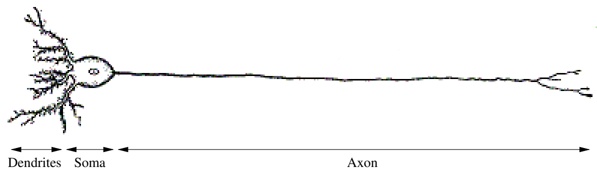
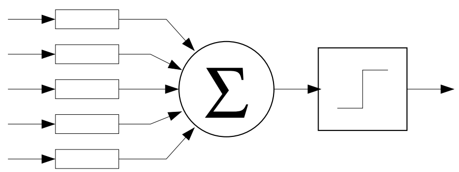
Classification with Separating Hyperplanes

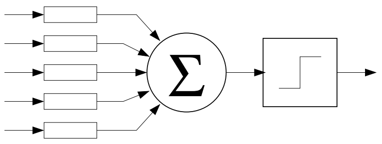


Neuron caricature, “artificial neuron”



- Weighted input signals
- Summing
- Thresholded output

What can a single "artificial neuron" compute?



$\vec{x}$ Input in vector format
$\vec{w}$ Weights in vector format
o Output

$$o = \operatorname{sign}\left(\sum_i x_i w_i\right)$$

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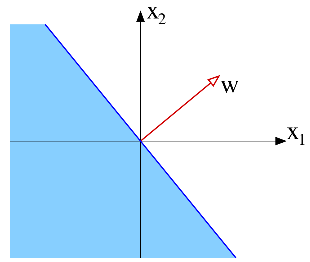
Geometrical interpretation



Variable threshold $\equiv$ Not anchored to origin
Common trick: treat the threshold as a weight

Training a linear separator

What does learning mean here?

Learning means finding the best weights w_i

Two good algorithms exist:

- Perceptron Learning
- Delta Rule

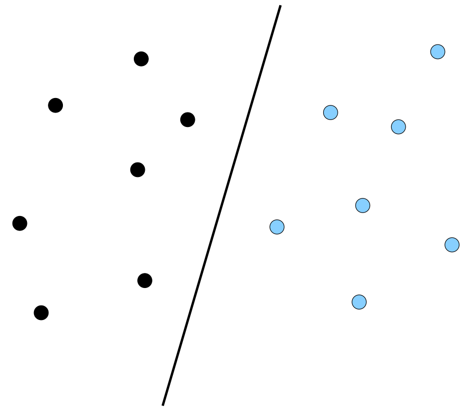
Perceptron Learning

- Incremental learning
- Weights only change when the output is wrong
- Update rule: $w_i \leftarrow w_i + \eta(t - o)x_i$
- Always converges if the problem is solvable

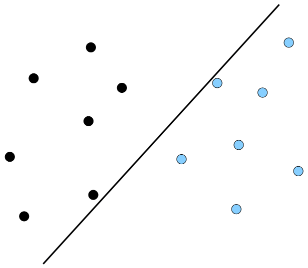
Delta Rule (LMS-rule)

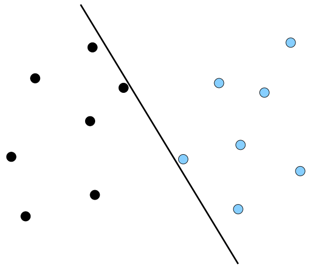
- Incremental learning
- Weights always change
- $w_i \leftarrow w_i + \eta(t - \vec{w}^T\vec{x})x_i$
- Converges only in the mean
- Will find an optimal solution even if the problem can not be fully solved

Linear Separation



Many acceptable solutions $\rightarrow$ bad generalization

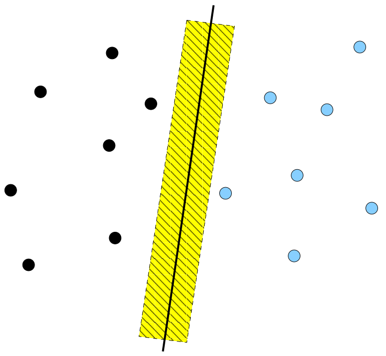




- Structural Risk

Hyperplane with margins

Training data points are *at least* a distance d from the plane



Less arbitrariness $\rightarrow$ better generalization

- Wide margins restrict the possible hyperplanes to choose from
- Less risk to choose a bad hyperplane by accident
- Reduced risk for bad generalization

Minimization of the structural risk $\equiv$ maximization of the margin

Out of all hyperplanes which solve the problem
the one with widest margin will probably generalize best

Mathematical Formulation

- Separating Hyperplane

$$\vec{w}^T\vec{x} = 0$$

- Hyperplane with a margin

$$\vec{w}^T\vec{x} \geq 1 \qquad \text{when } t = 1$$
$$\vec{w}^T\vec{x} \leq -1 \qquad \text{when } t = -1$$

- Combined

$$t\vec{w}^T\vec{x} \geq 1$$

How wide is the margin?

