# Model free approaches
# SVM: Support Vector Machines

## Formation ENSTA-ParisTech
## Conférence IA

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# Support Vector Machine (SVM)

Theory elaborated in the early 1990's (Vapnik *et al*) based on the idea of 'maximum margin'

- deterministic criterion learned on the training set ← supervised classification
- ☞ general, i.e. model free, linear classification rule
- ☞ classification rule is linear in a transformed space of higher (possible infinite) dimension than the original input feature/predictor space

## Supplementary materials

- Coursera online video with python notebook material (13mn) https://www.coursera.org/lecture/data-analytics-accountancy-2/introduction-to-support-vector-machine-dDP0v
- Wikipedia page (quite complete and detailed) https://en.wikipedia.org/wiki/Support_vector_machine
- Short and easy to understand Scikit-learn documentation (with examples) https://scikit-learn.org/stable/modules/svm.html

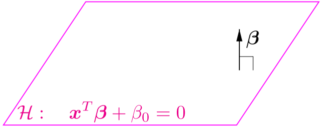
# Linear discrimination and Separating hyperplane

## Binary classification problem

- $X \in \mathbb{R}^p$
- $Y \in \{-1, 1\} \leftarrow 2$ classes
- Training set $(x_i, y_i)$, for $i = 1, \ldots, n$

Defining a linear discriminant function $h(x) \Leftrightarrow$ defining a separating hyperplane $\mathcal{H}$ with equation

$$\boldsymbol{x}^T \boldsymbol{\beta} + \beta_0 = 0,$$

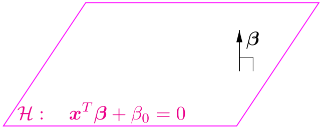



- $\boldsymbol{\beta} \in \mathbb{R}^p$ is the normal vector (vector normal to the hyperplane $\mathcal{H}$),
- $\beta_0 \in \mathbb{R}$ is the intercept (regression interpretation) or offset (geometrical interpretation)
- ☞ $\mathcal{H}$ is an *affine subspace* of dimension $p - 1$
- ☞ $h(x) \equiv \boldsymbol{x}^T \boldsymbol{\beta} + \beta_0$ is the associated (linear) discriminant function

# Separating hyperplane and prediction rule

For a given separating hyperplane $\mathcal{H}$ with equation

$$\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0,$$




the prediction rule can be expressed as

- $\widehat{y} = +1$, if $h(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 \geq 0$, ($\boldsymbol{x}$ is above $\mathcal{H}$)
- $\widehat{y} = -1$, otherwise, ($\boldsymbol{x}$ is below $\mathcal{H}$)

or in an equivalent way:

$$\widehat{y} \equiv G(\boldsymbol{x}) = \text{sign}\left[\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0\right]$$

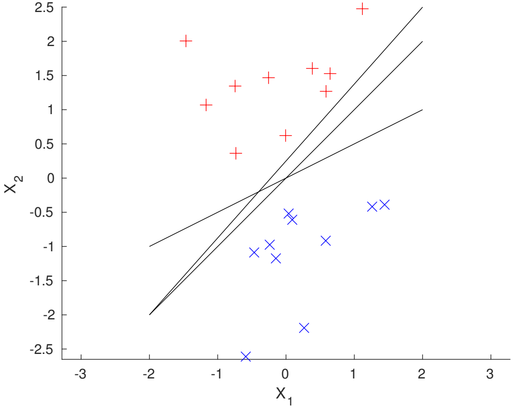
Rk: $\boldsymbol{x}$ is in class $y \in \{-1, 1\}$: prediction $G(\boldsymbol{x})$ is correct iff $y\left(\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0\right) \geq 0$

# Separating Hyperplane: separable case

Linear separability assumption: $\exists \boldsymbol{\beta} \in \mathbb{R}^p$ and $\beta_0 \in \mathbb{R}$ s.t. the hyperplane $\boldsymbol{x}^T \boldsymbol{\beta} + \beta_0 = 0$ perfectly separates the two classes on the training set:

$$y_k \left( x_k^T \boldsymbol{\beta} + \beta_0 \right) \geq 0, \quad \text{for } k = 1, \ldots, n,$$

## Separable case ($p = 2$ example)




Pb: infinitely many possible perfect separating hyperplanes $\boldsymbol{x}^T \boldsymbol{\beta} + \beta_0 = 0$

- Find the 'optimal' separating hyperplane?
- makes the 'biggest gap' from the samples

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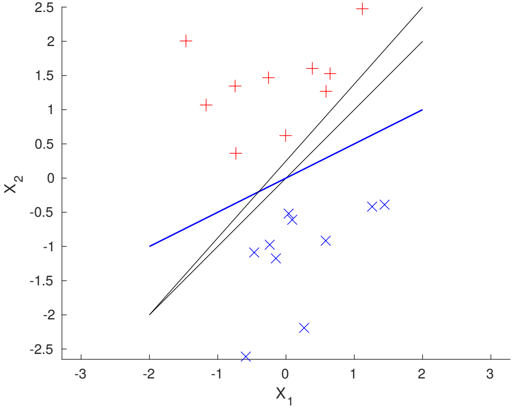



Pb: infinitely many possible perfect separating hyperplanes $\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0$

- ☞ Find the 'optimal' separating hyperplane?
- ☞ makes the 'biggest gap' from the samples

# Maximum margin separating hyperplane (separable case)

Distance of a point $\boldsymbol{x_k}$ to an hyperplane $\mathcal{H}$ s.t. $\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0$,

$$d(x_k, \mathcal{H}) \equiv \min_{x} \left\{ \|\boldsymbol{x} - \boldsymbol{x}_k\| \ : \ \boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0 \right\}$$

## Maximum margin principle

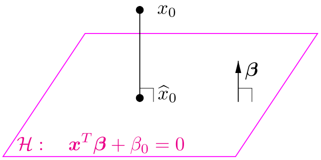
We are interested in the 'optimal' perfect separating hyperplane maximizing the distance $M > 0$, called the margin, between the samples of each class and the separating hyperplane

