Vietnam National University - Ho Chi Minh

Optimization, Machine Learning and Kernel Methods.

Machine Learning - Kernel Methods

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Regression, Classification and other Supervised Tasks

- **Two associated random variables**
  - A random variable x, taking values in $\mathcal{X}$,
  - A random variable y, taking values in $\mathcal{Y}$.
- **Two samples of (x, y) i.i.d. distributed from their joint law**
  - $\{(\mathbf{x}_1, \mathbf{y}_1), \cdots, (\mathbf{x}_n, \mathbf{y}_n)\}$, n couples of $\mathcal{X} \times \mathcal{Y}$.

Challenge: **predict** $\mathbf{y}$ when given only $\mathbf{x}$.

- In practice, **find** a function $\mathcal{X} \to \mathcal{Y}$ for which $f(\mathbf{x})$ is not too different from y on average.

Binary Classification

- $\mathcal{Y} = \{-1, 1\}$.
- f needs to be a functions that, given $\mathbf{x}$ predicts a label,

$$f : \mathcal{X} \mapsto \{-1, 1\}$$

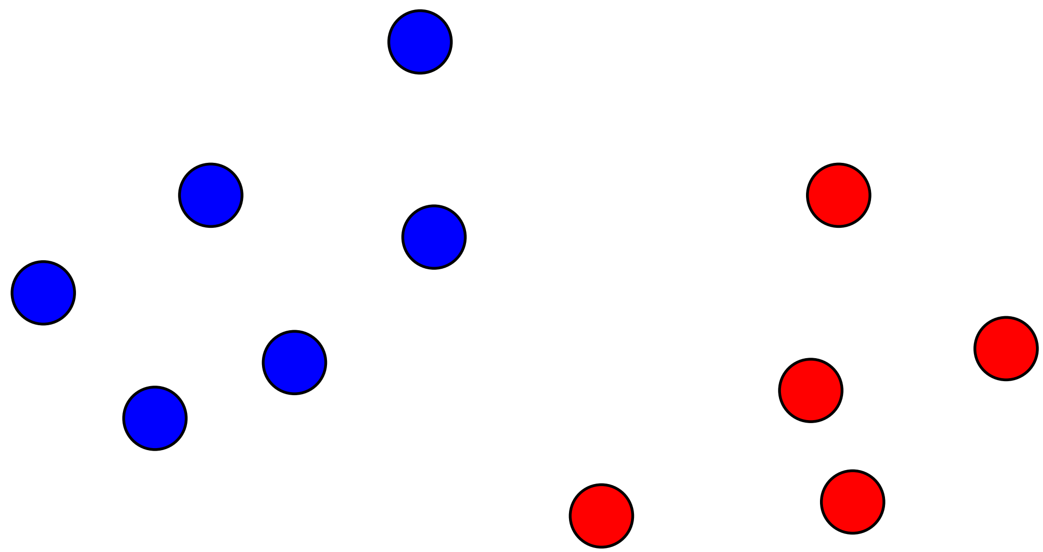
  of course, many possible choices for f's shape.
- We review here **linear** hyperplanes in $\mathcal{X} = \mathbb{R}^d$ first.
- We represent it in $\mathbb{R}^2$ for simplicity.

Next slides will cover an important algorithm, the **SVM** algorithm

- this algorithm can be naturally expressed in terms of *kernels*. we review later other algorithms for which this is also the case.

thanks to Jean-Philippe Vert for many of the following figures and slides.

Linear classifier, some degrees of freedom



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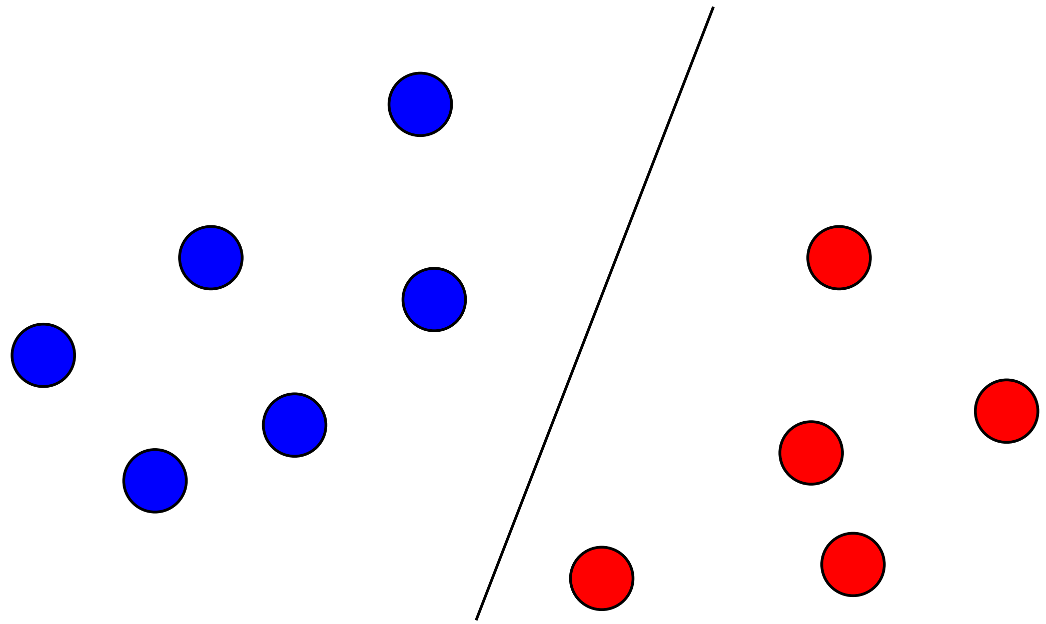

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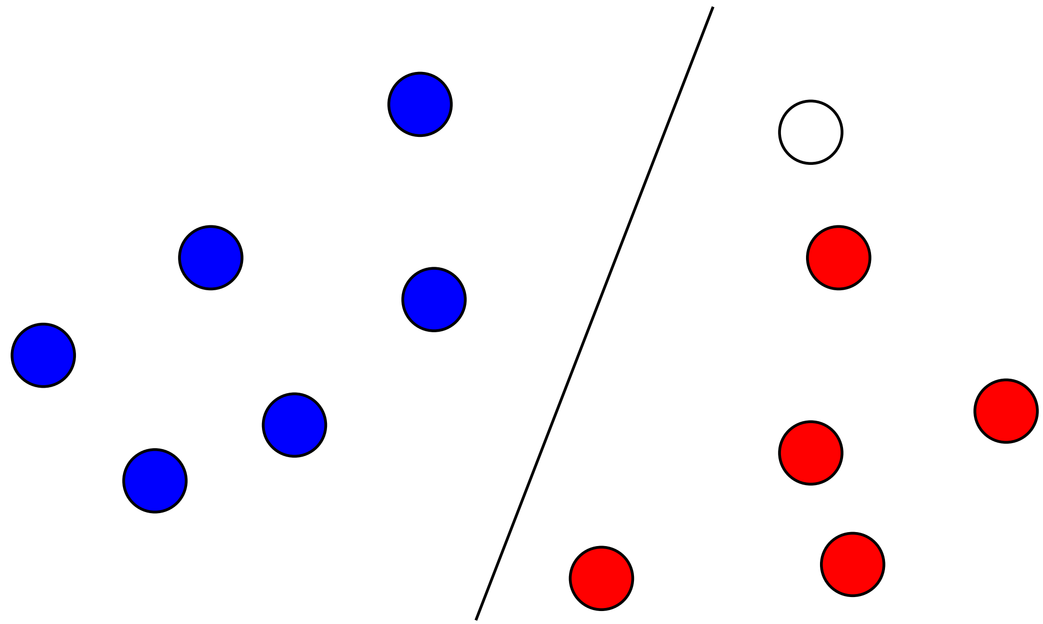

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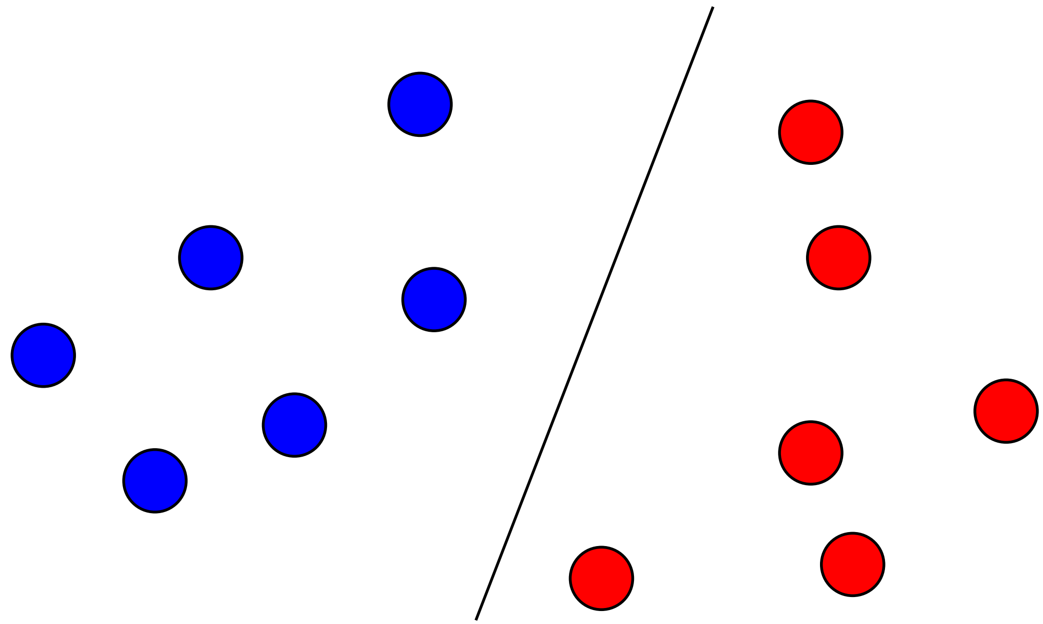