1. Select two points, $\vec{p}$ and $\vec{q}$, on the two margins:

$$\vec{w}^T\vec{p} = 1 \qquad \vec{w}^T\vec{q} = -1$$

2. Distance between $\vec{p}$ and $\vec{q}$ *along* $\vec{w}$:

$$2d = \frac{\vec{w}^T}{||\vec{w}||}(\vec{p} - \vec{q})$$

3. Simplify:

$$2d = \frac{\vec{w}^T\vec{p} - \vec{w}^T\vec{q}}{||\vec{w}||} = \frac{1 - (-1)}{||\vec{w}||} = \frac{2}{||\vec{w}||}$$

Maximal margin corresponds to minimal length of the weight vector

Best Separating Hyperplane

Minimize

$$\vec{w}^T\vec{w}$$

Constraints

$$t_i\vec{w}^T\vec{x}_i \geq 1 \qquad \forall i$$

Observation

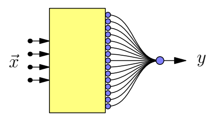
Almost everything becomes linearly separable
when represented in high-dimensional spaces

"Ordinary" low-dimensional data can be "scattered" into a high-dimensional space.

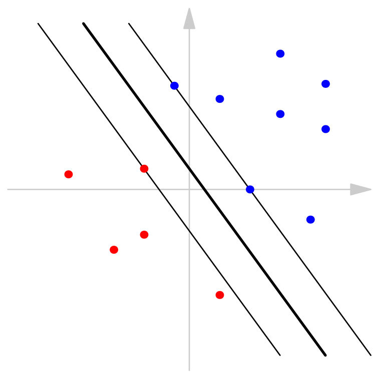
Two problems emerge

1. Many free parameters $\rightarrow$ bad generalization
2. Extensive computations

Support Vector Machines



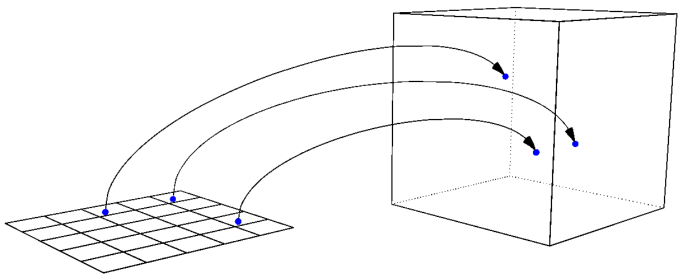
- Transform the input to a suitable high-dimensional space
- Choose the separation that has maximal margins



Support Vector Machines

- Advantages
  - Very good generalization
  - Works well even with few training samples
  - Fast classification
- Disadvantages
  - Non-local weight calculation
  - Hard to implement efficiently

Transform input data non-linearly into a high-dimensional feature space



Idea behind Kernels

Utilize the advantages of a high-dimensional space without actually representing anything high-dimensional

- Condition: The only operation done in the high-dimensional space is to compute *scalar products* between pairs of items
- Trick: The scalar product is computed using the original (low-dimensional) representation

Example

Points in 2D

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Transformation to 4D

$$\phi(\vec{x}) = \begin{bmatrix} x_1^3 \\ \sqrt{3}x_1^2 x_2 \\ \sqrt{3}x_1 x_2^2 \\ x_2^3 \end{bmatrix}$$

$$\begin{aligned}\phi(\vec{x})^T \cdot \phi(\vec{y}) &= x_1^3 y_1^3 + 3x_1^2 y_1^2 x_2 y_2 + 3x_1 y_1 x_2^2 y_2^2 + x_2^3 y_2^3 \\ &= (x_1 y_1 + x_2 y_2)^3 \\ &= (\vec{x}^T \cdot \vec{y})^3 \\ &= \mathcal{K}(\vec{x}, \vec{y})\end{aligned}$$

Common Kernels

Polynomials

$$\mathcal{K}(\vec{x}, \vec{y}) = (\vec{x}^T \vec{y} + 1)^p$$

Radial Bases

$$\mathcal{K}(\vec{x}, \vec{y}) = e^{-\frac{1}{2\sigma^2}||\vec{x}-\vec{y}||^2}$$

