Foundation of Intelligent Systems, Part I

SVM's & Kernel Methods

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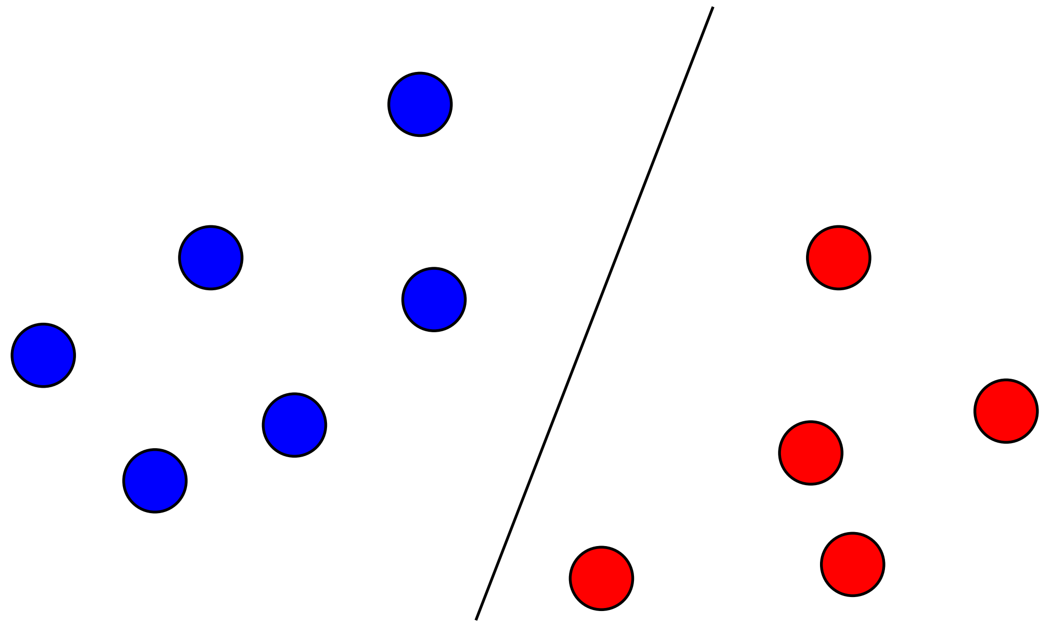
Support Vector Machines
The linearly-separable case

A criterion to select a linear classifier: the margin ?



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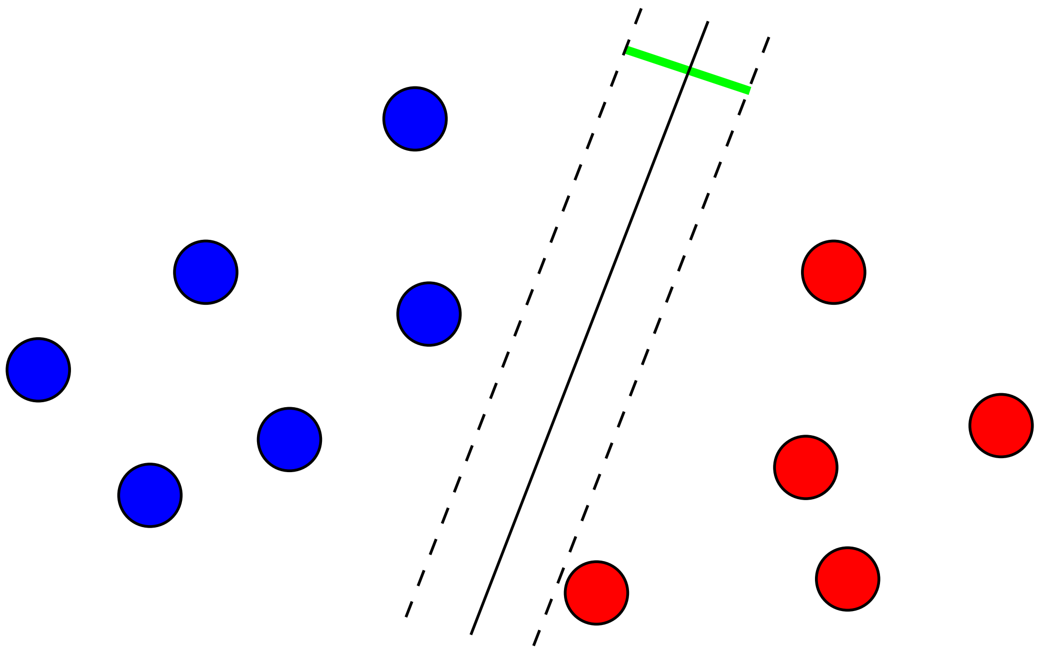

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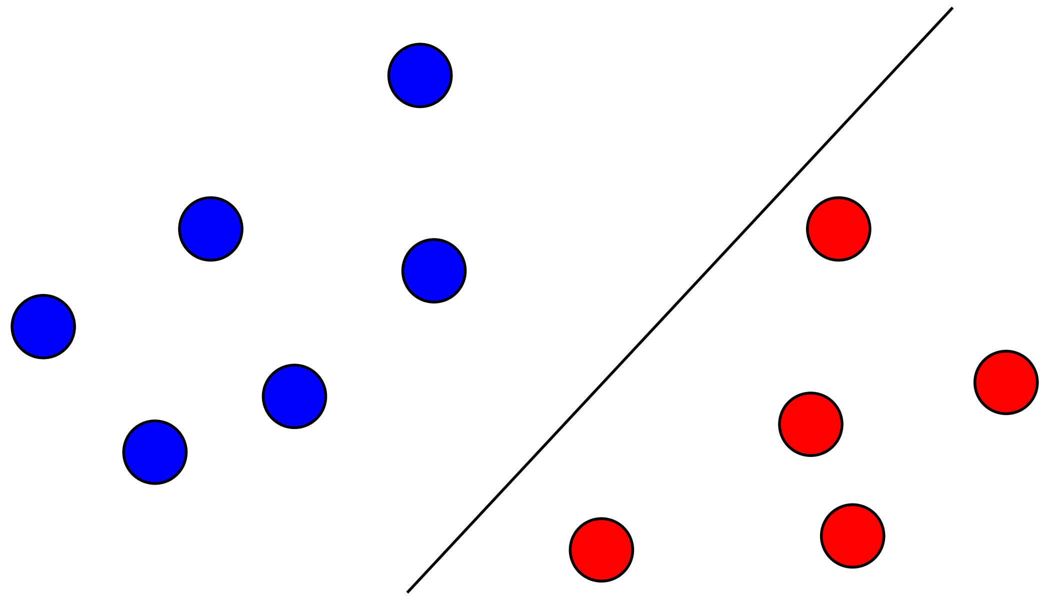

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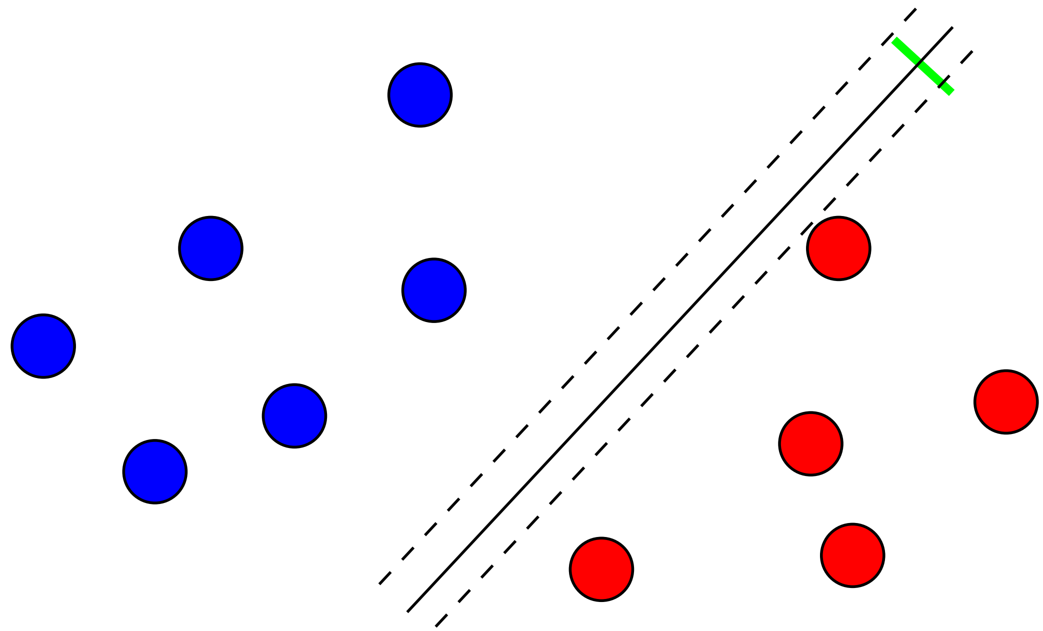

