# S1324:
# Support Vector Machines

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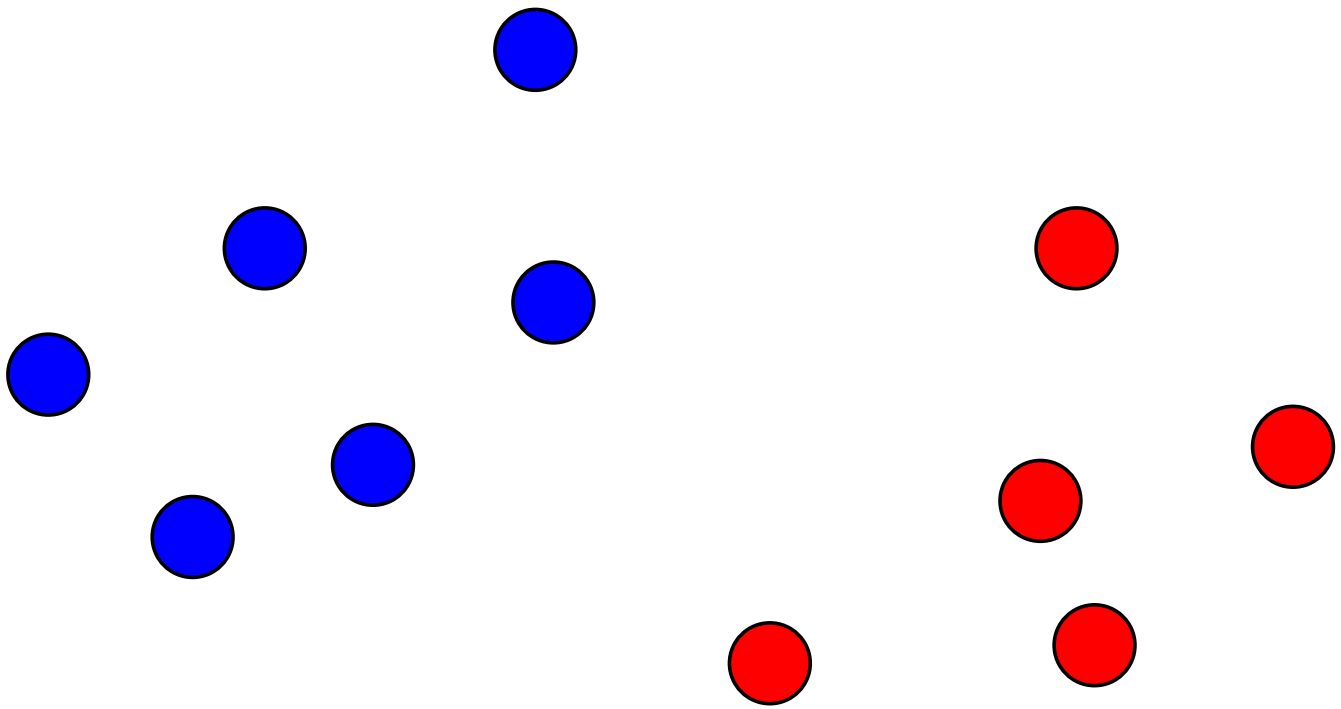
based on slides by J.-P. Vert

2015-05-22

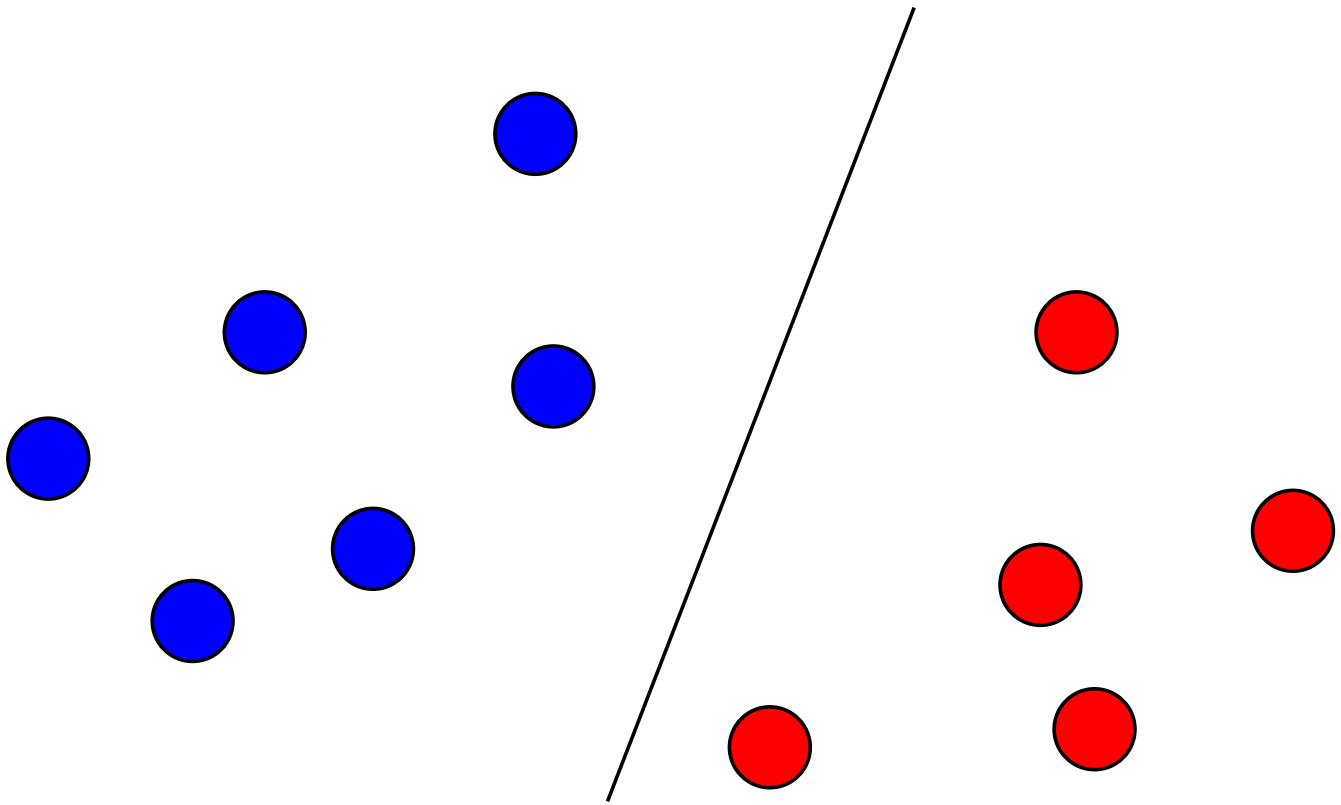


# Hard-margin Linear Support Vector Machines

# Linear classifier



# Linear classifier



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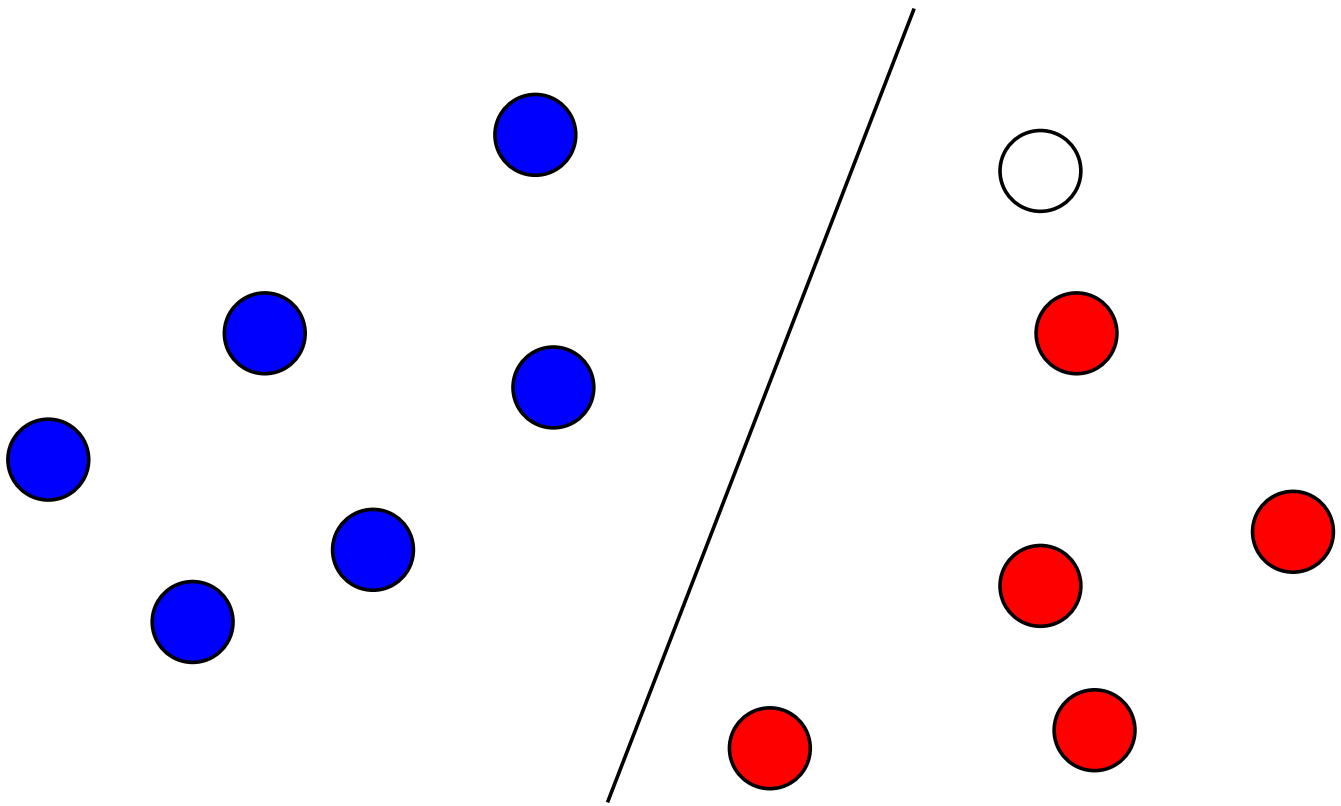

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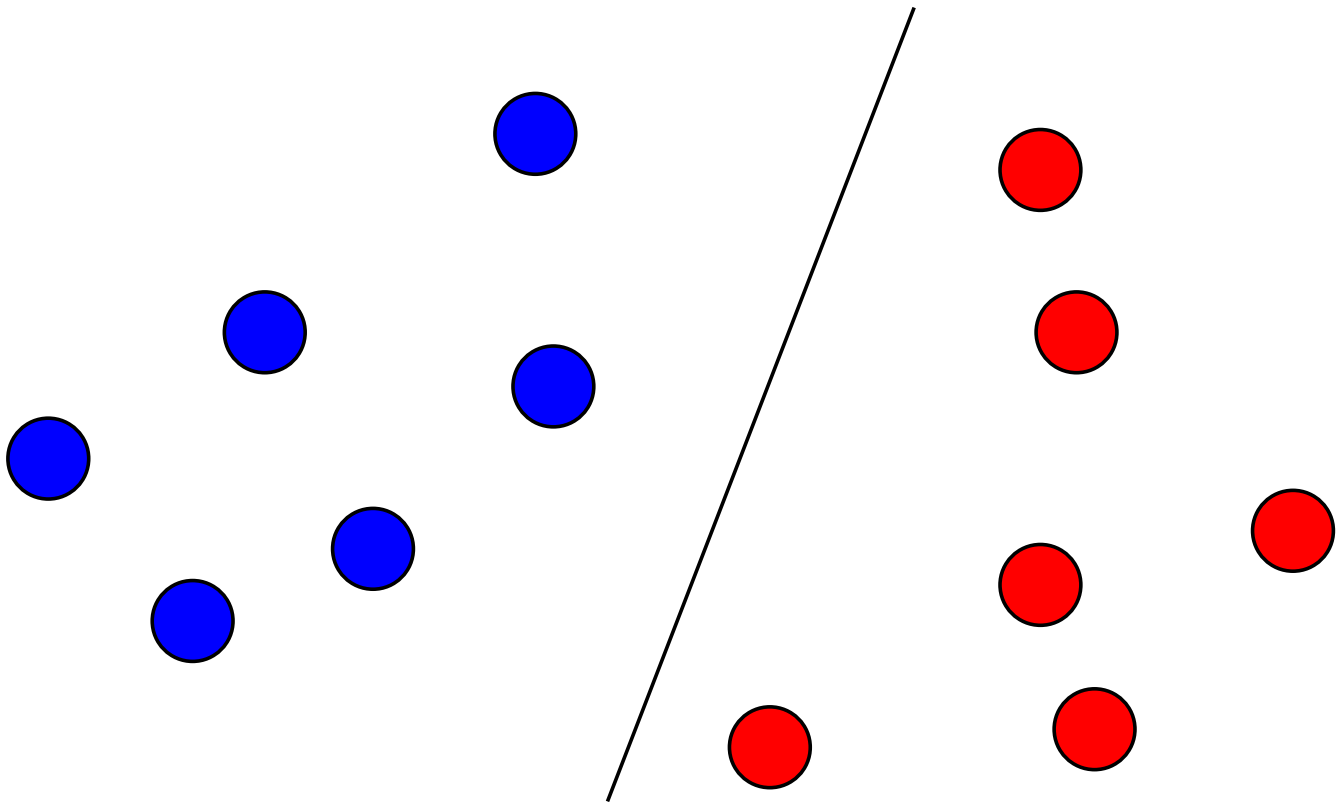

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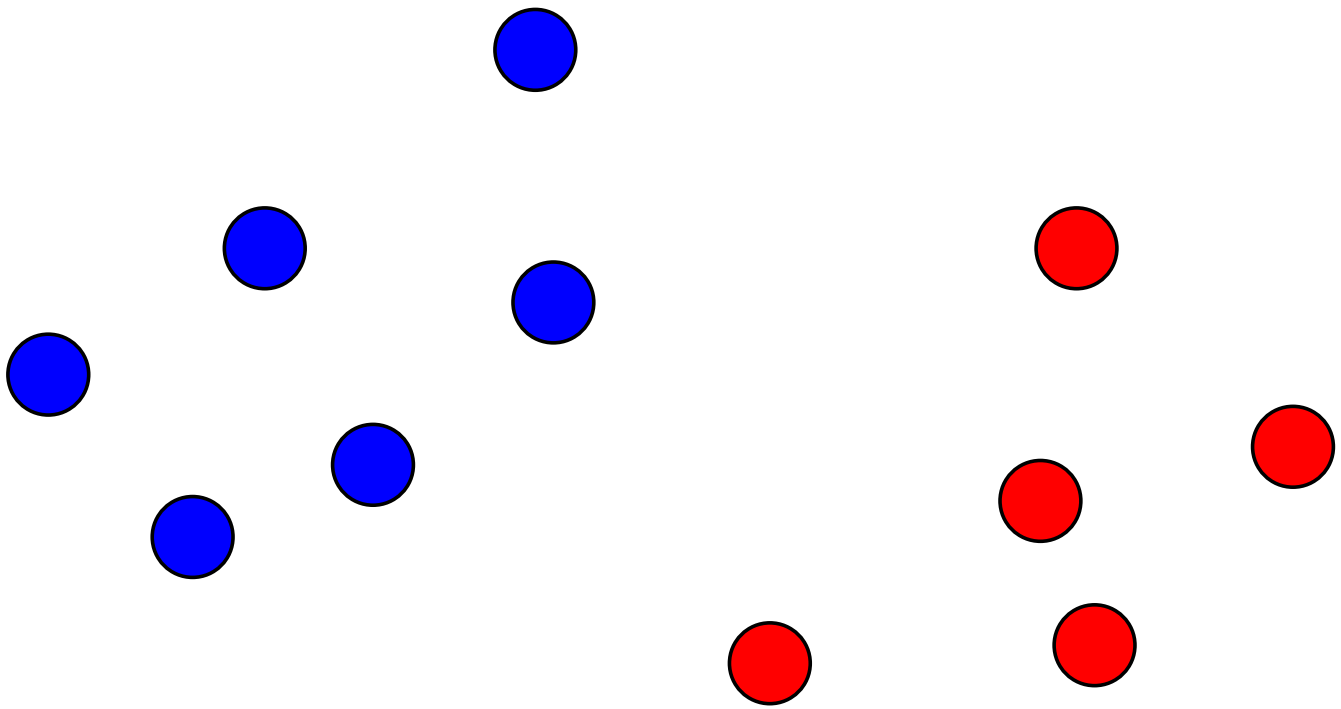

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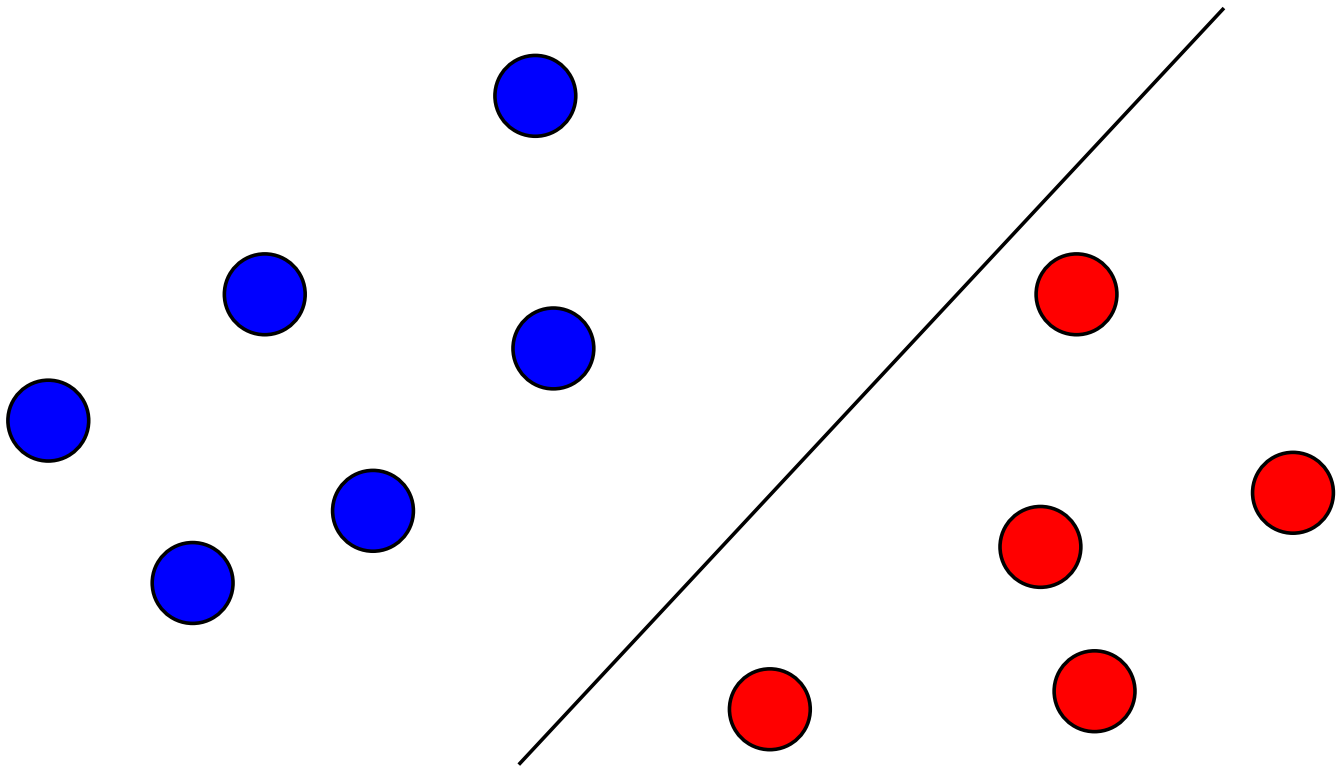

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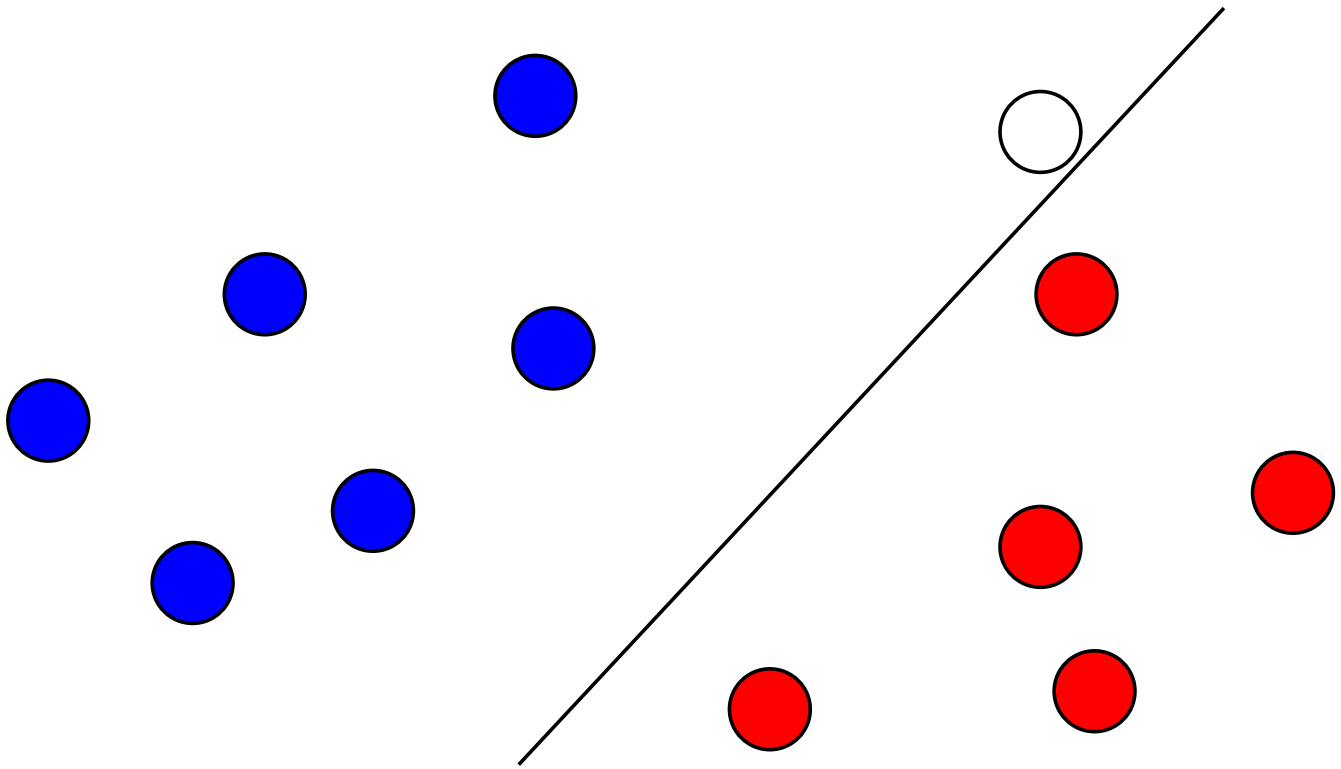

