Introduction to Machine Learning
NPFL 054

http://ufal.mff.cuni.cz/course/npfl054

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Lecture #9

Support Vector Machines (SVM)

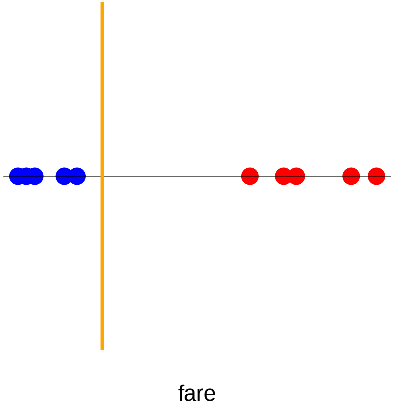
We focus on binary classification and separating the classes by a hyperplane

Key points

1. Hyperplane, Maximizing the margin
2. Quadratic programming, Duality optimization task, Dot product
3. Kernel trick

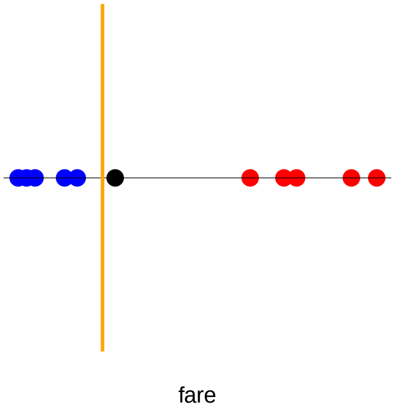
Basic idea

- Titanic data set
- Target class values: Survived, Not Survived
- Feature: Fare
- Separating hyperplane (point in 1D)



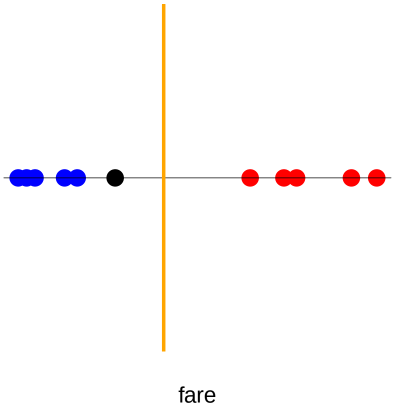
Basic idea

- New test example will by classified into Red. But the example is closer to Blue



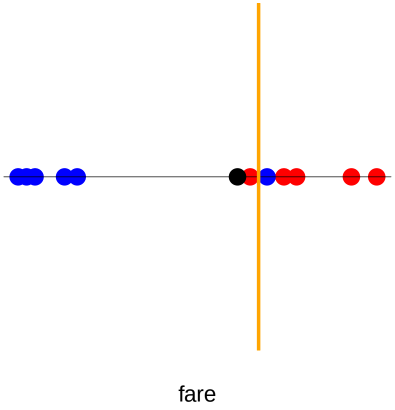
Basic idea

- Let separating hyperplane be the midpoint between the closest examples of the two clusters