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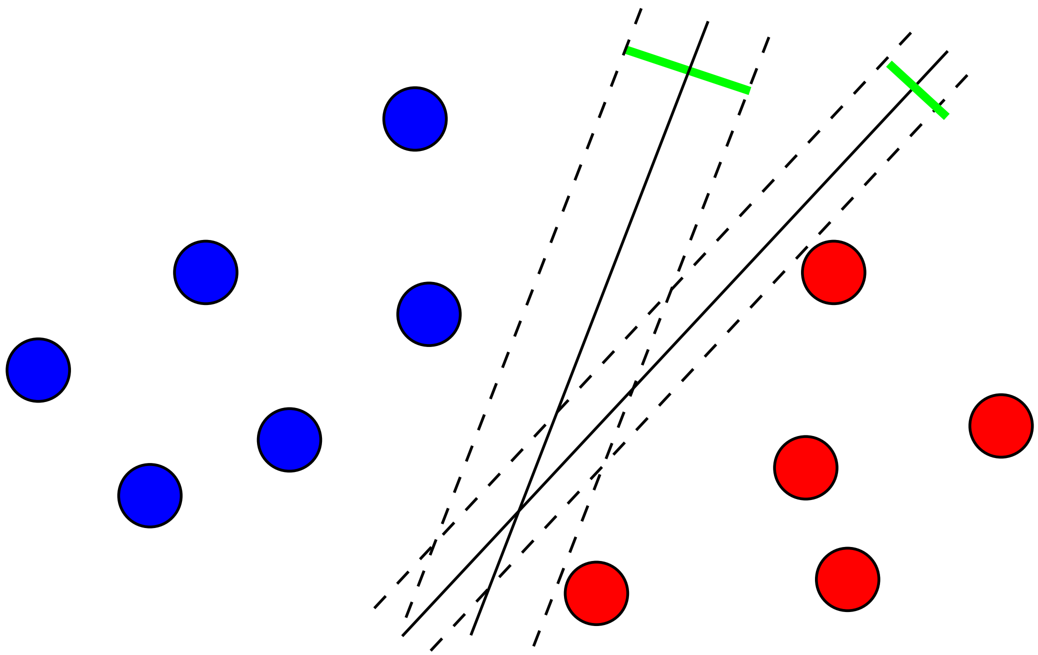
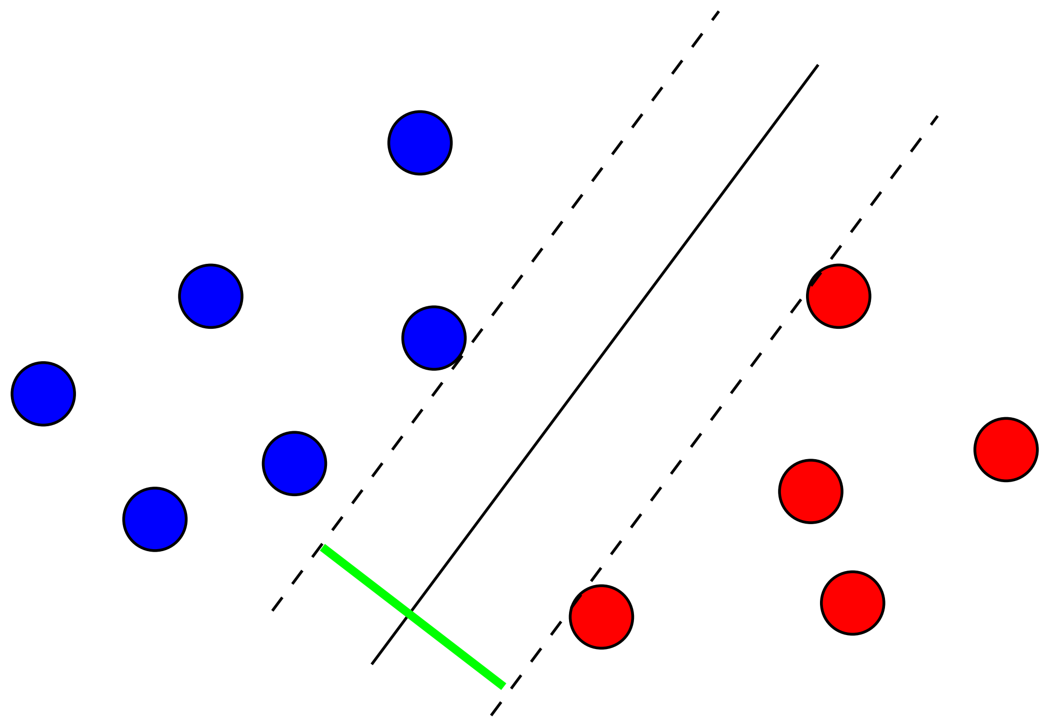
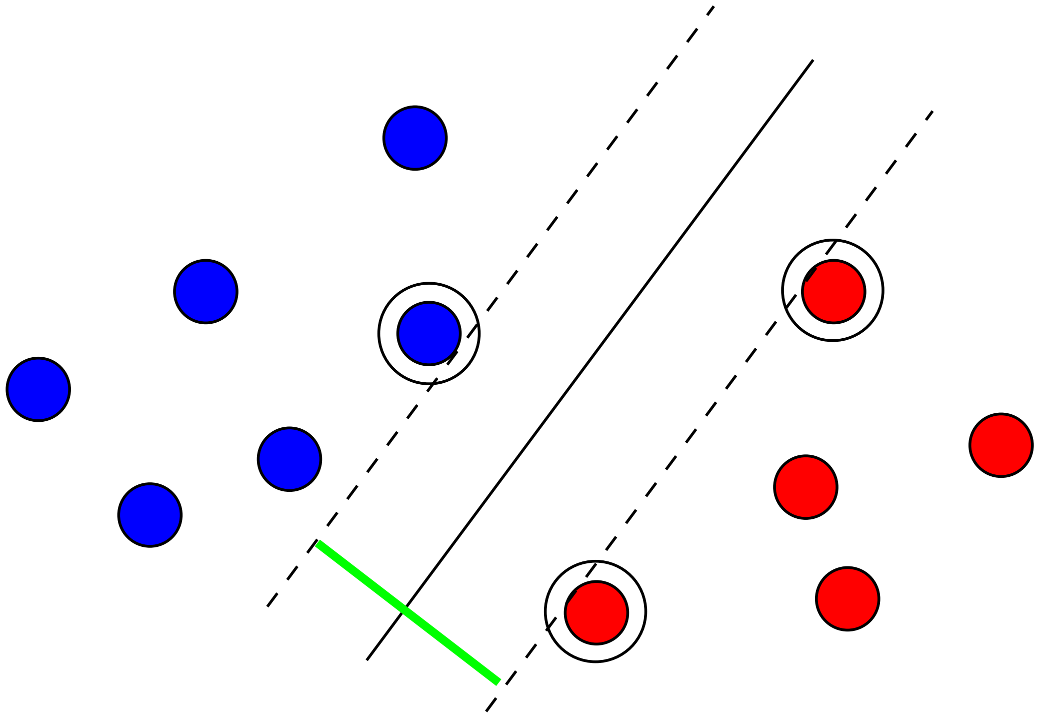


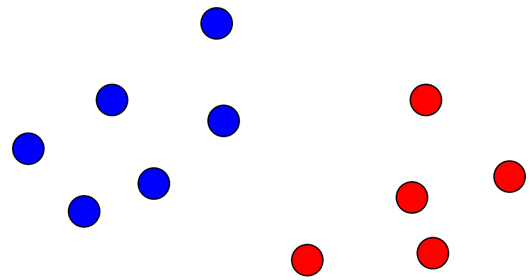
Largest Margin Linear Classifier ?



Support Vectors with Large Margin



In equations



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

$$\mathcal{T} = \{(\mathbf{x}_1, \mathbf{y}_1), \dots, (\mathbf{x}_N, \mathbf{y}_N)\},$$

  where $\mathbf{x}_i \in \mathbb{R}^d$ and $\mathbf{y}_i \in \{-1, 1\}$.

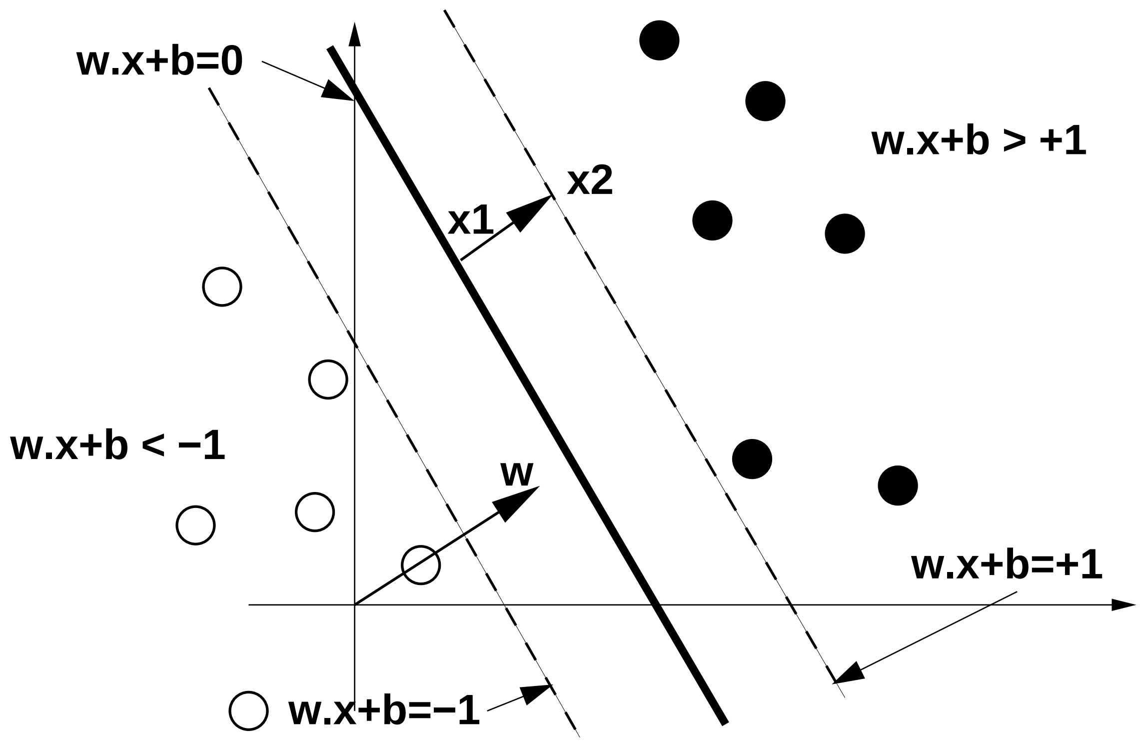
- We assume (for the moment) that the data are **linearly separable**, i.e., that there exists $(\mathbf{w}, b) \in \mathbb{R}^d \times \mathbb{R}$ such that:

$$\begin{cases} \mathbf{w}^T \mathbf{x}_i + b > 0 & \text{if } \mathbf{y}_i = 1\,, \\ \mathbf{w}^T \mathbf{x}_i + b < 0 & \text{if } \mathbf{y}_i = -1\,. \end{cases}$$

How to find the largest separating hyperplane?

For the linear classifier $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$ consider the *interstice* defined by the hyperplanes

- $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b = +1$
- $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b = -1$



The margin is $2/||\mathbf{w}||$

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

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

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

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

where γ is the margin.