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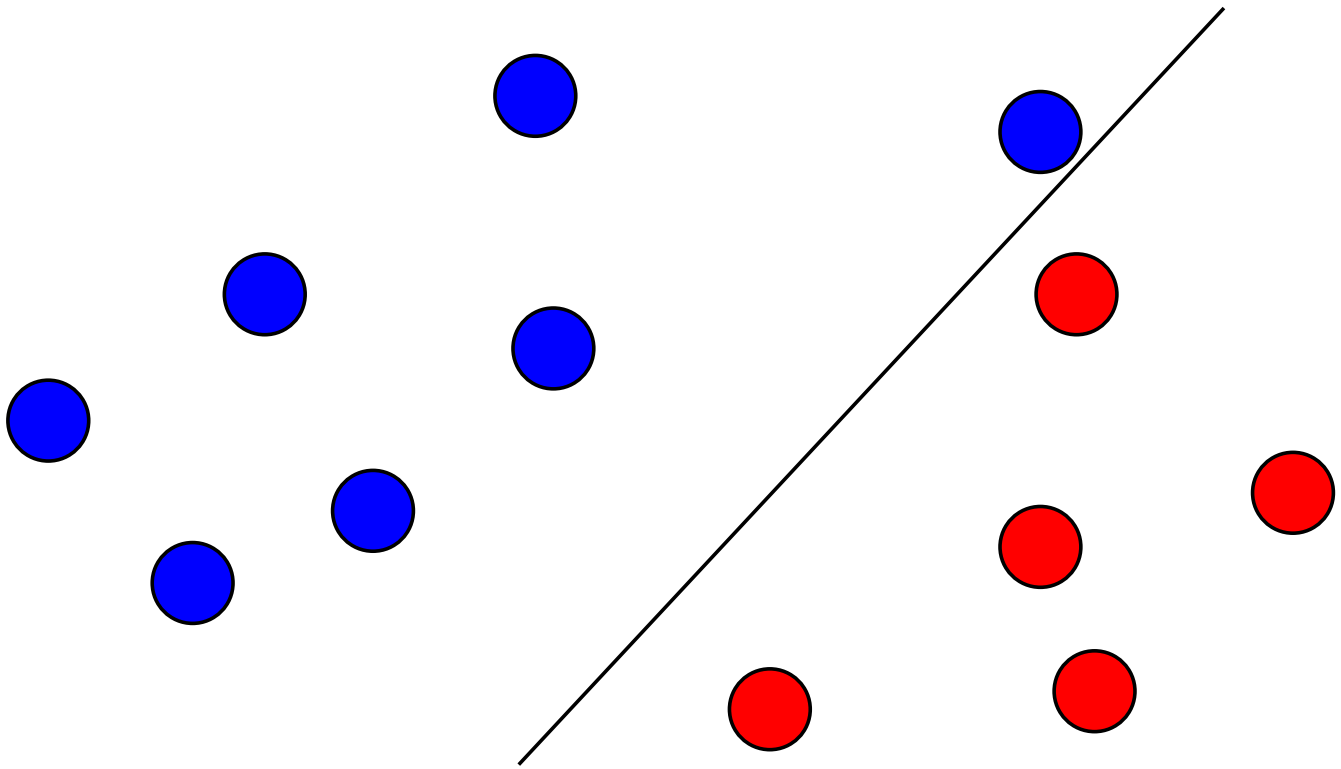
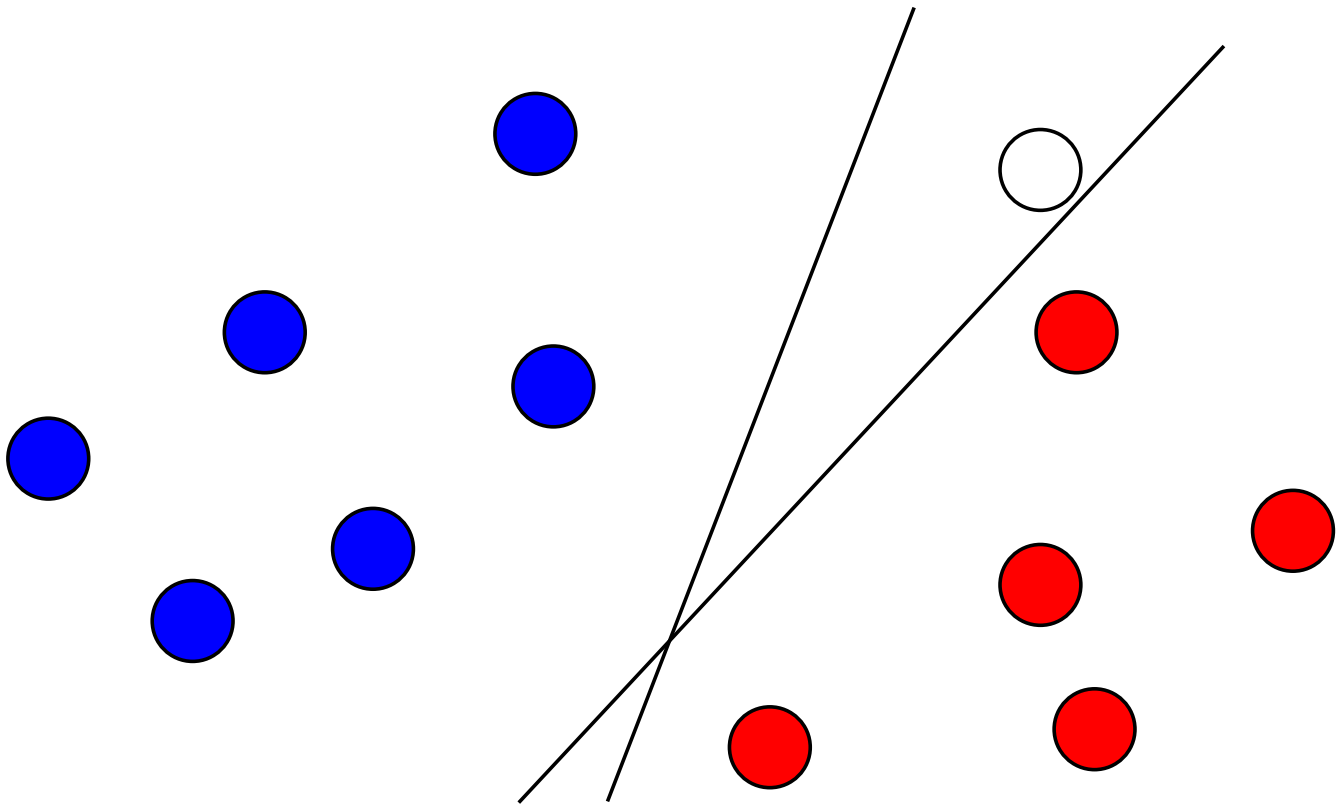
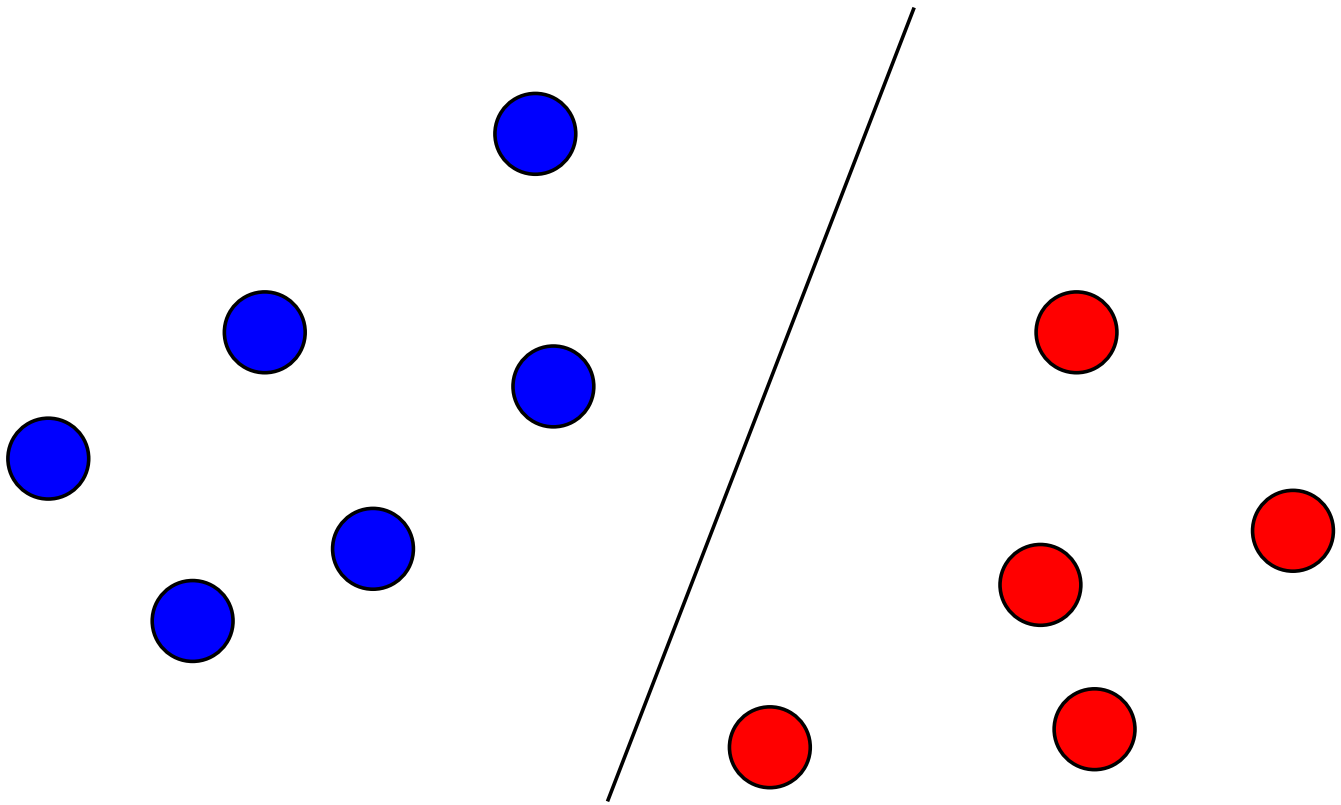


# Which one is better?



# The margin of a linear classifier



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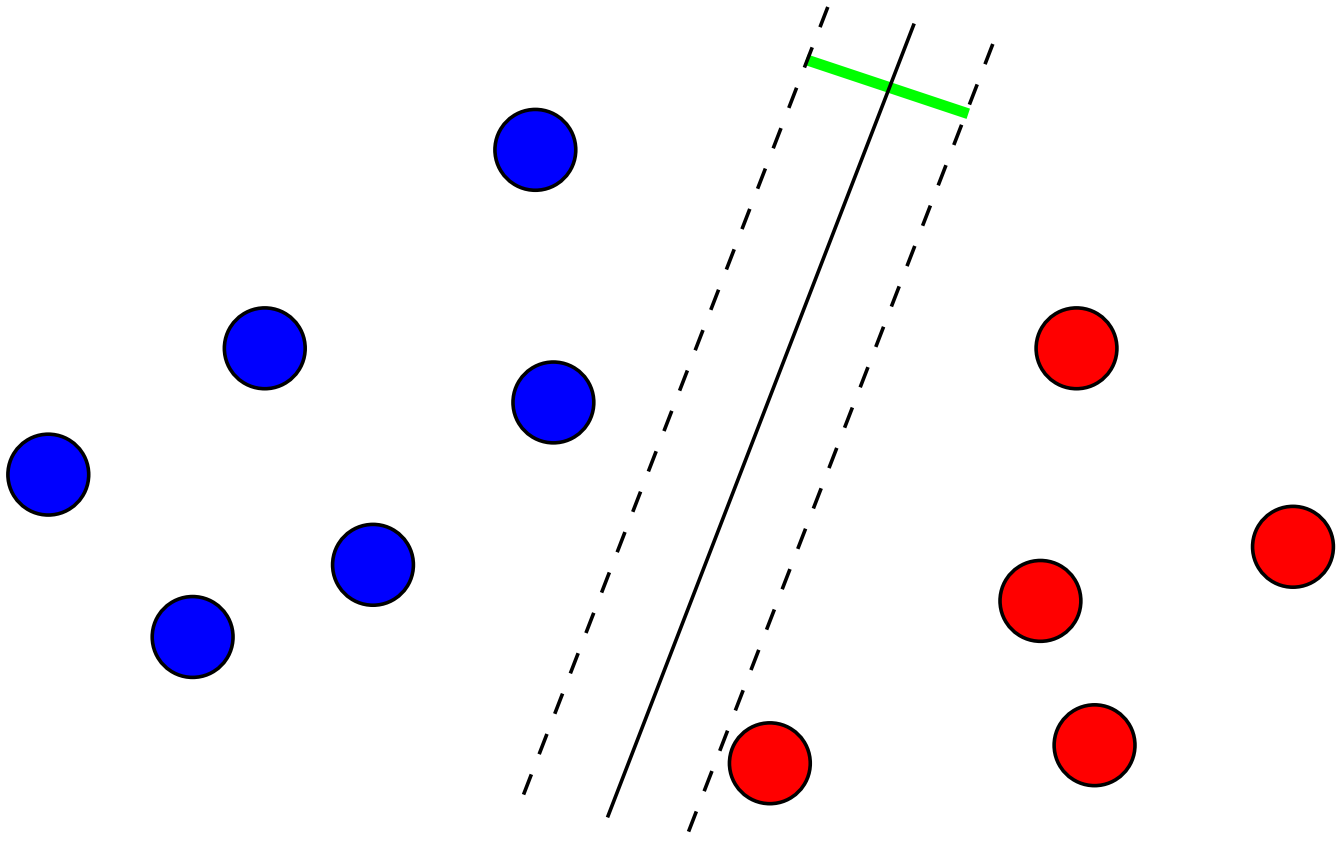

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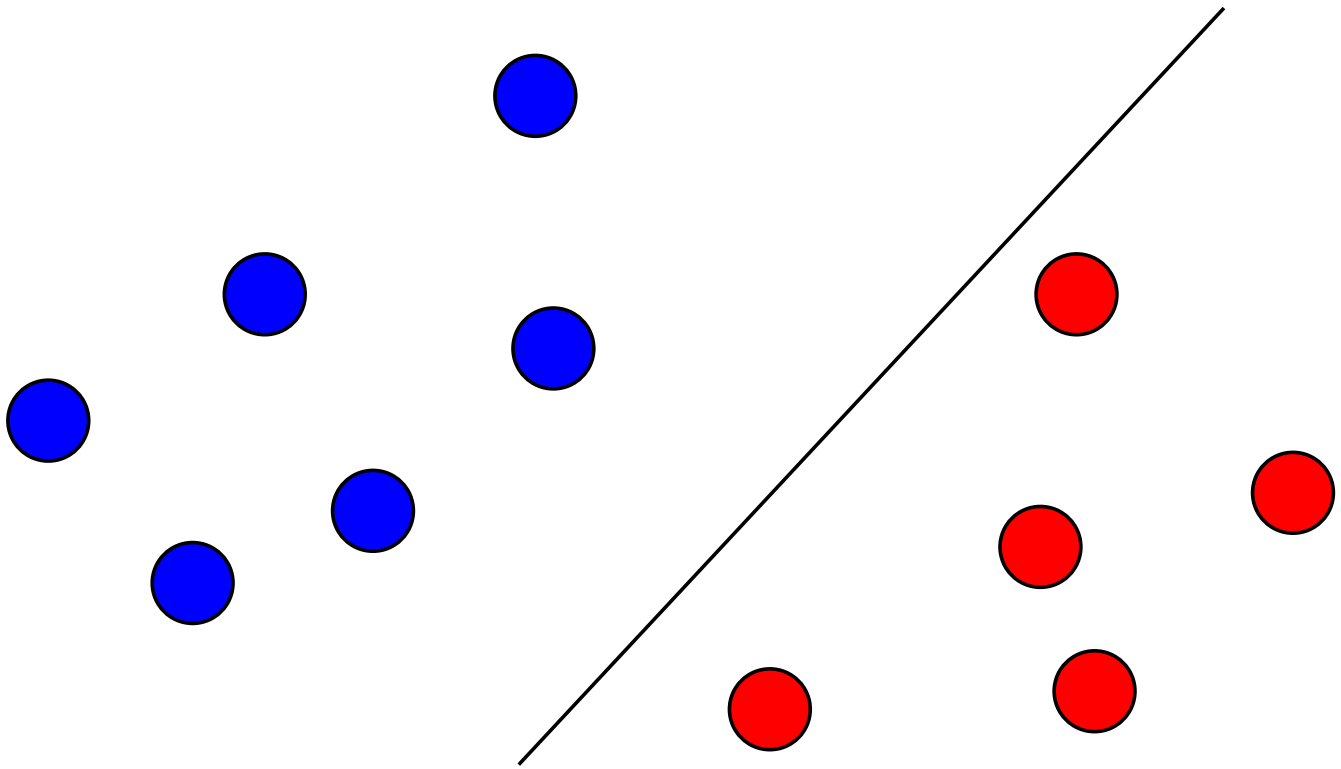

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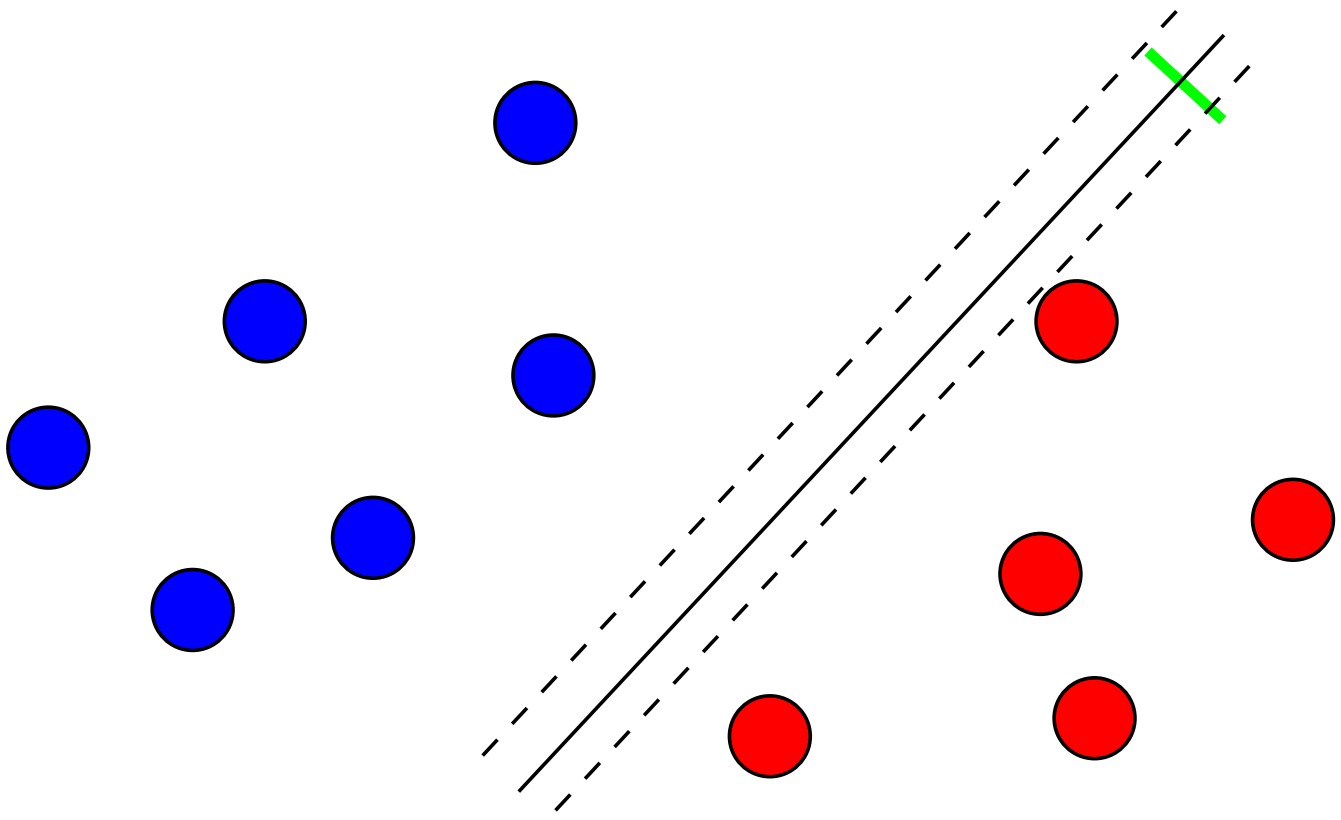

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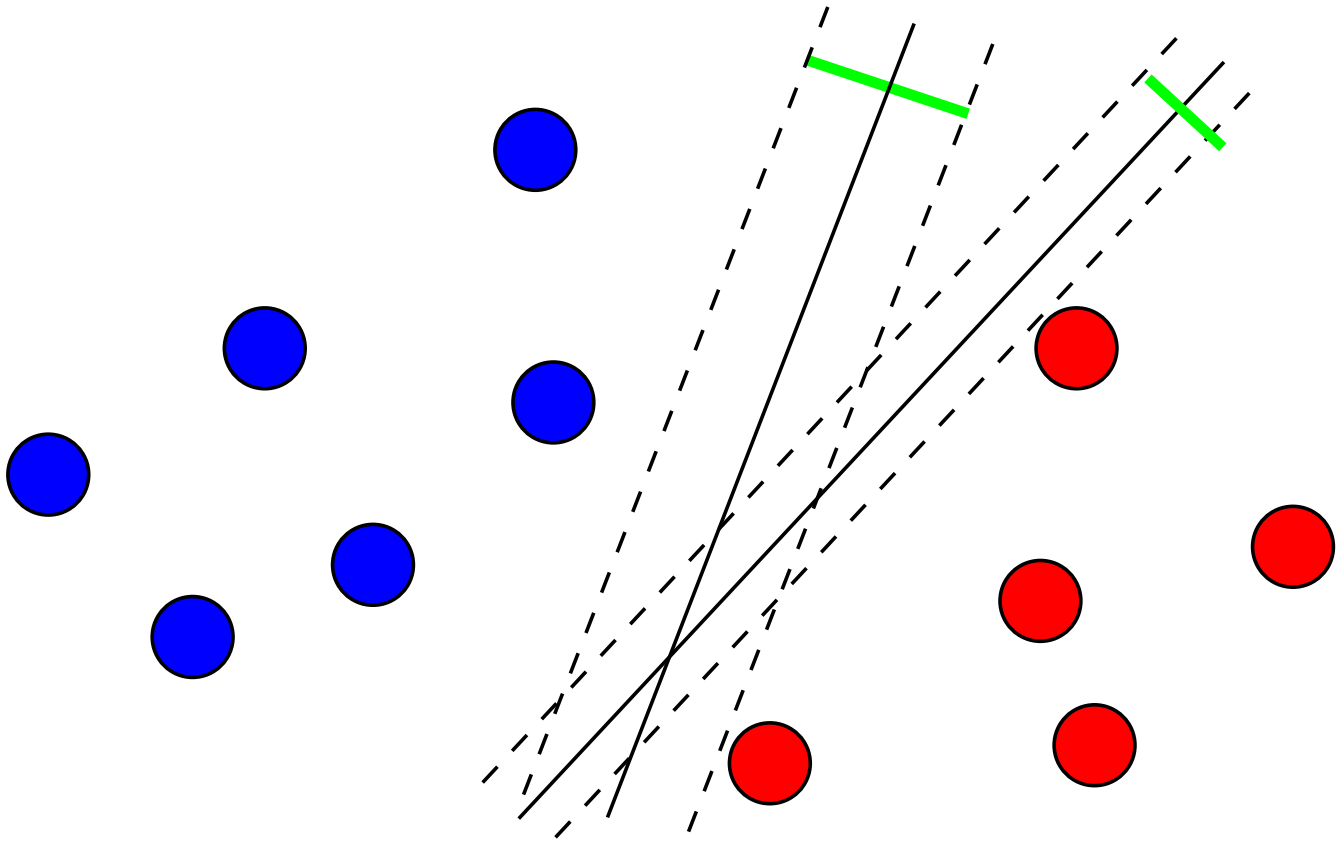
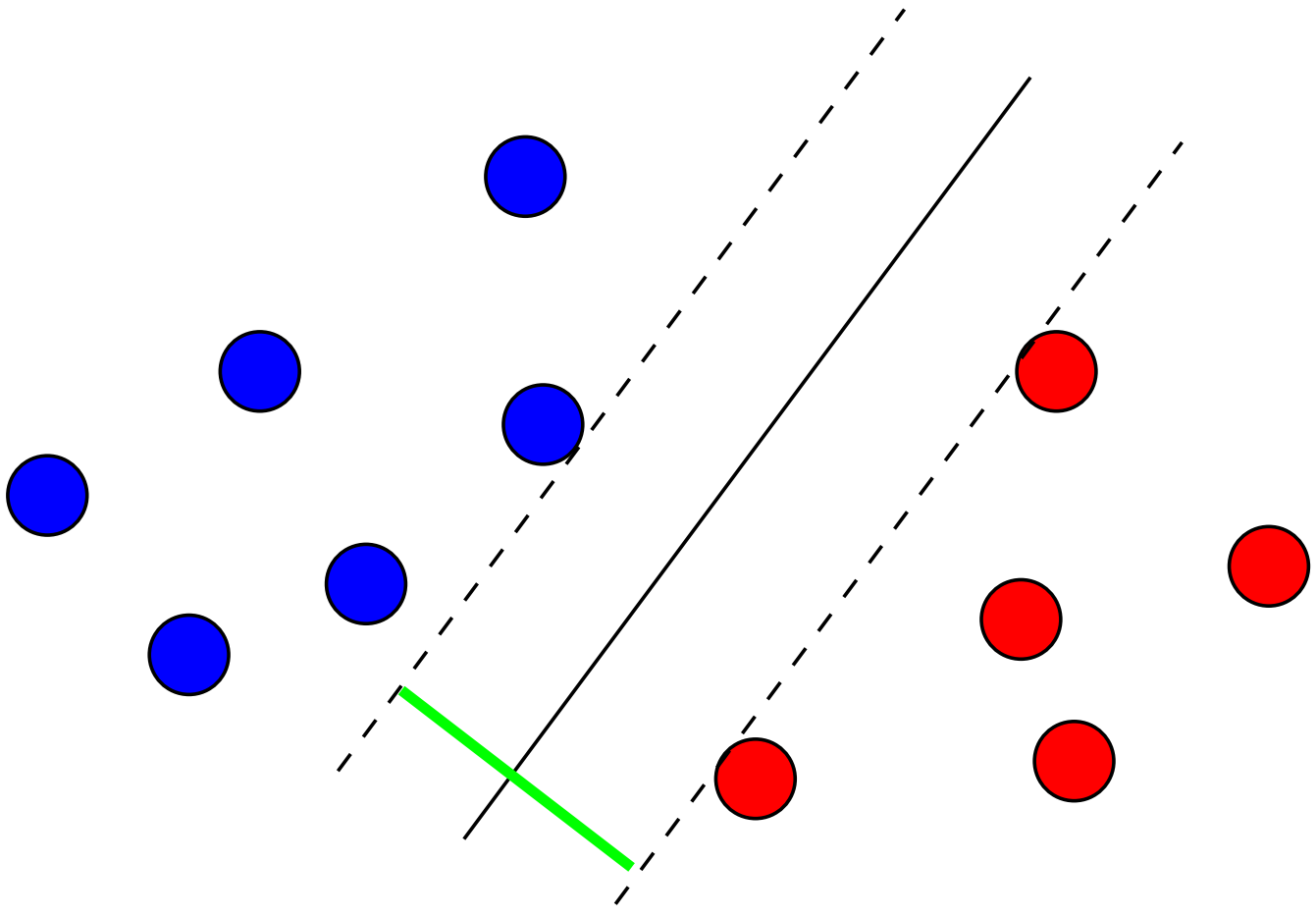
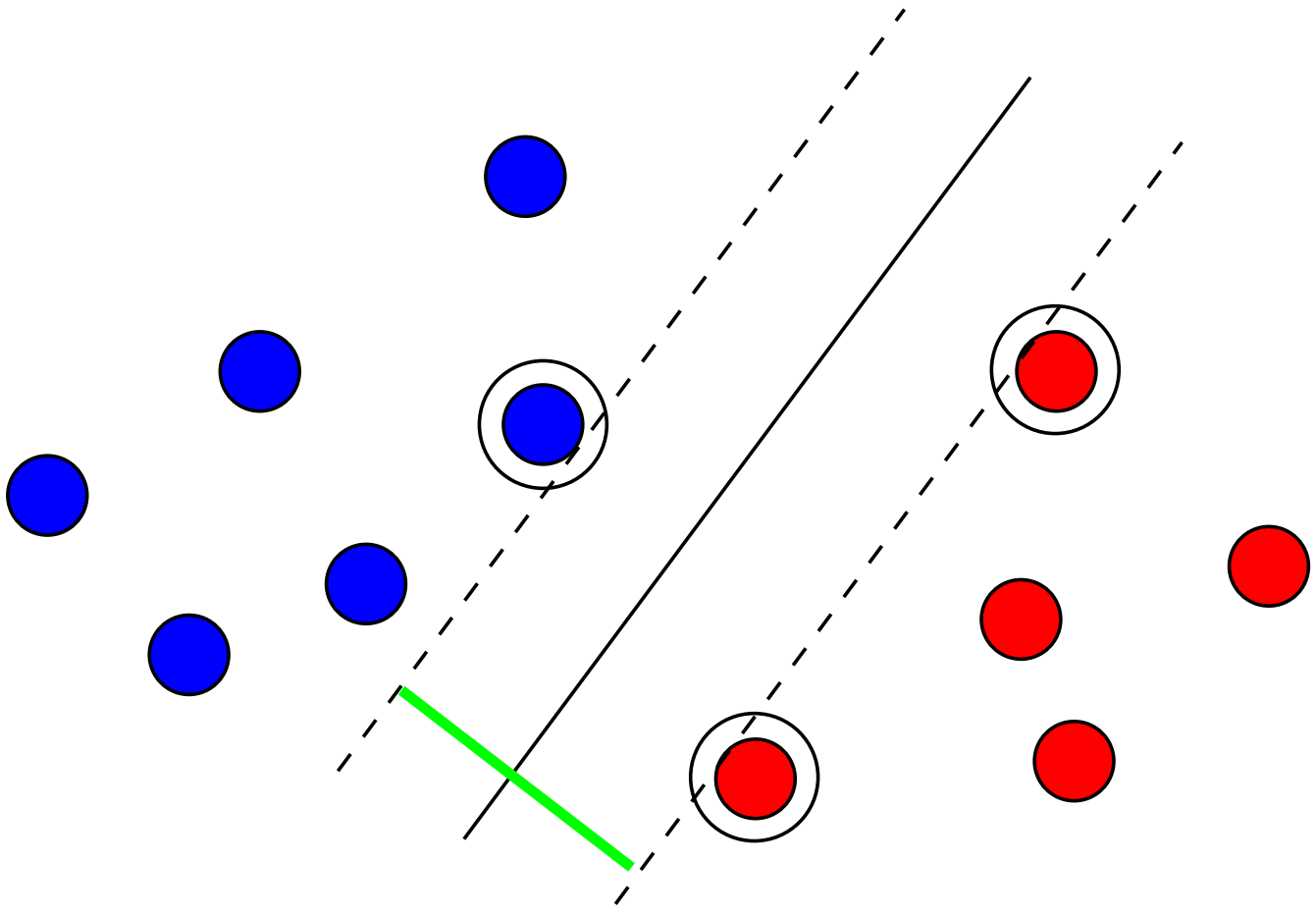