$\Rightarrow$ Find $\boldsymbol{\beta} \in \mathbb{R}^p$ and $\beta_0 \in \mathbb{R}$ s.t. the margin

$$M = \min_{1 \le k \le n} \{d(x_k, \mathcal{H})\}$$

is maximized

# Signed distance




$\widehat{\boldsymbol{x}}_0 \in \mathcal{H} \Rightarrow -\widehat{\boldsymbol{x}}_0^T \boldsymbol{\beta} = \beta_0$

From the orthogonality principle,

$$d(x_0, \mathcal{H}) = \|\boldsymbol{x}_0 - \widehat{\boldsymbol{x}}_0\|,$$

where $\widehat{\boldsymbol{x}}_0$ is the orthogonal projection of $\boldsymbol{x}_0$ on $\mathcal{H}$

$\Rightarrow$ $\boldsymbol{x}_0 - \widehat{\boldsymbol{x}}_0$ and $\boldsymbol{\beta}$ are collinear,

$\Rightarrow$ $\boldsymbol{x}_0 - \widehat{\boldsymbol{x}}_0 = \underbrace{\langle \boldsymbol{x}_0 - \widehat{\boldsymbol{x}}_0, \boldsymbol{\beta}^* \rangle}_{\text{unsigned distance}} \boldsymbol{\beta}^*$, where $\boldsymbol{\beta}^* = \frac{\boldsymbol{\beta}}{\|\boldsymbol{\beta}\|}$,

$$\Rightarrow \text{signed distance} = (\boldsymbol{x}_0 - \widehat{\boldsymbol{x}}_0)^T \frac{\boldsymbol{\beta}}{\|\boldsymbol{\beta}\|} = \frac{\boldsymbol{x}_0^T \boldsymbol{\beta} - \widehat{\boldsymbol{x}}_0^T \boldsymbol{\beta}}{\|\boldsymbol{\beta}\|} = \frac{\boldsymbol{x}_0^T \boldsymbol{\beta} + \beta_0}{\|\boldsymbol{\beta}\|},$$

## Remarks

- $|\langle \boldsymbol{x}_0 - \widehat{\boldsymbol{x}}_0, \boldsymbol{\beta}^* \rangle| = \|\boldsymbol{x}_0 - \widehat{\boldsymbol{x}}_0\| = d(\boldsymbol{x}_0, \mathcal{H}) \leftarrow$ "signed distance"
- for any perfect separating hyperplane $y_k \langle \boldsymbol{x}_k - \widehat{\boldsymbol{x}}_k, \boldsymbol{\beta}^* \rangle = \frac{1}{\|\boldsymbol{\beta}\|} y_k(\boldsymbol{x}_k^T \boldsymbol{\beta} + \beta_0) \geq 0$, for $k = 1, \ldots, n$,

# Canonical separating hyperplane

For any perfect separating hyperplane, for $k = 1, \dots, n$

$$y_k \langle \boldsymbol{x}_k - \widehat{\boldsymbol{x}}_k, \boldsymbol{\beta}^* \rangle = d(x_k, \mathcal{H})$$

Hence, the margin reads

$$M \equiv \min_{1 \le k \le n} \{d(x_k, \mathcal{H})\} = \frac{1}{\|\boldsymbol{\beta}\|} \min_{1 \le k \le n} \left\{ y_k (\boldsymbol{x}_k^T \boldsymbol{\beta} + \beta_0) \right\}$$

## Remarks

- The bound $M$ is reached (min of a countable set),
- ☞ the samples at the margin are denoted as $\boldsymbol{x}_{\mathrm{margin}}$

## Canonical expression of the separating hyperplane

$\boldsymbol{\beta}$ and $\beta_0$ are normalized s.t.

$$y_{\mathrm{margin}} (\boldsymbol{x}_{\mathrm{margin}}^T \boldsymbol{\beta} + \beta_0) = 1, \quad \text{thus } M = \frac{1}{\|\boldsymbol{\beta}\|}$$

# Primal problem (separable case)

Canonical hyperplane expression:

$$\begin{aligned} \text{maximizing the margin } M = \frac{1}{\|\boldsymbol{\beta}\|} \quad &\Leftrightarrow \quad \text{minimizing} \quad \|\boldsymbol{\beta}\| \\ &\Leftrightarrow \quad \text{minimizing} \quad \frac{1}{2}\|\boldsymbol{\beta}\|^2 \end{aligned}$$

## Primal optimization problem

$$\begin{cases} \min_{\boldsymbol{\beta}, \beta_0} & \frac{1}{2}\|\boldsymbol{\beta}\|^2, \\ \text{subject to} & y_k \left(\boldsymbol{x}_k^T \boldsymbol{\beta} + \beta_0\right) \geq 1, \text{ for } 1 \leq k \leq n. \end{cases}$$

- quadratic criterion + linear inequality constraints

☞ convex optimization problem for which standard numerical procedures are available

## Reminder on constrained optimization

- Concept of feasible descent direction
- Primal problem (constrained form) / Dual problem (Lagrangian form)
- KKT necessary conditions

# Reminder on constrained optimization

## Constrained problem: primal problem

$$\begin{cases} \min_x & f(\mathbf{x}) \\ \text{s.t.} & g(\mathbf{x}) \leq 0 \end{cases}$$

## Objective function $f(\mathbf{x})$

To decrease the objective function $f(\mathbf{x})$, a descent direction $\boldsymbol{d}$ must satisfy

$$f(\mathbf{x} + \epsilon \boldsymbol{d}) \approx J(\mathbf{x}) + \epsilon \nabla f(\mathbf{x})^T \boldsymbol{d} < f(\mathbf{x}),$$

hence $\boldsymbol{d}$ is a descent direction iff $\nabla f(\mathbf{x})^T \boldsymbol{d} < 0$

# Reminder on constrained optimization (Cont'd)

## Objective $f(\boldsymbol{x})$

$$\text{descent direction:} \quad \nabla f(\boldsymbol{x})^T \boldsymbol{d} < 0$$

## Constraint $g(\boldsymbol{x})$

To satisfy the constraint, a feasible descent direction $\boldsymbol{d}$ must satisfy