All training points should be on the appropriate side

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

$$\mathbf{w}^T \mathbf{x}_i + b \geq 1$$

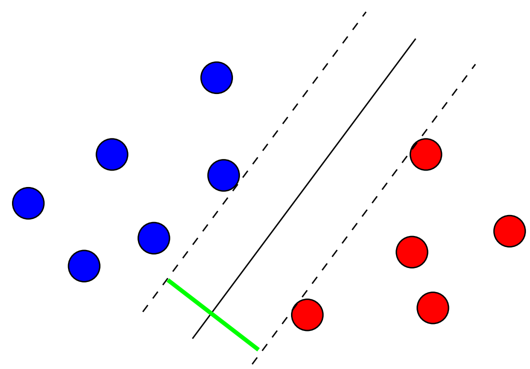
- For negative examples ($y_i = -1$) this means:

$$\mathbf{w}^T \mathbf{x}_i + b \leq -1$$

- in both cases:

$$\forall i = 1, \ldots, n, \qquad \mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b \right) \geq 1$$

Finding the optimal hyperplane



- Finding the optimal hyperplane is equivalent to finding $(\mathbf{w}, b)$ which minimize:

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

under the constraints:

$$\forall i = 1, \dots, n, \qquad \mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) - 1 \geq 0.$$

This is a classical quadratic program on $\mathbb{R}^{d+1}$
linear constraints - **quadratic objective**

Lagrangian

- In order to minimize:

$$\frac{1}{2}||\mathbf{w}||^2$$

under the constraints:

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

- introduce **one dual variable α_i for each constraint**,
- one constraint for **each training point**.
- the **Lagrangian** is, for $\alpha \succeq 0$ (that is for each $\alpha_i \geq 0$)

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

The Lagrange dual function

$$g(\alpha) = \inf_{\mathbf{w}\in\mathbb{R}^d, b\in\mathbb{R}} \left\{ \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \left(y_i \left(\mathbf{w}^T \mathbf{x}_i + b \right) - 1 \right) \right\}$$

the saddle point conditions give us that at the minimum in $\mathbf{w}$ and b

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i \mathbf{y}_i \mathbf{x}_i, \quad (\text{ derivating w.r.t } \mathbf{w}) \quad (*)$$

$$0 = \sum_{i=1}^{n} \alpha_i \mathbf{y}_i, \quad (\text{derivating w.r.t } b) \qquad (**)$$

substituting $(*)$ in g, and using $(**)$ as a constraint, get the dual function $g(\alpha)$.

- To solve the dual problem, **maximize** g w.r.t. α.
- **Strong duality holds** : primal and dual problems have the **same optimum**.
- KKT gives us $\alpha_i(\mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) - 1) = 0$,
  ...*hence*, either $\boldsymbol{\alpha_i = 0}$ or $\boldsymbol{\mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) = 1}$.
- $\alpha_i \neq 0$ **only** for points on the support hyperplanes $\{(\mathbf{x}, \mathbf{y}) |\, \mathbf{y}_i(\mathbf{w}^T \mathbf{x}_i + b) = 1\}$.

Dual optimum

The dual problem is thus

$$\begin{array}{ll}\text{maximize} & g(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} \alpha_i\alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j \\ \text{such that} & \alpha \succeq 0, \sum_{i=1}^{n} \alpha_i \mathbf{y}_i = 0.\end{array}$$

> This is a **quadratic program** in $\mathbb{R}^n$, with *box constraints*.
> α^* can be computed using optimization software
> ($e.g.$ built-in `matlab` function)

Recovering the optimal hyperplane

- With α^*, we recover $(\mathbf{w}^T, b^*)$ corresponding to the **optimal hyperplane**.
- $\mathbf{w}^T$ is given by $\mathbf{w}^T = \sum_{i=1}^n y_i \alpha_i \mathbf{x}_i^T$,
- b^* is given by the conditions on the support vectors $\alpha_i > 0$, $\mathbf{y}_i(\mathbf{w}^T \mathbf{x}_i + b) = 1$,

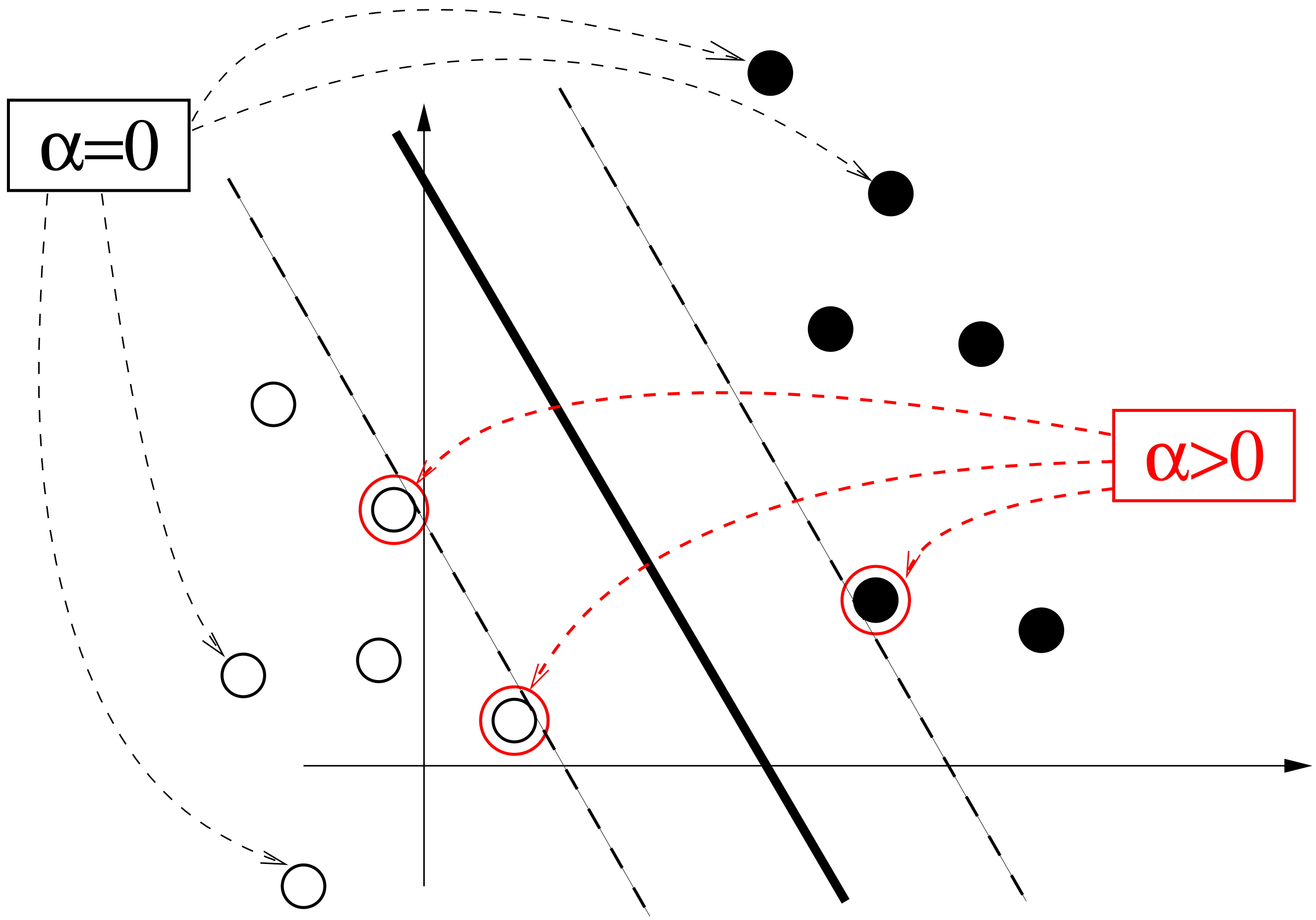
$$b^* = -\frac{1}{2}\left(\min_{\mathbf{y}_i=1,\alpha_i>0}(\mathbf{w}^T\mathbf{x}_i) + \max_{\mathbf{y}_i=-1,\alpha_i>0}(\mathbf{w}^T\mathbf{x}_i)\right)$$

- the **decision function** is therefore:

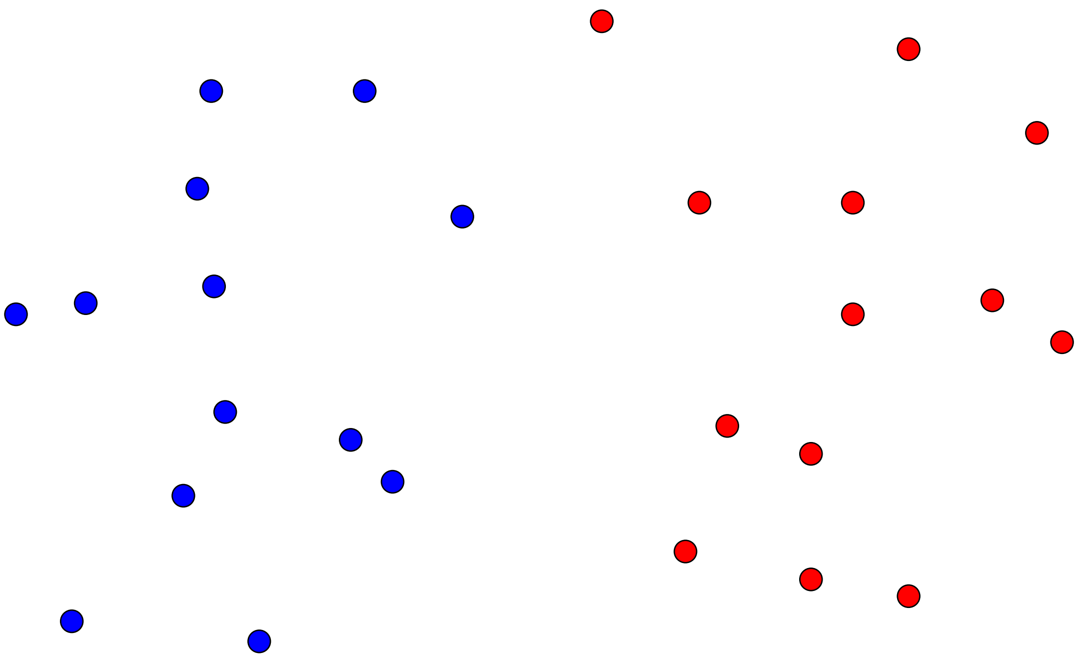
$$\begin{aligned} f^*(\mathbf{x}) &= \mathbf{w}^T\mathbf{x} + b^* \\ &= \left(\sum_{i=1}^n y_i\alpha_i\mathbf{x}_i^T\right)\mathbf{x} + b^*. \end{aligned}$$

- Here the **dual** solution gives us directly the **primal** solution.