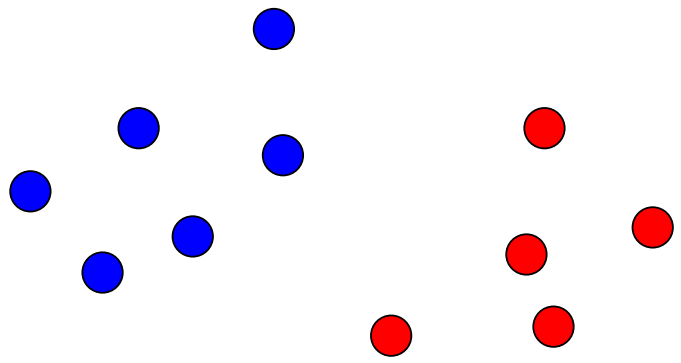
# Largest margin classifier (*hard-margin SVM*)



# Support vectors



# More formally



- The training set is a finite set of $n$ data/class pairs:

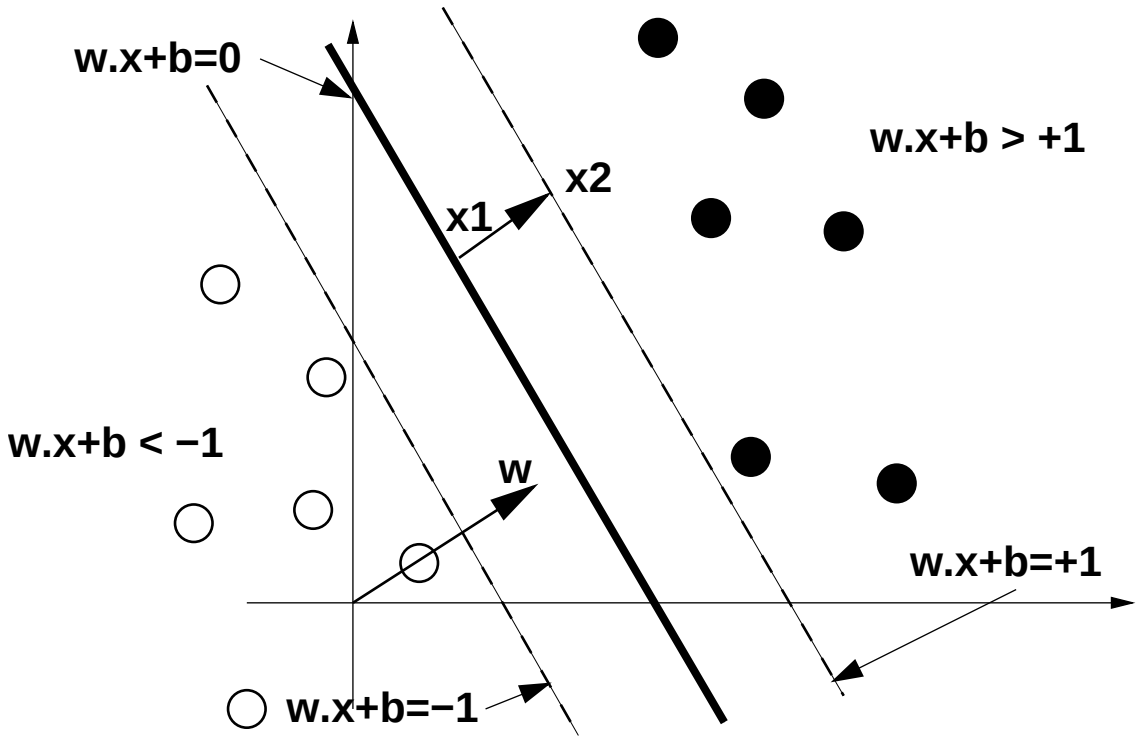
$$\mathcal{S} = \left\{(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n)\right\} ,$$

  where $\vec{x}_i \in \mathbb{R}^p$ and $y_i \in \{-1, 1\}$.
- We assume (for the moment) that the data are linearly separable, i.e., that there exists $(\vec{w}, b) \in \mathbb{R}^p \times \mathbb{R}$ such that:

$$\begin{cases} \vec{w}.\vec{x}_i + b > 0 & \text{if } y_i = 1 , \\ \vec{w}.\vec{x}_i + b < 0 & \text{if } y_i = -1 . \end{cases}$$

# How to find the largest separating hyperplane?

For a given linear classifier $f(x) = \vec{w}.\vec{x} + b$ consider the "tube" defined by the values $-1$ and $+1$ of the decision function:



# The margin is $2/\| \vec{w} \|$

Indeed, the points $\vec{x}_1$ and $\vec{x}_2$ satisfy:

$$\begin{cases} \vec{w}.\vec{x}_1 + b = 0\,, \\ \vec{w}.\vec{x}_2 + b = 1\,. \end{cases}$$

By subtracting we get $\vec{w}.(\vec{x}_2 - \vec{x}_1) = 1$, and therefore:

$$\gamma = 2\| \vec{x}_2 - \vec{x}_1 \| = \frac{2}{\| \vec{w} \|}\,.$$

# All training points should be on the correct side of the dotted line

For positive examples ($y_i = 1$) this means:

$$\vec{w}.\vec{x}_i + b \geq 1\,.$$

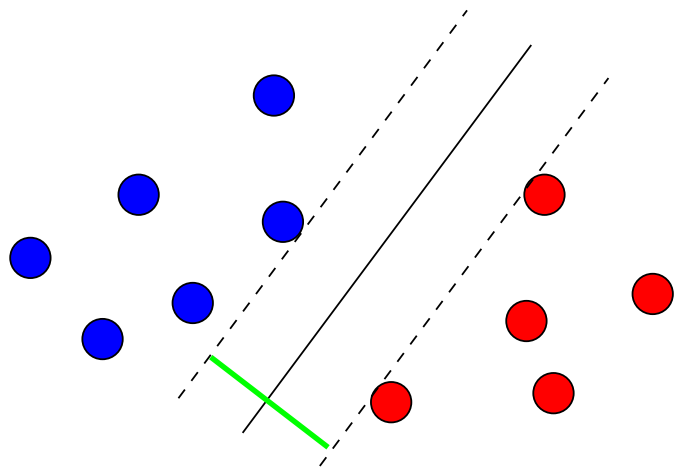
For negative examples ($y_i = -1$) this means:

$$\vec{w}.\vec{x}_i + b \leq -1\,.$$

Both cases are summarized by:

$$\forall i = 1, \ldots, n\,, \qquad y_i\left(\vec{w}.\vec{x}_i + b\right) \geq 1\,.$$

# Finding the optimal hyperplane



Find $(\vec{w}, b)$ which minimize:

$$\| \vec{w} \|^2$$

under the constraints:

$$\forall i = 1, \ldots, n, \qquad y_i \left( \vec{w}.\vec{x}_i + b \right) - 1 \geq 0 \, .$$

*This is a classical quadratic program on* $\mathbb{R}^{p+1}$.

# Lagrangian

In order to minimize:

$$\frac{1}{2}\| \vec{w} \|_2^2$$

under the constraints:

$$\forall i = 1, \ldots, n\,, \qquad y_i \left(\vec{w}.\vec{x}_i + b\right) - 1 \geq 0\,,$$

we introduce one dual variable $\alpha_i$ for each constraint, i.e., for each training point. The Lagrangian is:

$$L\left(\vec{w}, b, \vec{\alpha}\right) = \frac{1}{2}||\vec{w}||^2 - \sum_{i=1}^{n} \alpha_i \left(y_i \left(\vec{w}.\vec{x}_i + b\right) - 1\right)\,.$$

# Lagrangian

- $L\left(\vec{w}, b, \vec{\alpha}\right)$ is convex quadratic in $\vec{w}$. It is minimized for:

$$\nabla_{\vec{w}} L = \vec{w} - \sum_{i=1}^{n} \alpha_i y_i \vec{x}_i = 0 \quad \Longrightarrow \quad \vec{w} = \sum_{i=1}^{n} \alpha_i y_i \vec{x}_i \,.$$

- $L\left(\vec{w}, b, \vec{\alpha}\right)$ is affine in $b$. Its minimum is $-\infty$ except if:

$$\nabla_b L = \sum_{i=1}^{n} \alpha_i y_i = 0 \,.$$

# Dual function

- We therefore obtain the Lagrange dual function:

$$q(\vec{\alpha}) = \inf_{\vec{w}\in\mathbb{R}^p, b\in\mathbb{R}} L(\vec{w}, b, \vec{\alpha})$$
$$= \begin{cases} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \vec{x}_i . \vec{x}_j & \text{if } \sum_{i=1}^{n} \alpha_i y_i = 0\,, \\ -\infty & \text{otherwise.} \end{cases}$$

- The dual problem is:

$$\begin{aligned} \text{maximize} \quad & q(\vec{\alpha}) \\ \text{subject to} \quad & \vec{\alpha} \geq 0\,. \end{aligned}$$

# Dual problem

Find $\alpha^* \in \mathbb{R}^n$ which maximizes

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

under the (simple) constraints $\alpha_i \geq 0$ (for $i = 1, \ldots, n$), and

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

*This is a quadratic program on $\mathbb{R}^N$, with "box constraints". $\vec{\alpha}^*$ can be found efficiently using dedicated optimization softwares.*

# Recovering the optimal hyperplane

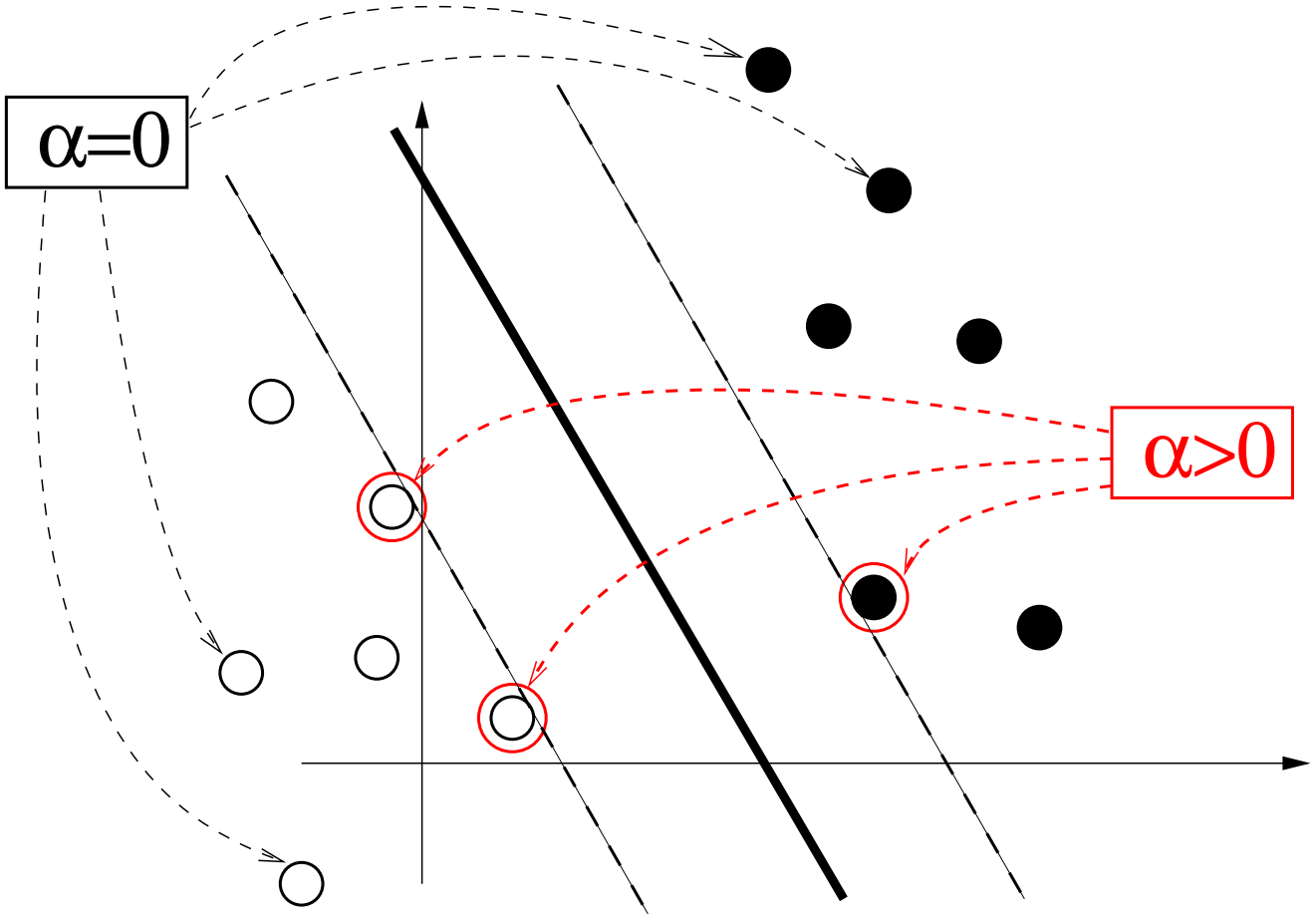
Once $\vec{\alpha}^*$ is found, we recover $(\vec{w}^*, b^*)$ corresponding to the optimal hyperplane. $w^*$ is given by:

$$\vec{w}^* = \sum_{i=1}^{n} \alpha_i \vec{x}_i,$$

and the decision function is therefore:

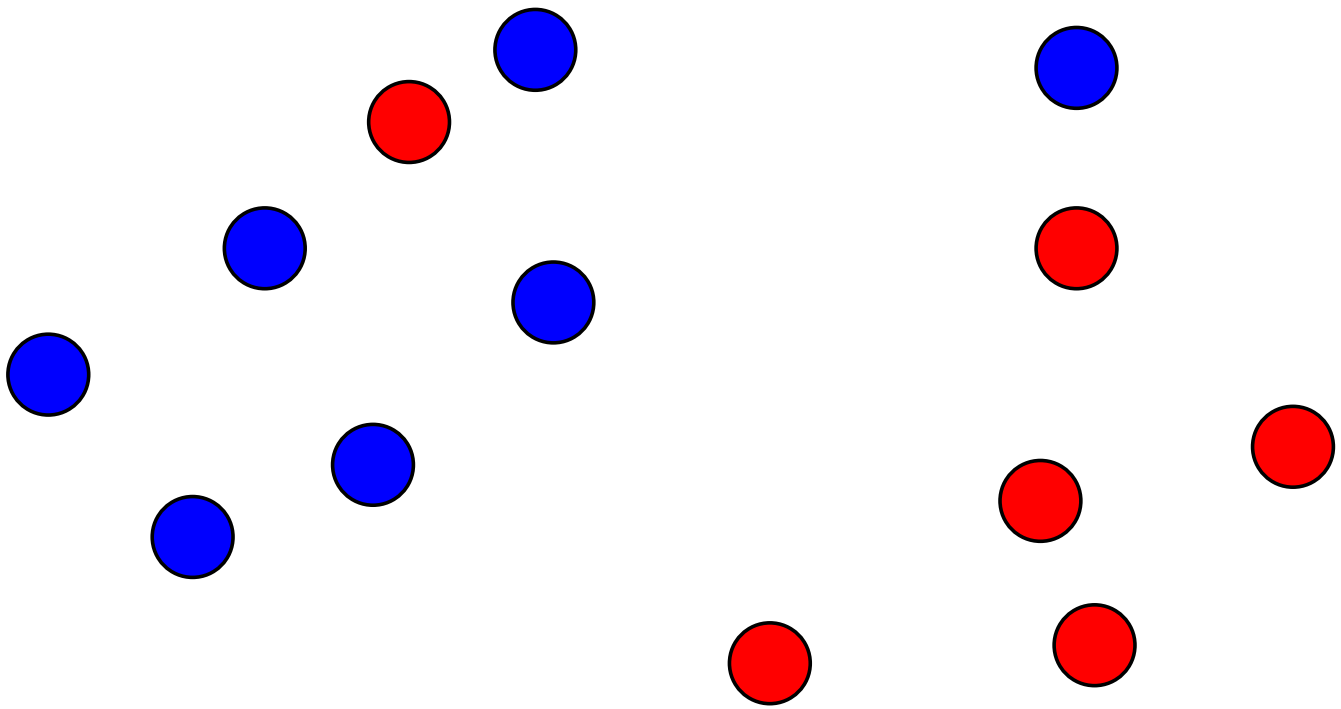
$$\begin{aligned} f^*(\vec{x}) &= \vec{w}^*.\vec{x} + b^* \\ &= \sum_{i=1}^{n} \alpha_i \vec{x}_i.\vec{x} + b^* \,. \end{aligned} \tag{1}$$

# Interpretation: support vectors



# Soft-Margin Linear Support Vector Machines

# What if data are not linearly separable?



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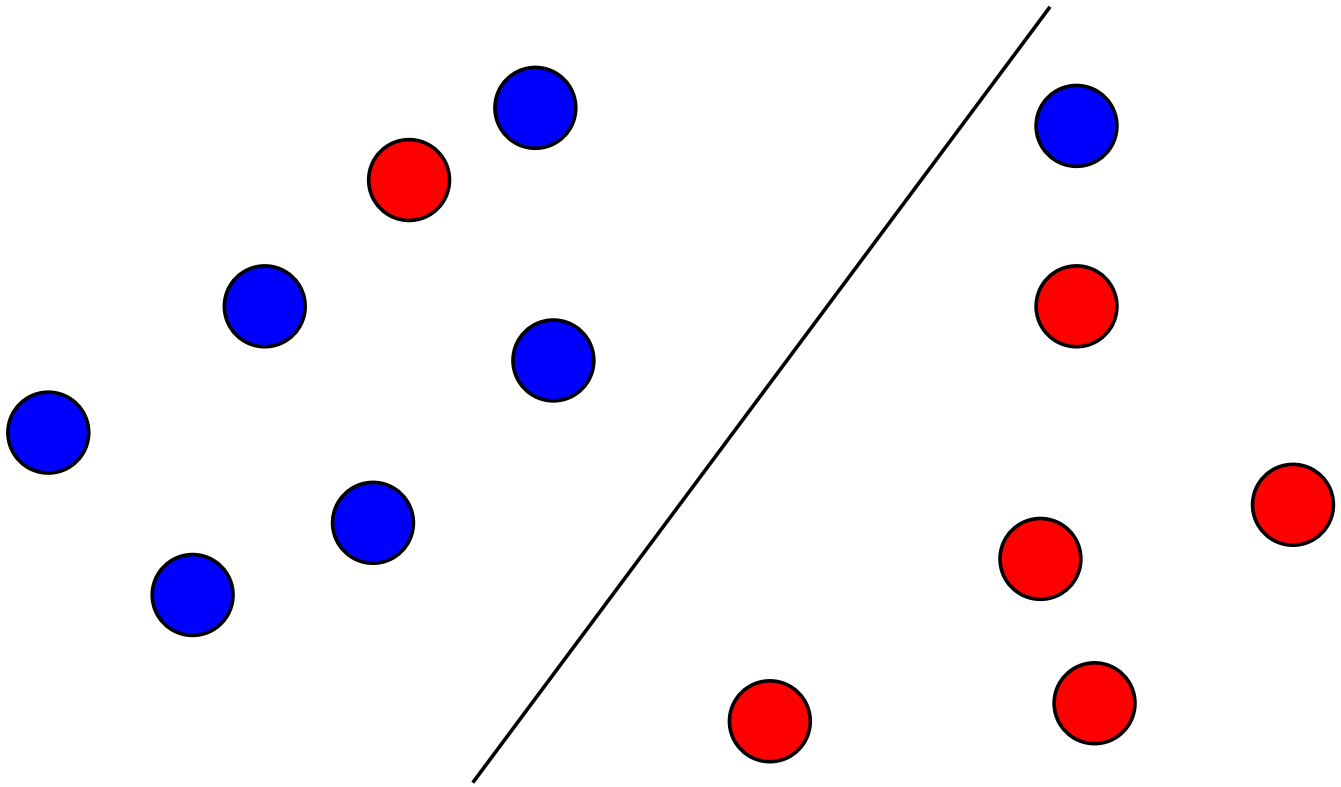