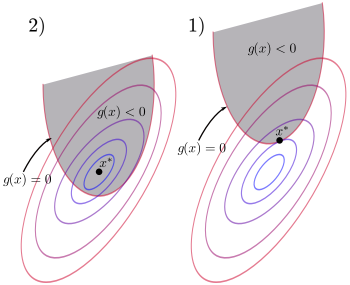
$$g(\boldsymbol{x} + \epsilon \boldsymbol{d}) \approx g(\boldsymbol{x}) + \epsilon \nabla g(\boldsymbol{x})^T \boldsymbol{d} \leq 0,$$

hence

$$\text{feasible direction:} \begin{cases} g(\boldsymbol{x}) < 0 & \Rightarrow \text{ no constraint on } \boldsymbol{d}, \\ g(\boldsymbol{x}) = 0 & \Rightarrow \nabla g(\boldsymbol{x})^T \boldsymbol{d} \leq 0 \end{cases}$$

# Reminder on constrained optimization (Cont'd)

## Necessary conditions: two possibilities for optimality




There is no feasible descent direction in $\boldsymbol{x}^*$ when either

1. $\nabla f(\boldsymbol{x}^*) = -\alpha \nabla g(\boldsymbol{x}^*)$, with $\alpha > 0$, $g(\boldsymbol{x}^*) = 0$
2. $\nabla f(\boldsymbol{x}^*) = 0$, i.e. $\alpha = 0$, $g(\boldsymbol{x}^*) < 0$

## Remarks

1. $\boldsymbol{x}^*$ lies at the limit of the feasible domain (i.e. $g(\boldsymbol{x}^*) = 0$) and the two gradients are collinear and in opposite direction
2. $\boldsymbol{x}^*$ belongs to the interior of the feasible domain (i.e. $g(\boldsymbol{x}^*) < 0$). Same 1st order necessary conditions as those obtained when there is no constraint

# Reminder on constrained optimization (Cont'd)

## Constrained form: primal problem

$$\begin{cases} \min_x & f(\boldsymbol{x}) \\ \text{s.t.} & g_j(\boldsymbol{x}) \leq 0, \text{ for all } j = 1, \ldots, q \end{cases}$$

## Lagrangian form: dual problem

Inequality convex constraints $\Rightarrow$ introduction of the Lagrange multipliers $\alpha_j$

$$\begin{cases} \min_x & f(\boldsymbol{x}) + \sum_j \alpha_j g_j(\boldsymbol{x}^*) \\ \text{s.t.} & \alpha_j \geq 0, \text{ for all } j = 1, \ldots, q \end{cases}$$

## Karush–Kuhn–Tucker (KKT) conditions

For $\boldsymbol{x}^*$ being a local min, it is necessary that

$$\begin{cases} \nabla f(\boldsymbol{x}^*) + \sum_{j=1}^{q} \alpha_j \nabla g_j(\boldsymbol{x}^*) = 0 & \leftarrow \text{first order conditions} \\ \text{s.t. } \alpha_j \geq 0 \text{ and } \alpha_j g_j(\boldsymbol{x}^*) = 0 & \leftarrow \text{complementary conditions} \end{cases}$$

## End of reminder on constrained optimization

☞ Dual form for SVM optimization problem

# Lagrangian (separable case)

Linear constraints of positivity $\Rightarrow$ introduction of the Lagrange multipliers

## Lagrangian

$$L(\boldsymbol{\beta}, \beta_0, \boldsymbol{\alpha}) = \frac{1}{2}\|\boldsymbol{\beta}\|^2 - \sum_{i=1}^{n} \alpha_i \underbrace{\left[y_i(\boldsymbol{x}_i^T\boldsymbol{\beta} + \beta_0) - 1\right]}_{\geq 0},$$

where $\alpha_i$ are the Lagrange multipliers

## First order Karush–Kuhn–Tucker necessary conditions

Setting the partial derivatives w.r.t. $\boldsymbol{\beta}$ and $\beta_0$ to zero yields

$$\begin{cases} \widehat{\boldsymbol{\beta}} & = \sum_{i=1}^n \alpha_i y_i \boldsymbol{x}_i, \\ 0 & = \sum_{i=1}^n \alpha_i y_i, \end{cases}$$

- plugging these expression in the Lagrangian yields the dual expression

# Dual problem (separable case)

## Dual optimization problem

$$\begin{cases} \max_{\boldsymbol{\alpha}} & \widetilde{L}(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \boldsymbol{x}_i^T \boldsymbol{x}_j, \\ \text{subject to} & \alpha_i \geq 0 \text{ and } \sum_{i=1}^{n} \alpha_i y_i = 0. \end{cases}$$

- ☞ simple convex optimization problem for which standard numerical procedures are available
- ☞ calculation of the optimum multipliers $\widehat{\alpha}_i$

# Support vectors and maximum margin hyperplane (separable case)

## Complementary slackness Karush–Kuhn–Tucker necessary conditions

$$\widehat{\alpha}_i[y_i h(\boldsymbol{x}_i) - 1] = 0 \quad \Rightarrow \quad \widehat{\alpha}_i = 0 \ \text{ as } \ y_i h(\boldsymbol{x}_i) > 1$$

- since $\widehat{\boldsymbol{\beta}} = \sum_{i=1}^n \widehat{\alpha}_i y_i \boldsymbol{x}_i$, $\widehat{\boldsymbol{\beta}}$ depends only on the points at the margin ← support vectors
- $\widehat{\beta}_0$ can be derived from the complementary slackness expression for any of support vectors $\boldsymbol{x}_{\text{margin}}$

$$\begin{aligned} y_{\text{margin}} h(\boldsymbol{x}_{\text{margin}}) - 1 = 0 \quad &\Rightarrow \quad \widehat{\boldsymbol{\beta}}^T \boldsymbol{x}_{\text{margin}} + \widehat{\beta}_0 = y_{\text{margin}}, \\ &\Rightarrow \quad \widehat{\beta}_0 = -\widehat{\boldsymbol{\beta}}^T \boldsymbol{x}_{\text{margin}} + y_{\text{margin}} \end{aligned}$$