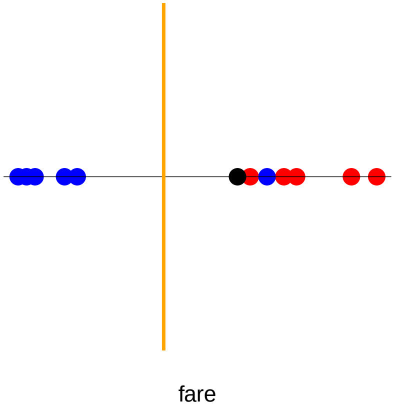
Basic idea

- But this idea is very sensitive to outliers



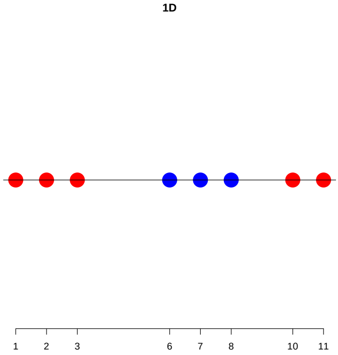
Basic idea

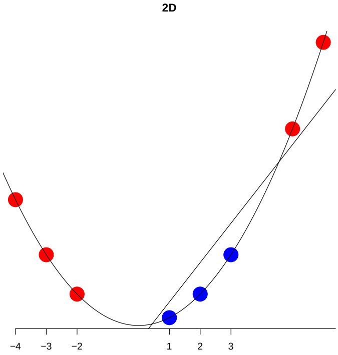
- Let's allow misclassification



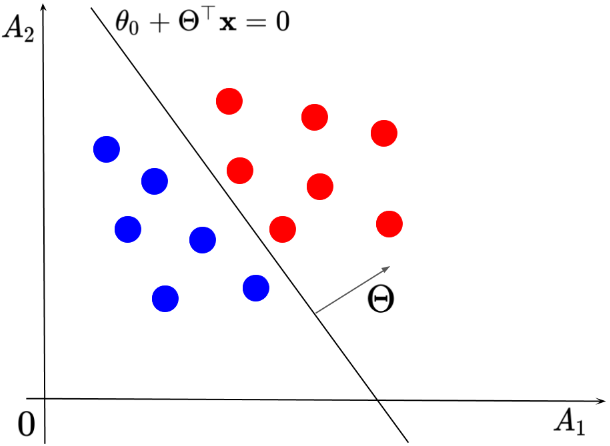
Basic idea

- Do separation with a hyperplane in a higher dimension space if not possible in an original space





Hyperplane



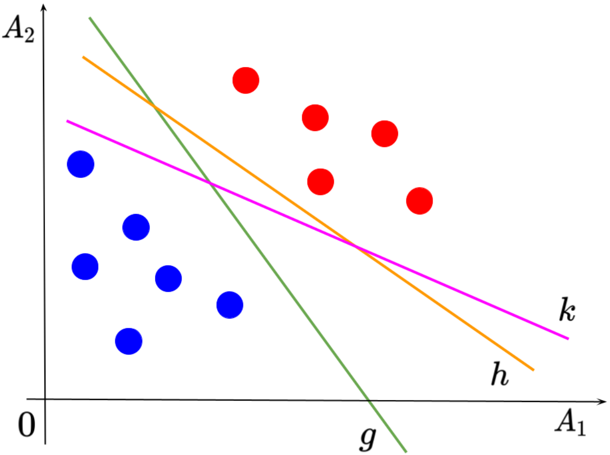
Classification using hyperplane

Recall the classification rule using $\theta_0 + \Theta^\top \mathbf{x} = 0$

$$f(\mathbf{x}) = \begin{cases} 1 \text{ if } \theta_0 + \theta_1 x_1 + \cdots + \theta_m x_m \geq 0 \\ 0 \text{ if } \theta_0 + \theta_1 x_1 + \cdots + \theta_m x_m < 0 \end{cases}$$

Classification using hyperplane

How to compare hyperplanes?



How to compare hyperplanes?

- training examples $D = \{\langle \mathbf{x}_i, y_i \rangle, \mathbf{x}_i \in X, y_i \in \{-1, +1\}\}$
- hyperplane g: $\theta_0 + \Theta^\top \mathbf{x} = 0$

1.

$$\overline{\rho}_g(D) = \min_{\langle \mathbf{x}, y \rangle \in D} (\theta_0 + \Theta^\top \mathbf{x})$$

But we work with negative values as well, therefore

2.

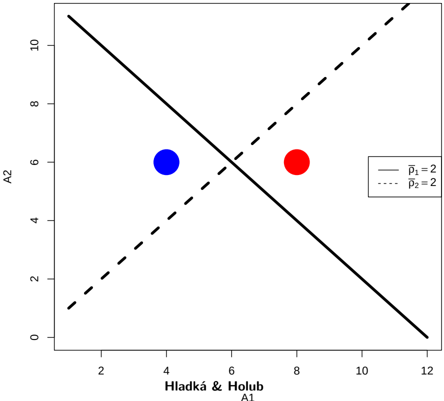
$$\overline{\rho}_g(D) = \min_{\langle \mathbf{x}, y \rangle \in D} |\theta_0 + \Theta^\top \mathbf{x}|$$

How to compare hyperplanes?

But

Example

- $g_1 : -12 + x_1 + x_2 = 0$
- $g_2 : -x_1 + x_2 = 0$, misclassification of the two examples



How to compare hyperplanes?