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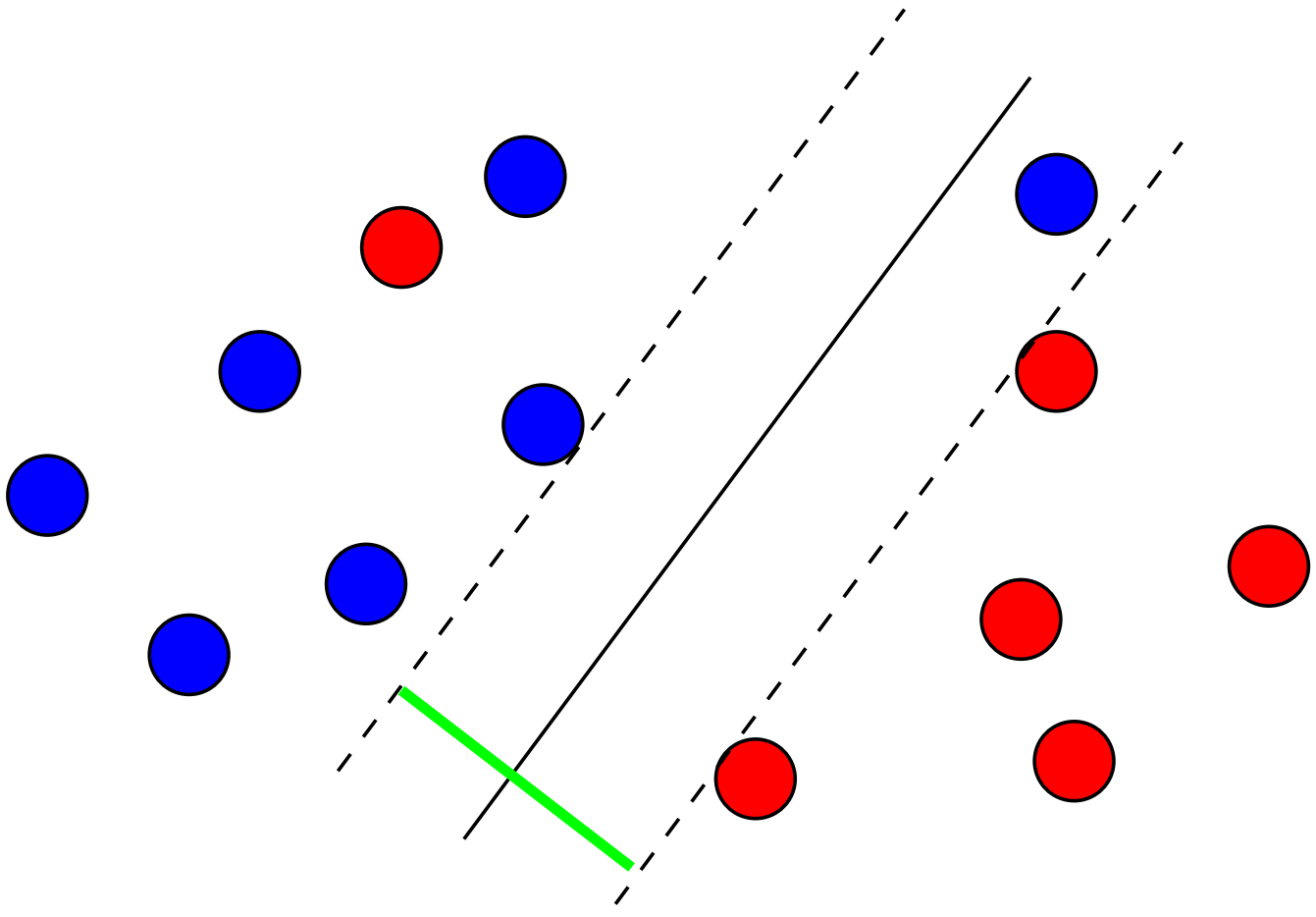

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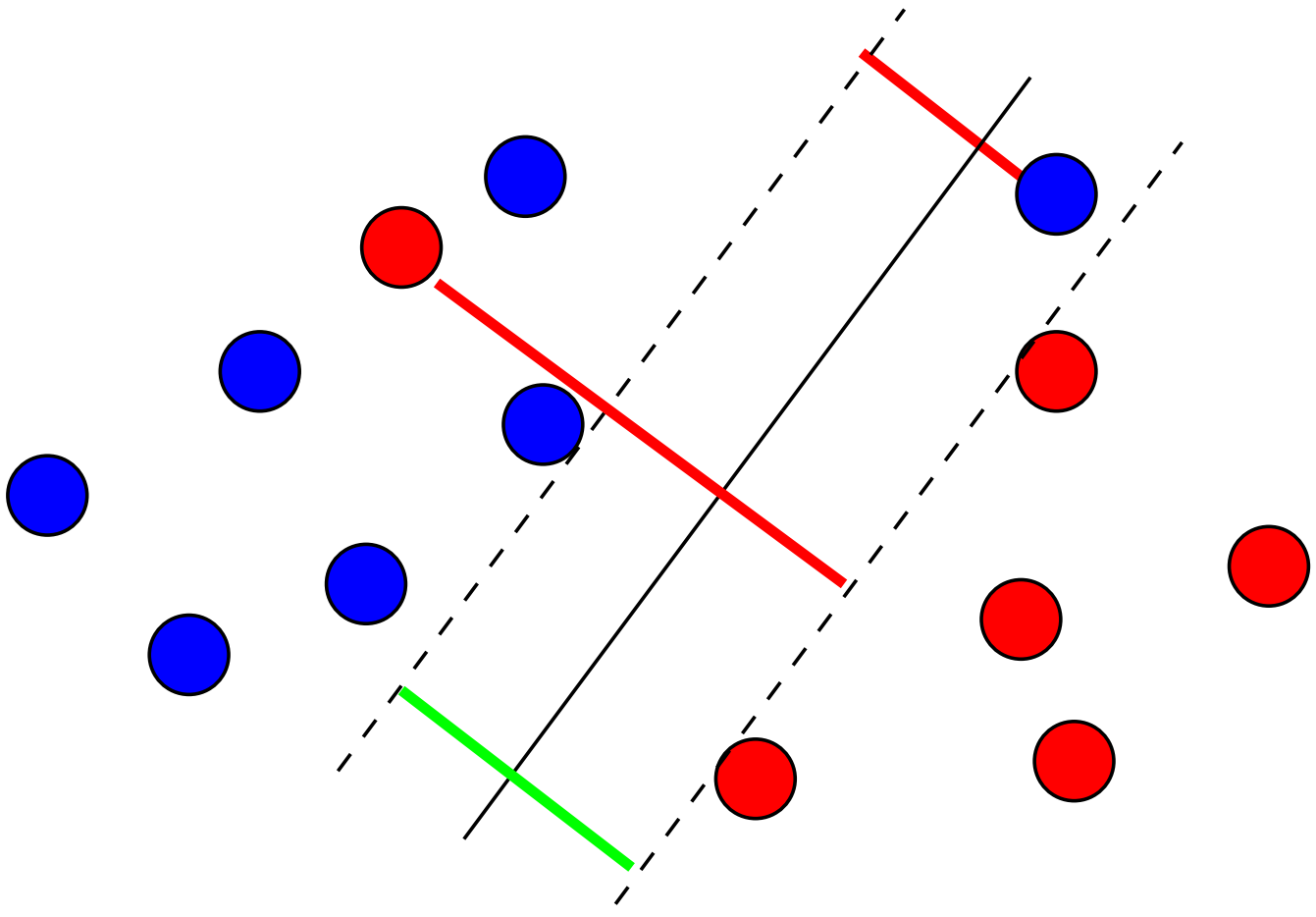
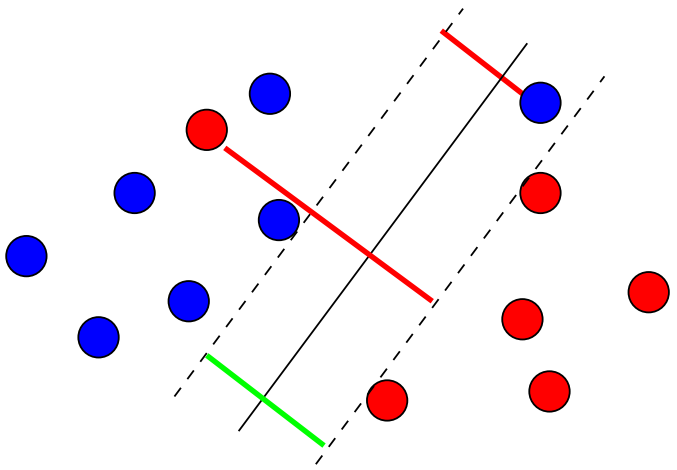


# Soft-margin SVM

- Find a trade-off between large margin and few errors.
- Mathematically:

$$\min_f \left\{ \frac{1}{margin(f)} + C \times errors(f) \right\}$$

- $C$ is a parameter



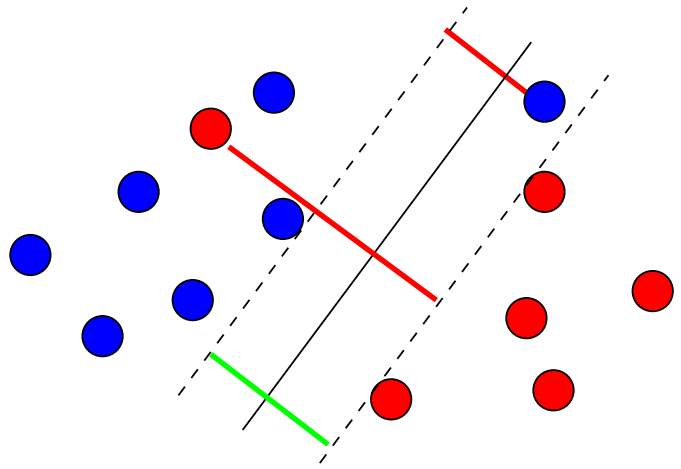
# Soft-margin SVM formulation

- The margin of a labeled point $(\vec{x}, y)$ is

$$margin(\vec{x}, y) = y\left(\vec{w}.\vec{x} + b\right)$$

- The error is
  - 0 if $margin(\vec{x}, y) > 1$,
  - $1 - margin(\vec{x}, y)$ otherwise.
- The soft margin SVM solves:

$$\min_{\vec{w},b} \left\{ ||\vec{w}||^2 + C \sum_{i=1}^{n} \max\left(0, 1 - y_i\left(\vec{w}.\vec{x}_i + b\right)\right) \right\}$$

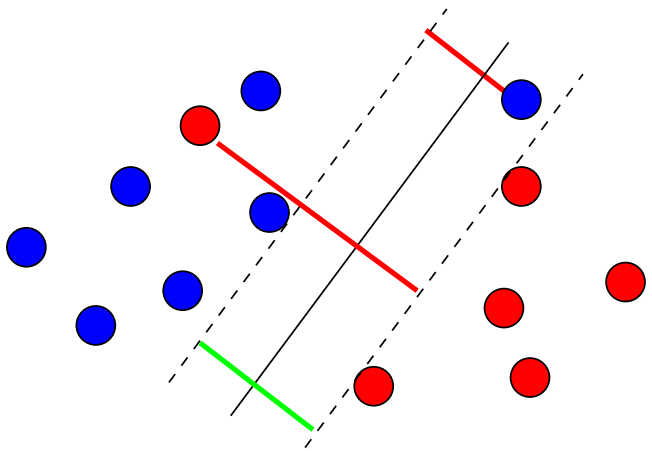


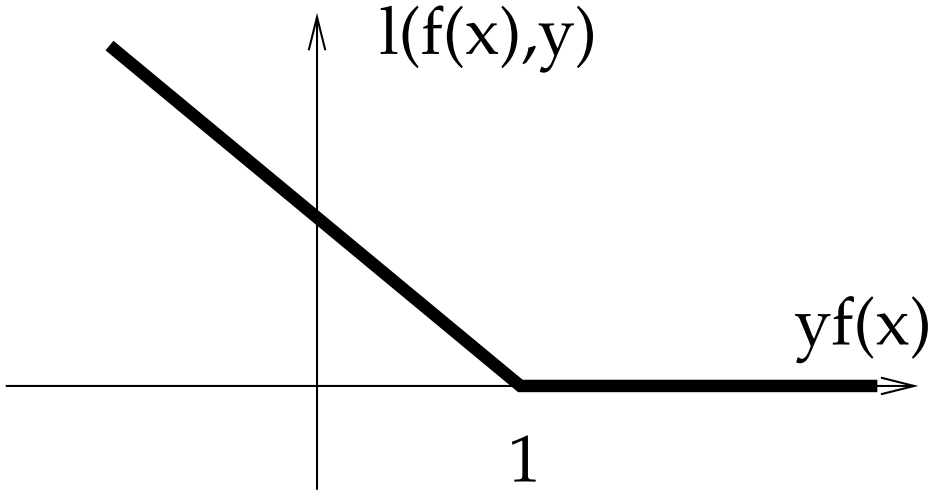
# Soft-margin SVM and hinge loss

$$\min_{\vec{w},b} \left\{ \sum_{i=1}^{n} \ell_{\text{hinge}} \left( \vec{w}.x_i + b, y_i \right) + \lambda \| \vec{w} \|_2^2 \right\} ,$$

for $\lambda = 1/C$ and the hinge loss function:

$$\ell_{\text{hinge}}(u, y) = \max(1 - yu, 0) = \begin{cases} 0 & \text{if } yu \geq 1, \\ 1 - yu & \text{otherwise.} \end{cases}$$





# Dual formulation of soft-margin SVM (*exercice*)

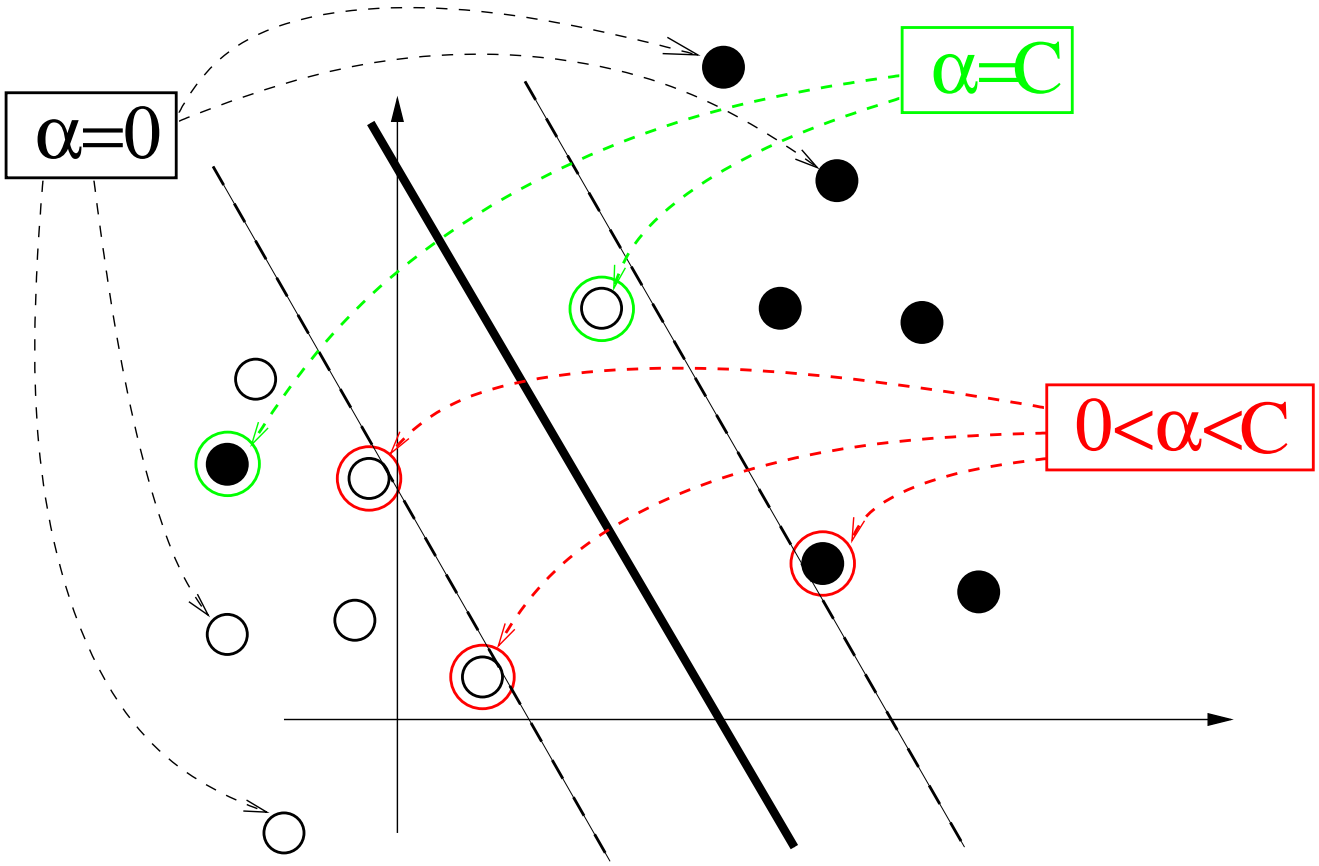
Maximize

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

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0. \end{cases}$$

# Interpretation: bounded and unbounded support vectors



# Primal (for large $n$) vs dual (for large $p$) optimization

1. Find $(\vec{w}, b) \in \mathbb{R}^{p+1}$ which solve:

$$\min_{\vec{w},b} \left\{ \sum_{i=1}^{n} \ell_{\text{hinge}} \left( \vec{w}.x_i + b, y_i \right) + \lambda \| \vec{w} \|_2^2 \right\} .$$

2. Find $\alpha^* \in \mathbb{R}^n$ which maximizes

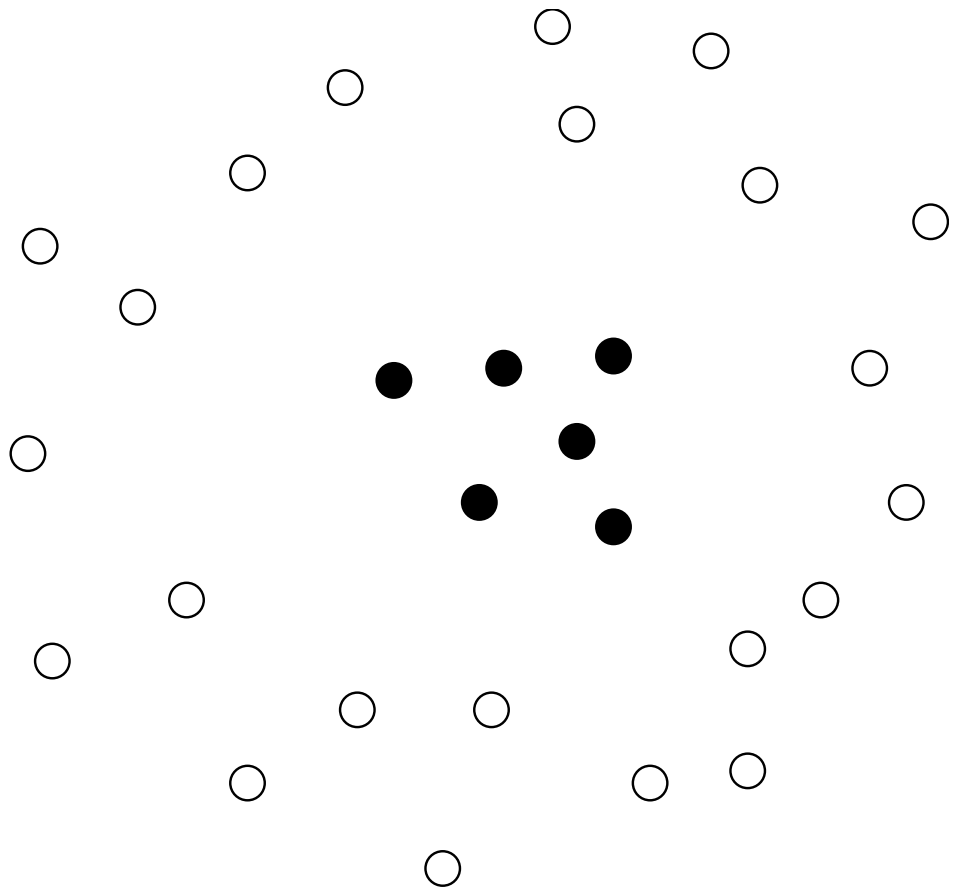
$$L(\vec{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \vec{x}_i . \vec{x}_j \, ,$$

under the constraints:

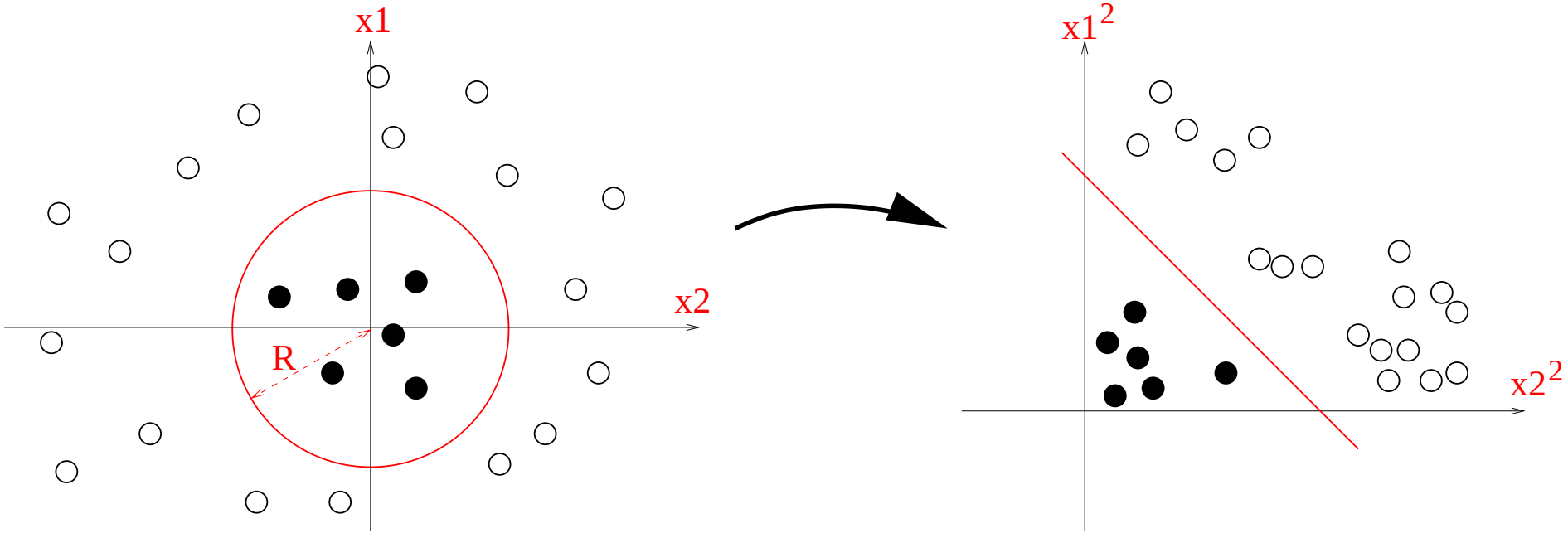
$$\begin{cases} 0 \leq \alpha_i \leq C, \quad \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0. \end{cases}$$

# Non-Linear Support Vector Machines and Kernels

# Sometimes linear methods are not interesting



# Solution: nonlinear mapping to a feature space




For $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ let $\Phi(x) = \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}$. The decision function is:

$$f(x) = x_1^2 + x_2^2 - R^2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}^\top \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix} - R^2 = \beta^\top \Phi(x) + b\,.$$

# Kernel = inner product in the feature space

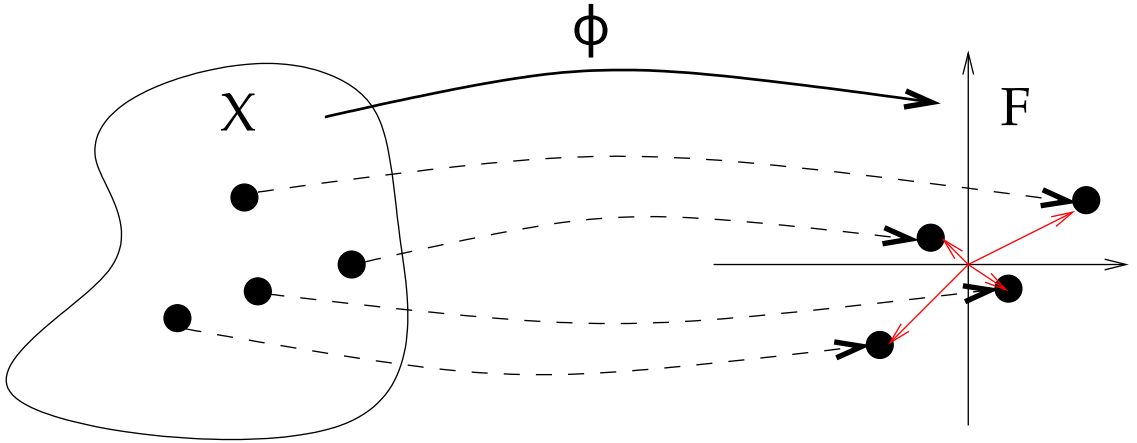
## Definition

For a given mapping

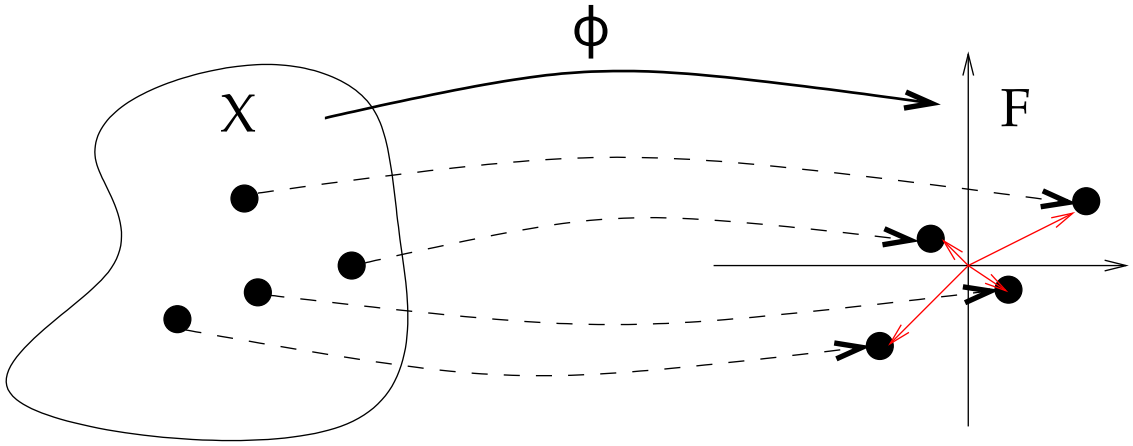
$$\Phi : \mathcal{X} \mapsto \mathcal{H}$$

from the space of objects $\mathcal{X}$ to some Hilbert space of features $\mathcal{H}$, the kernel between two objects $x$ and $x'$ is the inner product of their images in the features space:

$$\forall x, x' \in \mathcal{X}, \quad K(x, x') = \Phi(x)^\top \Phi(x') \,.$$



# Example

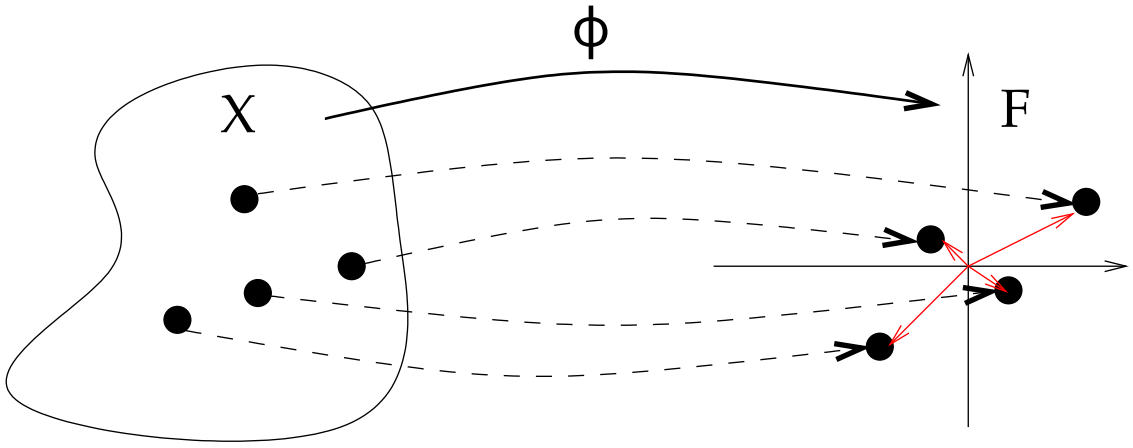



Let $\mathcal{X} = \mathcal{H} = \mathbb{R}^2$ and for $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ let $\Phi(x) = \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}$