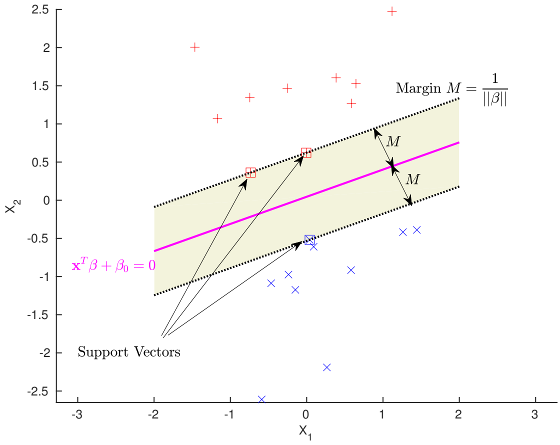
☞ the only inputs used to construct the maximum margin hyperplane are the support vectors and the discriminant function reads

$$h(\boldsymbol{x}) = \sum_{i=1}^n \widehat{\alpha}_i y_i (\boldsymbol{x} - \boldsymbol{x}_{\text{margin}})^T \boldsymbol{x}_i + y_{\text{margin}}$$

# Maximum margin separating hyperplane (separable case)

## Separable case

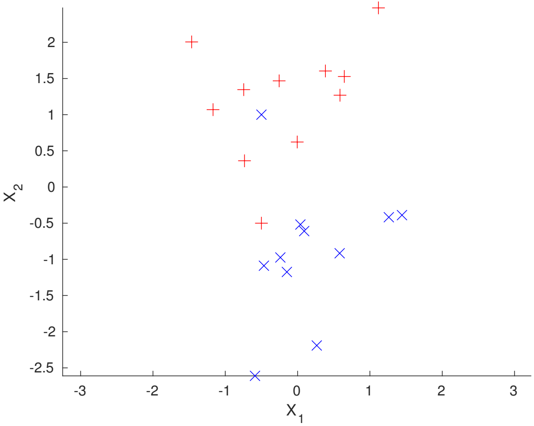
- Maximizing the *margin M* between the separating hyperplane and the training data:




The maximum margin hyperplane depends only on the points at the margin called the *support vectors*

# Nonseparable case

- in general, overlap of the 2 classes
- ☞ No hyperplane that perfectly separates the training data



# Maximum margin separating hyperplane (nonseparable case)

## Soft-Margin solution for the nonseparable case

Considering a *soft-margin* that allows wrong classifications

- introduction of *slack variables* $\xi_i \geq 0$ s.t.

$$y_i(\boldsymbol{x_i}^T \boldsymbol{\beta} + \beta_0) \geq (1 - \xi_i)$$

  Support vectors include now the wrong classified points, and the points inside the margins ($\xi_i > 0$)

- Primal problem: adding a penalty in the criterion

$$\begin{cases} \min_{\boldsymbol{\beta}, \beta_0, \xi} & \frac{1}{2}||\boldsymbol{\beta}||^2 + C \sum_{i=1}^{n} \xi_i, \\ \text{subject to} & y_i(\boldsymbol{x_i}^T \boldsymbol{\beta} + \beta_0) \geq 1 - \xi_i, \end{cases}$$

  where $C > 0$ is the "cost" or "regularization" parameter

# Regularization parameter (nonseparable case)

$$\text{Criterion to be minimized:} \quad \frac{1}{2}||\beta||^2 + C\sum_{i=1}^{n}\xi_i,$$

## Influence of the regularization parameter $C > 0$

$C$ drives the margin size, thus the number of support vectors

- $C \gg 0$ : small margin, less support vectors ($\sim$ overfitting)
- $C \to 0^+$ : large margin, more support vectors ($\sim$ underfitting)
- $C \to +\infty$ : converges in the separable case to the *Hard-Margin* solution

Rk: strength of the regularization is inversely proportional to $C$ (compared with the regularization parameter $\lambda$ for ridge penalty, $C \equiv \frac{1}{\lambda}$)

## Choosing the regularization parameter $C > 0$

- the optimal $C$ can be estimated by cross validation

☞ performance might not be very sensitive to choices of $C$ (due to the rigidity of a linear boundary)

☞ usually $C \approx 1$ yields a good trade-off

# Dual problem (nonseparable case)

Introducing the Lagrangian and substituting the first order KKT conditions w.r.t. $\boldsymbol{\beta}$, $\beta_0$, $\boldsymbol{\xi}$ yields the dual expression

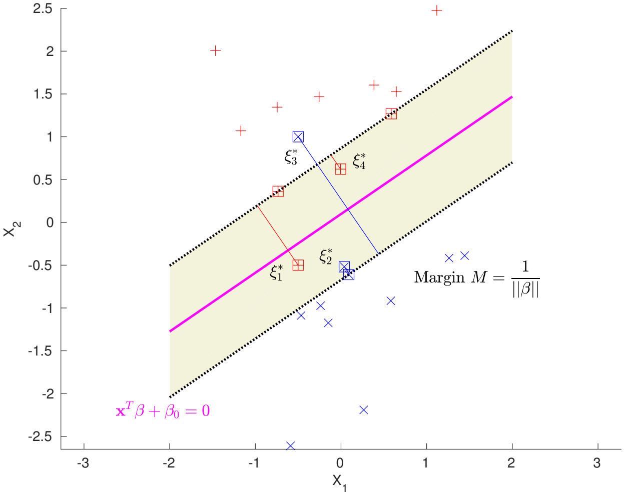
## Dual optimization problem

$$\begin{cases} \max_{\boldsymbol{\alpha}} & \widetilde{L}(\boldsymbol{\alpha}) = \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j=1}^n \alpha_i\alpha_j y_i y_j \boldsymbol{x}_i^T \boldsymbol{x}_j, \\ \text{subject to} & 0 \leq \alpha_i \leq C \text{ and } \sum_{i=1}^n \alpha_i y_i = 0. \end{cases}$$

- only difference w.r.t the separable case: $\alpha_i \leq C$ constraint!
- simple convex optimization problem for which standard numerical procedure are available

# Optimal separating hyperplane

## Soft-Margin example (nonseparable case)




### Vector Supports

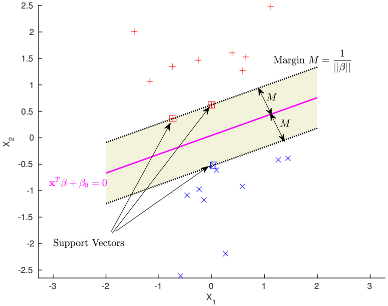
The support vectors are now the points at the margin, inside the margin, or wrongly classified.