Interpretation: support vectors

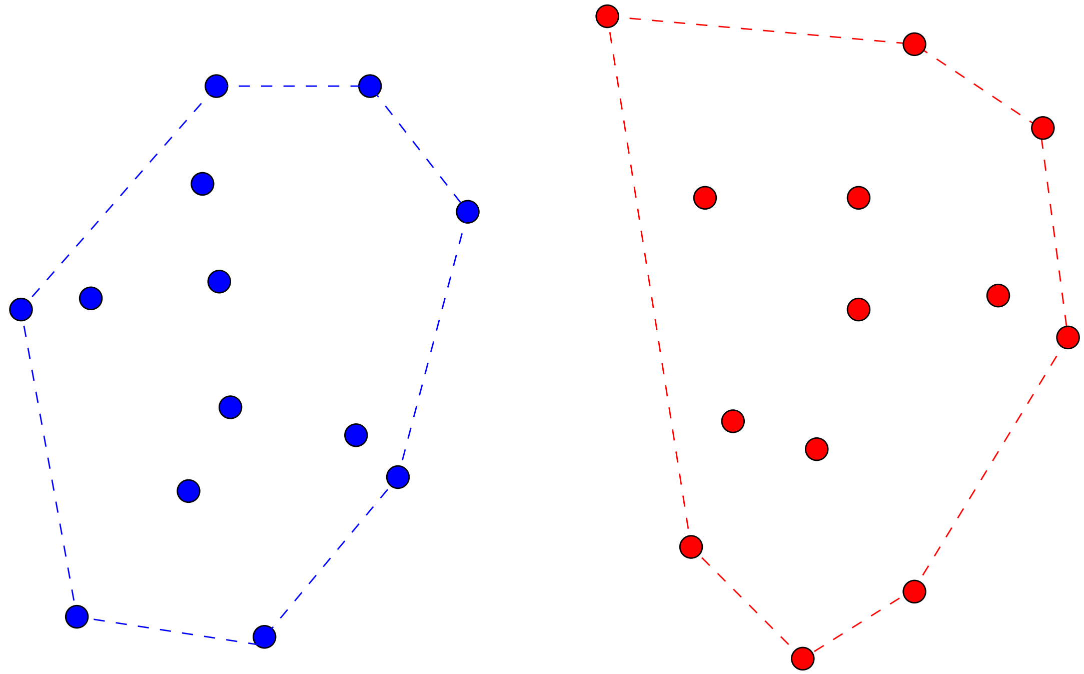


Another interpretation: Convex Hulls



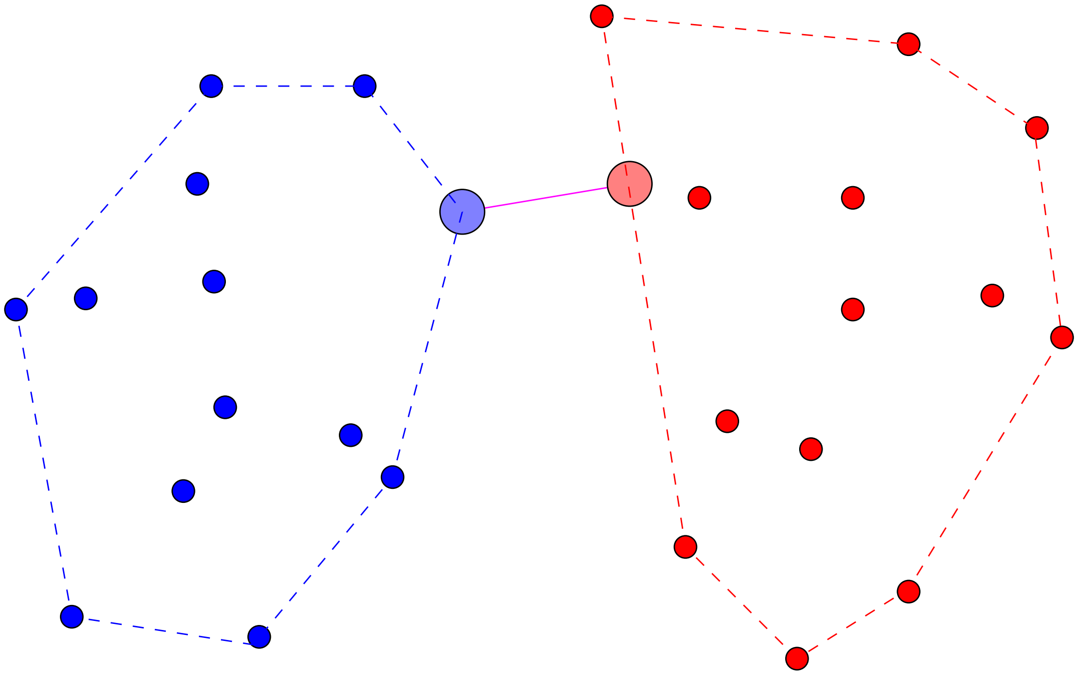
go back to 2 sets of points that are linearly separable

Another interpretation: Convex Hulls



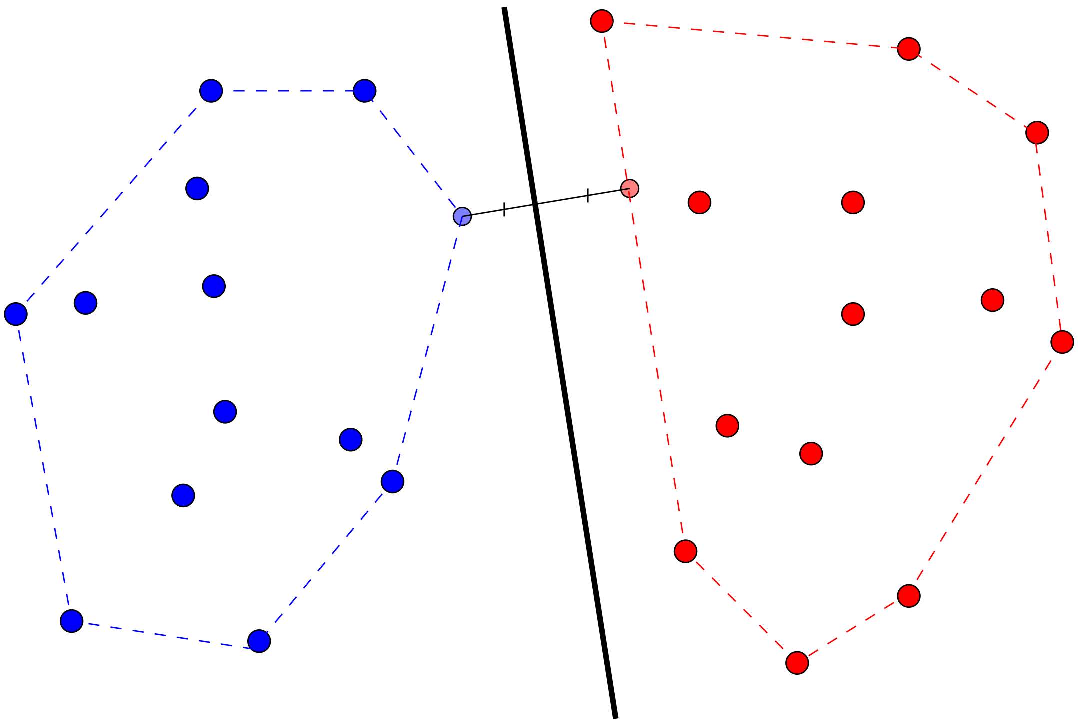
Linearly separable = convex hulls do not intersect

Another interpretation: Convex Hulls



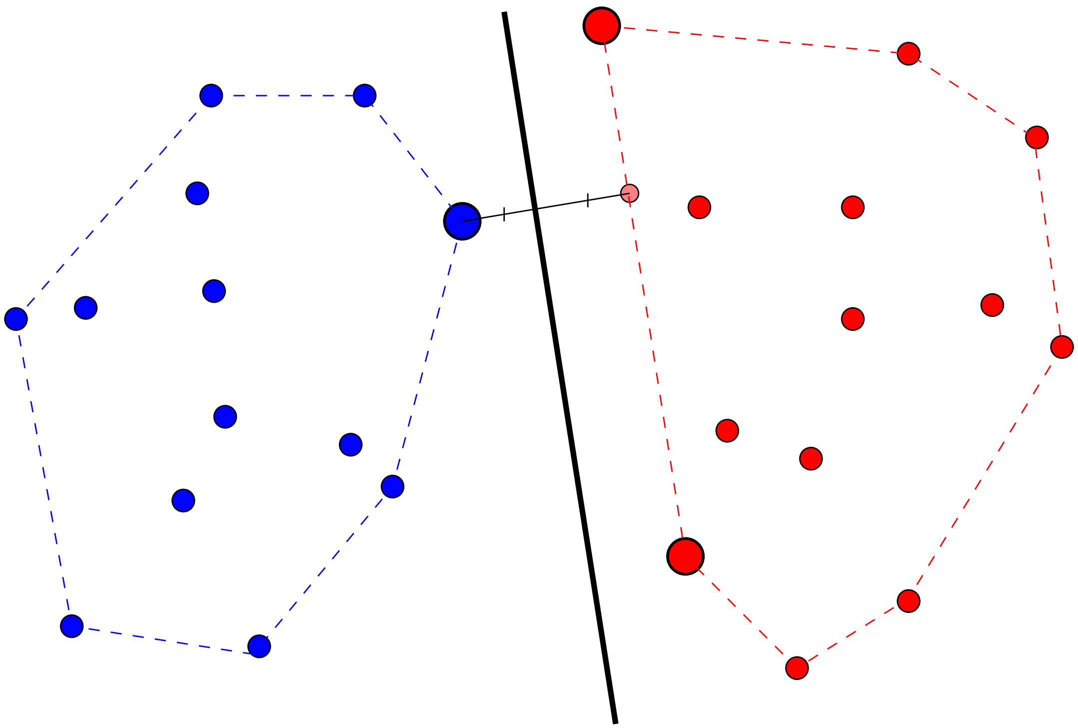
Find two closest points, one in each convex hull

Another interpretation: Convex Hulls



The SVM = bisection of that segment

Another interpretation: Convex Hulls

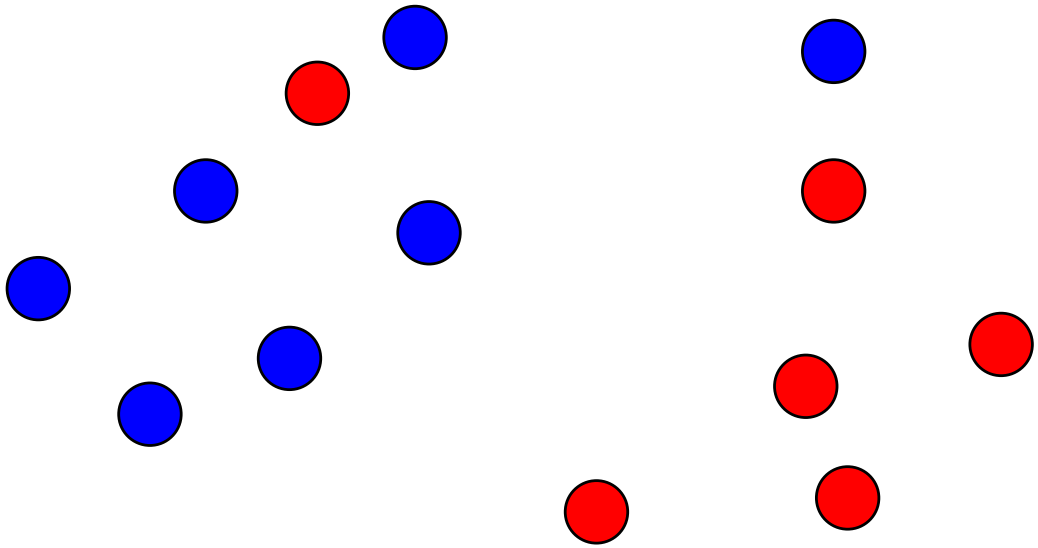


support vectors = extreme points of the faces on which the two points lie

The non-linearly separable case

(when convex hulls intersect)

What happens when the data is not linearly separable?