Then

$$K(x, x') = \Phi(x)^\top \Phi(x') = (x_1)^2 (x_1')^2 + (x_2)^2 (x_2')^2 \,.$$

# The kernel tricks




## 2 tricks

1. Many linear algorithms (in particular linear SVM) can be performed in the feature space of $\Phi(x)$ without explicitly computing the images $\Phi(x)$, but instead by computing kernels $K(x, x')$.
2. It is sometimes possible to easily compute kernels which correspond to complex large-dimensional feature spaces: $K(x, x')$ is often much simpler to compute than $\Phi(x)$ and $\Phi(x')$

# Trick 1 : SVM in the original space

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^\top x_j \,,$$

  under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C \,, \quad \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0 \,. \end{cases}$$

- Predict with the decision function

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i x_i^\top x + b^* \,.$$

# Trick 1 : SVM in the feature space

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \Phi(x_i)^\top \Phi(x_j) \ ,$$

  under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C \,, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0 \,. \end{cases}$$

- Predict with the decision function

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i \Phi(x_i)^\top \Phi(x) + b^* \,.$$

# Trick 1 : SVM in the feature space with a kernel

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K\left(x_i, x_j\right) \ ,$$

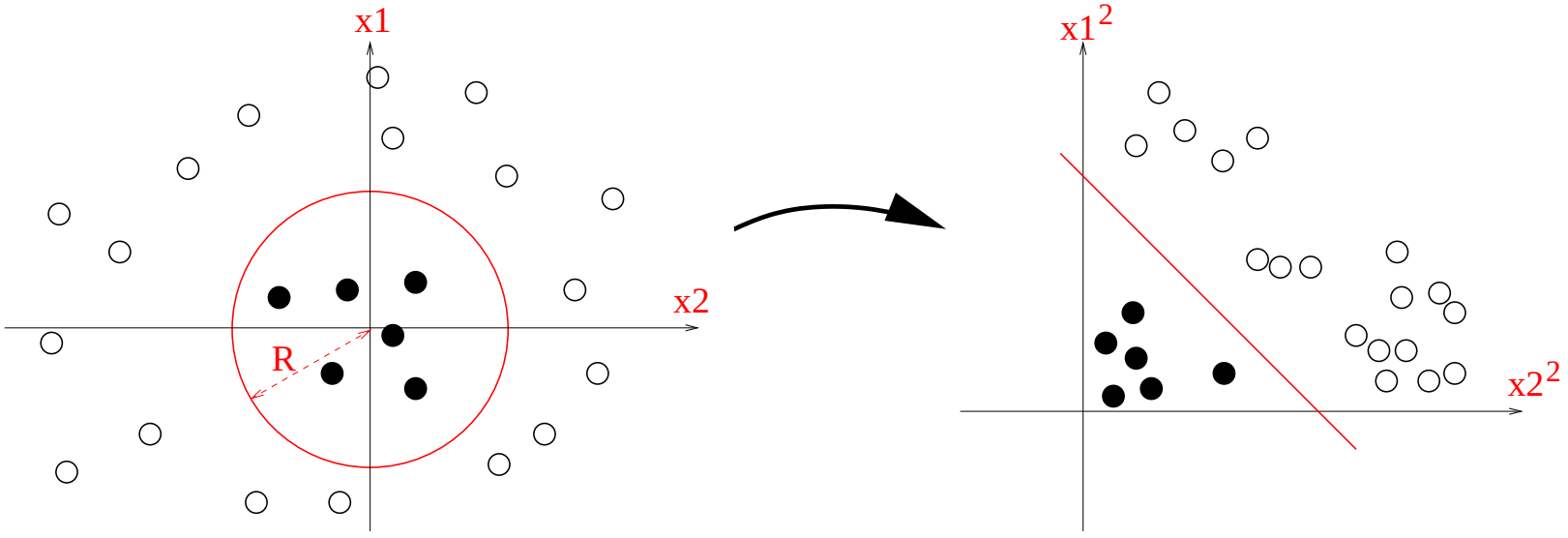
  under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C \,, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0 \,. \end{cases}$$

- Predict with the decision function

$$f(x) = \sum_{i=1}^{n} \alpha_i K\left(x_i, x\right) + b^* \,.$$

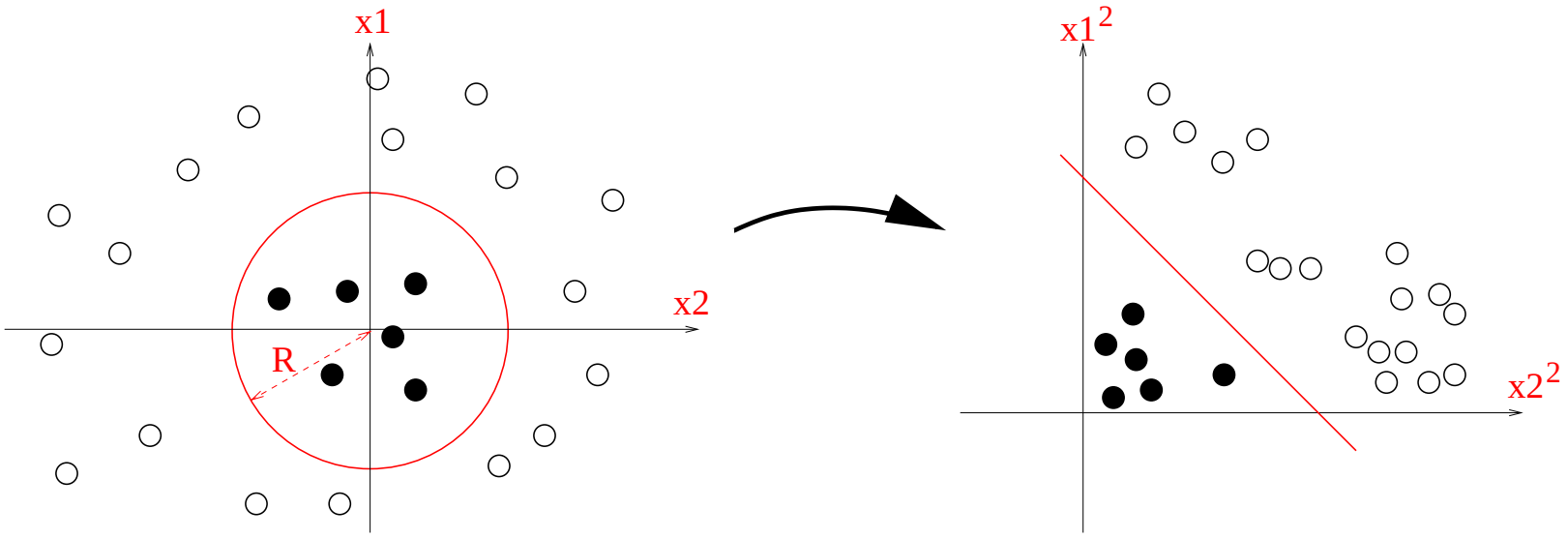
# Trick 2 illustration: polynomial kernel




For $x = (x_1, x_2)^\top \in \mathbb{R}^2$, let $\Phi(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$:

$$\begin{aligned} K(x, x') &= x_1^2 x_1'^2 + 2x_1x_2x_1'x_2' + x_2^2 x_2'^2 \\ &= \left(x_1x_1' + x_2x_2'\right)^2 \\ &= \left(x^\top x'\right)^2 . \end{aligned}$$

# Trick 2 illustration: polynomial kernel




More generally, for $x, x' \in \mathbb{R}^p$,

$$K(x, x') = \left(x^\top x' + 1\right)^d$$

is an inner product in a feature space of all monomials of degree up to $d$ *(left as exercice.)*

# Combining tricks: learn a polynomial discrimination rule with SVM

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \left( x_i^\top x_j + 1 \right)^d ,$$

  under the constraints:

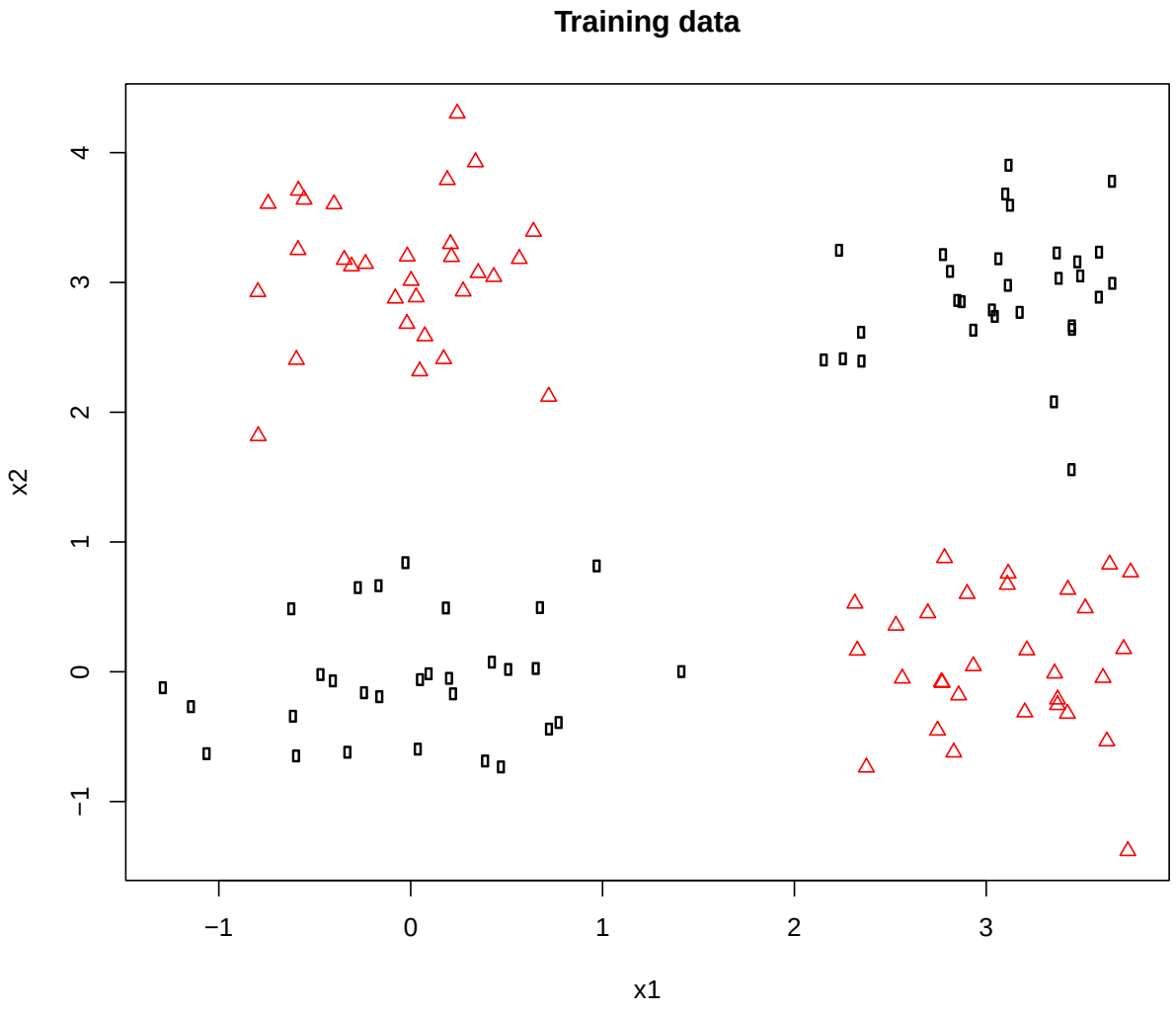
$$\begin{cases} 0 \leq \alpha_i \leq C , & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0 . \end{cases}$$

- Predict with the decision function

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i \left( x_i^\top x + 1 \right)^d + b^* .$$

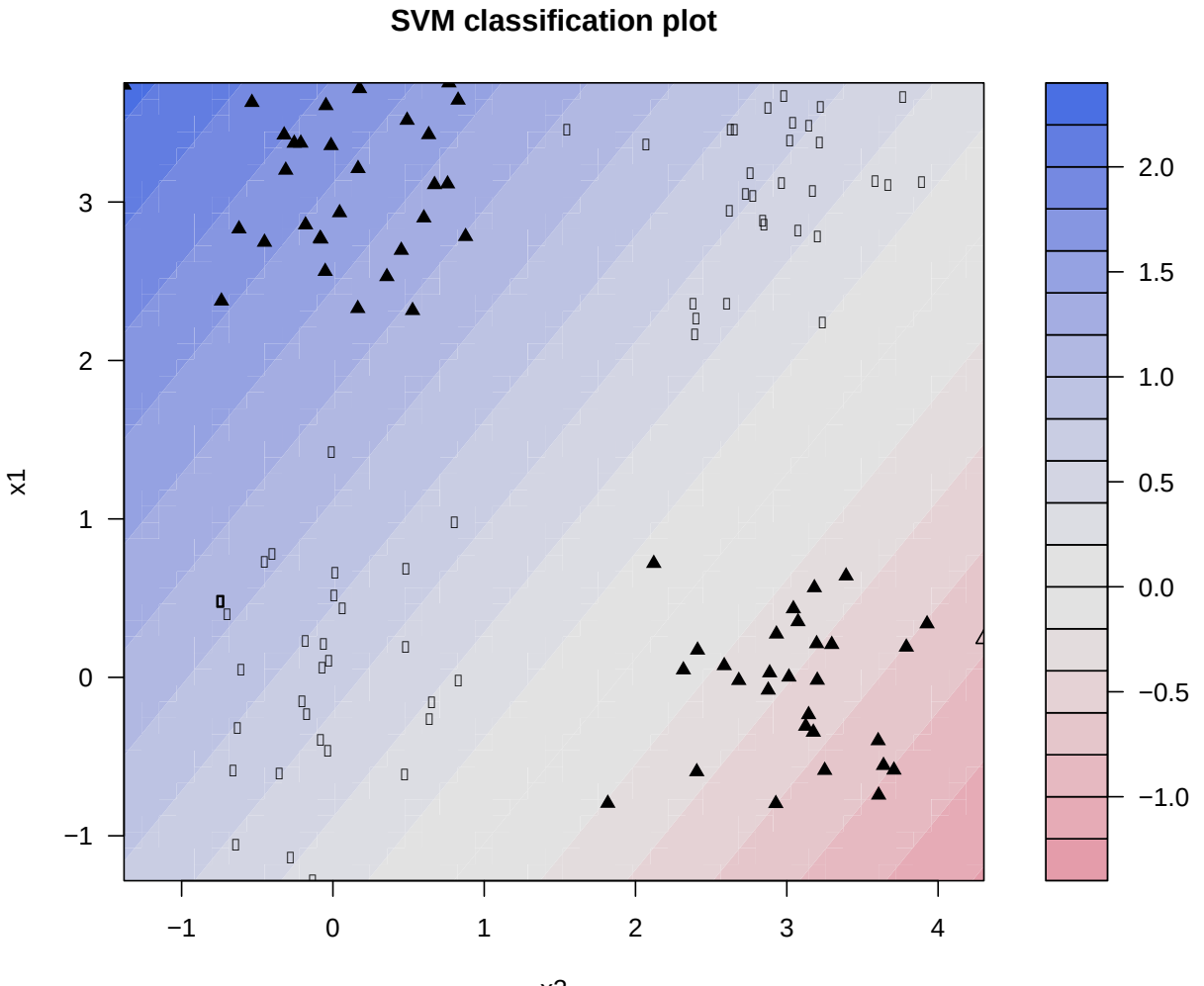
# Illustration: toy nonlinear problem

```
> plot(x,col=ifelse(y>0,1,2),pch=ifelse(y>0,1,2))
```



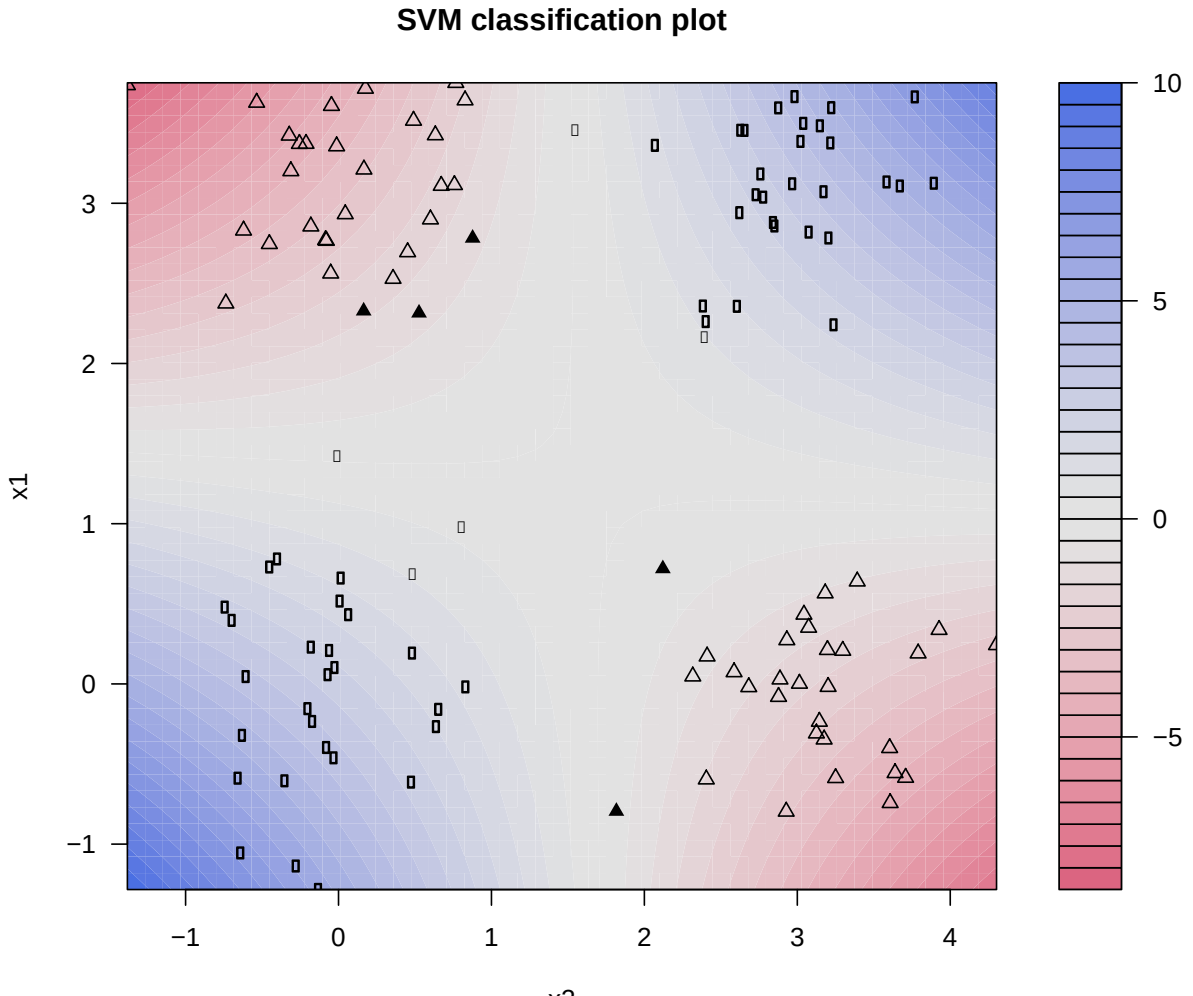
# Illustration: toy nonlinear problem, linear SVM

```
> library(kernlab)
> svp <- ksvm(x,y,type="C-svc",kernel='vanilladot')
> plot(svp,data=x)
```



# Illustration: toy nonlinear problem, polynomial SVM

```
> svp <- ksvm(x,y,type="C-svc", ...
                          kernel=polydot(degree=2))
> plot(svp,data=x)
```



# Which functions $K(x, x')$ are kernels?

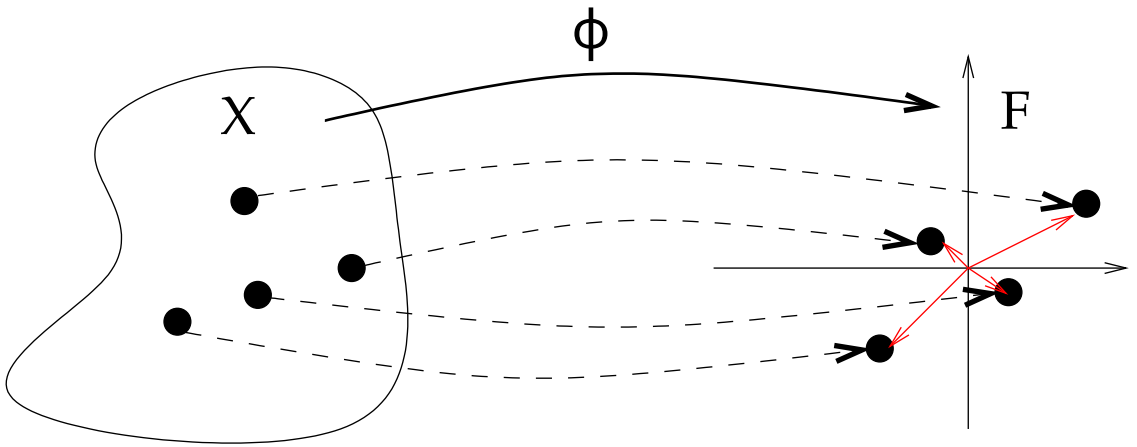
## Definition

A function $K(x, x')$ defined on a set $\mathcal{X}$ is a kernel if and only if there exists a features space (Hilbert space) $\mathcal{H}$ and a mapping

$$\Phi : \mathcal{X} \mapsto \mathcal{H} \ ,$$

such that, for any $x, x'$ in $\mathcal{X}$:

$$K\left(x, x'\right) = \left\langle \Phi\left(x\right), \Phi\left(x'\right) \right\rangle_{\mathcal{H}} \ .$$



# Positive Definite (p.d.) functions

## Definition

A positive definite (p.d.) function on the set $\mathcal{X}$ is a function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ symmetric:

$$\forall \left(\mathbf{x}, \mathbf{x}'\right) \in \mathcal{X}^2, \quad K\left(\mathbf{x}, \mathbf{x}'\right) = K\left(\mathbf{x}', \mathbf{x}\right),$$

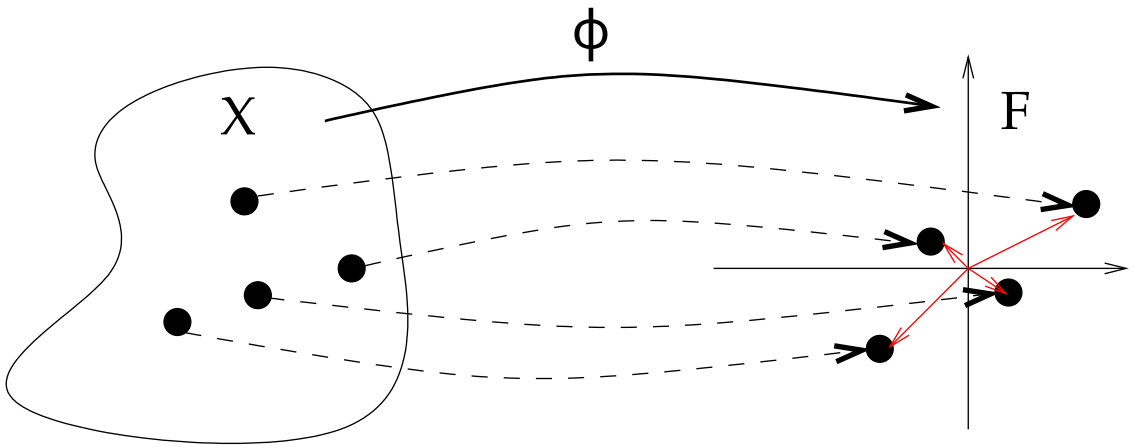
and which satisfies, for all $N \in \mathbb{N}$, $(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \in \mathcal{X}^N$ et $(a_1, a_2, \ldots, a_N) \in \mathbb{R}^N$:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j K\left(\mathbf{x}_i, \mathbf{x}_j\right) \geq 0.$$

# Kernels are p.d. functions

**Theorem (Aronszajn, 1950)**

*$K$ is a kernel if and only if it is a positive definite function.*



# Proof?

- Kernel $\Longrightarrow$ p.d. function:
  - $\langle \Phi(\mathbf{x}), \Phi(\mathbf{x}') \rangle_{\mathbb{R}^d} = \langle \Phi(\mathbf{x}'), \Phi(\mathbf{x})_{\mathbb{R}^d} \rangle$ ,
  - $\sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle_{\mathbb{R}^d} = \| \sum_{i=1}^{N} a_i \Phi(\mathbf{x}_i) \|^2_{\mathbb{R}^d} \geq 0$ .
- P.d. function $\Longrightarrow$ kernel: more difficult...