Therefore

3. **functional margin of D w.r.t. g**

$$\overline{\rho}_g(D) = \min_{\langle \mathbf{x}, y \rangle \in D} y \cdot (\theta_0 + \Theta^\top \mathbf{x})$$

But the functional margin is not scale invariant

How to compare hyperplanes?

Example

- g_1: $5 + 2x_1 + x_2 = 0$, $\Theta_1 = \langle 2, 1 \rangle$
- g_2: $50 + 20x_1 + 10x_2 = 0$, $\Theta_2 = \langle 20, 10 \rangle$
- Θ_1 and Θ_2 have the same unit vector $\langle \frac{2}{\sqrt{5}}, \frac{1}{\sqrt{5}} \rangle$, i.e. they represent the same hyperplane
- $\overline{\rho}_{g_2}(D) = 10 \cdot \overline{\rho}_{g_1}(D)$
- $||\Theta||$ does not matter
- Θ's direction matters, it's given by its unit vector

How to compare hyperplanes?

Therefore, instead of Θ we use its unit vector

4. **geometric margin of D w.r.t. g**

$$\rho_g(D) = \min_{\langle \mathbf{x}, y \rangle \in D} y \cdot \left(\frac{\theta_0}{||\Theta||} + \frac{\Theta^\top}{||\Theta||}\mathbf{x}\right) = \min_{\langle \mathbf{x}, y \rangle \in D} \frac{\overline{\rho}_g(D)}{||\Theta||}$$

Geometric margin of D

Example

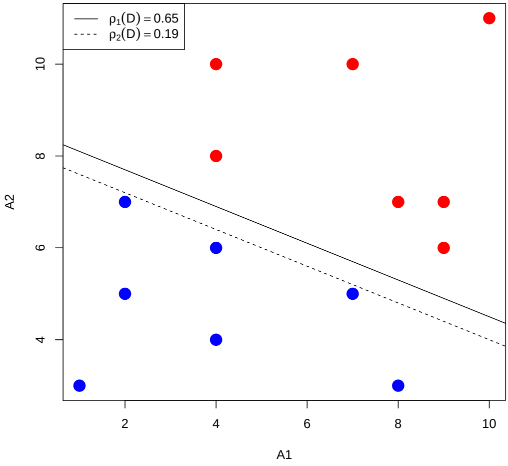
```
> A1 <- c(4,4,7,8,9,9,10, 1,2,2,4,4, 7,8)
> A2 <- c(8,10,10,7, 6,7,11,3,5,7,4,6,5,3)
> c <-  c(-1,-1,-1,-1,-1,-1,-1,1,1,1,1,1,1,1)
> d <- data.frame(A1,A2,c)

> t01 <- 8.5; t11 <- -0.4; t21 <- -1
> m.1 <- d[,3]*(t01 + t11*d[,1] + t21*d[,2])/sqrt(t11^2+t21^2)
> t02 <- 8; t12 <- -0.4; t22 <- -1
> m.2 <- d[,3]*(t02 + t12*d[,1] + t22*d[,2])/sqrt(t12^2+t22^2)

> min(m.1)
[1] 0.6499337
> min(m.2)
[1] 0.1856953
```

Geometric margin of D

Example (cntnd)



Margins of $\mathbf{x}$

- **Margin of $\mathbf{x}$** w.r.t. g is distance of $\mathbf{x}$ to g

$$\rho_g(\mathbf{x}) = \frac{|\theta_0 + \Theta^\top \mathbf{x}|}{||\Theta||}$$

- **Functional margin of** $\langle \mathbf{x}, y \rangle$ w.r.t. g is

$$\overline{\rho}_g(\mathbf{x}, y) = y \cdot (\Theta_0 + \Theta^\top \mathbf{x})$$