$\xi_i^* \equiv M\xi_i \leftarrow$ distance between a support vector and the margin

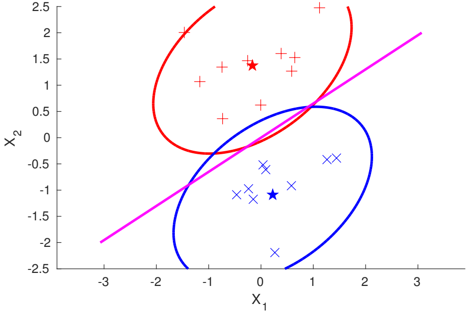
# Linear discrimination: SVM vs LDA

## Linear discrimination

- Linear Discriminant Analysis (LDA): Gaussian generative model
- SVM: criterion optimization (maximizing the margin)



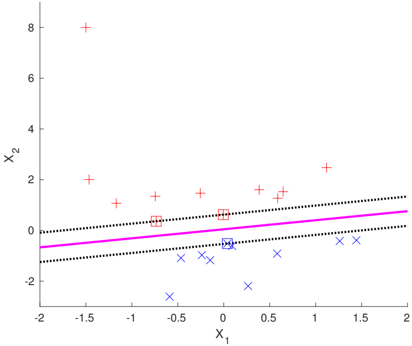

SVM



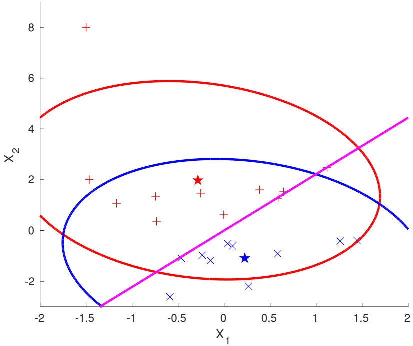

LDA

# Linear discrimination: SVM vs LDA (Cont'd)

## Adding one atypical data




SVM



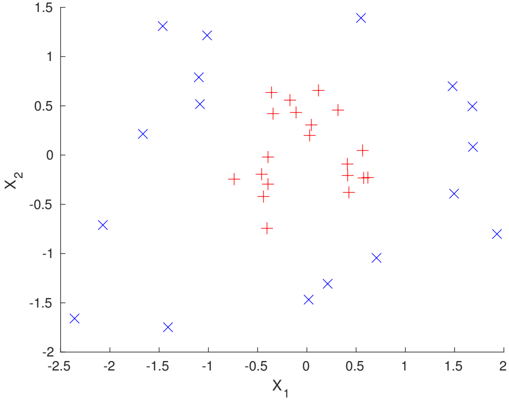

LDA

## SVM property

- Nonsensitive to atypical points (outliers) far from the margin

☞ sparse method (information ≡ support vectors)

# Nonlinear discrimination in the input space




Sometimes a linear separation won't work, whatever the slack variables...

## Transformed space $\mathcal{F}$

- Choice of a transformed space $\mathcal{F}$ (expansion space) where the linear separation assumption is more relevant
- Nonlinear expansion map $\phi \ : \mathbb{R}^p \rightarrow \mathcal{F}$, $\boldsymbol{x} \mapsto \phi(\boldsymbol{x}) \leftarrow$ enlarged features

# Nonlinear discrimination in the input space

- Non-linear transformation: 'projection' in the space of monomials of order 2.

$$\begin{aligned} \phi : \mathbb{R}^2 &\to \mathbb{R}^3 \\ \mathrm{x} &\mapsto \phi(\mathrm{x}) \\ (\mathrm{x}_1, \mathrm{x}_2) &\mapsto (\mathrm{x}_1^2, \mathrm{x}_2^2, \sqrt{2}\mathrm{x}_1\mathrm{x}_2) \end{aligned}$$

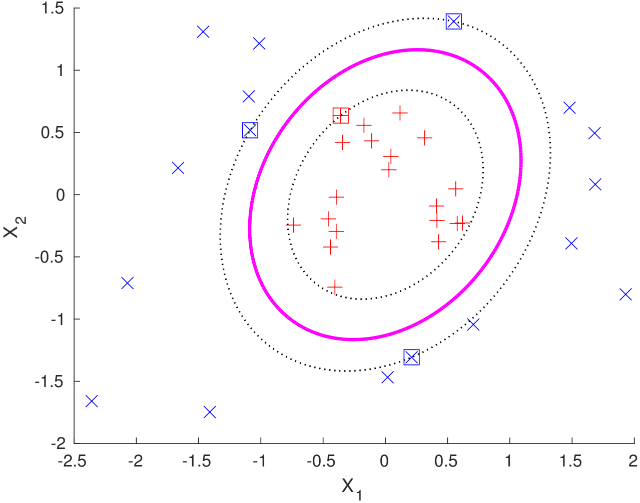
- In $\mathbb{R}^3$, the inner product can be expressed as

$$\begin{aligned} \langle \phi(\mathrm{x}), \phi(\mathrm{x}') \rangle_{\mathbb{R}^3} &= \sum_{i=1}^{3} \phi(\mathrm{x})_i \phi(\mathrm{x}')_i \\ &= \phi(\mathrm{x})_1\phi(\mathrm{x}')_1 + \phi(\mathrm{x})_2\phi(\mathrm{x}')_2 + \phi(\mathrm{x})_3\phi(\mathrm{x}')_3 \\ &= \mathrm{x}_1^2 \mathrm{x'}_1^2 + \mathrm{x}_2^2 \mathrm{x'}_2^2 + 2\mathrm{x}_1\mathrm{x}_2\mathrm{x'}_1\mathrm{x'}_2 \\ &= (\mathrm{x}_1\mathrm{x'}_1 + \mathrm{x}_2\mathrm{x'}_2)^2 \\ &= \langle \mathrm{x}, \mathrm{x}' \rangle_{\mathbb{R}^2}^2 \\ &= k(\mathrm{x}, \mathrm{x}'). \end{aligned}$$

Remark: $k(\mathrm{x}, \mathrm{x}')$ can be computed directly from the input data without computing $\phi(\mathrm{x})$ (see later the 'Kernel Trick')!