# Kernel examples

- **Polynomial** $\mathcal{X} = \mathbb{R}^m$

$$K(u, v) = (u.v + c)^d$$

- **Gaussian Radial Basis Function (RBF)** $\mathcal{X} = \mathbb{R}^m$

$$K(u, v) = \exp\left(-\frac{|u - v|^2}{2\sigma^2}\right)$$

- **Min** $\mathcal{X} = \mathbb{R}_+$

$$K(u, v) = \min(u, v)$$

# Example: SVM with a Gaussian kernel

- Training:

$$\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \exp\left( -\frac{||\vec{x}_i - \vec{x}_j||^2}{2\sigma^2} \right)$$

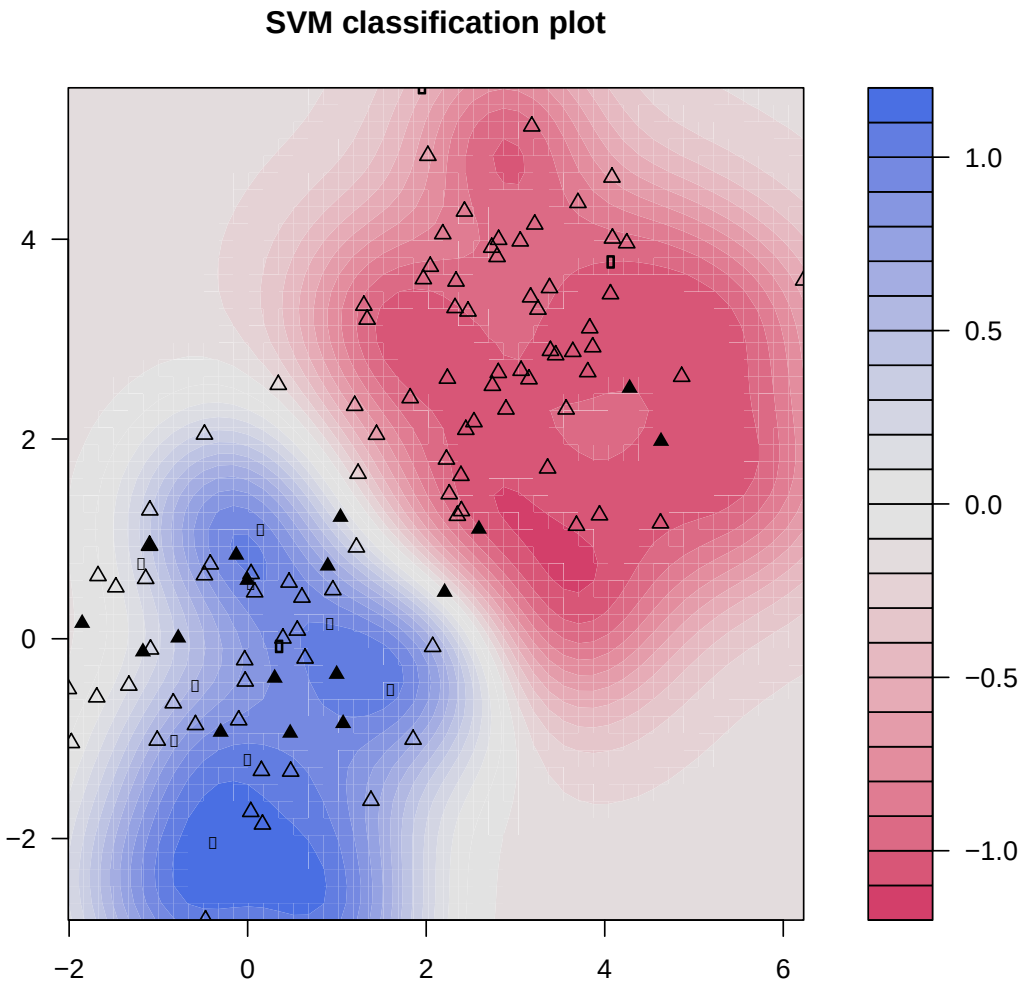
$$\text{s.t. } 0 \leq \alpha_i \leq C, \quad \text{and } \sum_{i=1}^{n} \alpha_i y_i = 0.$$

- Prediction

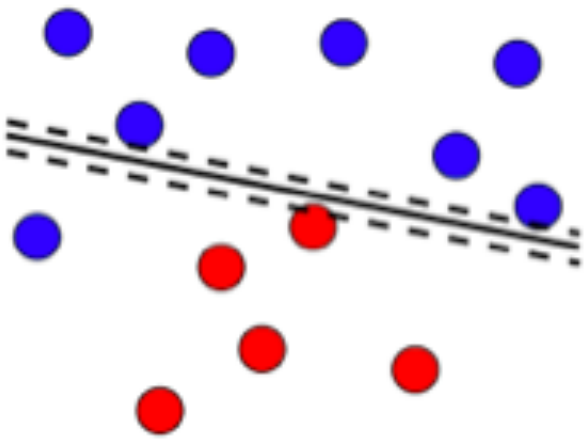
$$f(\vec{x}) = \sum_{i=1}^{n} \alpha_i \exp\left( -\frac{||\vec{x} - \vec{x}_i||^2}{2\sigma^2} \right)$$

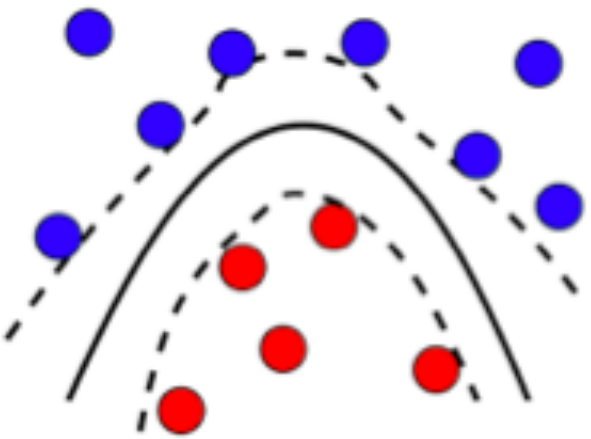
# Example: SVM with a Gaussian kernel

$$f(\vec{x}) = \sum_{i=1}^{n} \alpha_i \exp\left(-\frac{||\vec{x} - \vec{x}_i||^2}{2\sigma^2}\right)$$

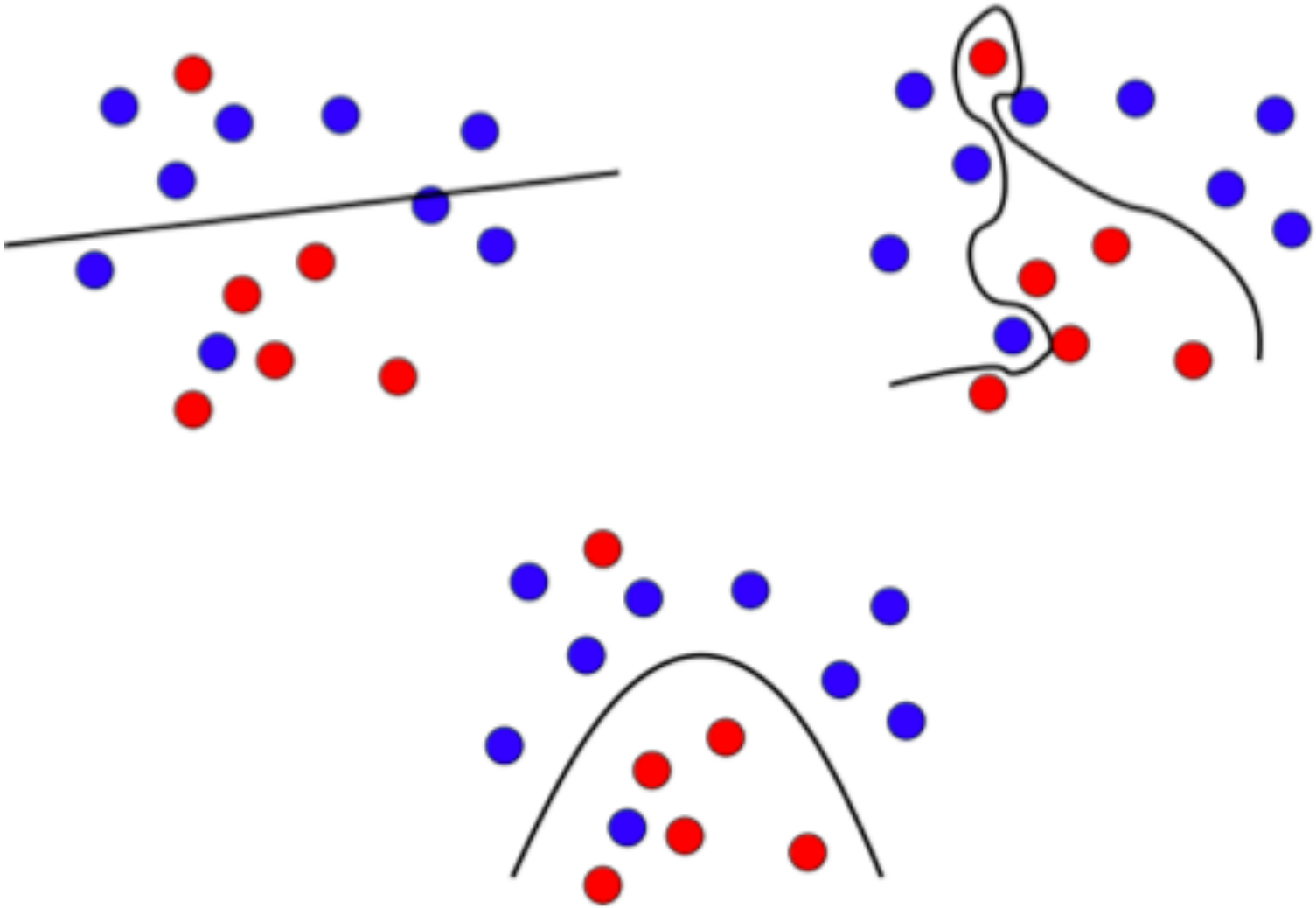


# Linear vs nonlinear SVM





# Regularity vs data fitting trade-off

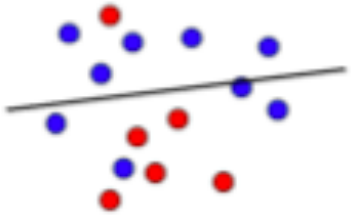


# $C$ controls the trade-off

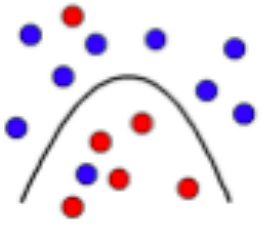
$$\min_f \left\{ \frac{1}{margin(f)} + C \times errors(f) \right\}$$

- Large C :
  - makes few errors

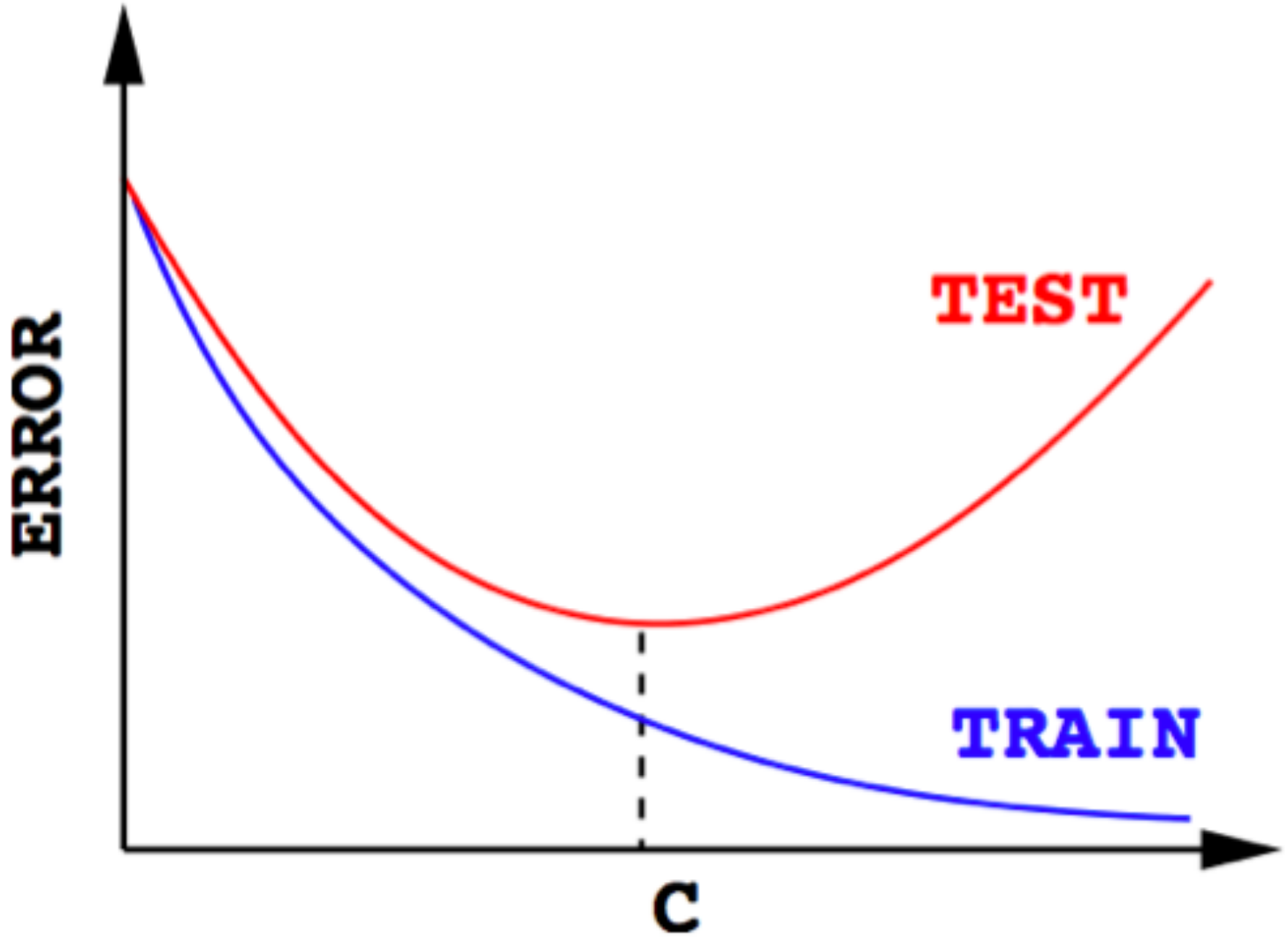
- Small C :
  - ensure a large margin



- Intermediate C:
  - finds a trade-off



# Why it is important to control the trade-off



# How to choose $C$ in practice

- Split your dataset in two ("train" and "test")
- Train SVM with different $C$ on the "train" set
- Compute the accuracy of the SVM on the "test" set
- Choose the $C$ which minimizes the "test" error
- (you may repeat this several times = cross-validation)

# Kernels for Strings

# Supervised sequence classification

## Data (training)

- Secreted proteins:

```
MASKATLLLAFTLLFATCIARHQQRQQQQNQCQLQNIEA...
MARSSLFTFLCLAVFINGCLSQIEQQSPWEFQGSEVW...
MALHTVLIMLSLLPMLEAQNPEHANITIGEPITNETLGWL...
...
```

- Non-secreted proteins:

```
MAPPSVFAEVPQAQPVLVFKLIADFREDPDPRKVNLGVG...
MAHTLGLTQPNSTEPHKISFTAKEIDVIEWKGDILVVG...
MSISESYAKEIKTAFRQFTDFPIEGEQFEDFLPIIGNP..
...
```

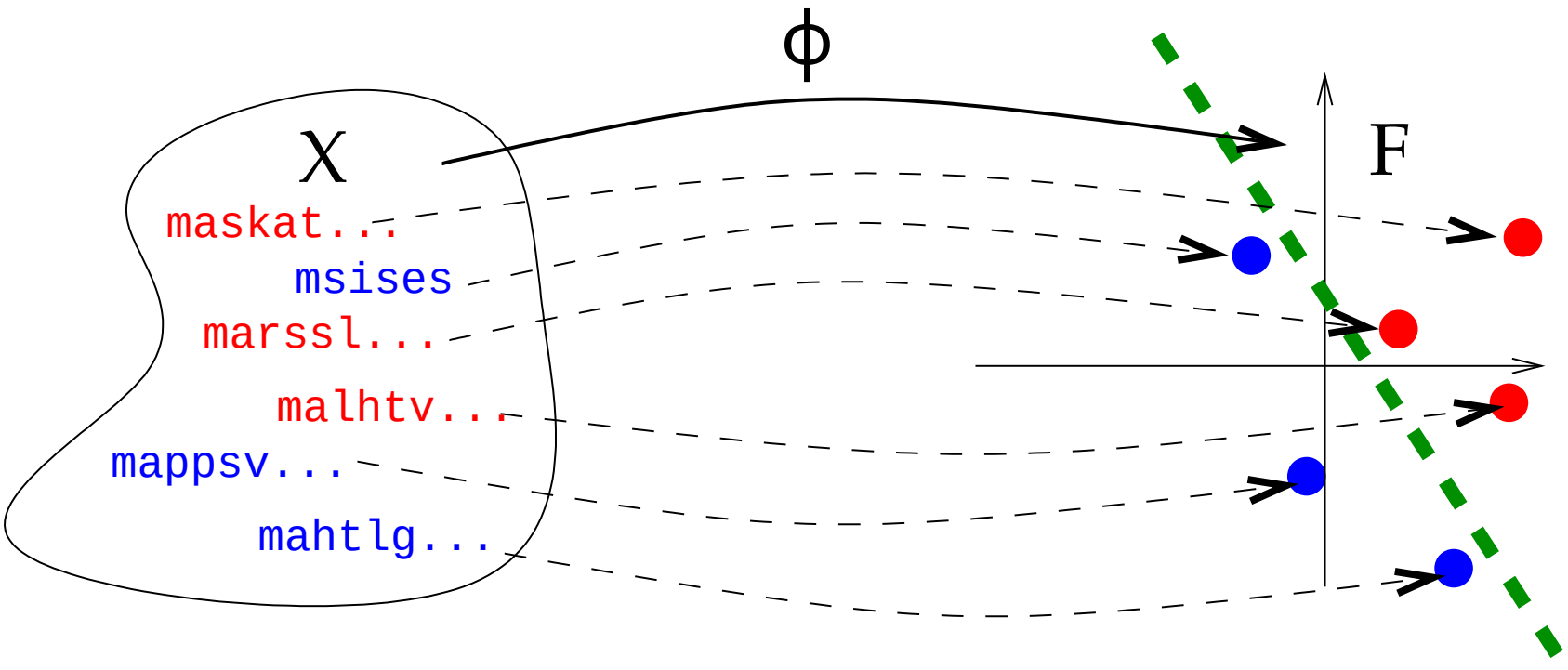
## Goal

- Build a classifier to predict whether new proteins are secreted or not.

# String kernels

## The idea

- Map each string $x \in \mathcal{X}$ to a vector $\Phi(x) \in \mathcal{F}$.
- Train a classifier for vectors on the images $\Phi(x_1), \ldots, \Phi(x_n)$ of the training set (nearest neighbor, linear perceptron, logistic regression, support vector machine...)



# Example: substring indexation

## The approach

Index the feature space by fixed-length strings, i.e.,

$$\Phi(\mathbf{x}) = (\Phi_u(\mathbf{x}))_{u \in \mathcal{A}^k}$$

where $\Phi_u(\mathbf{x})$ can be:

- the number of occurrences of $u$ in $\mathbf{x}$ (without gaps) : spectrum kernel (Leslie et al., 2002)
- the number of occurrences of $u$ in $\mathbf{x}$ up to $m$ mismatches (without gaps) : mismatch kernel (Leslie et al., 2004)
- the number of occurrences of $u$ in $\mathbf{x}$ allowing gaps, with a weight decaying exponentially with the number of gaps : substring kernel (Lohdi et al., 2002)

# Spectrum kernel (1/2)

## Kernel definition

- The 3-spectrum of

$$\mathbf{x} = \texttt{CGGSLIAMMWFGV}$$

is:

$$(\texttt{CGG}, \texttt{GGS}, \texttt{GSL}, \texttt{SLI}, \texttt{LIA}, \texttt{IAM}, \texttt{AMM}, \texttt{MMW}, \texttt{MWF}, \texttt{WFG}, \texttt{FGV}) \ .$$

- Let $\Phi_u(\mathbf{x})$ denote the number of occurrences of $u$ in $\mathbf{x}$. The $k$-spectrum kernel is:

$$K(\mathbf{x}, \mathbf{x}') := \sum_{u \in \mathcal{A}^k} \Phi_u(\mathbf{x}) \Phi_u(\mathbf{x}') \ .$$

# Spectrum kernel (2/2)

## Implementation

- The computation of the kernel is formally a sum over $|\mathcal{A}|^k$ terms, but at most $|\mathbf{x}| - k + 1$ terms are non-zero in $\Phi(\mathbf{x}) \implies$ Computation in $O(|\mathbf{x}| + |\mathbf{x}'|)$ with pre-indexation of the strings.
- Fast classification of a sequence $\mathbf{x}$ in $O(|\mathbf{x}|)$:

$$f(\mathbf{x}) = \mathbf{w} \cdot \Phi(\mathbf{x}) = \sum_u w_u \Phi_u(\mathbf{x}) = \sum_{i=1}^{|\mathbf{x}|-k+1} w_{x_i \ldots x_{i+k-1}}.$$

## Remarks

- Work with any string (natural language, time series...)
- Fast and scalable, a good default method for string classification.
- Variants allow matching of $k$-mers up to $m$ mismatches.