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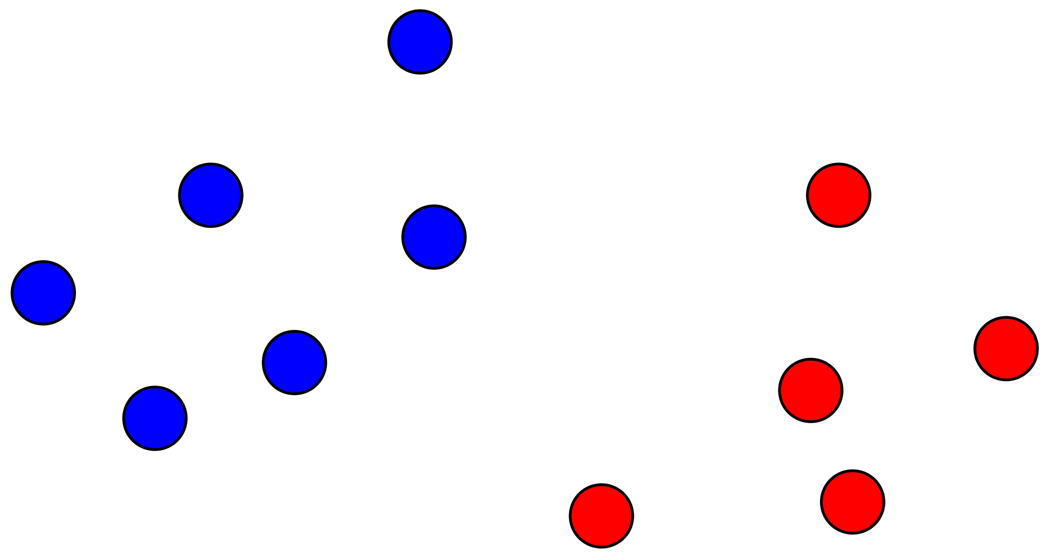

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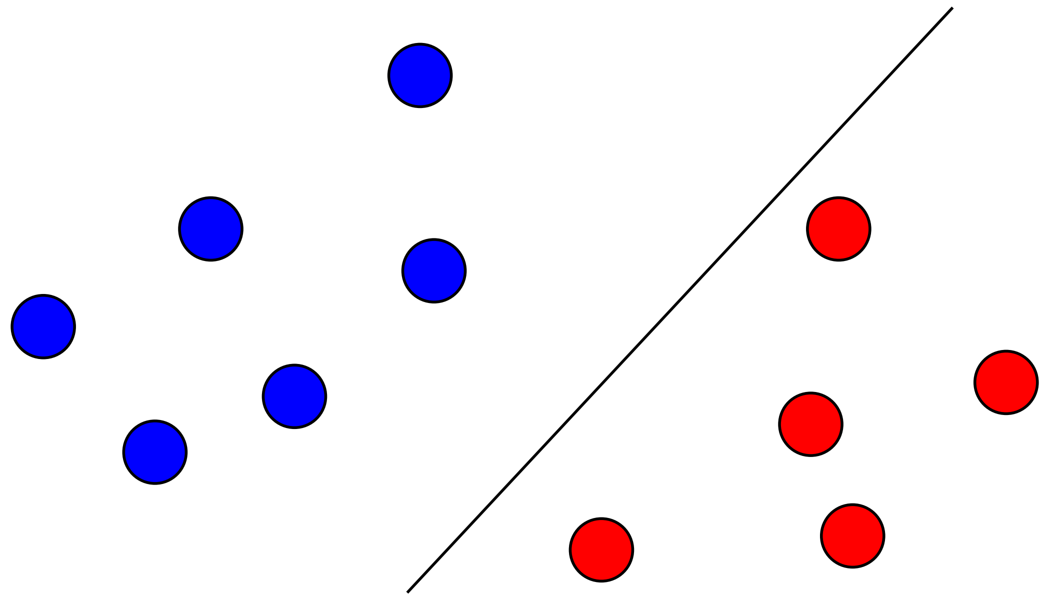

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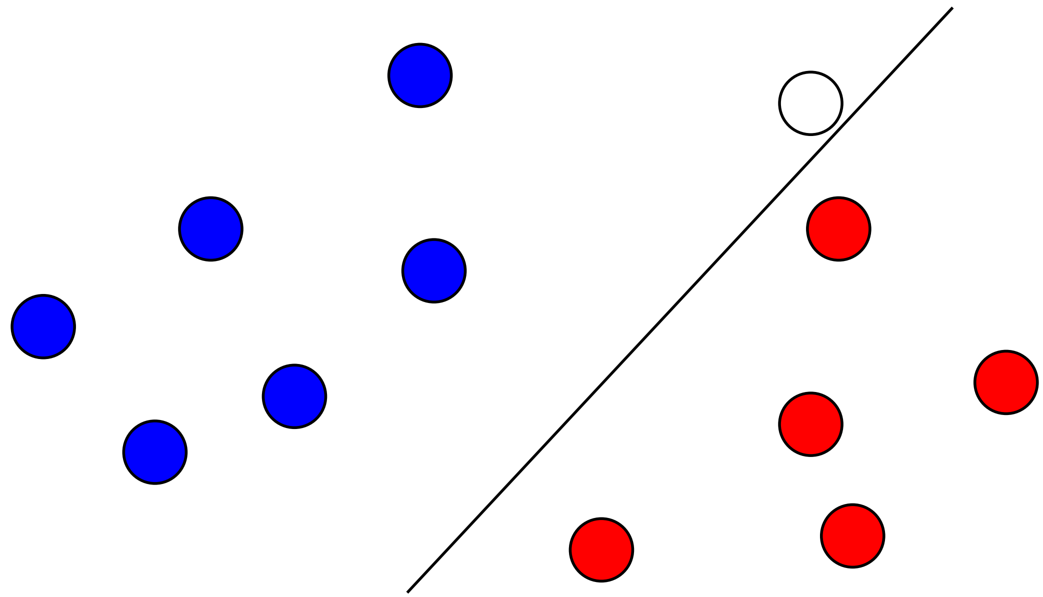