# Nonlinear discrimination in the input space

- $X \in \mathbb{R}^2$, $\phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)^T$




Linear separation in the feature space $\mathcal{F}$ $\Rightarrow$ Nonlinear separation in the input space

# Kernel trick

The SVM solution depends only on the inner product between the input features $\phi(\boldsymbol{x})$ and the support vectors $\phi(\boldsymbol{x}_{\mathrm{margin}})$

## Kernel trick

Use of a kernel function $k$ associated with an expansion/feature map $\phi$:

$$\begin{array}{rccc} k: & \mathbb{R}^p \times \mathbb{R}^p & \to & \mathbb{R} \\ & (\boldsymbol{x}, \boldsymbol{x}') & \mapsto & k(\boldsymbol{x}, \boldsymbol{x}') \equiv \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{x}') \rangle \end{array}$$

and the separating hyperplane reads $h(\boldsymbol{x}) = \sum_{i=1}^{n} \widehat{\alpha}_i y_i k(\boldsymbol{x}_i, \boldsymbol{x}) + \widehat{\beta}_0$

## Advantages

- computations are performed in the original input space: less expensive than in a high dimensional transformed space $\mathcal{F}$
- explicit representations of the feature map $\phi$ and enlarged feature space $\mathcal{F}$ are not necessary, the only expression of $k$ is required!
- ☞ possibility of complex transformations in possible infinite space $\mathcal{F}$
- ☞ standard trick in machine learning not limited to SVM (kernel ridge regression, gaussian process, spectral clustering, kernel-PCA ...)

# Kernel function

### Definition (Positive semi-definite kernel)

$k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is positive semi-definite is

- $\forall (\mathrm{x}, \mathrm{x}') \in \mathbb{R}^d \times \mathbb{R}^d, k(\mathrm{x}_i, \mathrm{x}_j) = k(\mathrm{x}_j, \mathrm{x}_i)$.
- $\forall n \in \mathbb{N}, \forall \xi_1 \ldots \xi_n \in \mathbb{R}, \forall \mathrm{x}_1 \ldots \mathrm{x}_n \in \mathbb{R}^d, \sum_{i,j}^n \xi_i \xi_j k(\mathrm{x}_i, \mathrm{x}_j) \geq 0$.

### Theorem (Mercer Theorem)

*To every positive semi-definite kernel $k$, there exists a Hilbert space $\mathcal{F}$ and a feature map $\phi : \mathbb{R}^d \to \mathcal{H}$ such that for all $\mathrm{x}_i, \mathrm{x}_j$ we have $k(\mathrm{x}_i, \mathrm{x}_j) = \langle \phi(\mathrm{x}_i), \phi(\mathrm{x}_j) \rangle_{\mathcal{H}}$.*

# Operations on kernels

Let $k_1$ and $k_2$ be positive semi-definite, and $\lambda_{1,2} > 0$ then:

1. $\lambda_1 k_1$, (multiplication by a positive scalar)
2. $\lambda_1 k_1 + \lambda_2 k_2$, (sum of kernels),
3. $k_1 k_2$, (product of kernels),
4. $\exp(k_1)$, (exponential of kernel),
5. $(\mathrm{x}_i, \mathrm{x}_j) \mapsto g(\mathrm{x}_i) g(\mathrm{x}_j) k_1(\mathrm{x}_i, \mathrm{x}_j)$, with $g : \mathbb{R}^d \to \mathbb{R}$, (multiplication by a function)

are all positive semi-definite, hence valid kernels.

☞ These operations allow us to create more complicated kernels by combining simple ones.

# Choosing the Kernel function

## Usual kernel functions

- Linear kernel ( $\mathcal{F} \equiv \mathbb{R}^p$) : $k(x, x') = x^T x'$
- Polynomial kernel (dimension of $\mathcal{F}$ increases with the order $d$)

$$k(x, x') = (x^T x')^d \quad \text{or} \quad (x^T x' + 1)^d$$

- Gaussian radial function ($\mathcal{F}$ with infinite dimension)

$$k(x, x') = \exp\left(-\gamma ||x - x'||^2\right)$$

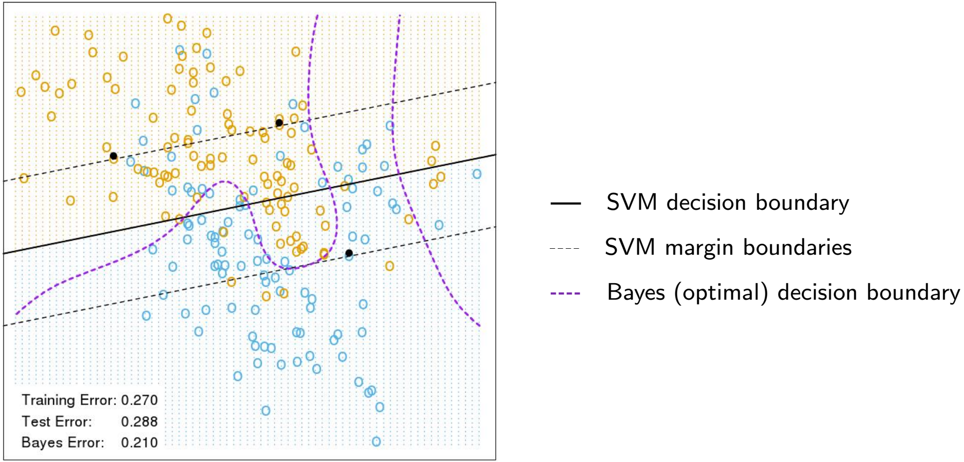
- Neural net kernel ($\mathcal{F}$ with infinite dimension)

$$k(x, x') = \tanh\left(\kappa_1 x^T x' + \kappa_2\right)$$

☞ standard practice is to estimate the optimal kernel parameters by cross-validation