Structural Risk Minimization

Minimize

$$\vec{w}^T \vec{w}$$

Constraints

$$t_i \vec{w}^T \vec{x}_i \geq 1 \qquad \forall i$$

- Non-linear transformation ϕ of input $\vec{x}$

New formulation

Minimize

$$\frac{1}{2}\vec{w}^T \vec{w}$$

Constraints

$$t_i \vec{w}^T \phi(\vec{x}_i) \geq 1 \qquad \forall i$$

Structural Risk Minimization

Minimize

$$\frac{1}{2}\vec{w}^T \vec{w}$$

Constraints

$$t_i \vec{w}^T \phi(\vec{x}_i) \geq 1 \qquad \forall i$$

Lagranges Multiplier Method

$$L = \frac{1}{2}\vec{w}^T \vec{w} - \sum_i \alpha_i \left[t_i \vec{w}^T \phi(\vec{x}_i) - 1 \right]$$

Minimize w.r.t. $\vec{w}$, maximize w.r.t. $\alpha_i \geq 0$

$$\frac{\partial L}{\partial \vec{w}} = 0$$

$$L = \frac{1}{2}\vec{w}^T\vec{w} - \sum_i \alpha_i \left[t_i \vec{w}^T \phi(\vec{x}_i) - 1\right]$$

$$\frac{\partial L}{\partial \vec{w}} = 0 \implies \vec{w} - \sum_i \alpha_i t_i \phi(\vec{x}_i) = 0$$

$$\vec{w} = \sum_i \alpha_i t_i \phi(\vec{x}_i)$$

Use

$$\vec{w} = \sum_i \alpha_i t_i \phi(\vec{x}_i)$$

to eliminate $\vec{w}$

$$L = \frac{1}{2}\vec{w}^T\vec{w} - \sum_i \alpha_i \left[t_i \vec{w}^T \phi(\vec{x}_i) - 1\right]$$

$$L = \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j t_i t_j \phi(\vec{x}_i)^T \phi(\vec{x}_j) - \sum_{i,j} \alpha_i \alpha_j t_i t_j \phi(\vec{x}_i)^T \phi(\vec{x}_j) + \sum_i \alpha_i$$

$$L = \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j t_i t_j \phi(\vec{x}_i)^T \phi(\vec{x}_j)$$

The Dual Problem

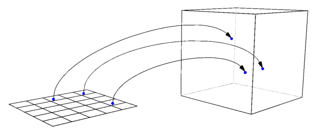
Maximize

$$\sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j t_i t_j \phi(\vec{x}_i)^T \phi(\vec{x}_j)$$

Under the constraints

$$\alpha_i \geq 0 \quad \forall i$$

- $\vec{w}$ has disappeared
- $\phi(\vec{x})$ only appear in scalar product pairs

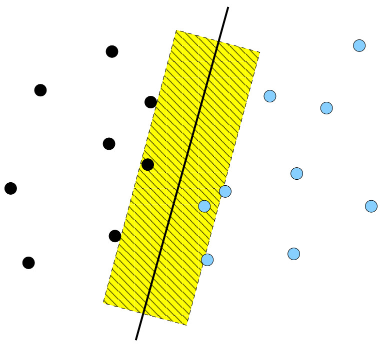


1. Choose a suitable kernel function
2. Compute α_i (solve the maximization problem)
3. $\vec{x}_i$ corresponding to $\alpha_i \neq 0$ are called support vectors
4. Classify new data points via

$$\sum_i \alpha_i t_i \mathcal{K}(\vec{x}, \vec{x}_i) > 0$$

None-Separable Training Samples

Allow for Slack



Linear separation
Structural Risk Minimization
Support Vector Machines
Kernels
Non-separable Classes

Re-formulation of the minimization problem

Minimize

$$\frac{1}{2}\vec{w}^T\vec{w} + C\sum_i \xi_i$$

Constraints

$$t_i\vec{w}^T\phi(\vec{x}_i) \geq 1 - \xi_i$$

ξ_i are called *slack variables*

Örjan Ekeberg Machine Learning

Linear separation
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Dual Formulation with Slack

Maximize

$$\sum_i \alpha_i - \frac{1}{2}\sum_{i,j}\alpha_i\alpha_j t_i t_j \phi(\vec{x}_i)^T\phi(\vec{x}_j)$$

With constraints

$$0 \leq \alpha_i \leq C \quad \forall i$$

Otherwise, everything remains as before

Örjan Ekeberg Machine Learning