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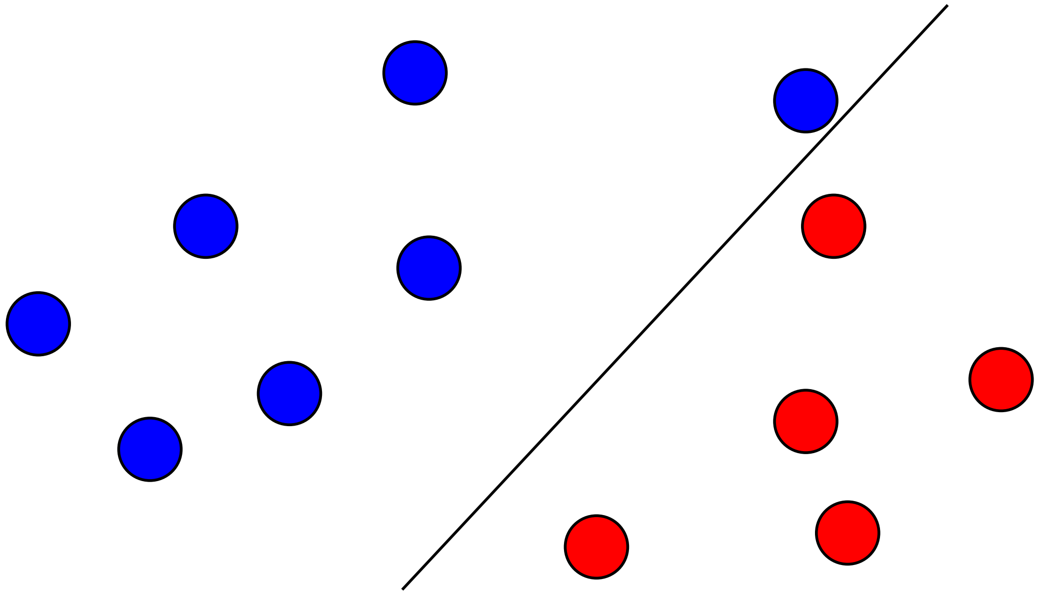
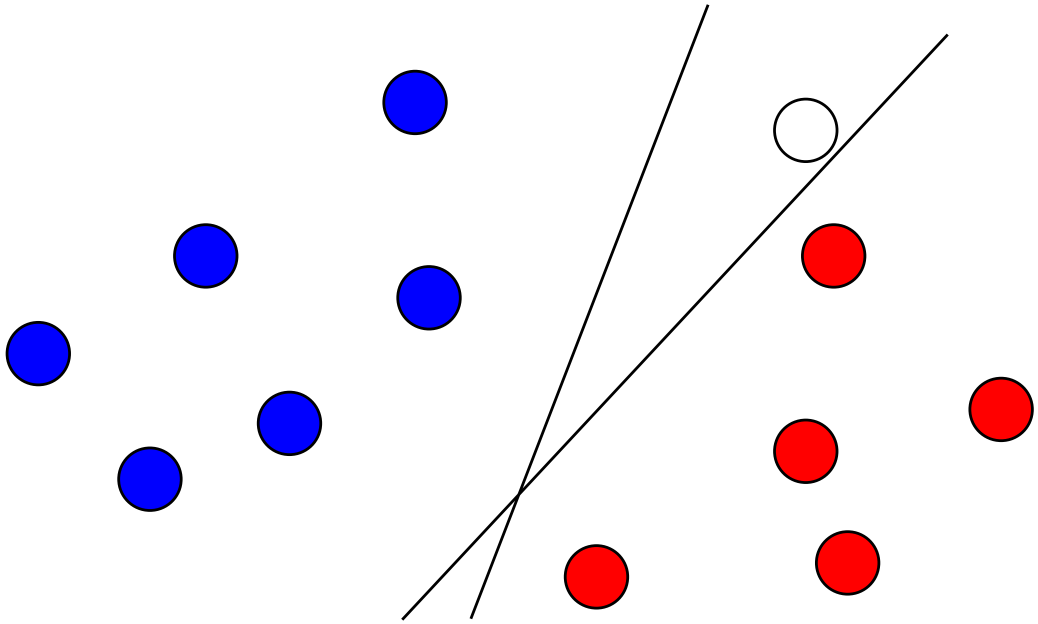
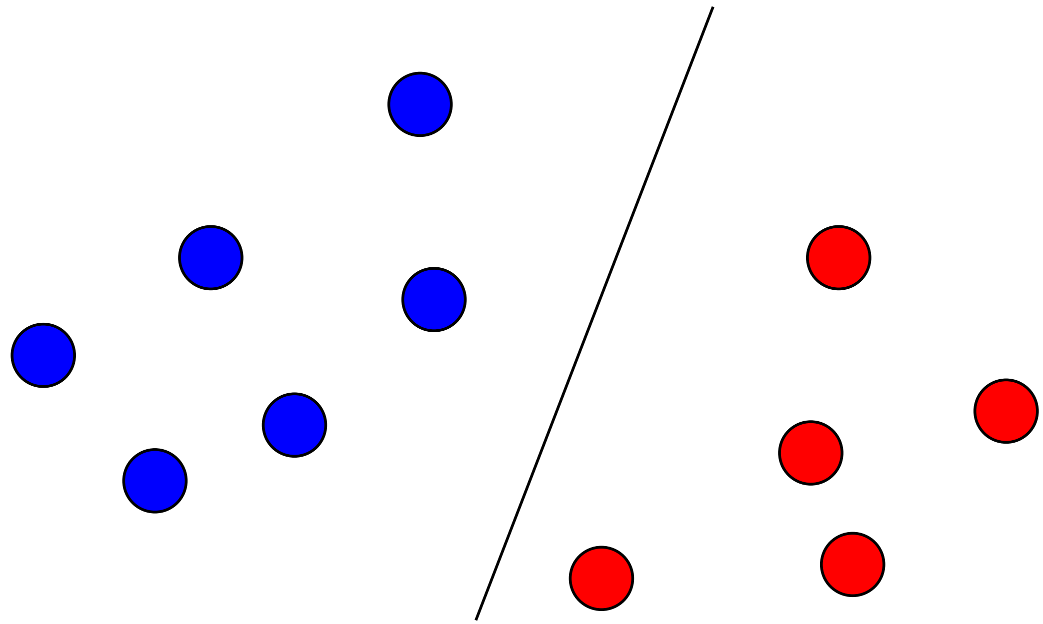


Which one is better?



A criterion to select a linear classifier: the margin



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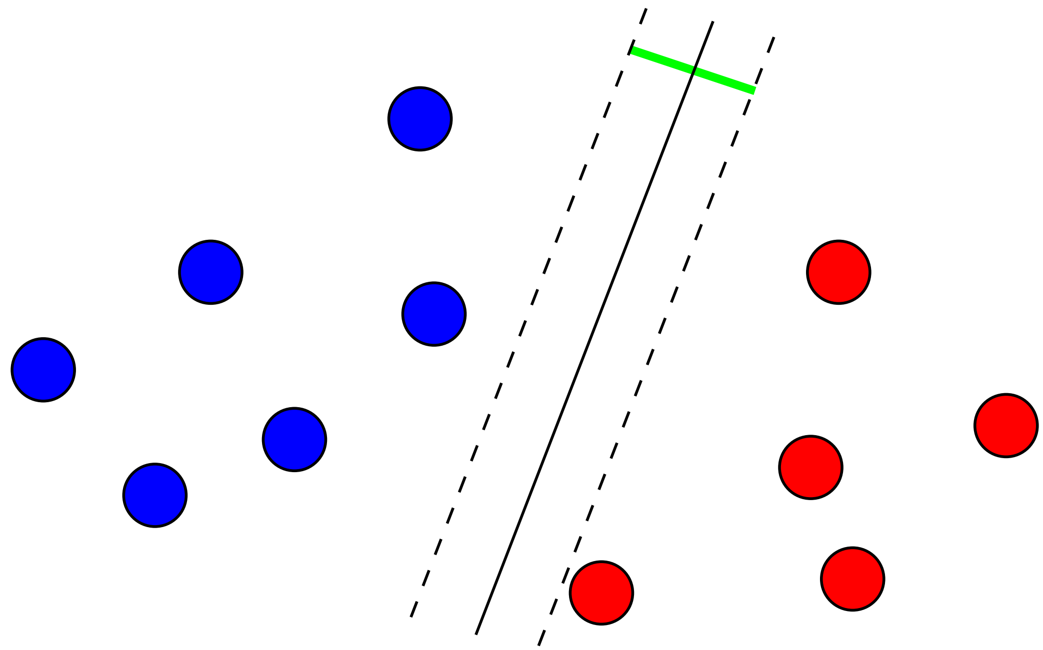

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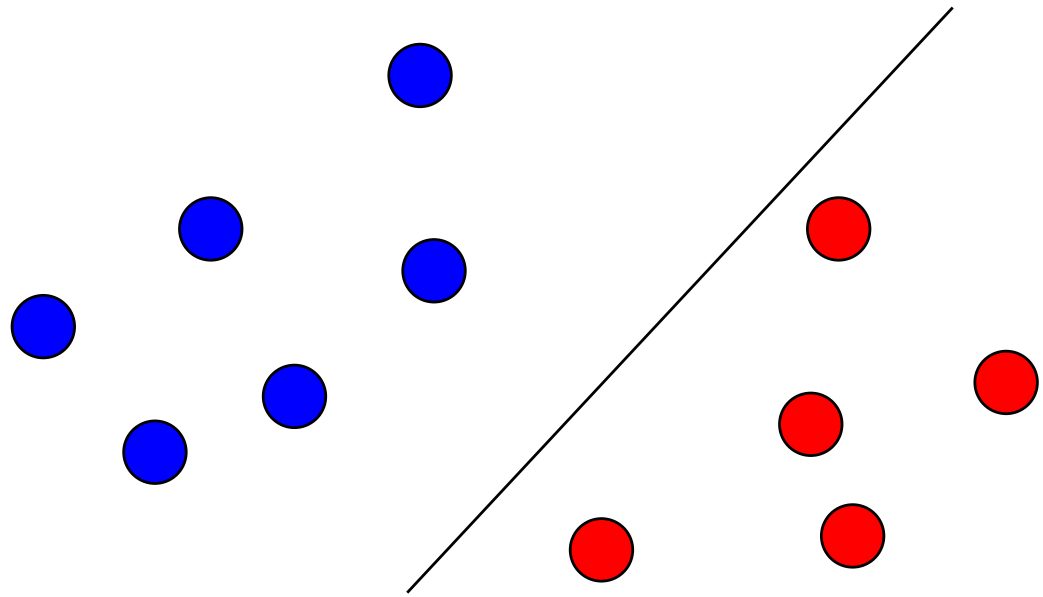