# Application: binary data (cf course 2 example)

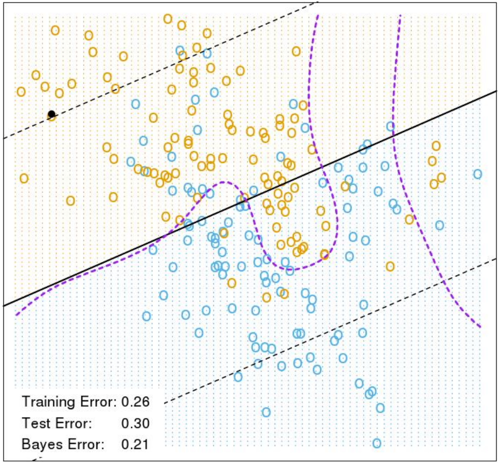
## Linear kernel




$C = 10000$

# Application: binary data (cf course 2 example)

## Linear kernel




$C = 0.01$

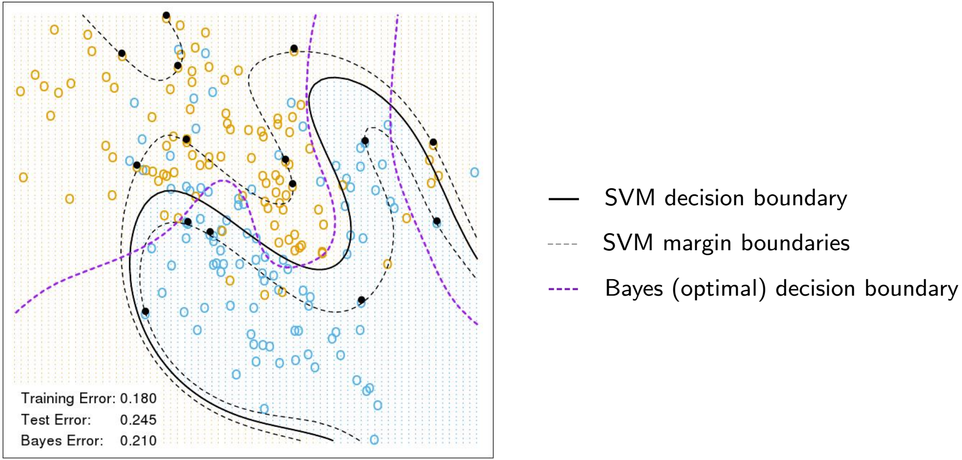
— SVM decision boundary

---- SVM margin boundaries

---- Bayes (optimal) decision boundary

# Application: binary data (cf course 2 example)

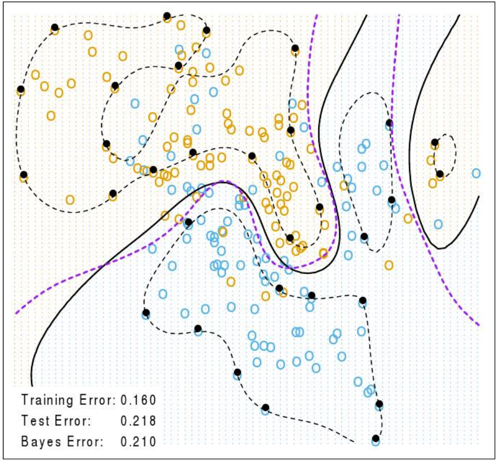
## Polynomial kernel ($d = 4$)




$C \approx 1$

# Application: binary data (cf course 2 example)

## Gaussian radial kernel ($\gamma = 1$)




$C \approx 1$

- SVM decision boundary
- SVM margin boundaries
- Bayes (optimal) decision boundary

# Scale your data!

## Scaling of the variables matters!

For instance, with Gaussian kernel

$$\begin{aligned} k(x, x') &= \exp\left(-\gamma \|x - x'\|^2\right) \\ &= \exp\left(-\gamma \sum_{i=1}^{p} (x_i - x_i')^2\right), \end{aligned}$$

the variables that have the greatest magnitudes are favored to compute distances or inner-products.

## Practical advices

- If the variables are in different units, scaling each is strongly recommended.
- If they are in the same units, you might or might not scale the variables (depend on your problem)

## Usual scaling methods

- normalization in $[0, 1]$: $\tilde{x}_i = \dfrac{x_i - \min_i}{\max_i - \min_i}$
- standardization to get zero mean and unit variance: $\tilde{x}_i = \dfrac{x_i - \mu_i}{\sigma_i}$

# Multiclass SVM

- $Y \in \{1, \ldots, K\} \leftarrow K$ classes

Standard approach: direct generalization by using multiple binary SVMs

## OVA: one-versus-all strategy

- $K$ classifiers between one class ($+1$ label) versus all the other classes ($-1$ label)

☞ classifier with the highest confidence value (e.g. the maximum distance to the separator hyperplane) assigns the class

## OVO: one-versus-one strategy

- $\binom{K}{2} = K(K-1)/2$ classifiers between every pair of classes

☞ majority vote rule: the class with the most votes determines the instance classification

Which to choose? if $K$ is not too large, choose OVO

# SVM vs Logistic regression (LR)

- When classes are nearly separable, SVM does better than LR. So does LDA.
- When not, LR (with ridge penalty) and SVM are very similar
- If one wants to estimate probabilities for each class, LR is the natural choice
- For non linear boudaries, kernel SVMs are popular. Can use kernels with LR and LDA as well, but computations are more expensive.