- **Geometric margin of** $\langle \mathbf{x}, y \rangle$ w.r.t. g is functional margin scaled by $||\Theta||$

$$\rho_g(\mathbf{x}, y) = \overline{\rho}_g(\mathbf{x}, y)/||\Theta||$$

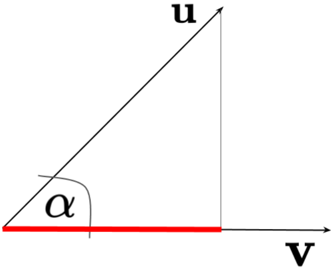
Linearly separable data

Data set $D = \{\langle \mathbf{x}_i, y_i \rangle, \mathbf{x}_i \in X, y_i \in \{-1, +1\}\}$ is **linearly separable** if there exists a hyperplane $g : \theta_0 + \Theta^\top \mathbf{x} = 0$ that separates the two classes completly, i.e.

$$\forall \langle \mathbf{x}, y \rangle \in D : \quad \overline{\rho_g}(\mathbf{x}, y) > 0$$

Dot product

- $\mathbf{u} = \langle u_1, \ldots, u_m \rangle$, $\mathbf{v} = \langle v_1, \ldots, v_m \rangle$
- algebraic definition $\mathbf{u} \cdot \mathbf{v} = u_1 v_1 + \cdots + u_m v_m$
- geometric definition $\mathbf{u} \cdot \mathbf{v} = ||\mathbf{u}|| \cdot ||\mathbf{v}|| \cdot \cos \alpha$



$$||\mathbf{v}|| = 1 \rightarrow \mathbf{u} \cdot \mathbf{v} = ||\mathbf{u}|| \cdot \cos \alpha$$

Quadratic programming

Quadratic programming

optimizes a quadratic objective function f

$$\min_{\mathbf{x}} / \max_{\mathbf{x}} f(\mathbf{x})$$

subject to constraints

$$g_i(\mathbf{x}) \leq 0, i = 1, \ldots, G$$

$$h_j(\mathbf{x}) = 0, j = 1, \ldots, H$$

Support Vector Machines
Binary classification task $Y = \{+1, -1\}$

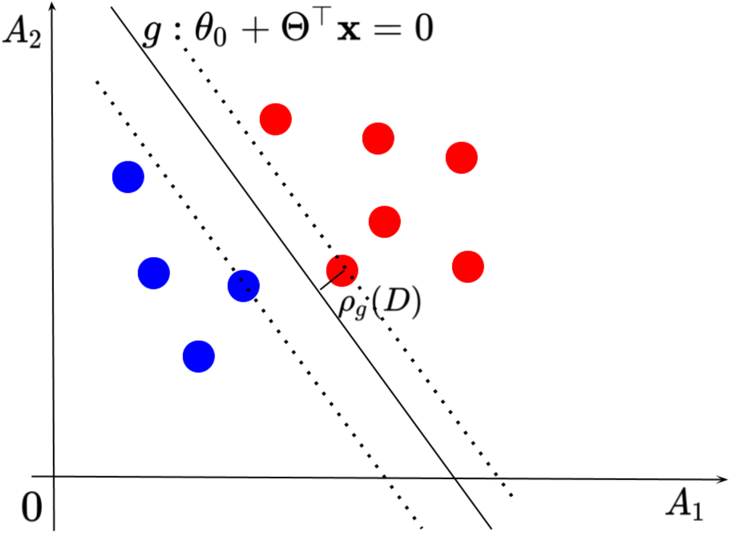
1. Large margin classifier (linear separability)
2. Soft margin classifier (not linear separability)
3. Kernels (non-linear class boundaries)

Large Margin Classifier
Training data is linearly separable

Optimization task

$$g^\star = \mathrm{argmax}_g \rho_g(D)$$

Large Margin Classifier
Training data is linearly separable



Large Margin Classifier
Training data is linearly separable

$\Theta_0 + \Theta^\top \mathbf{x}$ and $k\Theta_0 + (k\Theta)^\top \mathbf{x}$ define the same hyperplane.

$$\frac{y_i(\Theta_0 + \Theta^\top \mathbf{x}_i)}{||\Theta||} = \frac{y_i(k\Theta_0 + (k\Theta)^\top \mathbf{x}_i)}{||k\Theta||}$$