# Local alignmnent kernel (Saigo et al., 2004)

```
CGGSLIAMM----WFGV
|...|||||....||||
C---LIVMMNRLMWFGV
```

$$s_{S,g}(\pi) = S(C,C) + S(L,L) + S(I,I) + S(A,V) + 2S(M,M) + S(W,W) + S(F,F) + S(G,G) + S(V,V) - g(3) - g(4)$$

$$SW_{S,g}(x,y) := \max_{\pi \in \Pi(x,y)} s_{S,g}(\pi) \quad \text{is not a kernel}$$

$$K_{LA}^{(\beta)}(x,y) = \sum_{\pi \in \Pi(x,y)} \exp\left(\beta s_{S,g}(x,y,\pi)\right) \quad \text{is a kernel}$$

# LA kernel is p.d.: proof (1/2)

## Definition: Convolution kernel (Haussler, 1999)

Let $K_1$ and $K_2$ be two p.d. kernels for strings. The convolution of $K_1$ and $K_2$, denoted $K_1 \star K_2$, is defined for any $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$ by:

$$K_1 \star K_2(\mathbf{x}, \mathbf{y}) := \sum_{\mathbf{x}_1\mathbf{x}_2=\mathbf{x}, \mathbf{y}_1\mathbf{y}_2=\mathbf{y}} K_1(\mathbf{x}_1, \mathbf{y}_1) K_2(\mathbf{x}_2, \mathbf{y}_2).$$

## Lemma

*If $K_1$ and $K_2$ are p.d. then $K_1 \star K_2$ is p.d..*

# LA kernel is p.d.: proof (2/2)

$$K_{LA}^{(\beta)} = \sum_{n=0}^{\infty} K_0 \star \left( K_a^{(\beta)} \star K_g^{(\beta)} \right)^{(n-1)} \star K_a^{(\beta)} \star K_0 \,,$$

with

- The constant kernel:

$$K_0 (\mathbf{x}, \mathbf{y}) := 1 \,.$$

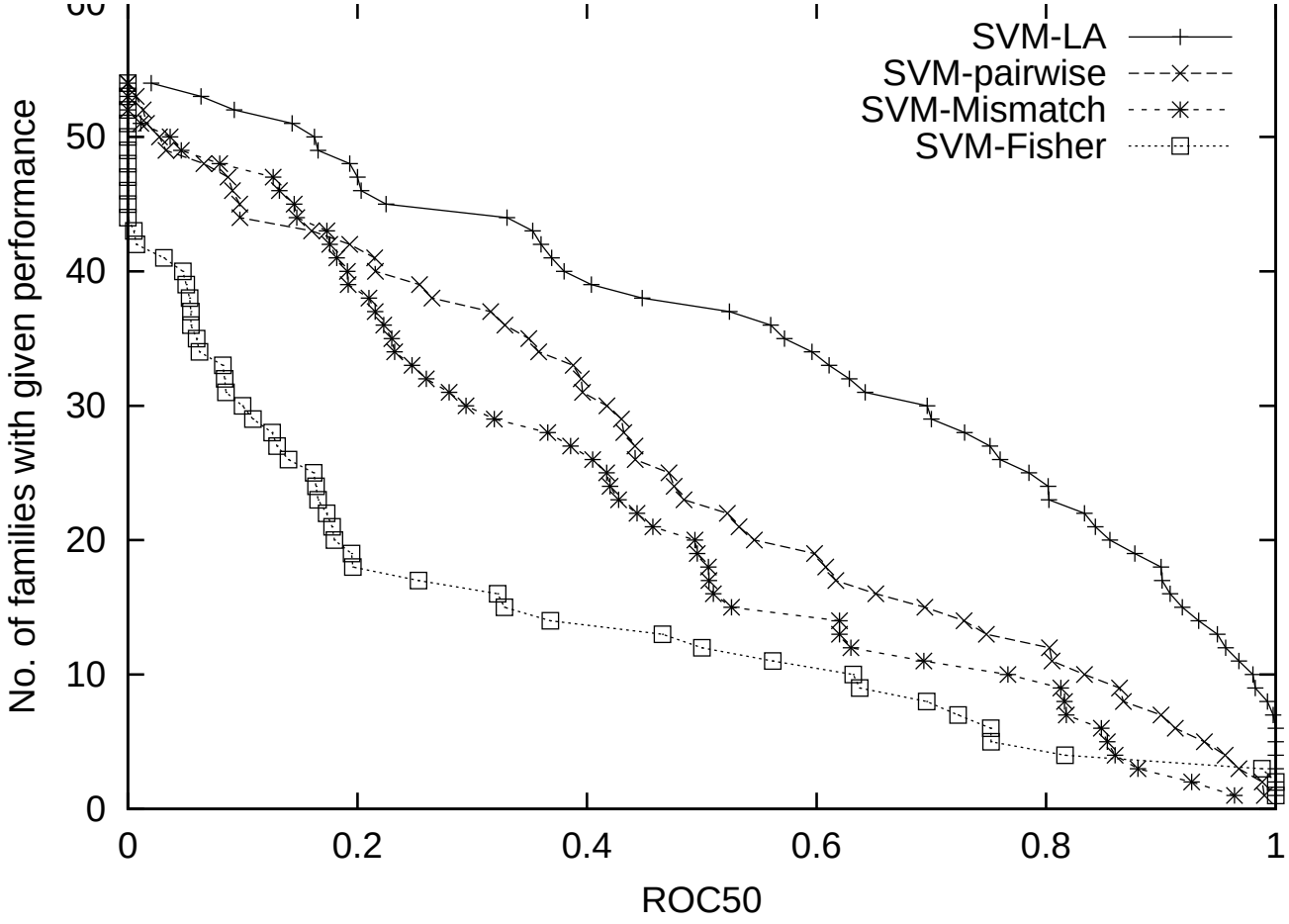
- A kernel for letters:

$$K_a^{(\beta)} (\mathbf{x}, \mathbf{y}) := \begin{cases} 0 & \text{if } |\mathbf{x}| \neq 1 \text{ where } |\mathbf{y}| \neq 1 \,, \\ \exp(\beta S(\mathbf{x}, \mathbf{y})) & \text{otherwise} \,. \end{cases}$$

- A kernel for gaps:

$$K_g^{(\beta)} (\mathbf{x}, \mathbf{y}) = \exp\left[\beta \left( g(|\mathbf{x}|) + g(|\mathbf{x}|) \right)\right] \,.$$

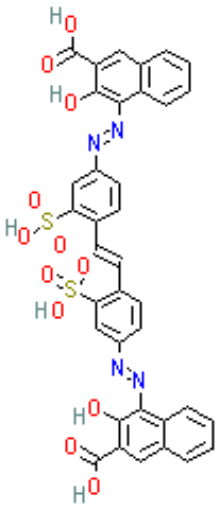
# The choice of kernel matters



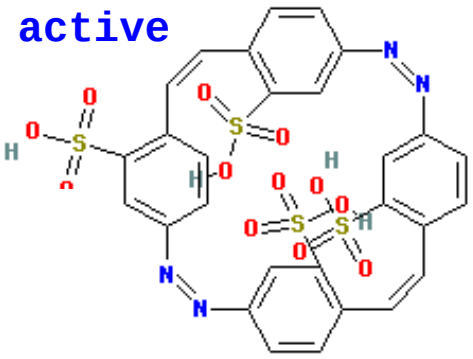

Performance on the SCOP superfamily recognition benchmark (from Saigo et al., 2004).

# Kernels for Graphs

# Virtual screening for drug discovery



active



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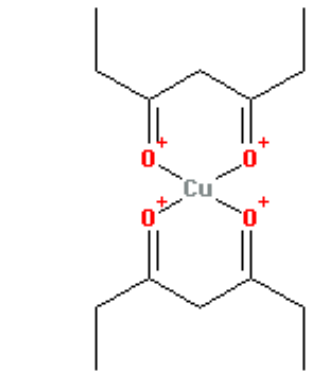

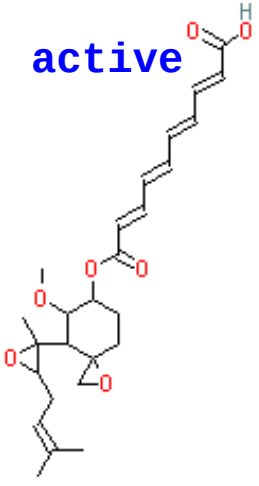

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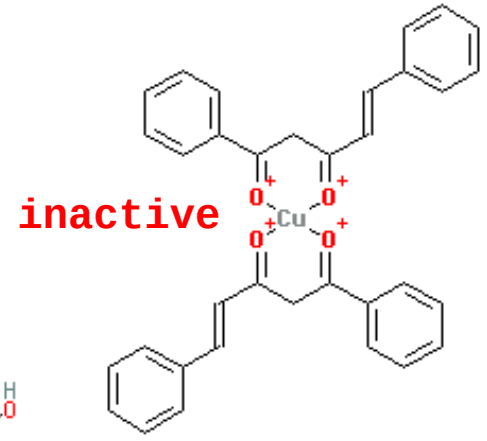

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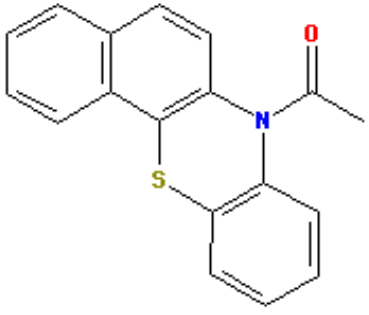
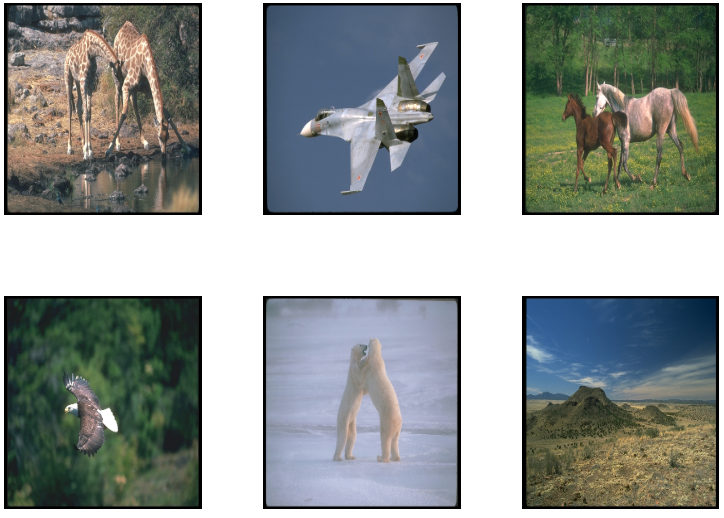
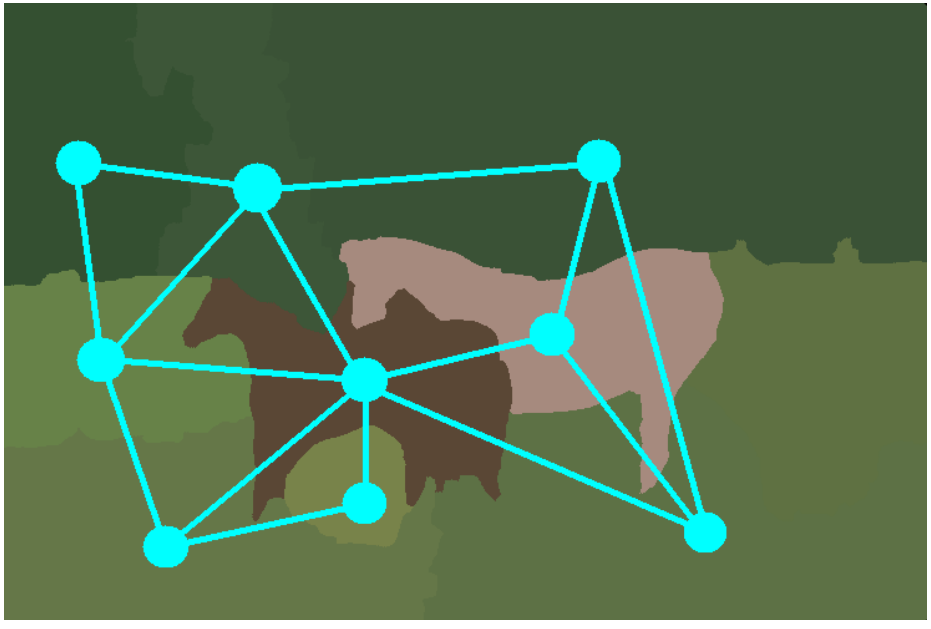


inactive

*NCI AIDS screen results (from http://cactus.nci.nih.gov).*

# Image retrieval and classification





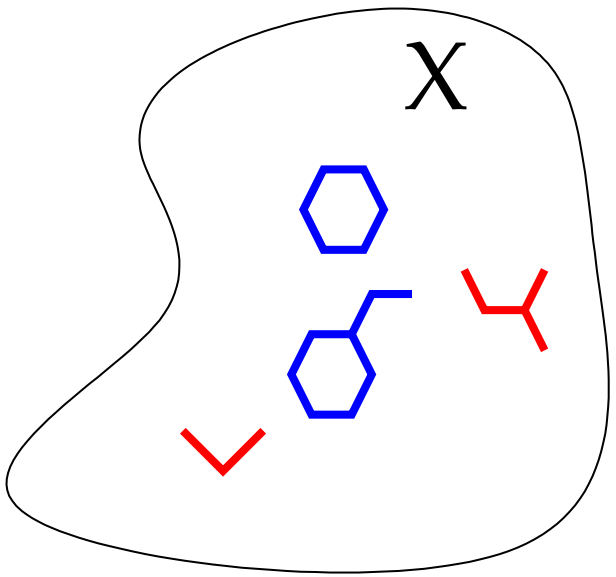
*From Harchaoui and Bach (2007).*

# Graph kernels

1. Represent each graph $x$ by a vector $\Phi(x) \in \mathcal{H}$, either explicitly or implicitly through the kernel

$$K(x, x') = \Phi(x)^\top \Phi(x') \,.$$

2. Use a linear method for classification in $\mathcal{H}$.



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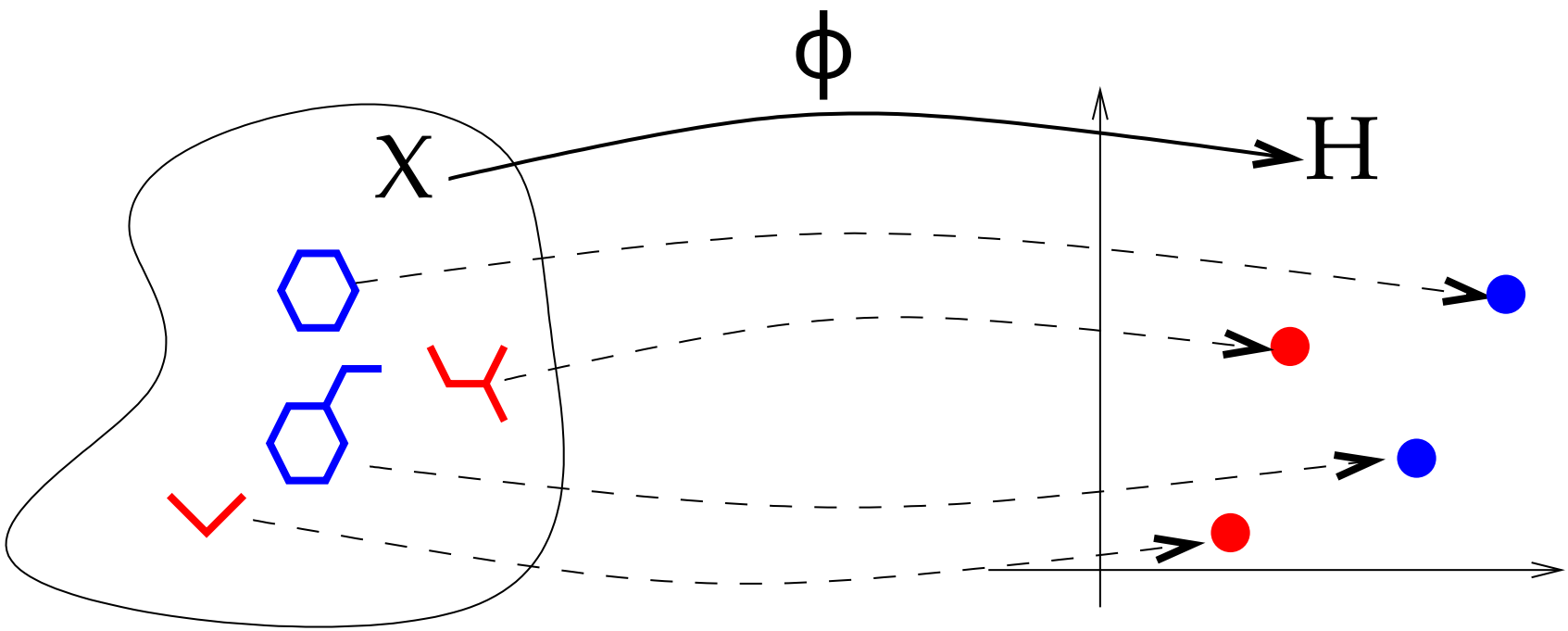

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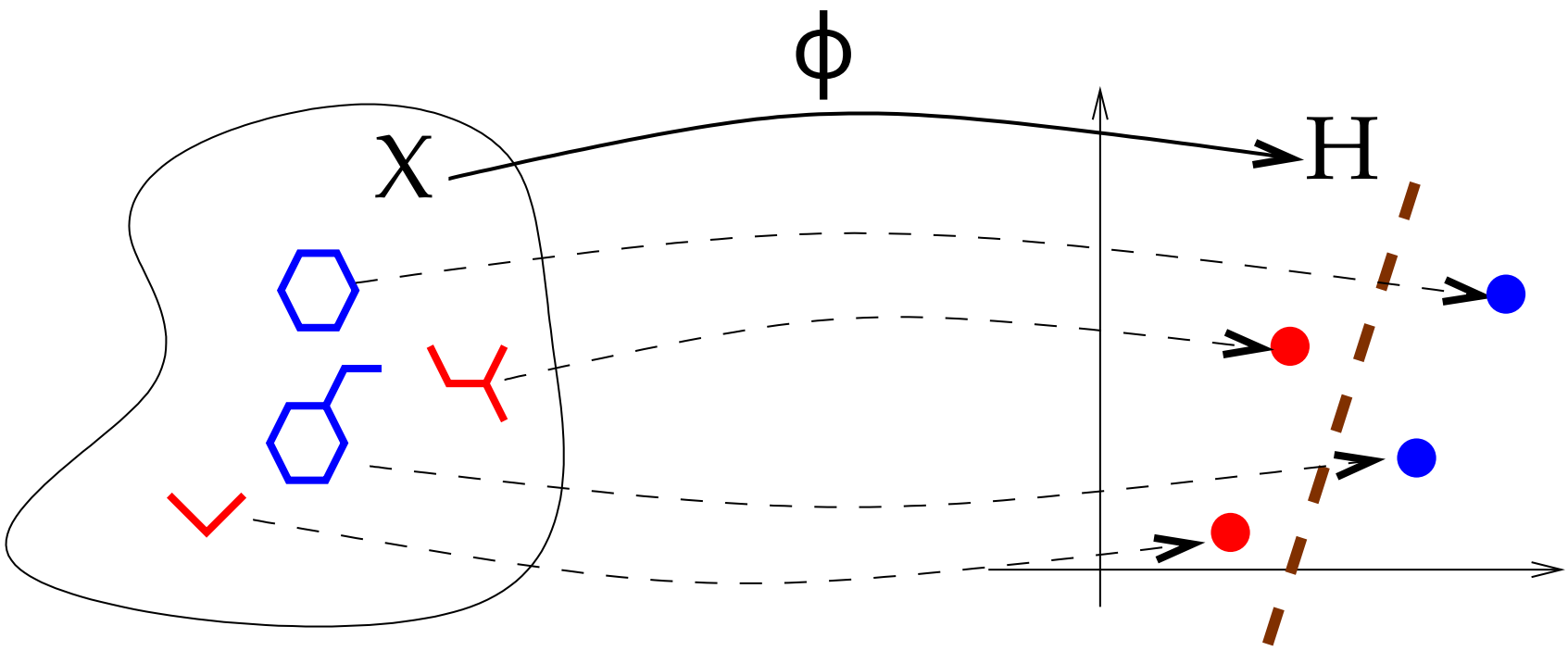
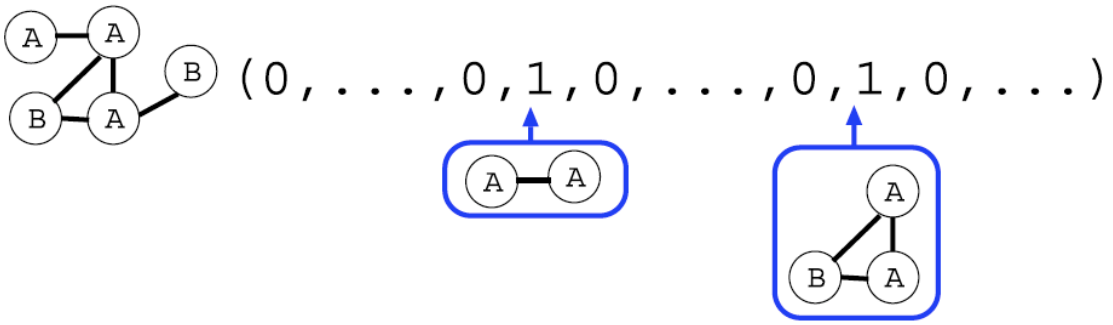


# Indexing by all subgraphs?




**Theorem**

*Computing all subgraph occurrences is NP-hard.*

**Proof.**

- The linear graph of size $n$ is a subgraph of a graph $X$ with $n$ vertices iff $X$ has an Hamiltonian path
- The decision problem whether a graph has a Hamiltonian path is NP-complete.

□

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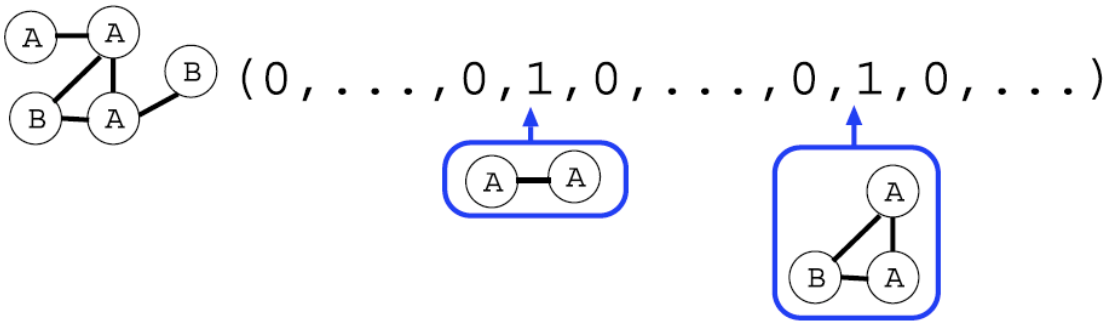


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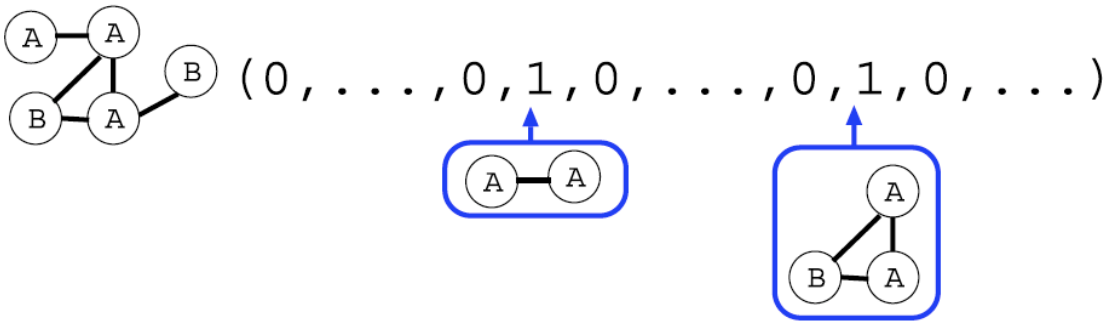


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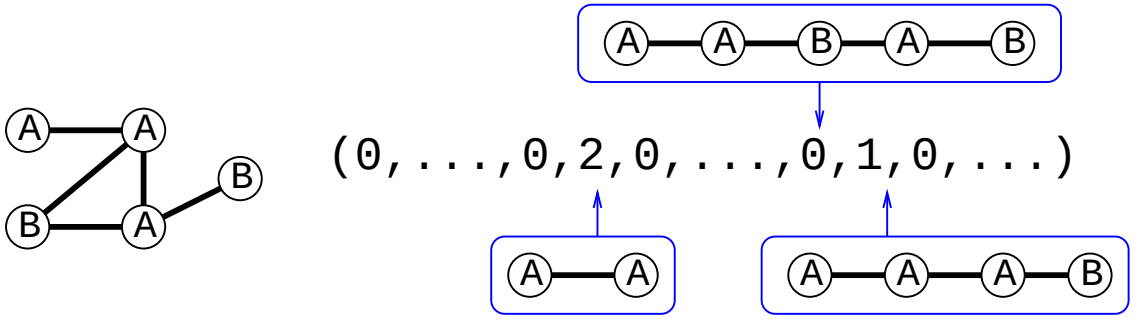
# Indexing by specific subgraphs

## Substructure selection

We can imagine more limited sets of substuctures that lead to more computationnally efficient indexing (non-exhaustive list)

- substructures selected by domain knowledge (MDL fingerprint)
- all path up to length $k$ (Openeye fingerprint, Nicholls 2005)
- all shortest paths (Borgwardt and Kriegel, 2005)
- all subgraphs up to $k$ vertices (graphlet kernel, Sherashidze et al., 2009)
- all frequent subgraphs in the database (Helma et al., 2004)

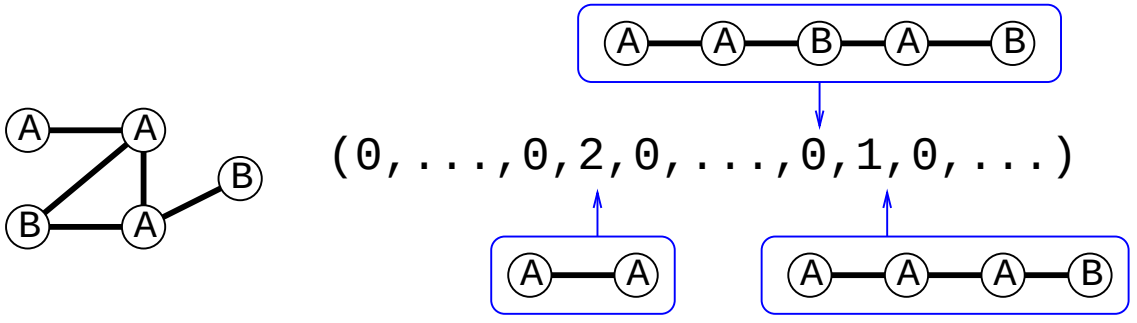
# Example : Indexing by all shortest paths




## Properties (Borgwardt and Kriegel, 2005)

- There are $O(n^2)$ shortest paths.
- The vector of counts can be computed in $O(n^4)$ with the Floyd-Warshall algorithm.