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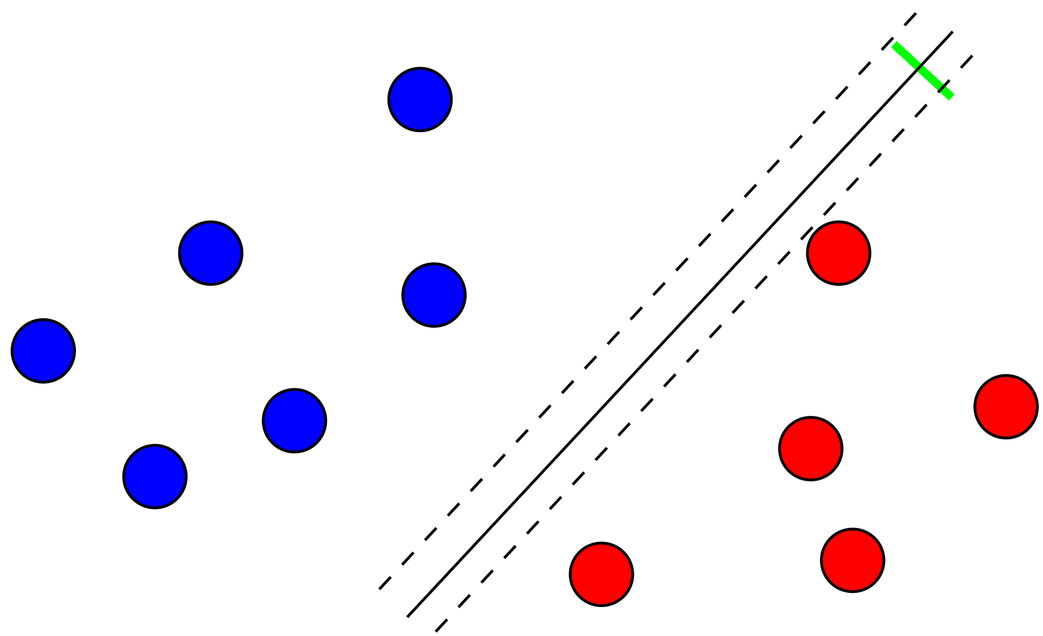

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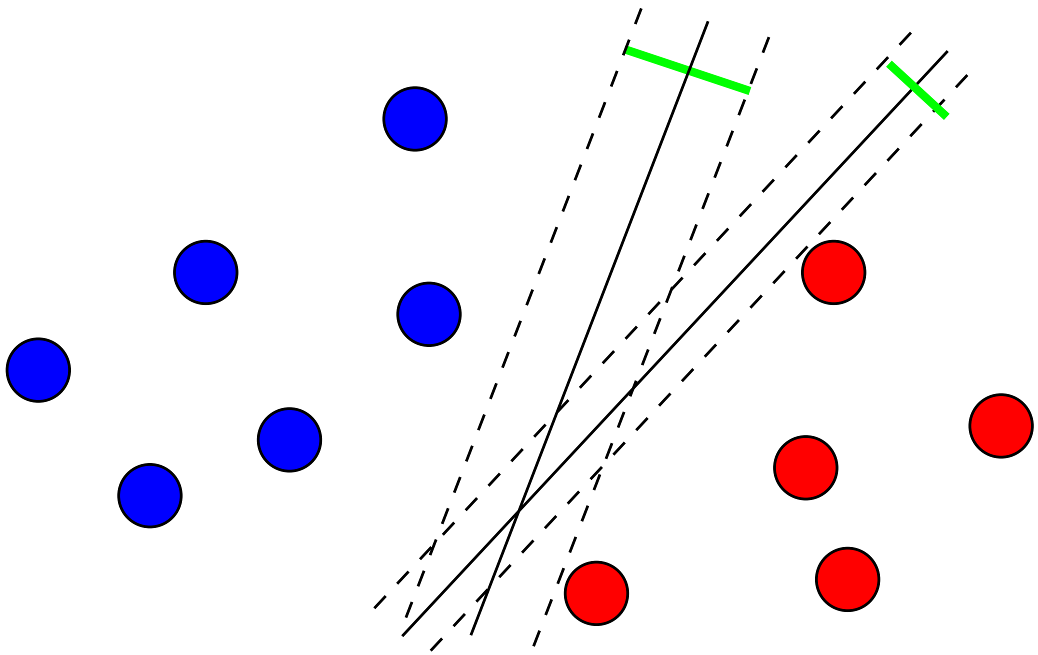
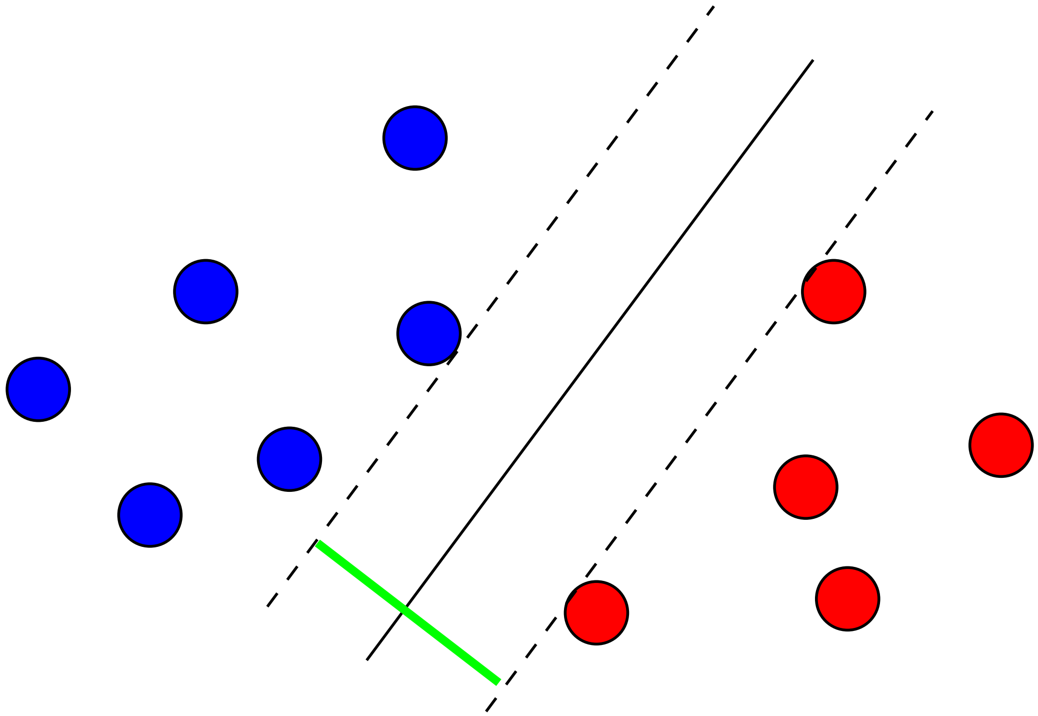
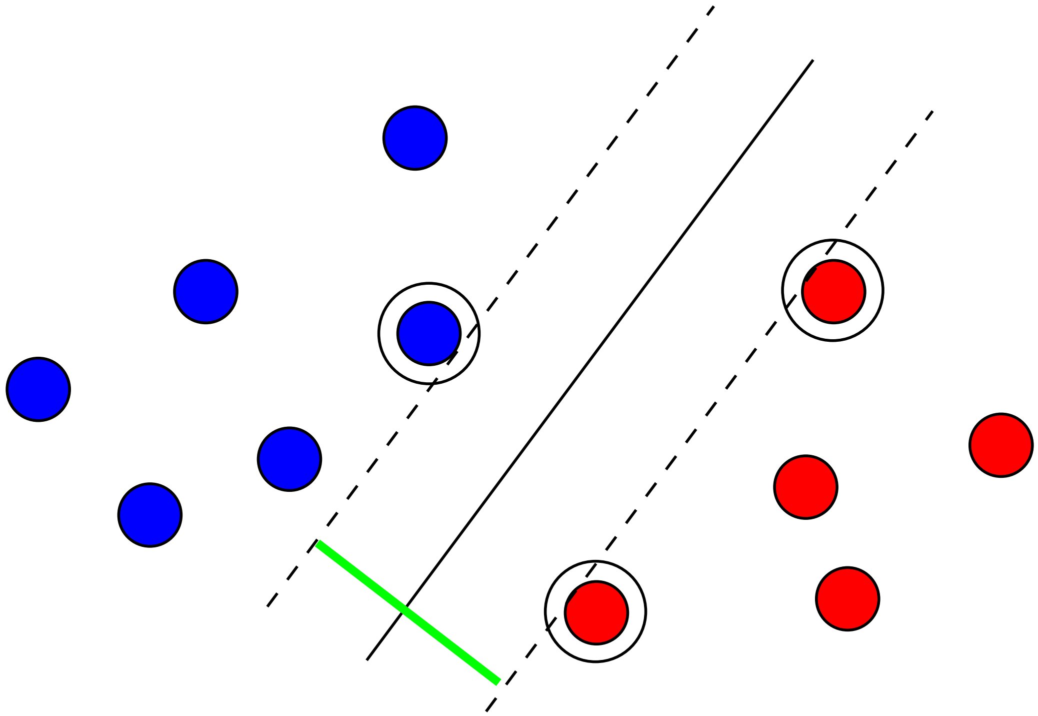