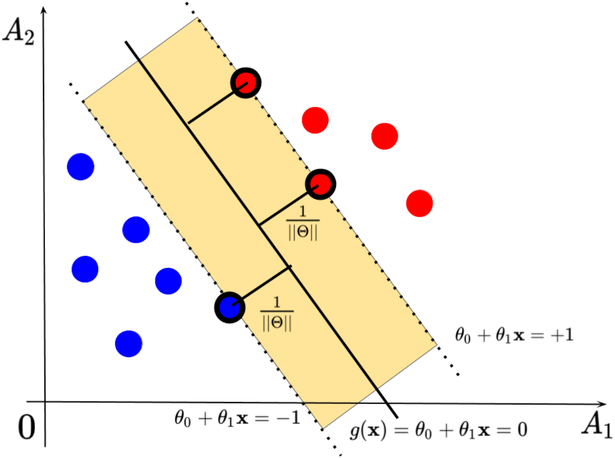
Therefore we can scale Θ so that $\overline{\rho}_g(D) = 1$.

Then

$$g^\star = \mathrm{argmax}_g \rho_g(D) = \max_\Theta \frac{2}{||\Theta||}$$

Large Margin Classifier
Training data is linearly separable

Supporting hyperplanes $\theta_0 + \Theta^\top \mathbf{x} = -1$ and $\theta_0 + \Theta^\top \mathbf{x} = +1$.
Support vectors are the instances touching the supporting hyperplanes.



Large Margin Classifier
Training data is linearly separable

Primal problem

Minimize

$$\frac{1}{2}||\Theta||^2$$

subject to

$$y_i(\theta_0 + \Theta^\top \mathbf{x}_i) \geq 1, i = 1, \ldots, n$$

quadratic function $+$ linear constraints $\rightarrow$ quadratic programming

Large Margin Classifier
Quadratic programming

For each constraint $y_i(\theta_0 + \Theta^\top \mathbf{x}_i) \geq 1$ introduce Lagrange multiplier $\alpha_i \geq 0$;
let $\boldsymbol{\alpha} = \langle \alpha_1, \ldots, \alpha_n \rangle$.

Lagrangian function $\mathcal{L}_P(\Theta, \theta_0, \boldsymbol{\alpha})$

$$\mathcal{L}_P(\Theta, \theta_0, \boldsymbol{\alpha}) = \frac{1}{2}||\Theta||^2 + \sum_{i=1}^{n} \alpha_i (1 - y_i(\theta_0 + \Theta^\top \mathbf{x}_i)) \tag{1}$$

To get the solution of the primal problem we need to solve the **Lagrangian problem** $\rightarrow$

Large Margin Classifier
Quadratic programming

$$\min_{\Theta,\theta_0} \max_{\boldsymbol{\alpha}} \mathcal{L}_P(\Theta, \theta_0, \boldsymbol{\alpha}) \tag{2}$$

$$\max_{\boldsymbol{\alpha}} \min_{\Theta,\theta_0} \mathcal{L}_P(\Theta, \theta_0, \boldsymbol{\alpha}) \tag{3}$$

subject to
$$\alpha_i \geq 0, i = 1, \ldots n$$

1. Minimize $\mathcal{L}_P$ w.r.t. Θ
   Therefore differentiate $\mathcal{L}_P$ w.r.t. Θ and $\frac{\partial \mathcal{L}}{\partial \Theta} = 0$. It gives
$$\Theta = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \tag{4}$$
2. Minimize $\mathcal{L}_P$ w.r.t. θ_0
   Therefore differentiate $\mathcal{L}_P$ w.r.t. θ_0 and $\frac{\partial \mathcal{L}}{\partial \theta_0} = 0$. It gives
$$\sum_{i=1}^{n} \alpha_i y_i = 0 \tag{5}$$

Large Margin Classifier
Quadratic programming

3. Substitute (4) into the primal form (1) and solve **Wolfe dual optimization problem**

$$\max_{\boldsymbol{\alpha}} \mathcal{L}_D(\boldsymbol{\alpha}) = \max_{\boldsymbol{\alpha}} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

subject to

$$\alpha_i \geq 0, i = 1 \ldots n$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

4. Get $\boldsymbol{\alpha}^\star$
5. Get $\Theta^\star = \sum_{i=1}^{n} \alpha_i^\star y_i \mathbf{x}_i$. Assume that $\mathbf{x}_i$ is a support vector. Then $1 = y_i(\theta_0^\star + {\Theta^\star}^\top \mathbf{x}_i) \rightarrow \theta_0^\star = y_i - {\Theta^\star}^\top \mathbf{x}_i$