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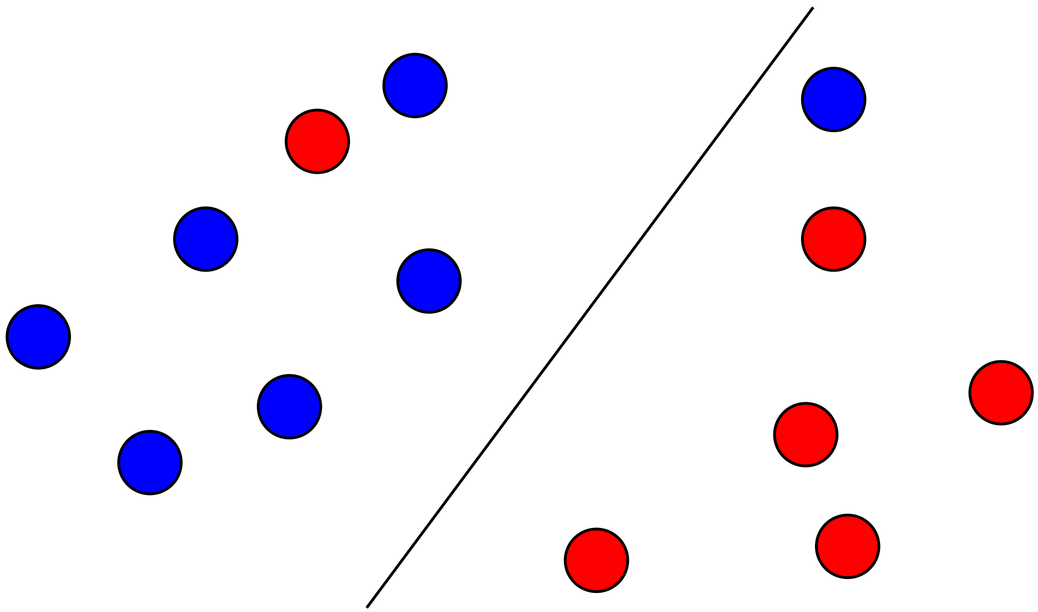

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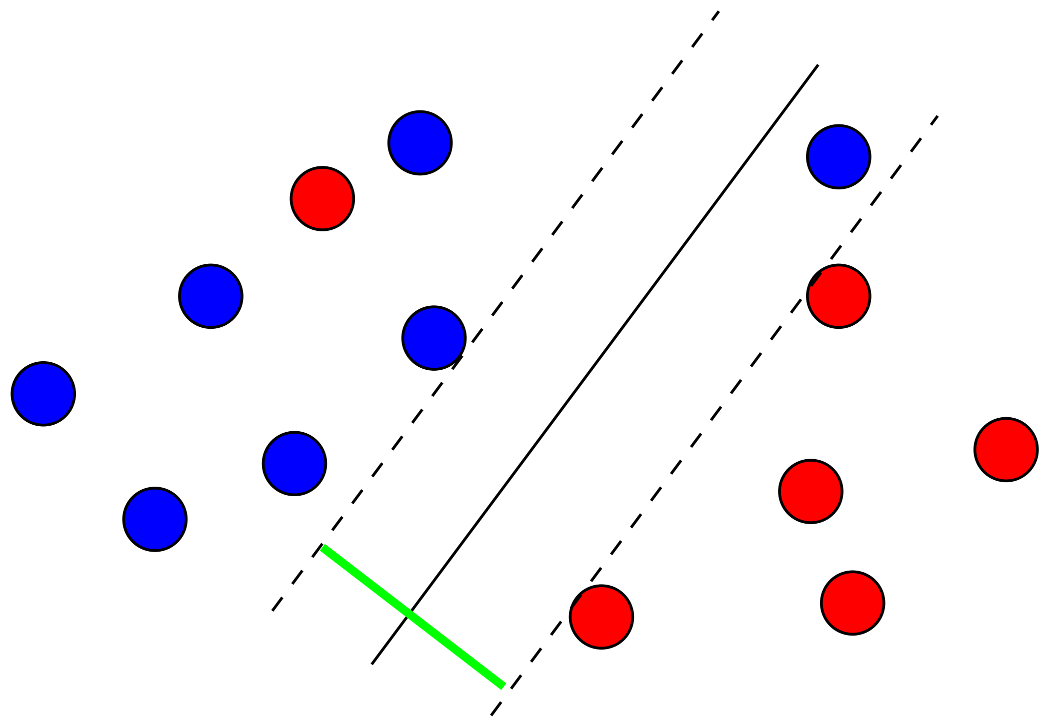

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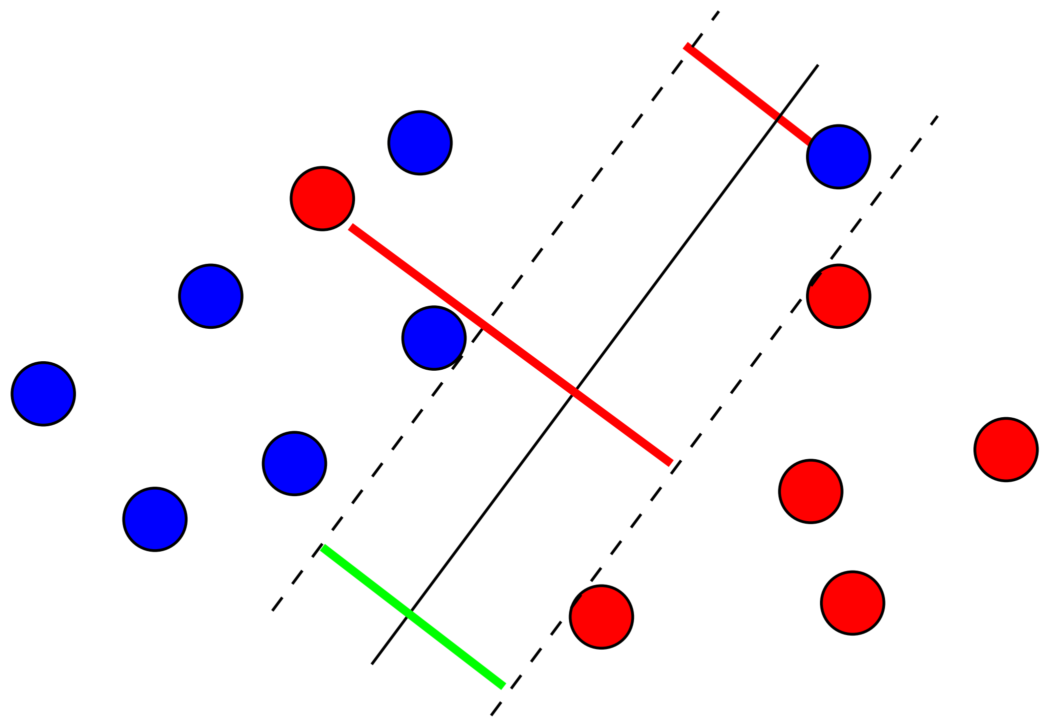


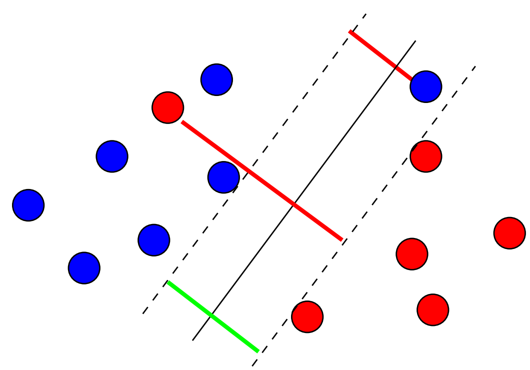
Soft-margin SVM ?

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

- Mathematically:

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

- C is a parameter



Soft-margin SVM formulation ?

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

$$\text{margin}(\mathbf{x}, \mathbf{y}) = \mathbf{y}\left(\mathbf{w}^T\mathbf{x} + b\right)$$

- The **error** is
  - 0 if $\text{margin}(\mathbf{x}, \mathbf{y}) > 1$,
  - $1 - \text{margin}(\mathbf{x}, \mathbf{y})$ otherwise.

- The soft margin SVM solves:

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

- $c(u, y) = \max\{0, 1 - yu\}$ is known as the **hinge loss**.

- $c(\mathbf{w}^T\mathbf{x}_i + b, \mathbf{y}_i)$ associates a mistake cost to the decision $\mathbf{w}, b$ for example $\mathbf{x}_i$.