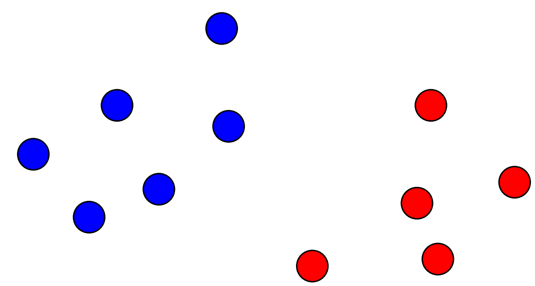
Largest Margin Linear Classifier



Support Vectors with Large Margin



In equations



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

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

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

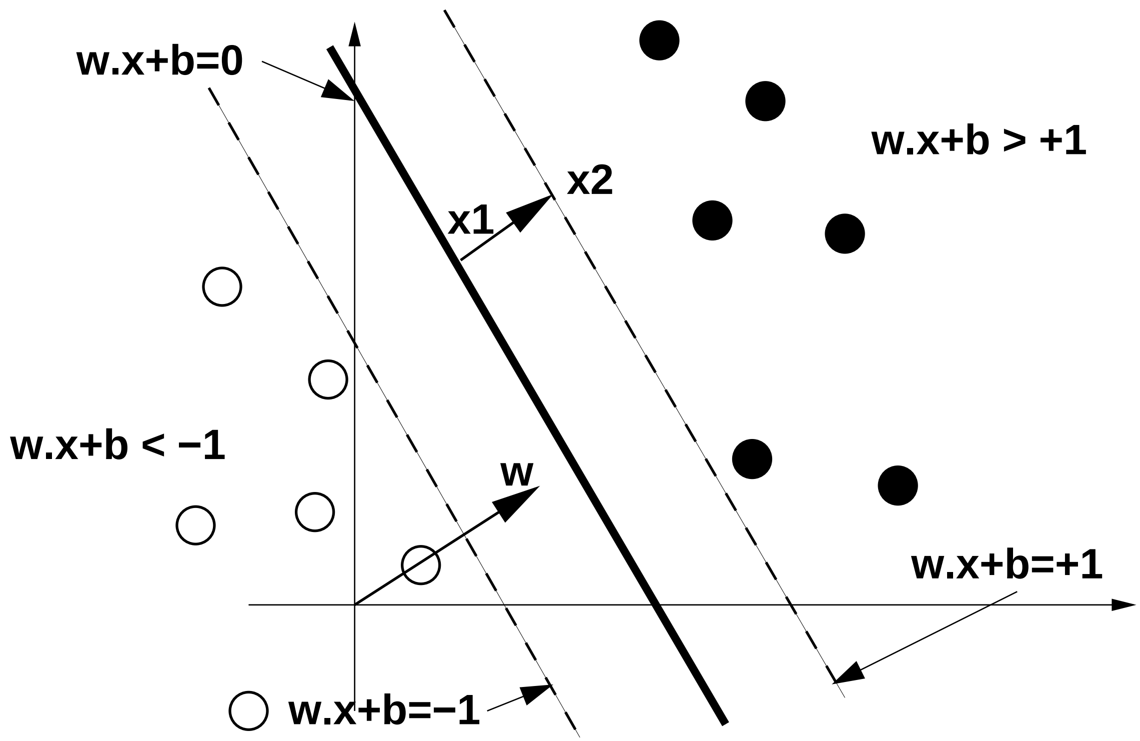
- We assume (for the moment) that the data are **linearly separable**, i.e., that there exists $(\mathbf{w}, b) \in \mathbb{R}^d \times \mathbb{R}$ such that:

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

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:

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

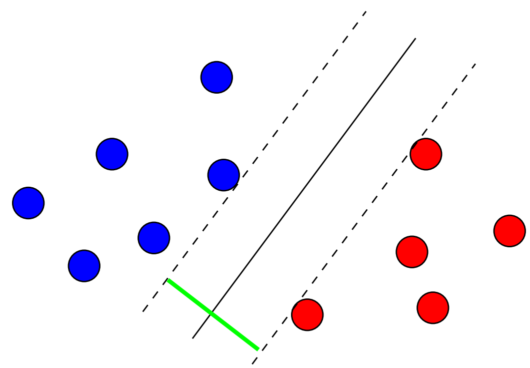
- For negative examples ($y_i = -1$) this means:

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

- 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



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

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

under the constraints:

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

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**,
- namely, for **each training point**. The Lagrangian is, for $\alpha \succeq 0$,

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

The Lagrange dual function

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

is only defined when

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

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

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. KKT gives us $\alpha_i(\mathbf{y}_i \left(\mathbf{w}^T\mathbf{x}_i + b\right) - 1) = 0$, either $\alpha_i = 0$ or $\mathbf{y}_i \left(\mathbf{w}^T\mathbf{x}_i + b\right) = 1$.
- $\alpha_i \neq 0$ **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 on $\mathbb{R}^n$, with *box constraints*.
α^* can be found efficiently using dedicated optimization softwares

Recovering the optimal hyperplane

- Once α^* is found, 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 $\alpha_i > 0$, $\mathbf{y}_i(\mathbf{w}^T \mathbf{x}_i + b) = 1$,

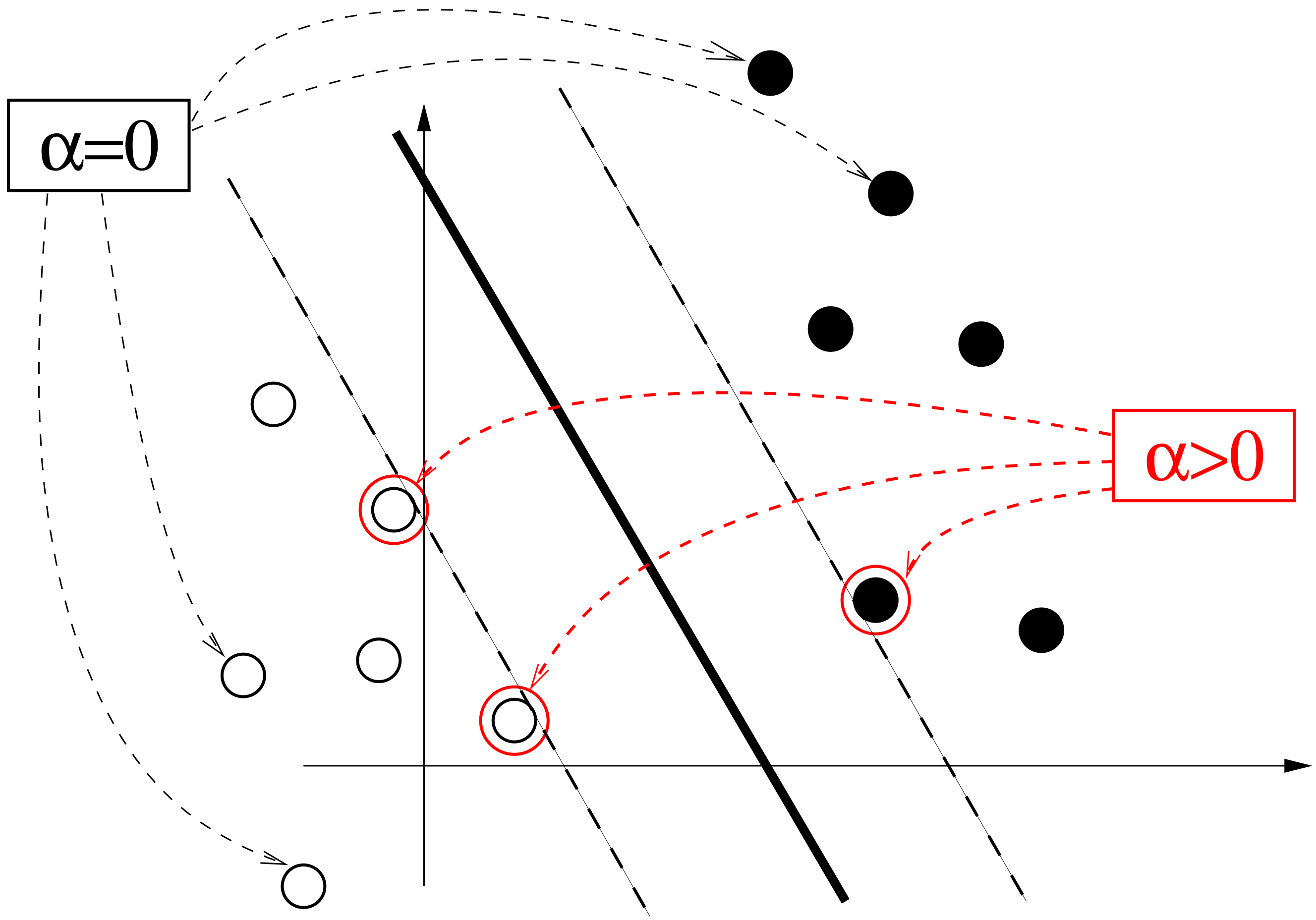
$$b^* = -\frac{1}{2}\left(\min_{\mathbf{y}_i=1,\alpha_i>0}(\mathbf{w}^T\mathbf{x}_i) + \max_{\mathbf{y}_i=-1,\alpha_i>0}(\mathbf{w}^T\mathbf{x}_i)\right)$$