# Conclusions on Support Vector Machines

## SVM properties

- model free approach based on a maximum margin criterion: may be very efficient for real-word data (but do not directly provide probability estimates nor variable importance weights)
- memory efficient sparse solution characterized by the only support vectors
- versatile algorithm: different choices of kernels to make a nonlinear classification in the original input space by performing an implicit linear classification in a higher dimensional space
- Possible extensions to other tasks than classification like regression (*support vector regression*) or anomaly detection (*one-class SVM*)
- effective in high dimensional spaces even when $p > n$.
- computionally expensive to train for large $n$ data sets: cost of the optimization procedure to solve the quadratic problem scales from $O(pn^2)$ to $O(pn^3)$ operations depending on the training set.
- popular algorithm, with a large literature

# Perspectives on 'Black Box' (model free) approaches

## Random Forests

- involve decision tree to split the prediction space in simple regions
- combine multiple decision trees to yield a single consensus prediction
- ☞ method able to scale efficiently to high dimensional data and large data sets

## Deep Neural Nets

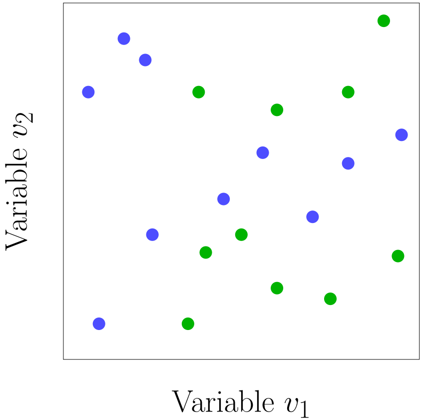
- Neural Nets with multiple hidden layers between input and output ones
- many variants of deep architectures (Recurrent, Convolutional,...) used in specific domains (speech, vision, ...)
- very computationally expensive to train due to the high number of parameters
- supported by empirical evidence
- ☞ dramatic performance jump for some big data applications

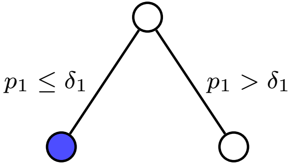
# Outline for model free approaches

# Random Forests

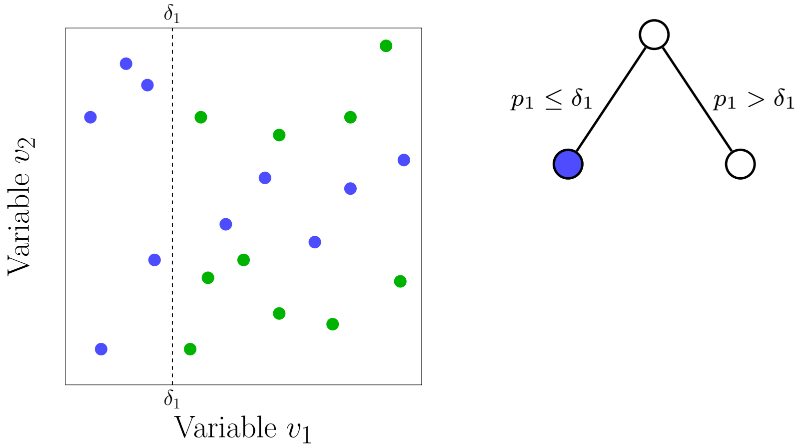
- Introduced in 2001 (Breiman)
- Model free and non linear
- Build a large collection of de-correlated trees and average them
- Combination of weak learners

# Decision trees

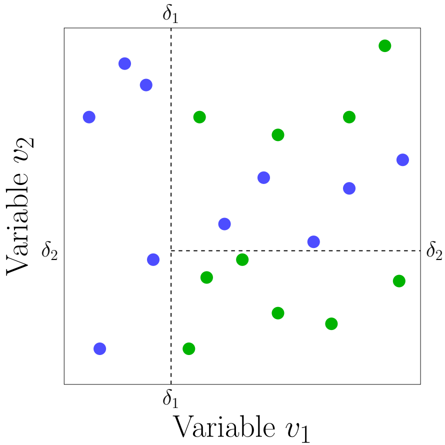


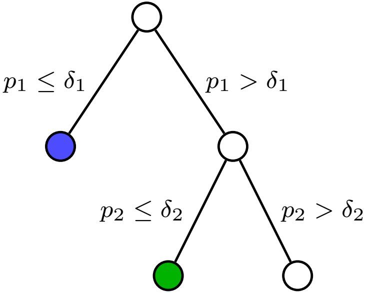



## Decision trees

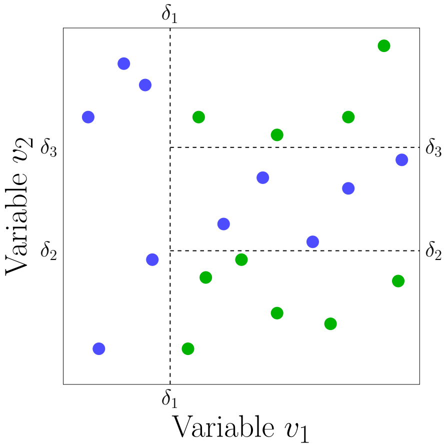


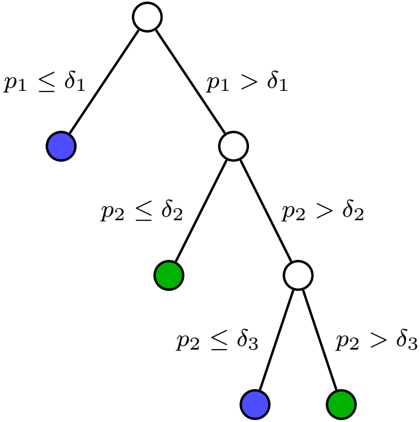
# Decision trees



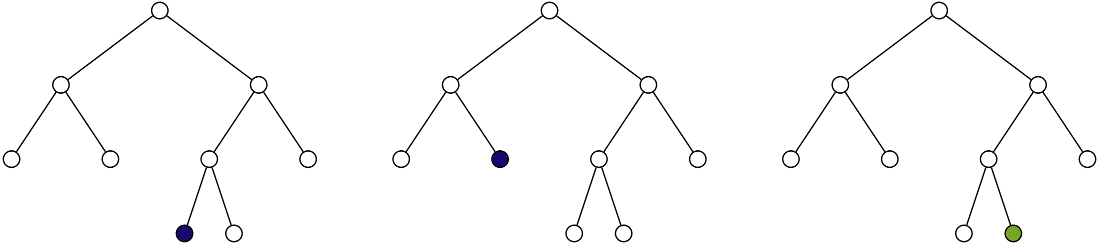
# Decision trees



# Random Forests

- For each tree:
  - Draw bootstrap sample $X^b$ for training sample
  - Learn tree, for each node
    - select $m$ features from the initial $p$ features
    - Find the best split (e.g. Gini index, entropy ...)



# Application: binary data