Dual formulation of soft-margin SVM

- The soft margin SVM program

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

can be rewritten as

$$\begin{array}{cc} \text{minimize} & \|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i \\ \text{such that} & \mathbf{y}_i\left(\mathbf{w}^T\mathbf{x}_i + b\right) \geq 1 - \xi_i \end{array}$$

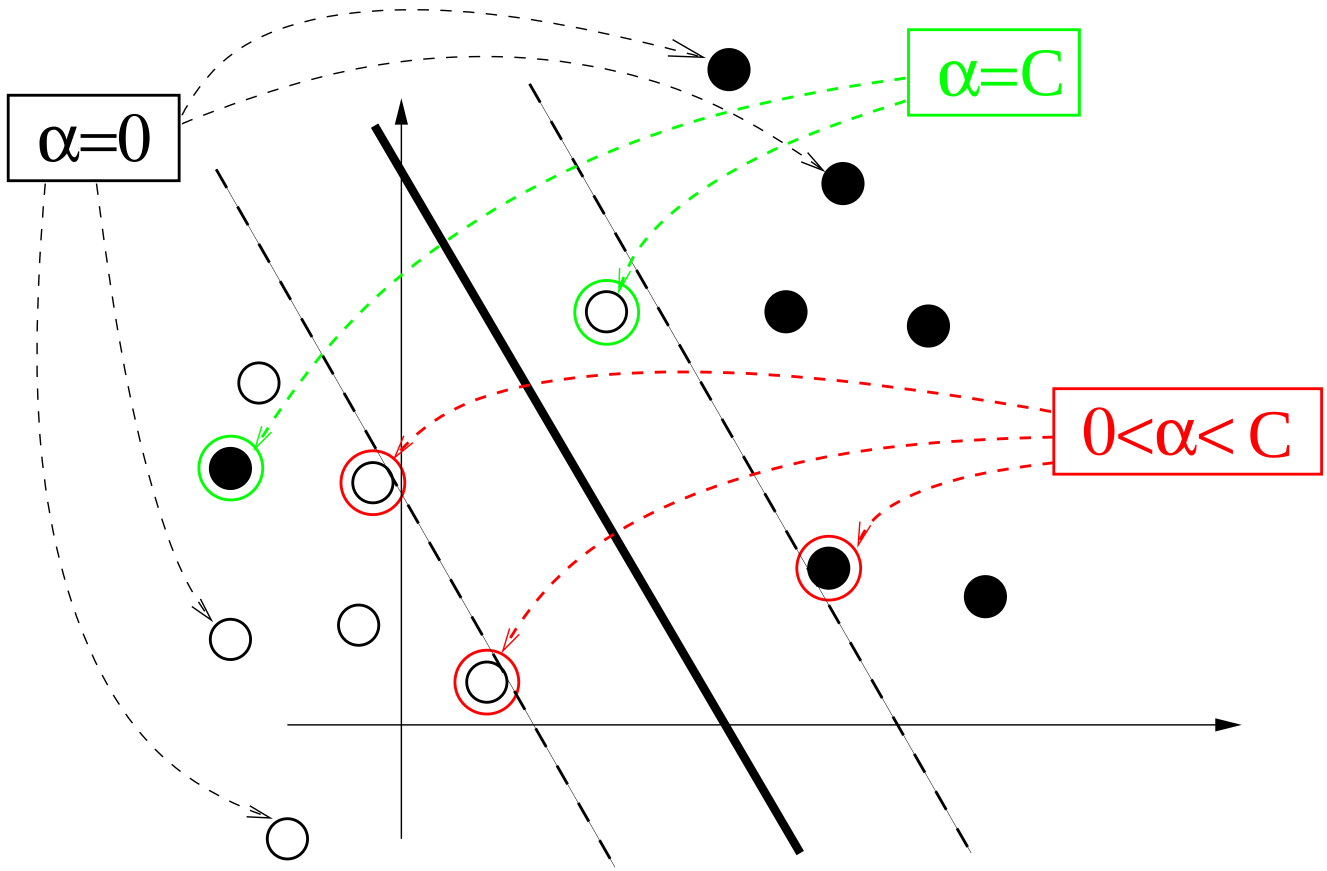
- In that case the dual function

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

which is finite under the constraints:

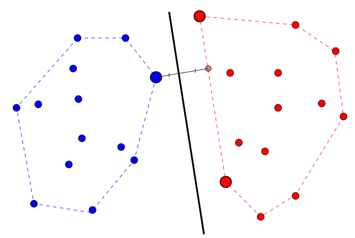
$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n}\alpha_i\mathbf{y}_i = 0. \end{cases}$$

Interpretation: bounded and unbounded support vectors

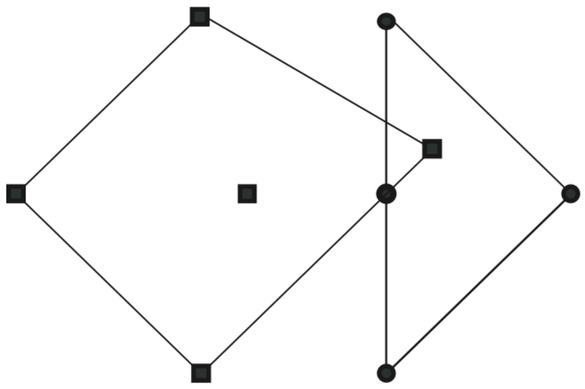


What about the convex hull analogy?

- Remember the separable case



- Here we consider the case where the two sets are not linearly separable, $i.e.$ their convex hulls **intersect.**



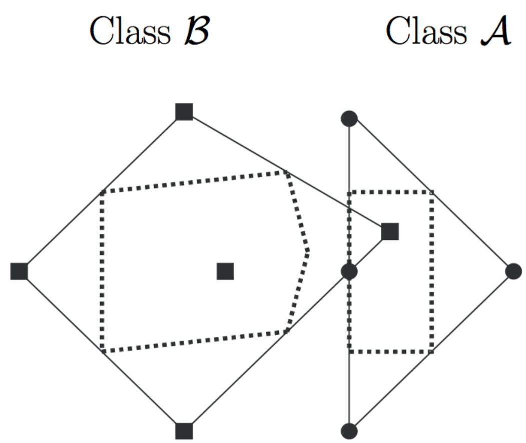
What about the convex hull analogy?

Definition 1. *Given a set of n points $\mathcal{A}$, and $0 \leq C \leq 1$, the set of finite combinations*

$$\sum_{i=1}^{n} \lambda_i \mathbf{x}_i, 1 \leq \lambda_i \leq C, \sum_{i=1}^{n} \lambda_i = 1,$$

is the (C) reduced convex hull of $\mathcal{A}$

- Using $C = 1/2$, the reduced convex hulls of $\mathcal{A}$ and $\mathcal{B}$,



- Soft-SVM with C = closest two points of C-reduced convex hulls.

Kernels

Kernel trick for SVM's

- use a mapping ϕ from $\mathcal{X}$ to a feature space,
- which corresponds to the **kernel** k:

$$\forall \mathbf{x}, \mathbf{x}' \in \mathcal{X}, \quad k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$$

- Example: if $\phi(\mathbf{x}) = \phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} x_1^2 \\ x_2^2 \end{bmatrix}$, then

$$k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle = (x_1)^2(x_1')^2 + (x_2)^2(x_2')^2.$$

Training a SVM in the feature space

Replace each $\mathbf{x}^T\mathbf{x}'$ in the SVM algorithm by $\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle = k(\mathbf{x}, \mathbf{x}')$

- **Reminder**: the dual problem is to maximize

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

under the constraints:

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

- The **decision function** becomes:

$$\begin{aligned} f(\mathbf{x}) &= \langle \mathbf{w}, \phi(x) \rangle + b^* \\ &= \sum_{i=1}^{n} y_i \alpha_i \boldsymbol{k(\mathbf{x}_i, \mathbf{x})} + b^*. \end{aligned} \tag{1}$$

The Kernel Trick ?

The explicit computation of $\phi(\mathbf{x})$ is not necessary.
The kernel $k(\mathbf{x}, \mathbf{x}')$ is enough.

- the SVM optimization for α works **implicitly** in the feature space.
- the SVM is a kernel algorithm: only need to input $\boldsymbol{K}$ and $\mathbf{y}$:

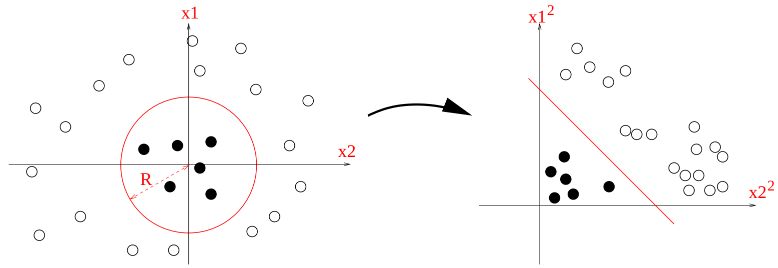
$$\begin{array}{ll} \text{maximize} & g(\alpha) = \alpha^T \mathbf{1} - \frac{1}{2}\alpha^T (\boldsymbol{K} \odot \mathbf{y}\mathbf{y}^T)\alpha \\ \text{such that} & 0 \leq \alpha_i \leq C, \quad \text{for } i = 1, \ldots, n \\ & \sum_{i=1}^{n} \alpha_i \mathbf{y}_i = 0. \end{array}$$

- $\boldsymbol{K}$'s **positive definite** $\Leftrightarrow$ **problem has an unique optimum**
- the decision function is $f(\cdot) = \sum_{i=1}^{n} \alpha_i \boldsymbol{k}(\mathbf{x}_i, \cdot) + b$.