# Example : Indexing by all shortest paths

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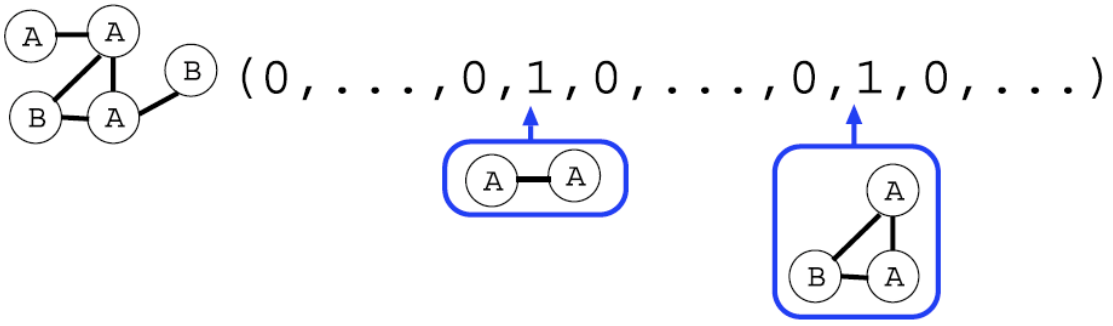
# Example : Indexing by all subgraphs up to $k$ vertices




## Properties (Shervashidze et al., 2009)

- Naive enumeration scales as $O(n^k)$.
- Enumeration of connected graphlets in $O(nd^{k-1})$ for graphs with degree $\leq d$ and $k \leq 5$.
- Randomly sample subgraphs if enumeration is infeasible.

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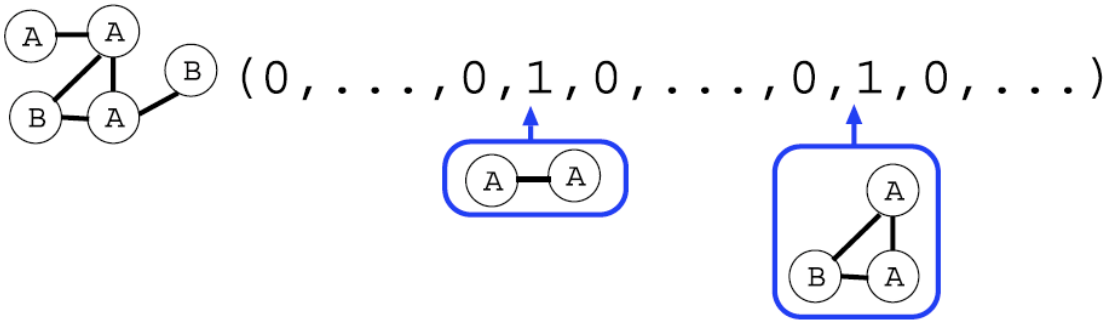


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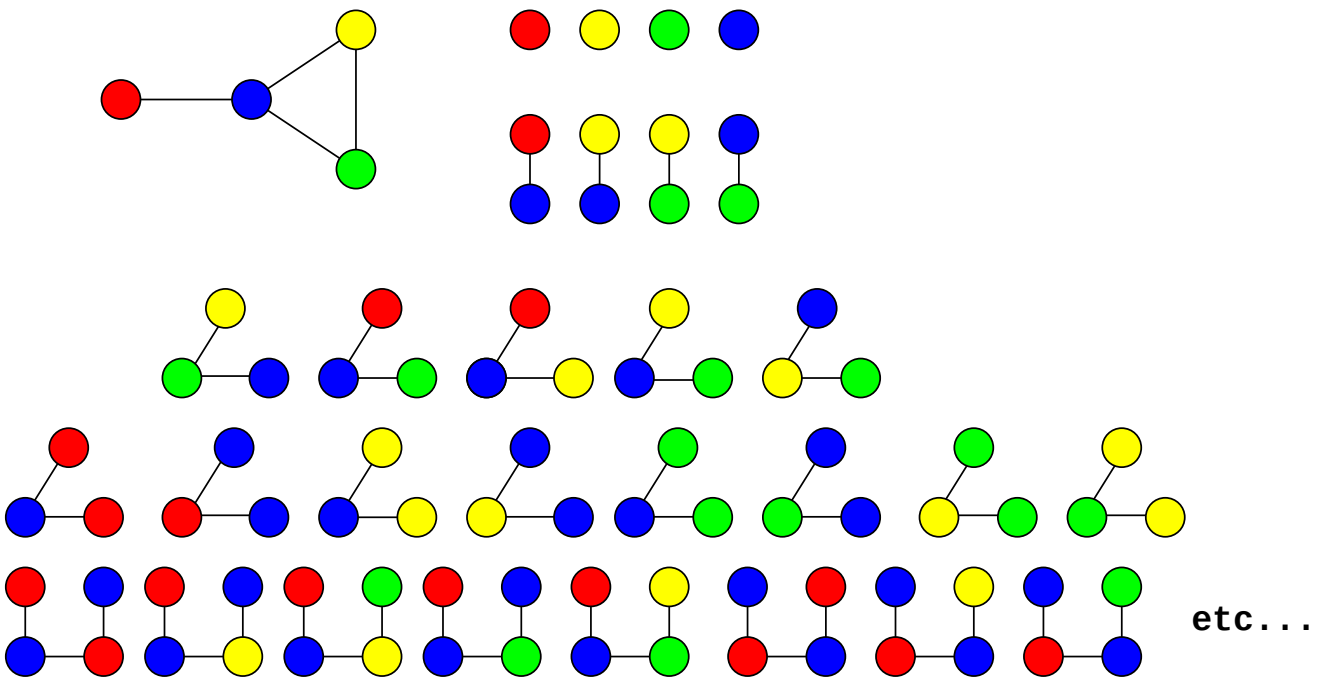
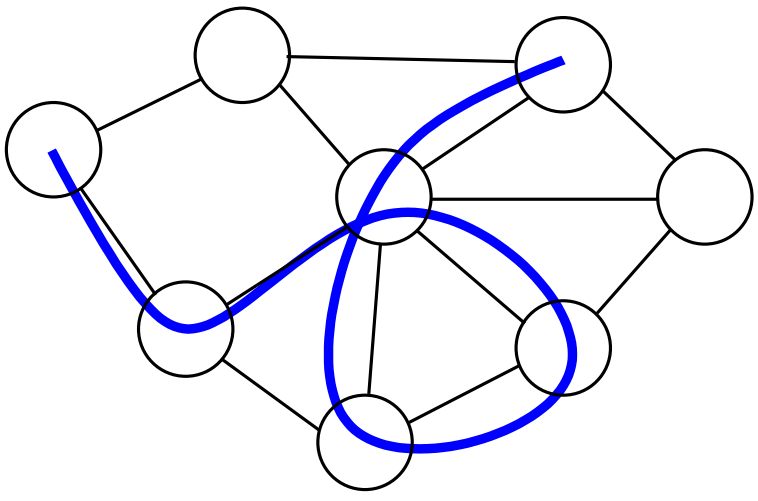
# Walks

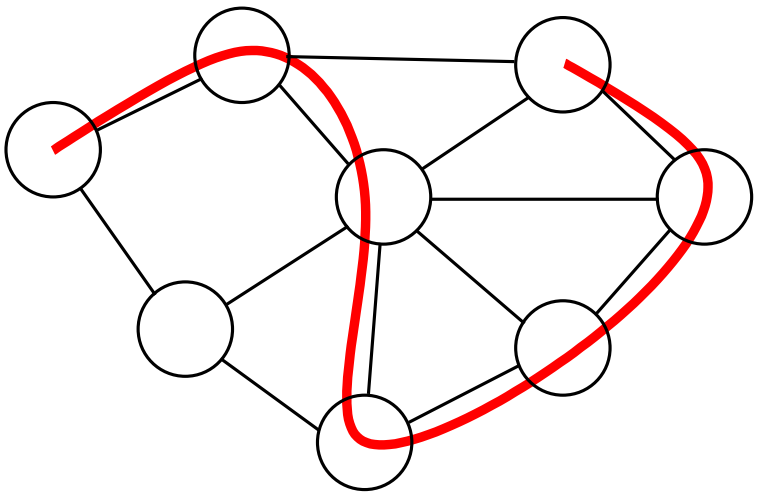
## Definition

- A walk of a graph $(V, E)$ is sequence of $v_1, \ldots, v_n \in V$ such that $(v_i, v_{i+1}) \in E$ for $i = 1, \ldots, n-1$.
- We note $\mathcal{W}_n(G)$ the set of walks with $n$ vertices of the graph $G$, and $\mathcal{W}(G)$ the set of all walks.



# Walks $\neq$ paths





# Walk kernel

## Definition

- Let $\mathcal{S}_n$ denote the set of all possible label sequences of walks of length $n$ (including vertices and edges labels), and $\mathcal{S} = \cup_{n \geq 1} \mathcal{S}_n$.
- For any graph $\mathcal{X}$ let a weight $\lambda_G(w)$ be associated to each walk $w \in \mathcal{W}(G)$.
- Let the feature vector $\Phi(G) = (\Phi_s(G))_{s \in \mathcal{S}}$ be defined by:

$$\Phi_s(G) = \sum_{w \in \mathcal{W}(G)} \lambda_G(w) \mathbf{1}\left(s \text{ is the label sequence of } w\right) .$$

- A walk kernel is a graph kernel defined by:

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# Walk kernel examples

- The *n*th-order walk kernel is the walk kernel with $\lambda_G(w) = 1$ if the length of $w$ is $n$, 0 otherwise. It compares two graphs through their common walks of length $n$.
- The random walk kernel is obtained with $\lambda_G(w) = P_G(w)$, where $P_G$ is a Markov random walk on $G$. In that case we have:

$$K(G_1, G_2) = P(label(W_1) = label(W_2)),$$

where $W_1$ and $W_2$ are two independant random walks on $G_1$ and $G_2$, respectively (Kashima et al., 2003).

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# Computation of walk kernels

**Proposition**

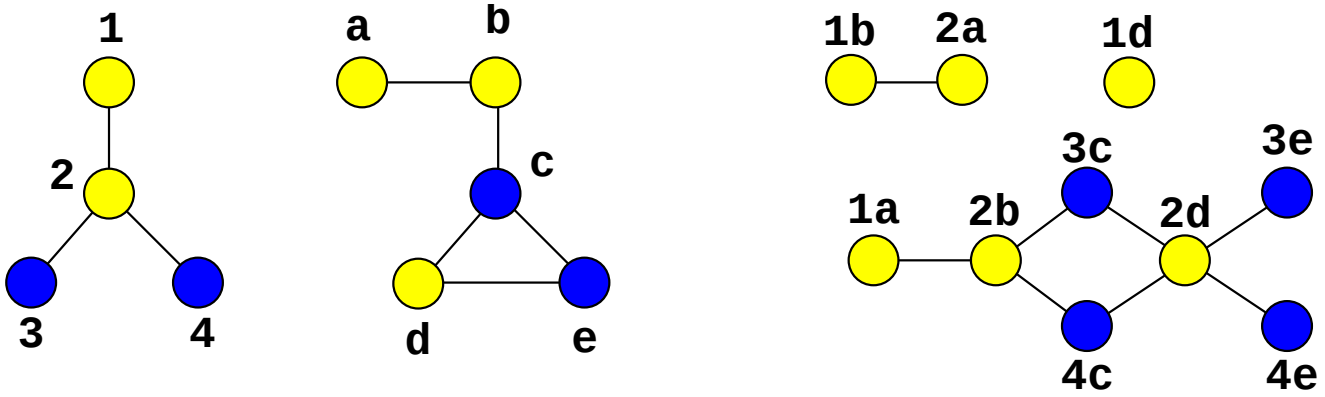
These three kernels (*n*th-order, random and geometric walk kernels) can be computed efficiently in polynomial time.

# Product graph

## Definition

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs with labeled vertices. The product graph $G = G_1 \times G_2$ is the graph $G = (V, E)$ with:

1. $V = \{(v_1, v_2) \in V_1 \times V_2 \ : \ v_1 \text{ and } v_2 \text{ have the same label}\}$ ,
2. $E = \left\{\left((v_1, v_2), (v_1', v_2')\right) \in V \times V \ : \ (v_1, v_1') \in E_1 \text{ and } (v_2, v_2') \in E_2\right\}$.




**G1** **G2** **G1 x G2**

# Walk kernel and product graph

## Lemma

There is a bijection between:

1. The pairs of walks $w_1 \in \mathcal{W}_n(G_1)$ and $w_2 \in \mathcal{W}_n(G_2)$ with the same label sequences,
2. The walks on the product graph $w \in \mathcal{W}_n(G_1 \times G_2)$.

## Corollary

$$
\begin{aligned}
K_{walk}(G_1, G_2) &= \sum_{s \in \mathcal{S}} \Phi_s(G_1)\Phi_s(G_2) \\
&= \sum_{(w_1, w_2) \in \mathcal{W}(G_1) \times \mathcal{W}(G_1)} \lambda_{G_1}(w_1)\lambda_{G_2}(w_2)\mathbf{1}(l(w_1) = l(w_2)) \\
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# Computation of the *n*th-order walk kernel

- For the *n*th-order walk kernel we have $\lambda_{G_1 \times G_2}(w) = 1$ if the length of $w$ is $n$, 0 otherwise.
- Therefore:

$$K_{nth-order}(G_1, G_2) = \sum_{w \in \mathcal{W}_n(G_1 \times G_2)} 1 \,.$$

- Let $A$ be the adjacency matrix of $G_1 \times G_2$. Then we get:

$$K_{nth-order}(G_1, G_2) = \sum_{i,j} [A^n]_{i,j} = \mathbf{1}^\top A^n \mathbf{1} \,.$$

- Computation in $O(n|G_1||G_2|d_1 d_2)$, where $d_i$ is the maximum degree of $G_i$.

# Computation of random and geometric walk kernels

- In both cases $\lambda_G(w)$ for a walk $w = v_1 \dots v_n$ can be decomposed as:

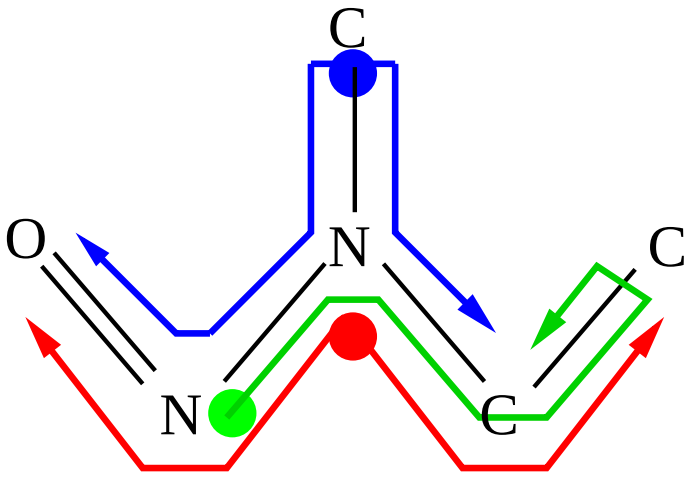
$$\lambda_G(v_1 \dots v_n) = \lambda^i(v_1) \prod_{i=2}^{n} \lambda^t(v_{i-1}, v_i)\,.$$

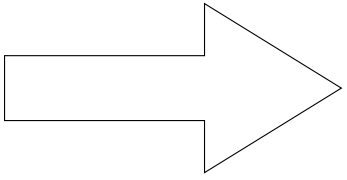
- Let $\Lambda_i$ be the vector of $\lambda^i(v)$ and $\Lambda_t$ be the matrix of $\lambda^t(v, v')$:

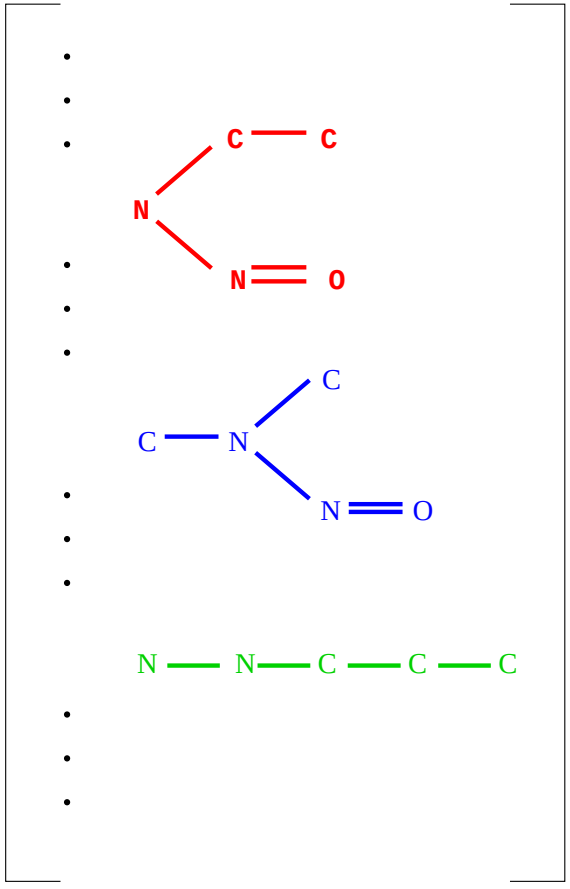
$$\begin{aligned} K_{walk}(G_1, G_2) &= \sum_{n=1}^{\infty} \sum_{w \in \mathcal{W}_n(G_1 \times G_2)} \lambda^i(v_1) \prod_{i=2}^{n} \lambda^t(v_{i-1}, v_i) \\ &= \sum_{n=0}^{\infty} \Lambda_i \Lambda_t^n \mathbf{1} \\ &= \Lambda_i \left(I - \Lambda_t\right)^{-1} \mathbf{1} \end{aligned}$$

- Computation in $O(|G_1|^3 |G_2|^3)$

# Extension: branching walks (Ramon and Gärtner, 2003; Mahé and Vert, 2009)

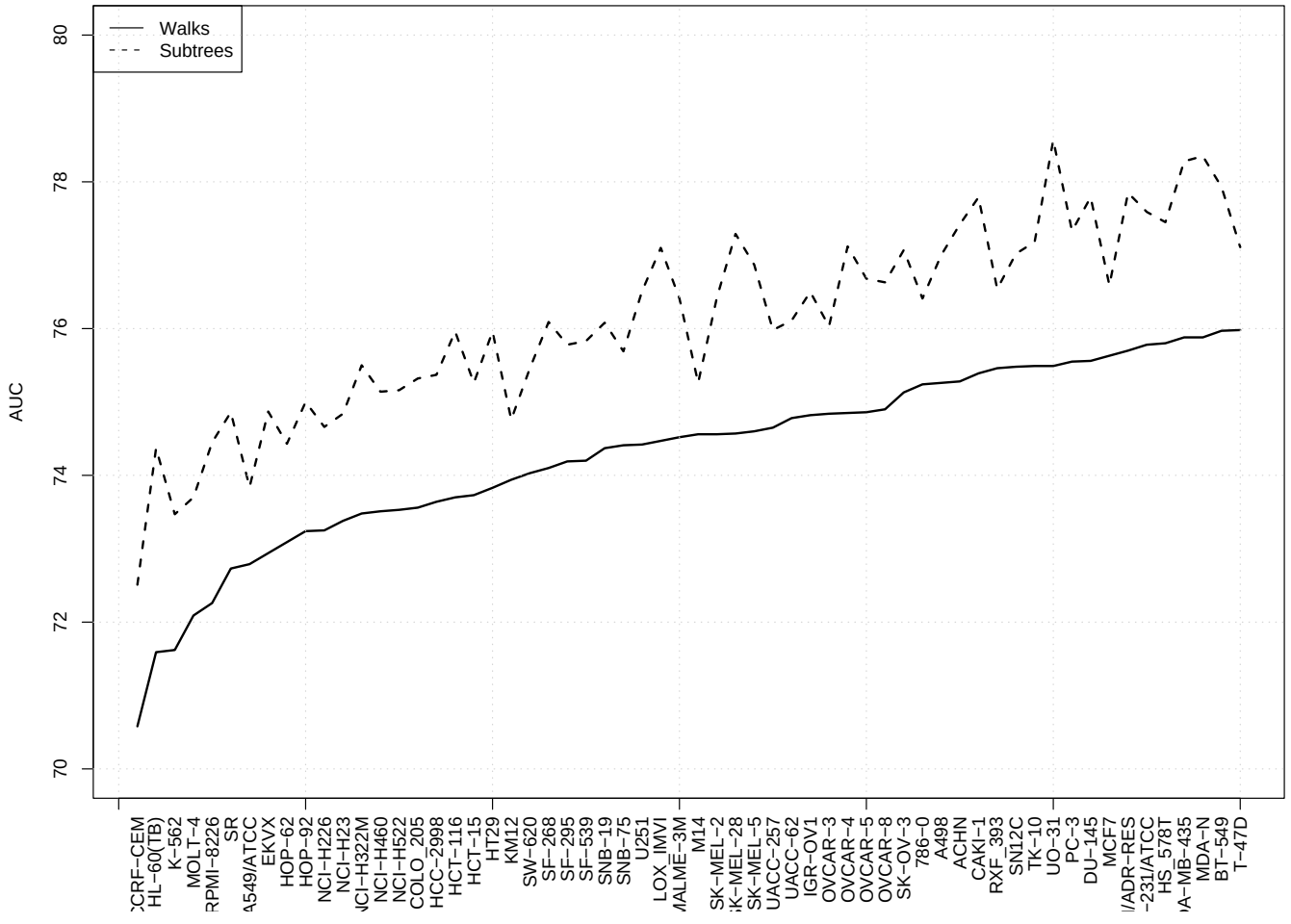





$$\mathcal{T}(v, n+1) = \sum_{R \subset \mathcal{N}(v)} \prod_{v' \in R} \lambda_t(v, v') \mathcal{T}(v', n)\,,$$

# 2D Subtree vs walk kernels

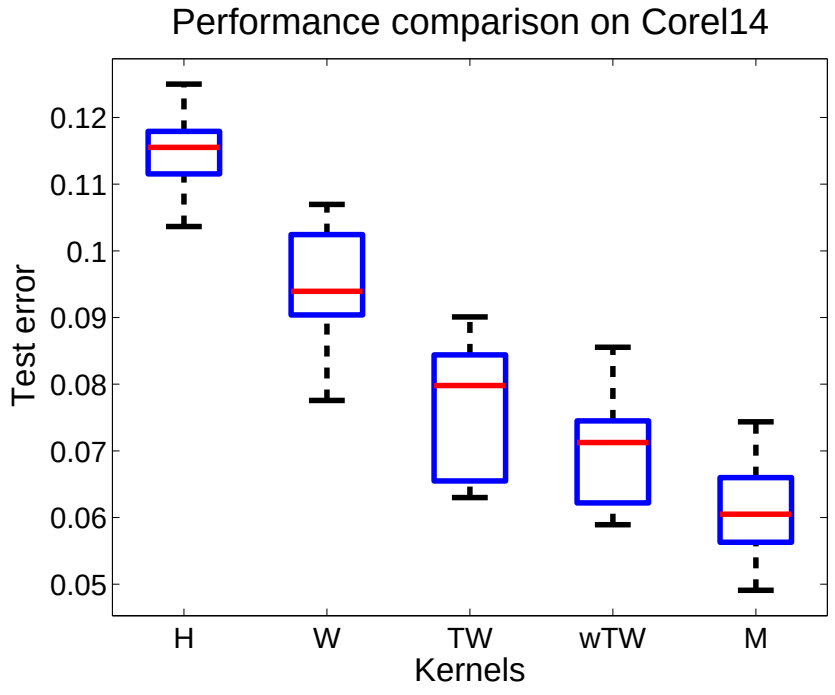



Screening of inhibitors for 60 cancer cell lines.

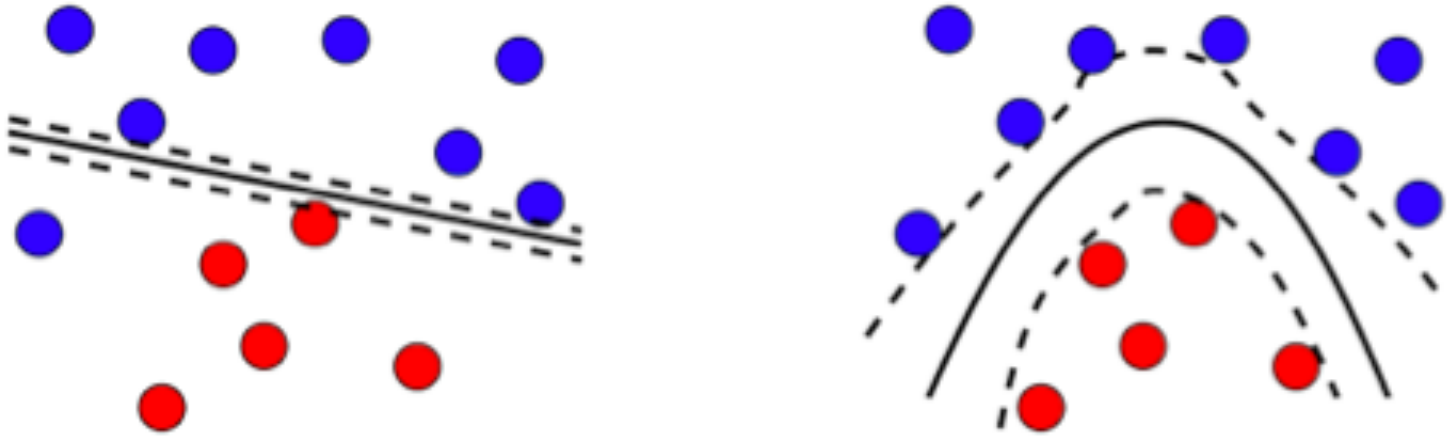
# Image classification (Harchaoui and Bach, 2007)

## COREL14 dataset

- 1400 natural images in 14 classes
- Compare kernel between histograms (H), walk kernel (W), subtree kernel (TW), weighted subtree kernel (wTW), and a combination (M).



# SVM summary



- Large margin classifier
- Control of the regularization / data fitting trade-off with $C$
- Linear or nonlinear (with the kernel trick)
- Extension to strings, graphs... and many other

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