Large Margin Classifier
Quadratic programming

- $\boldsymbol{\alpha}^\star$ is the solution to the dual problem
- $\Theta^\star$ is the solution to the primal problem
- the solutions $\boldsymbol{\alpha}^\star$ and $\Theta^\star$ must satisfy the Karush-Kuhn-Tucker conditions where one of them is *KKT dual complementarity*:

$$\alpha_i^\star \cdot (1 - y_i(\theta_0^\star + {\Theta^\star}^\top \mathbf{x}_i)) = 0$$

  - $y_i(\theta_0^\star + {\Theta^\star}^\top \mathbf{x}_i) \neq 1$, i.e., $\mathbf{x}_i$ is not support vector $\Rightarrow \alpha_i^\star = 0$
  - $\alpha_i^\star \neq 0 \Rightarrow y_i(\theta_0^\star + {\Theta^\star}^\top \mathbf{x}_i) = 1$, i.e., $\mathbf{x}_i$ is support vector

I.e., finding $\Theta^\star$ is equivalent to finding support vectors and their weights

Large Margin Classifier
Prediction

Prediction for a new instance $\mathbf{x}$

$$f(\mathbf{x}) = \mathrm{sign}(\sum_{i=1}^{n} \alpha_i^\star y_i \mathbf{x}_i \cdot \mathbf{x} + \theta_0^\star)$$

- similarity between $\mathbf{x}$ and support vector $\mathbf{x}_i$: a support vector that is more similar contributes more to the classification
- support vector that is more important, i.e. has larger α_i, contributes more to the classification
- if y_i is positive, than the contribution is positive, otherwise negative

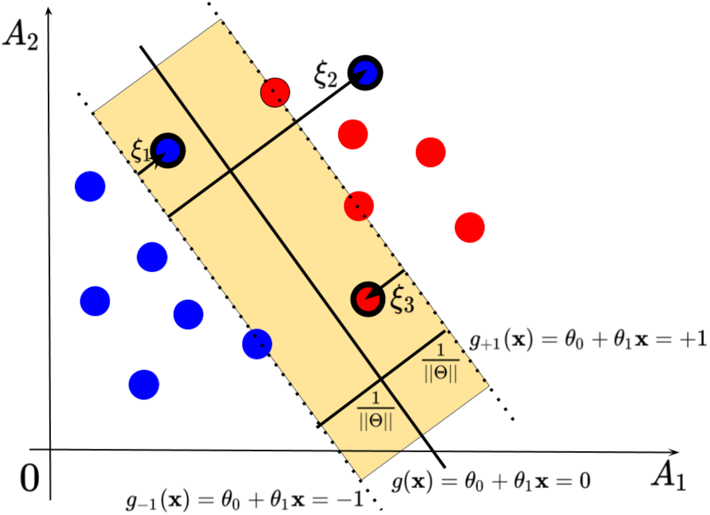
Soft Margin Classifier
Training data is not linearly separable

In a real problem it is unlikely that a hyperplane will exactly separate the data – even if a curved decision boundary is possible. So exactly separating the data is probably not desirable – if the data has noise and outliers, a smooth decision boundary that ignores a few data points is better than one that loops around the outliers.

Therefore

minimize $||\mathbf{\Theta}||^2$ **AND** the number of training mistakes

Soft Margin Classifier
Training data is not linearly separable



Soft Margin Classifier
Slack variables

$\xi_i \geq 0$

- $\xi_i = 0$ if $\mathbf{x}_i$ is correctly classified
- ξ_i is distance to y_i's supporting hyperplane" otherwise
    - margin violation – $0 < \xi_i \leq 1/||\Theta||$, see ξ_1, ξ_3 above
    - misclassification – $\xi_i > 1/||\Theta||$, see ξ_2 above

Soft Margin Classifier
Optimization problem

Minimize

$$\frac{1}{2}||\Theta||^2 + C\sum_{i=1}^{n}\xi_i$$

subject to

$$\xi_i \geq 0, y_i(\theta_0 + \Theta^\top \mathbf{x}_i) \geq 1 - \xi_i, i = 1, \dots n$$