Kernel example: polynomial kernel

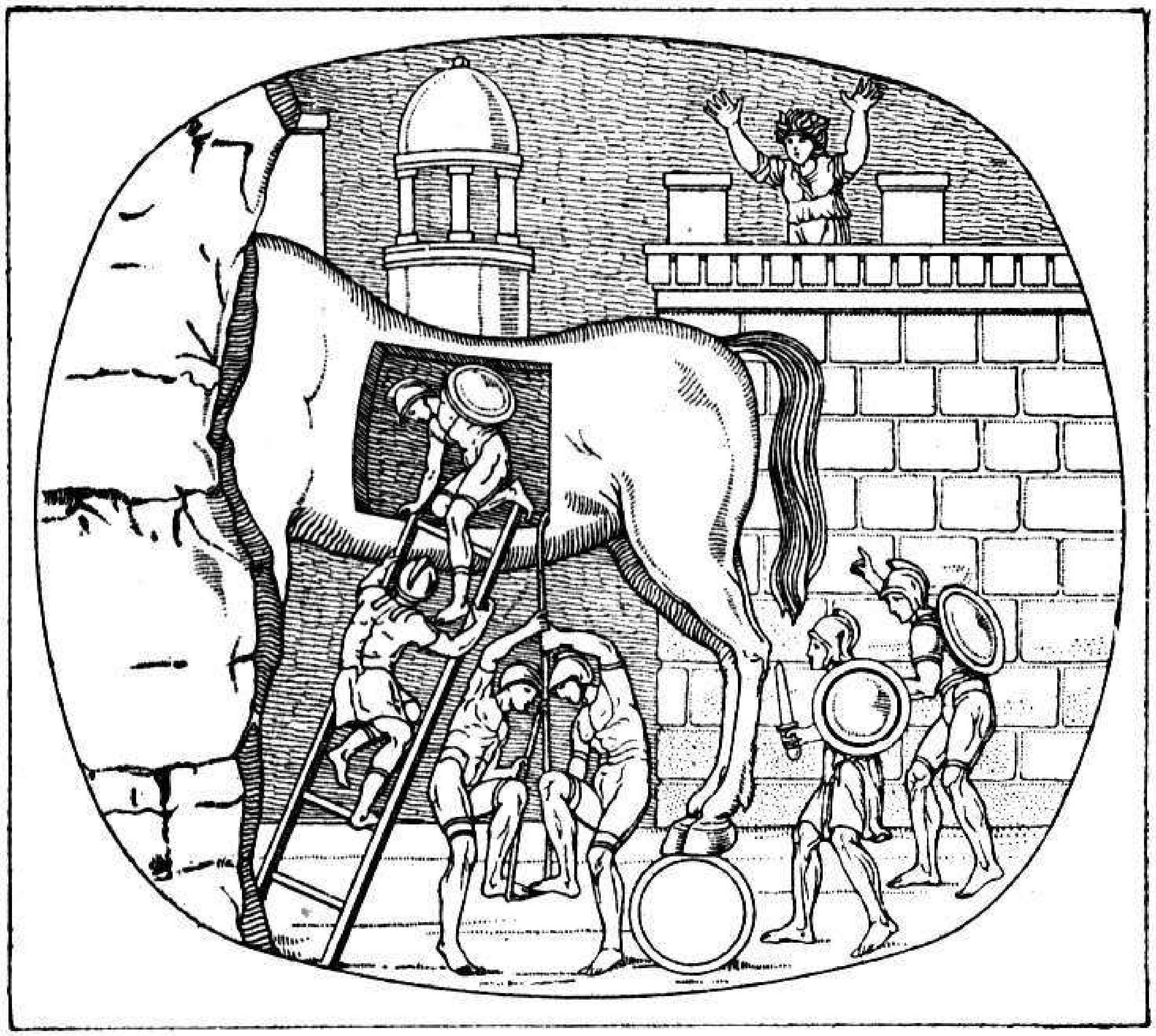
- For $\mathbf{x} = (x_1, x_2)^\top \in \mathbb{R}^2$, let $\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$:

$$\begin{aligned} \boldsymbol{K}(\mathbf{x}, \mathbf{x}') &= x_1^2 x_1'^2 + 2x_1x_2x_1'x_2' + x_2^2 x_2'^2 \\ &= \{x_1x_1' + x_2x_2'\}^2 \\ &= \{\mathbf{x}^T\mathbf{x}'\}^2 \,. \end{aligned}$$



Kernels are Trojan Horses onto Linear Models

- With kernels, complex structures can enter the realm of linear models

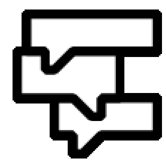
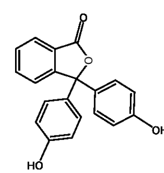


What is a kernel

In the context of these lectures...

- A kernel k is a function

$$\begin{array}{rccc} k: & \mathcal{X} \times \mathcal{X} & \longmapsto & \mathbb{R} \\ & (\mathbf{x}, \mathbf{y}) & \longrightarrow & k(\mathbf{x}, \mathbf{y}) \end{array}$$

- which compares two objects of a space $\mathcal{X}$, *e.g.*...
  - strings, texts and sequences, 
  - images, audio and video feeds,  
  - graphs, interaction networks and 3D structures 

- whatever actually... time-series of graphs of images? graphs of texts?...

Fundamental properties of a kernel

symmetric

$$k(\mathbf{x},\mathbf{y}) = k(\mathbf{y},\mathbf{x}).$$

positive-(semi)definite

for any *finite* family of points $\mathbf{x}_1, \cdots, \mathbf{x}_n$ of $\mathcal{X}$, the matrix

$$K = \begin{bmatrix} k(\mathbf{x}_1,\mathbf{x}_1) & k(\mathbf{x}_1,\mathbf{x}_2) & \cdots & k(\mathbf{x}_1,\mathbf{x}_i) & \cdots & k(\mathbf{x}_1,\mathbf{x}_n) \\ k(\mathbf{x}_2,\mathbf{x}_1) & k(\mathbf{x}_2,\mathbf{x}_2) & \cdots & k(\mathbf{x}_2,\mathbf{x}_i) & \cdots & k(\mathbf{x}_2,\mathbf{x}_n) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ k(\mathbf{x}_i,\mathbf{x}_1) & k(\mathbf{x}_i,\mathbf{x}_2) & \cdots & k(\mathbf{x}_i,\mathbf{x}_i) & \cdots & k(\mathbf{x}_2,\mathbf{x}_n) \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ k(\mathbf{x}_n,\mathbf{x}_1) & k(\mathbf{x}_n,\mathbf{x}_2) & \cdots & k(\mathbf{x}_n,\mathbf{x}_i) & \cdots & k(\mathbf{x}_n,\mathbf{x}_n) \end{bmatrix} \succeq 0$$

is positive semidefinite (has a nonnegative spectrum).

K is often called the **Gram matrix** of $\{\mathbf{x}_1, \cdots, \mathbf{x}_n\}$ using k

What can we do with a kernel?

The setting

- Pretty simple setting: a set of objects $\mathbf{x}_1, \cdots, \mathbf{x}_n$ of $\mathcal{X}$
- **Sometimes** additional information on these objects
  - labels $\mathbf{y}_i \in \{-1, 1\}$ or $\{1, \cdots, \#(\text{classes})\}$,
  - scalar values $\mathbf{y}_i \in \mathbb{R}$,
  - associated object $\mathbf{y}_i \in \mathcal{Y}$
- A kernel $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$.

A few intuitions on the possibilities of kernel methods

Important concepts and perspectives

- The functional perspective: represent **points as functions**.
- **Nonlinearity** : linear combination of kernel evaluations.
- Summary of a sample through its **kernel matrix**.

Represent any point in $\mathcal{X}$ as a function

For every **x**, the map
$$\mathbf{x} \longrightarrow k(\mathbf{x}, \cdot)$$
associates to **x** a function $k(\mathbf{x}, \cdot)$ from $\mathcal{X}$ to $\mathbb{R}$.

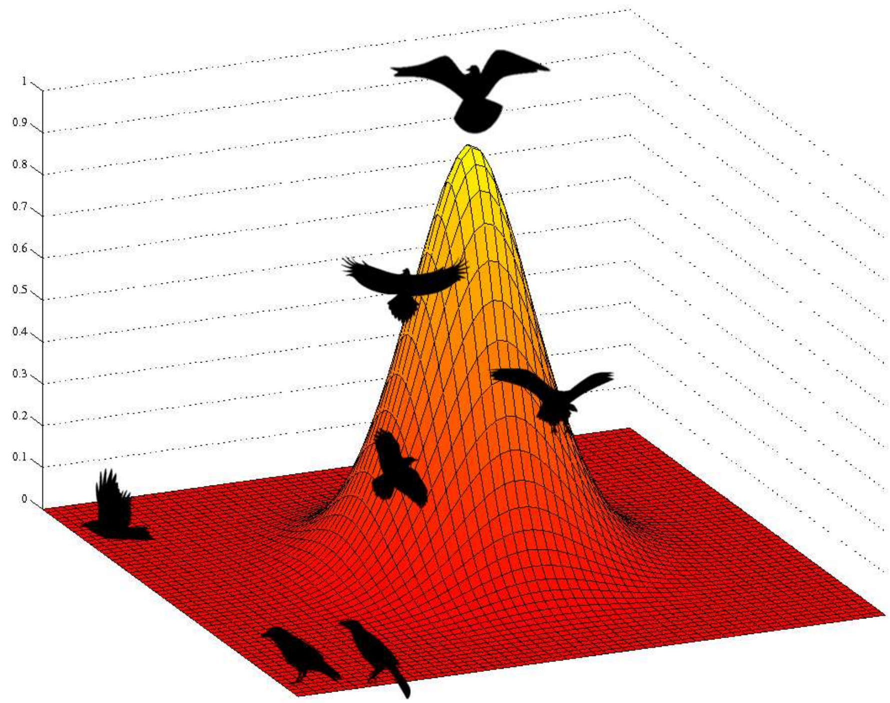
- Suppose we have a kernel k on bird images

- Suppose for instance

k ( , ) $= .32$

Represent any point in $\mathcal{X}$ as a function

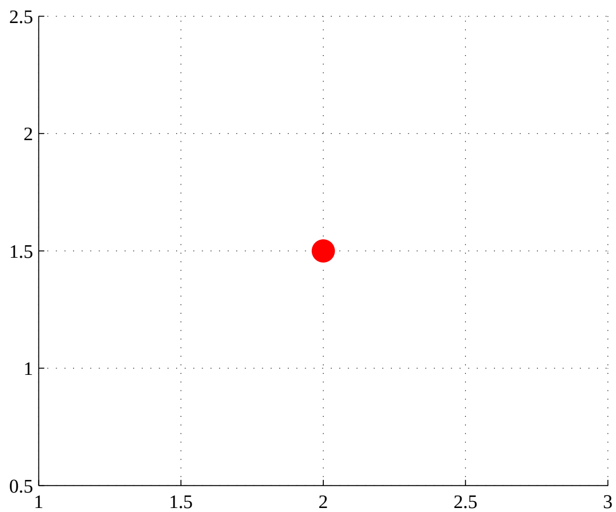
- We examine one image in particular: 
- With kernels, we get a **representation** of that bird as a real-valued function, defined on the space of birds, represented here as $\mathbb{R}^2$ for simplicity.



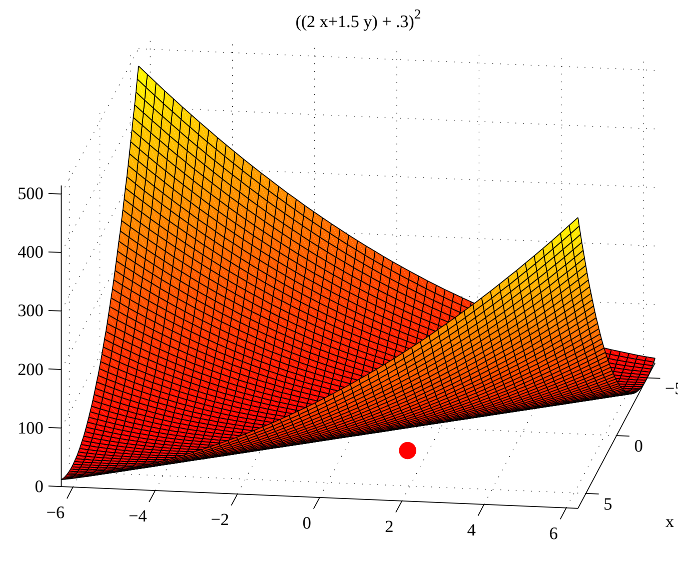
schematic plot of $k($  $, \cdot \,)$.