- the **decision function** is therefore:

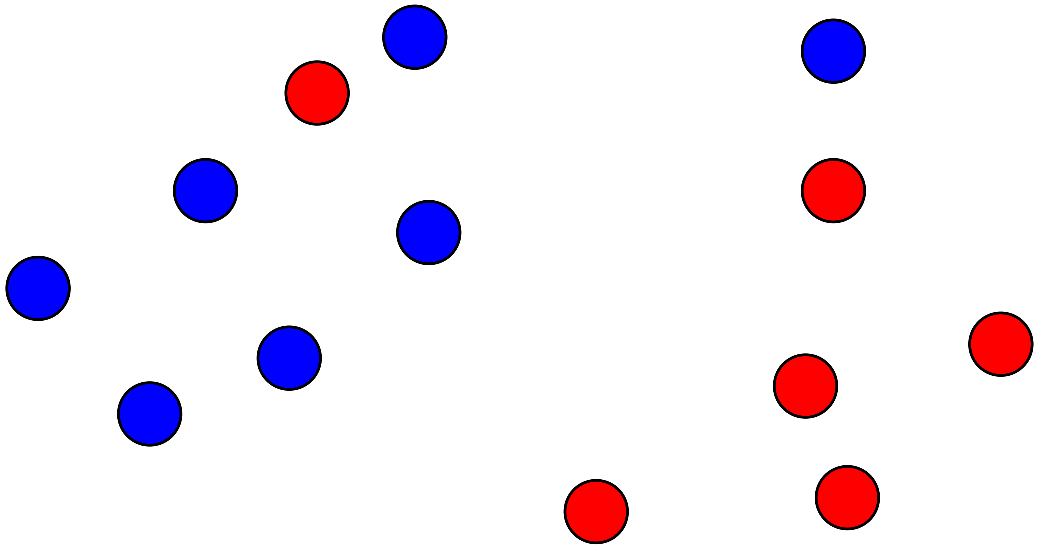
$$\begin{aligned} f^*(\mathbf{x}) &= \mathbf{w}^T\mathbf{x} + b^* \\ &= \sum_{i=1}^n y_i \alpha_i \mathbf{x}_i^T \mathbf{x} + b^*. \end{aligned}$$

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

Interpretation: support vectors



What happens when the data is not linearly separable?



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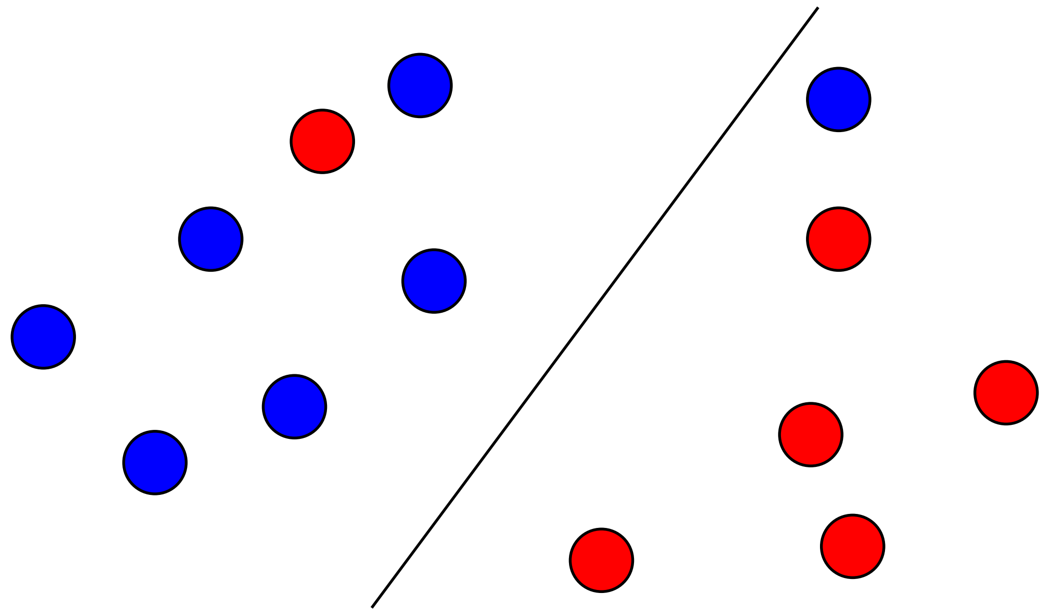

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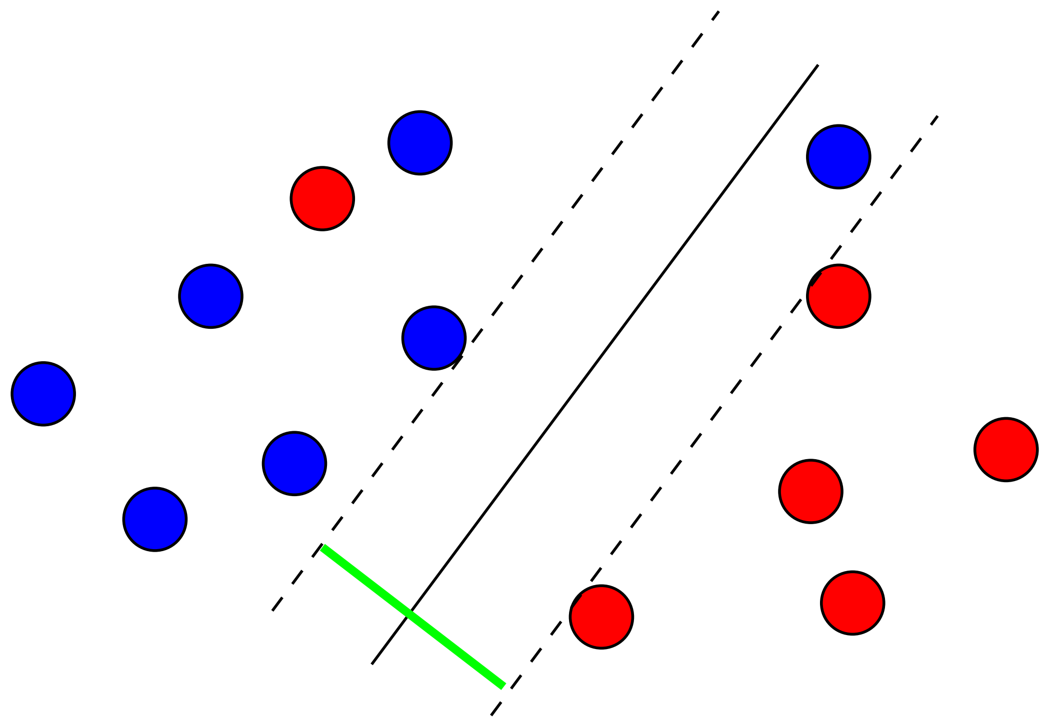

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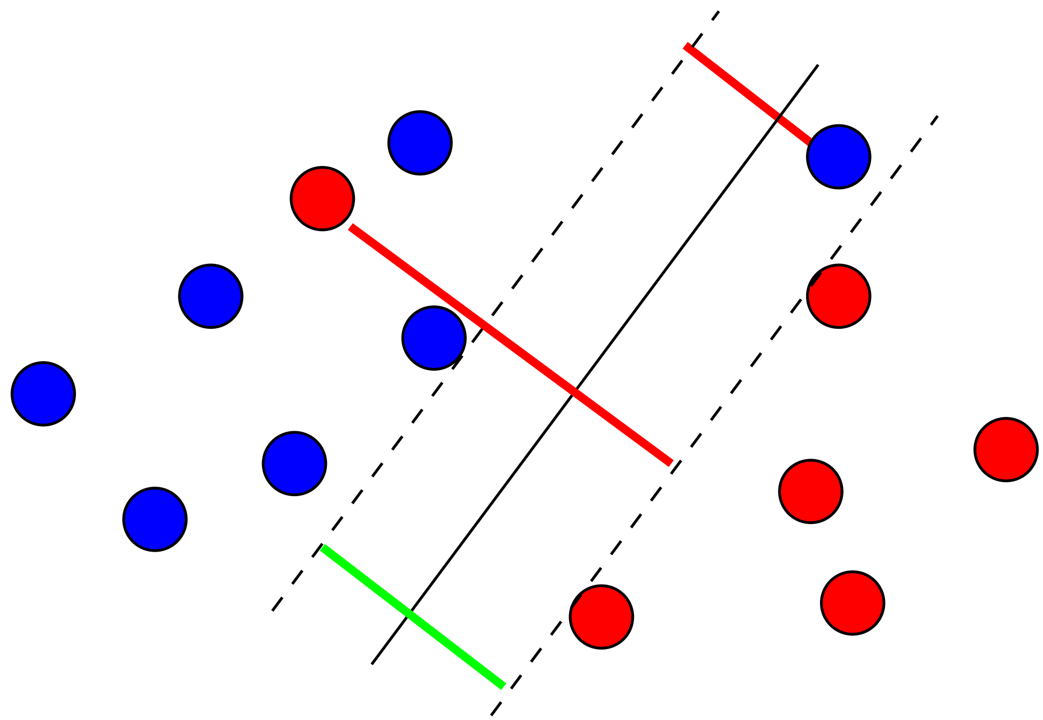
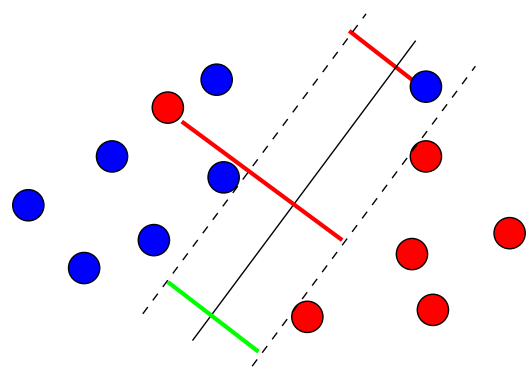