$C \geq 0$ trade-off parameter

- small $C \Rightarrow$ large margin
  relaxed model; misclassifications are not penalized
- large $C \Rightarrow$ narrow margin
  misclassifications are penalized strongly
  the model will not generalize much

Soft Margin Classifier
Quadratic programming

For each constraint $y_i(\theta_0 + \Theta^\top \mathbf{x}_i) \geq 1 - \xi_i$ introduce Lagrange multiplier $\alpha_i \geq 0$; let $\boldsymbol{\alpha} = \langle \alpha_1, ..., \alpha_n \rangle$.

Primal Lagrangian $\mathcal{L}_P(\Theta, \theta_0, \xi, \boldsymbol{\alpha})$ is given by

$$\mathcal{L}_P(\Theta, \theta_0, \xi, \boldsymbol{\alpha}) = \frac{1}{2}||\Theta||^2 + C \sum_{i=1}^{n} \xi_i + \sum_{i=1}^{n} \alpha_i (1 - \xi_i - y_i(\theta_0 + \Theta^\top \mathbf{x}_i)) \quad (6)$$

Soft Margin Classifier
Quadratic programming

Primal Lagrangian problem

$$\min_{\Theta,\theta_0,\xi} \max_{\boldsymbol{\alpha}} \mathcal{L}_P(\Theta, \theta_0, \xi, \boldsymbol{\alpha}) \tag{7}$$

$$\max_{\boldsymbol{\alpha}} \min_{\Theta,\theta_0,\xi} \mathcal{L}_P(\Theta, \theta_0, \xi, \boldsymbol{\alpha}) \tag{8}$$

subject to

$$\alpha_i \geq 0, \xi_i \geq 0, i = 1, \dots, n$$

1. Minimize $\mathcal{L}_P$ w.r.t. Θ. Therefore $\frac{\partial \mathcal{L}}{\partial \Theta} = 0$. It gives
$$\Theta = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \tag{9}$$
2. Minimize $\mathcal{L}_P$ w.r.t. θ_0. Therefore $\frac{\partial \mathcal{L}}{\partial \theta_0} = 0$. It gives
$$\sum_{i=1}^{n} \alpha_i y_i = 0 \tag{10}$$

Soft Margin Classifier
Quadratic programming

3. Minimize $\mathcal{L}_P$ w.r.t. ξ. Therefore $\frac{\partial L}{\partial \xi} = 0$. It gives

$$C\xi - \alpha = 0 \tag{11}$$

4. Substitute (9) into the primal form (6) and solve **Wolfe dual opt. problem**

$$\max_{\boldsymbol{\alpha}} \mathcal{L}_D(\boldsymbol{\alpha}) = \max_{\boldsymbol{\alpha}} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1, j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

subject to

$$\alpha_i \geq 0, \quad i = 1, \dots, n$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

5. Get $\boldsymbol{\alpha}^\star$
6. Get $\Theta^\star$

Soft Margin Classifier
Prediction

Prediction for a new instance $\mathbf{x}$

$$f(\mathbf{x}) = \mathrm{sign}(\sum_{i=1}^{n} \alpha_i^\star y_i \mathbf{x}_i \cdot \mathbf{x} + \theta_0^\star)$$

Non-linear boundary

Recall polynomial regression

Polynomial regression is an extension of linear regression where the relationship between features and target value is modelled as a d-th order polynomial.

Simple regression
$y = \theta_0 + \theta_1 x_1$

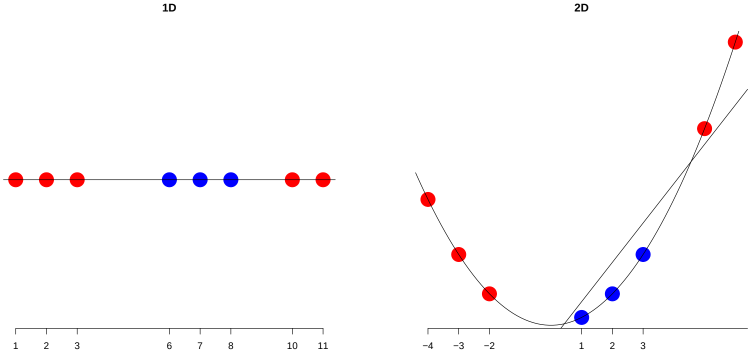
Polynomial regression
$y = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \ldots \theta_d x_1^d$

It is still a linear model with features $A_1, A_1^2, \ldots, A_1^d$.