Represent any point in $\mathcal{X}$ as a function

- If the bird example was confusing...
- $k\left(\begin{bmatrix} x \\ y \end{bmatrix}, \begin{bmatrix} x' \\ y' \end{bmatrix}\right) = \left(\begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} x' \\ y' \end{bmatrix} + .3\right)^2$
- From a point in $\mathbb{R}^2$ to a function defined over $\mathbb{R}^2$.



$\rightarrow$



- We assume implicitly that the **functional representation** will be more useful than the **original representation**.

Decision functions as linear combination of kernel evaluations

- Linear decisions functions are a major tool in statistics, that is functions

$$f(\mathbf{x}) = \beta^T \mathbf{x} + \beta_0.$$

- Implicitly, a point $\mathbf{x}$ is processed depending on its characteristics x_i,

$$f(\mathbf{x}) = \sum_{i=1}^{d} \boldsymbol{\beta_i} x_i + \boldsymbol{\beta_0}.$$

  the free parameters are scalars $\boldsymbol{\beta_0, \beta_1, \cdots, \beta_d}$.

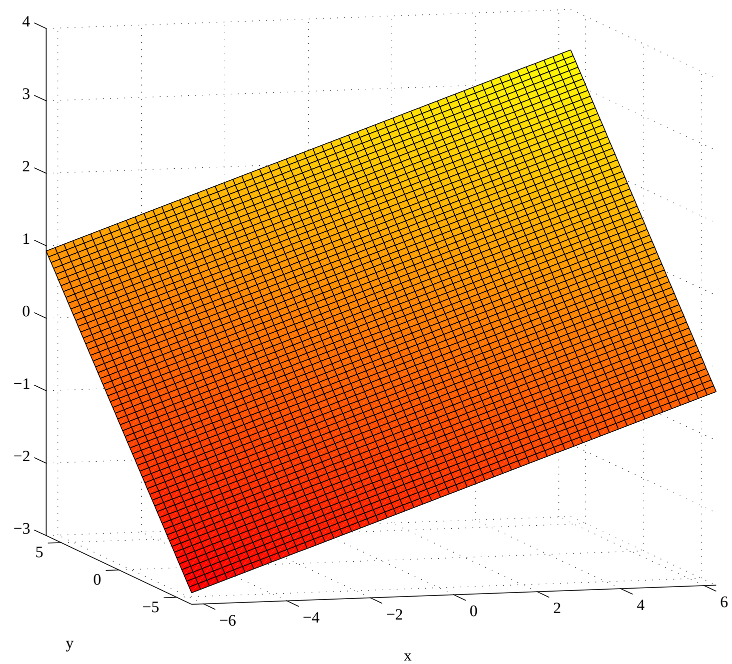
- Kernel methods yield candidate decision functions

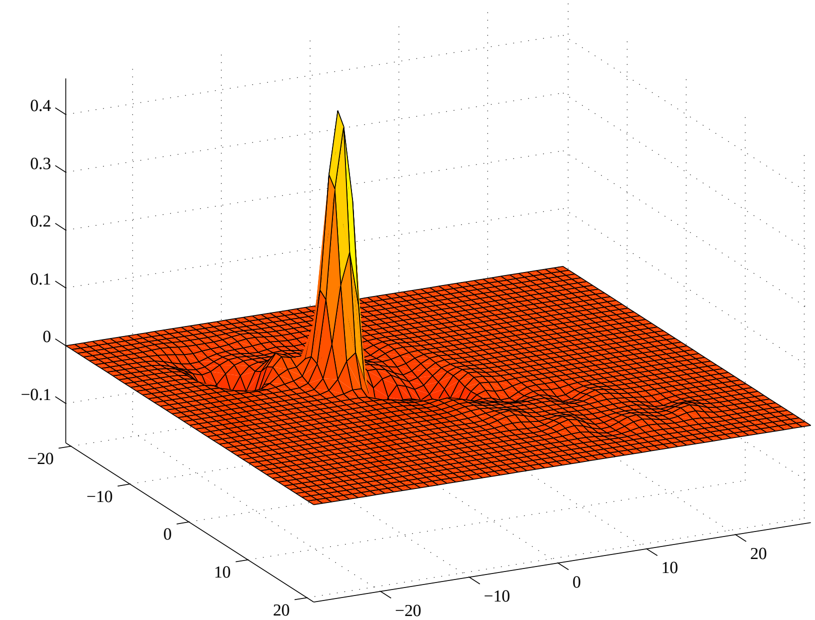
$$f(\mathbf{x}) = \sum_{j=1}^{\boldsymbol{n}} \boldsymbol{\alpha_j} k(\mathbf{x}_j, \mathbf{x}) + \boldsymbol{\alpha_0}.$$

  the free parameters are scalars $\boldsymbol{\alpha_0, \alpha_1, \cdots, \alpha_n}$.

Decision functions as linear combination of kernel evaluations

- linear decision surface / linear expansion of **kernel surfaces** (here $k_G(\mathbf{x}_i, \cdot)$)





- Kernel methods are considered **non-linear** tools.
- Yet not completely "nonlinear" $\rightarrow$ only one-layer of nonlinearity.

kernel methods use the data as a functional base to define decision functions

Decision functions as linear combination of kernel evaluations

database $\{\mathbf{x}_i, i = 1, \ldots, N\}$

$$f(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i \; k(\mathbf{x}_i, \mathbf{x})$$

kernel definition

weights α estimated
with a kernel machine

- f is any predictive function of interest of a new point **x**.
- Weights α are **optimized** with a kernel machine (*e.g.* support vector machine)

intuitively, kernel methods provide decisions based on how *similar* a point x is to each instance of the training set

The Gram matrix perspective

- Imagine a little task: you have read 100 novels so far.

- You would like to know whether you will enjoy reading a **new** novel.
- A few options:
  - read the book...
  - have friends read it for you, read reviews.
  - try to guess, based on the novels you read, if you will like it

The Gram matrix perspective

Two distinct approaches

- Define what **features** can characterize a book.
  - Map each book in the library onto vectors

$$\longrightarrow \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$$

typically the x_i's can describe...

▷ # pages, language, year 1st published, country,
▷ coordinates of the main action, keyword counts,
▷ author's prizes, popularity, booksellers ranking

- Challenge: find a decision function using 100 ratings and features.

The Gram matrix perspective

- Define what makes **two novels similar**,
  - Define a kernel k which quantifies novel similarities.
  - Map the library onto a Gram matrix

$$\longrightarrow \quad K = \begin{bmatrix} k(b_1,b_1) & k(b_1,b_2) & \cdots & k(b_1,b_{100}) \\ k(b_2,b_1) & k(b_2,b_2) & \cdots & k(b_2,b_{100}) \\ \vdots & \vdots & \ddots & \vdots \\ k(b_n,b_1) & k(b_n,b_2) & \cdots & k(b_{100},b_{100}) \end{bmatrix}$$

- Challenge: find a decision function that takes this 100×100 matrix as an input.

The Gram matrix perspective

Given a new novel,

- with the **features approach**, the prediction can be rephrased as **what are the features of this new book**? what **features** have I found in the past that were good indicators of my taste?

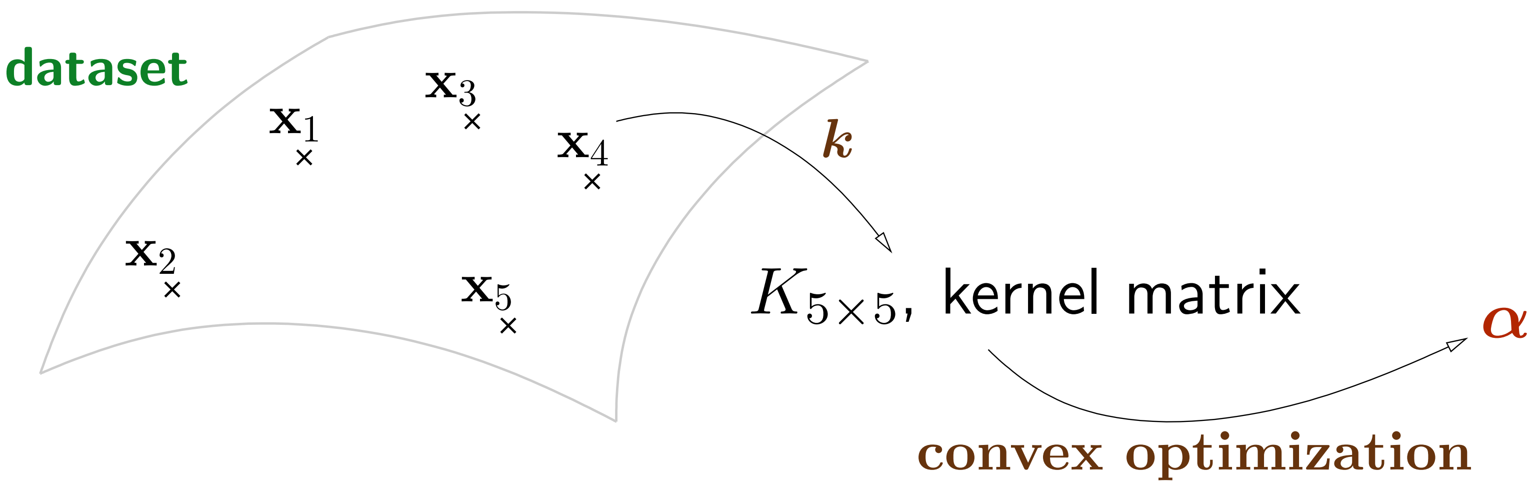
- with the **kernel approach**, the prediction is rephrased as **which novels this book is similar or dissimilar to?** what **pool of books** did I find the most influentials to define my tastes accurately?

kernel methods **only use kernel similarities**, do not consider features.

Features can help define similarities, but **never considered elsewhere**.

The Gram matrix perspective

in kernel methods, clear separation between the kernel...



and **Convex optimization** (thanks to psdness of K, more later) to output the α's.