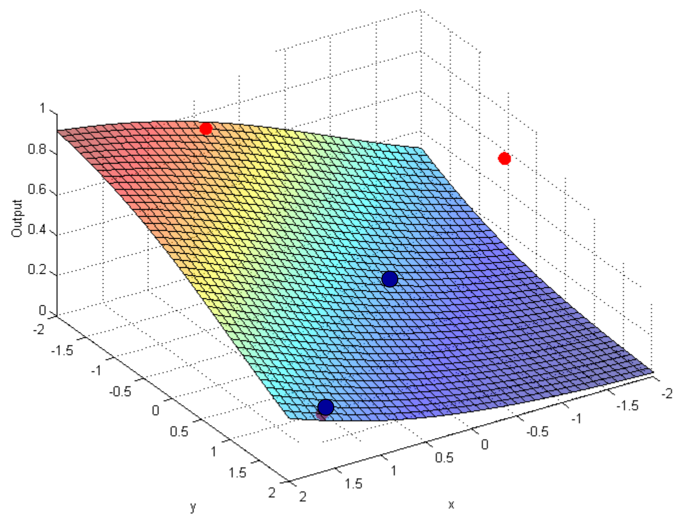
end for
return weights **w**

Xor Example.

- linear decision boundary does not exist



Xor example. Linear unit



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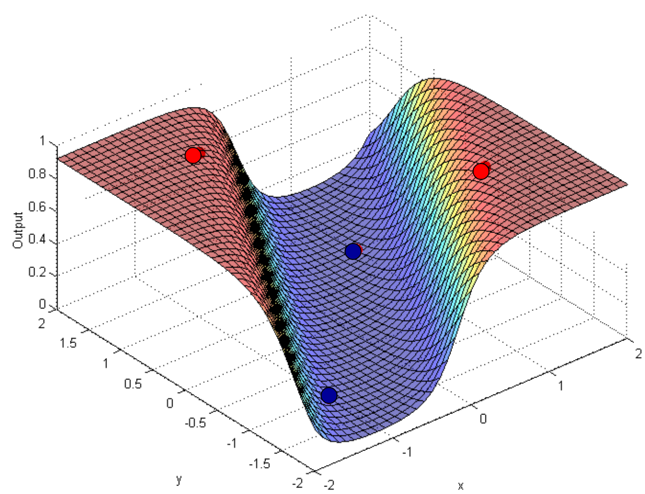
Xor example. Neural network with 2 hidden units



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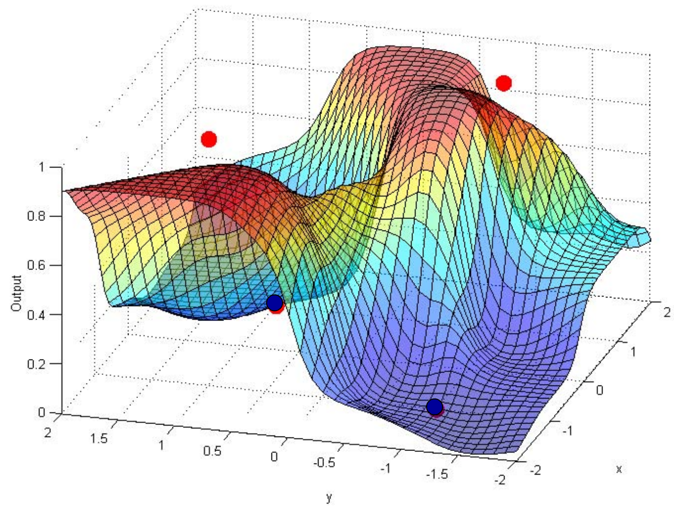
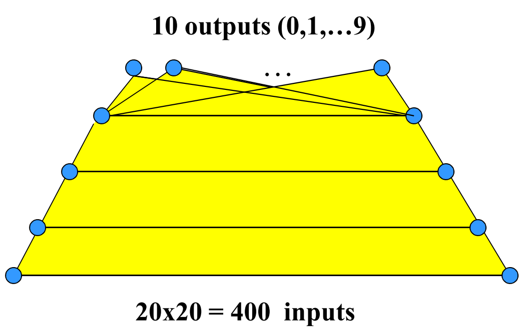
Xor example.
Neural network with 10 hidden units



MLP in practice

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



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