This defines a feature mapping $\phi(x_1) = [x_1, x_1^2, \ldots, x_1^d]$

Non-linear boundary

- for example $\phi(x_1) = [x_1 - 5, (x_1 - 5)^2]$

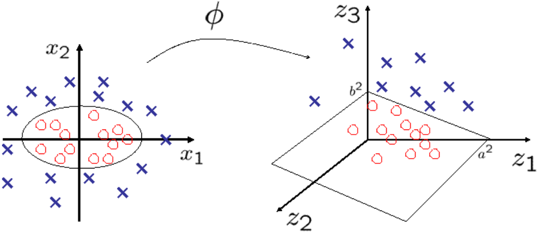


Kernels

Idea

- Apply Large/Soft margin classifier not to the orginal features but to the features obtained by the feature mapping $\phi(\mathbf{x}) : \mathcal{R}^m \rightarrow \mathcal{F}$
- Large/Soft margin classifier uses dot product $\mathbf{x}_i \cdot \mathbf{x}_j$.
  Replace it with $\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j)$.

Kernels



$$\phi : (x_1, x_2) \longrightarrow (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

$$\left(\frac{x_1}{a}\right)^2 + \left(\frac{x_2}{b}\right)^2 = 1 \longrightarrow \frac{z_1}{a^2} + \frac{z_3}{b^2} = 1$$

Source: `http://omega.albany.edu:8008/machine-learning-dir/notes-dir/ker1/ker1-l.html`

Kernels

However, finding ϕ could be expensive.

Kernel trick

- No need to know what ϕ is and what the new feature space is, i.e. no need to explicitly map the data to the new feature space
- Define a kernel function $K : \mathcal{R}^m \times \mathcal{R}^m \rightarrow \mathcal{R}$
- Replace the dot product $\mathbf{x}_i \cdot \mathbf{x}_j$ with a Kernel function $K(\mathbf{x}_i, \mathbf{x}_j)$:

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

Kernels
Prediction

Prediction for a new instance $\mathbf{x}$

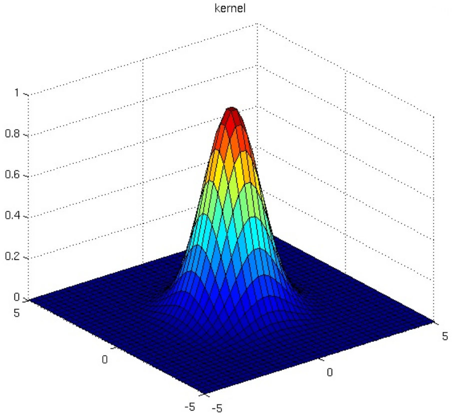
$$f(\mathbf{x}) = \mathrm{sign}(\sum_{i=1}^{n} \alpha_i^\star y_i K(\mathbf{x}_i, \mathbf{x}) + \theta_0^\star)$$

Common Kernel functions

- **Linear**
  $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i \cdot \mathbf{x}_j$
- **Polynomial**
  $K(\mathbf{x}_i, \mathbf{x}_j) = (\gamma \mathbf{x}_i \cdot \mathbf{x}_j + c)^d$
  – smaller degree can generalize better
  – higher degree can fit (only) training data better
- **Radial basis function**
  $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\gamma(||\mathbf{x}_i - \mathbf{x}_j||^2))$
  – very robust
  – use it when polynomial kernel is weak to fit data
- **Sigmoid**
  $K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\gamma \mathbf{x}_i \cdot \mathbf{x}_j + c)$, where $\tanh(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$

Radial Basis Function Kernel

- $K(\mathbf{x}_i, \mathbf{x}_j) = e^{-\gamma ||\mathbf{x}_i - \mathbf{x}_j||^2}$



Source: `http://www.cs.toronto.edu/~duvenaud/cookbook/index.html`