Soft-margin SVM

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

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

- 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

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

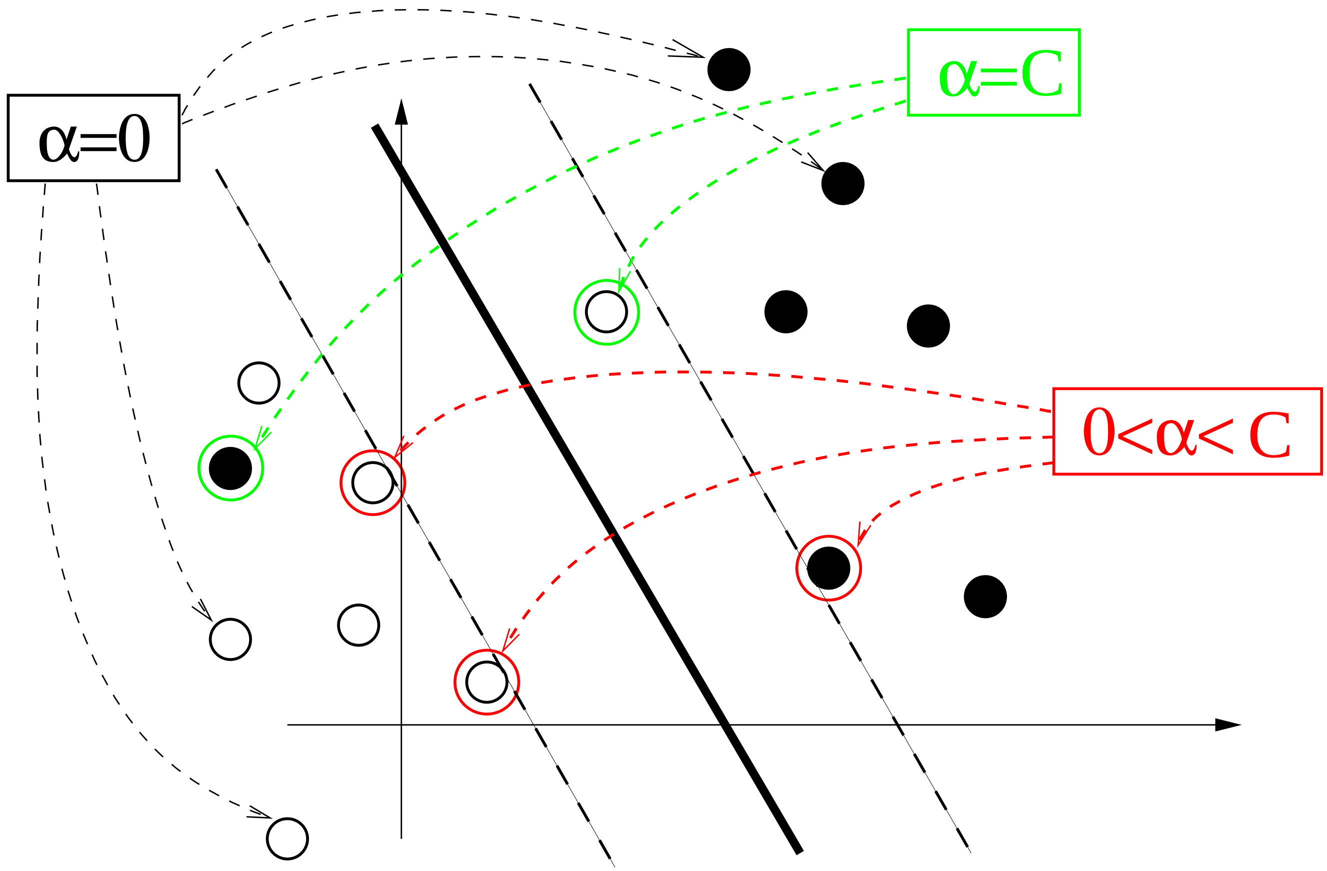
- In that case the dual function

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

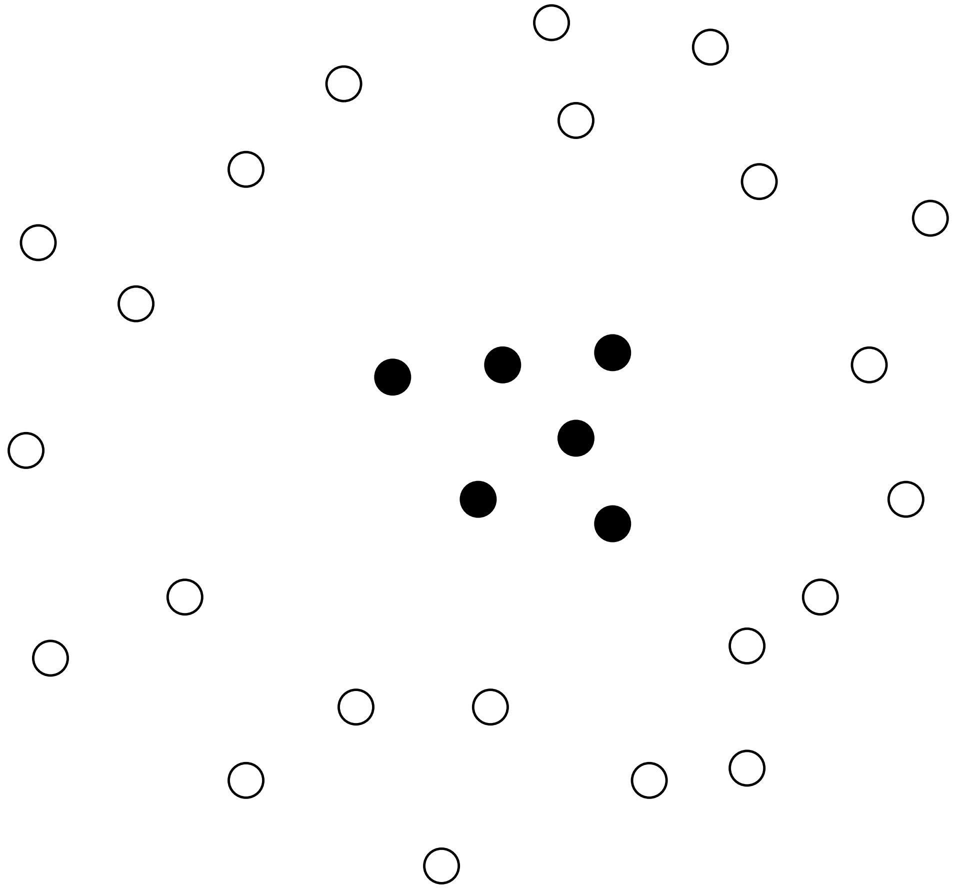
which is finite under the constraints:

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

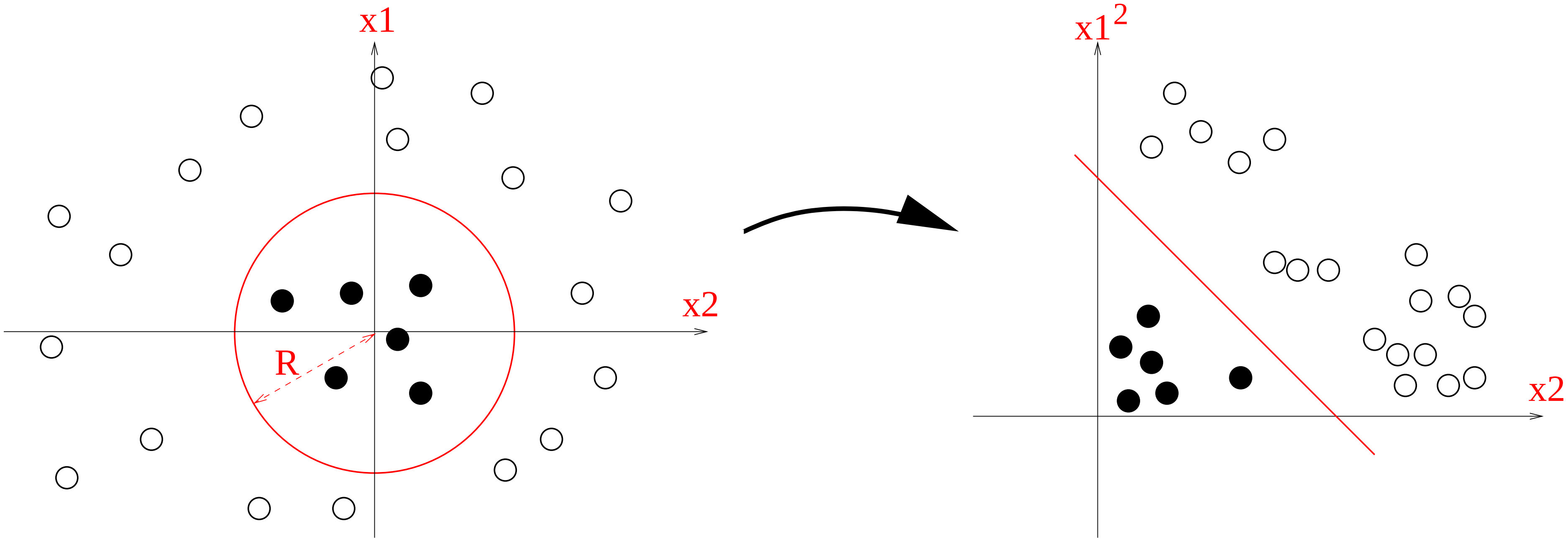
Interpretation: bounded and unbounded support vectors



Sometimes linear classifiers are not interesting



Solution: non-linear mapping to a feature space



Let $\phi(\mathbf{x}) = (x_1^2, x_2^2)'$, $\mathbf{w} = (1,1)'$ and $b = 1$. Then the decision function is:

$$f(\mathbf{x}) = x_1^2 + x_2^2 - R^2 = \langle \mathbf{w}, \phi(\mathbf{x}) \rangle + b,$$

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 $\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle = k(\mathbf{x}, \mathbf{x}')$

- 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:

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

- 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 K and $\mathbf{y}$:

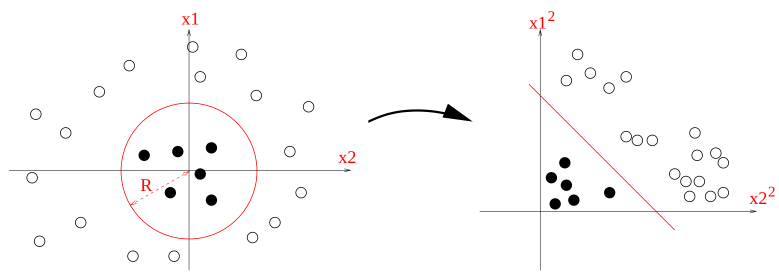
$$\begin{array}{ll} \text{maximize} & g(\alpha) = \alpha^T \mathbf{1} - \frac{1}{2}\alpha^T(\mathbf{y}^T \boldsymbol{K} \mathbf{y})\alpha \\ \text{such that} & 0 \leq \alpha_i \leq C, \quad \text{for } i = 1, \ldots, n \\ & \sum_{i=1}^n \alpha_i \mathbf{y}_i = 0. \end{array}$$

- in the end the solution $f(\mathbf{x}) = \sum_{i=1}^n y_i \alpha_i k(\mathbf{x}_i, \mathbf{x}) + b$.

Kernel example: polynomial kernel

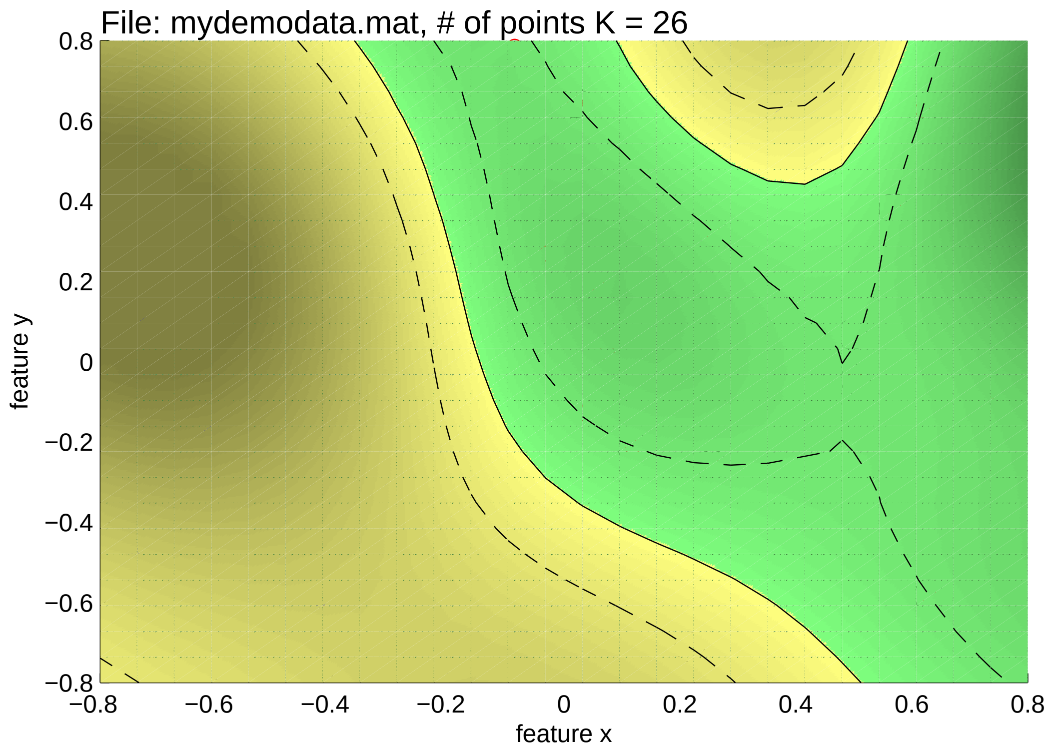
- For $\mathbf{x} = (x_1, x_2)^\top \in \mathbb{R}^2$, let $\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$:

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



Some demonstrations using Matlab

- playing with a few kernels and a few points



SVM's: a particular case of a more general framework, penalized estimation

Empirical Risk Minimization

- Starting with $\{(\mathbf{x}_1, \mathbf{y}_1), \cdots, (\mathbf{x}_n, \mathbf{y}_n)\}$, n couples of $\mathcal{X} \times \mathcal{Y}$,
- A class of functions $\mathcal{F}$,
- A cost function $\boldsymbol{c} : \mathcal{Y} \times \mathcal{Y}$, $c \geq 0$, which penalizes discrepancies (hinge, least squares *etc.*)
- find a function which minimizes

$$\hat{f} = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{c}(f(\mathbf{x}_i), y_i)$$

  and use this f as a decision function.
- As usual in minimizations, we like:
  - Convex problems, unique minimizers
  - Stable solutions numerically.

Linear least squares

- When $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \mathbb{R}$,
- $\boldsymbol{\mathcal{F} = \{\mathbf{x} \mapsto \beta^T \mathbf{x} + b\,, \beta \in \mathbb{R}^d, b \in \mathbb{R}\}}$, $\boldsymbol{c(\mathbf{y}_1, \mathbf{y}_2) = \|\mathbf{y}_1 - \mathbf{y}_2\|^2}$,
- The problem is known as **regression** with the **least squares criterion**.
- In this case, the minimizer

$$\operatorname*{argmin}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \|f(\mathbf{x}_i) - \mathbf{y}_i\|^2 = \operatorname*{argmin}_{\beta \in \mathbb{R}^d, b \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^{n} \|\beta^T \mathbf{x}_i + b - \mathbf{y}_i\|^2$$

  is **unique assuming** $n > d$ and no degeneracy.

- Why?

$$R : (b, \beta) \rightarrow \frac{1}{n} \sum_{i=1}^{n} \|\beta^T \mathbf{x}_i + b - \mathbf{y}_i\|^2 = \frac{1}{n} \|X^T \left[\begin{smallmatrix} b \\ \beta \end{smallmatrix}\right] - y\|^2$$

  is convex, where $X = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \cdots & \vdots \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \in \mathbb{R}^{d+1 \times n}$ and $y = \begin{bmatrix} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_n \end{bmatrix} \in \mathbb{R}^n$.

Linear least squares

- Notice that

$$R(b,\beta) = \frac{1}{n}\left(\left[\begin{smallmatrix} b \\ \beta \end{smallmatrix}\right]^T XX^T \left[\begin{smallmatrix} b \\ \beta \end{smallmatrix}\right] - 2y^T X^T \left[\begin{smallmatrix} b \\ \beta \end{smallmatrix}\right] + \|y\|^2 \right)$$

- Let us take the gradient of that function

$$n\nabla R = 2XX^T \left[\begin{smallmatrix} b \\ \beta \end{smallmatrix}\right] - 2Xy$$

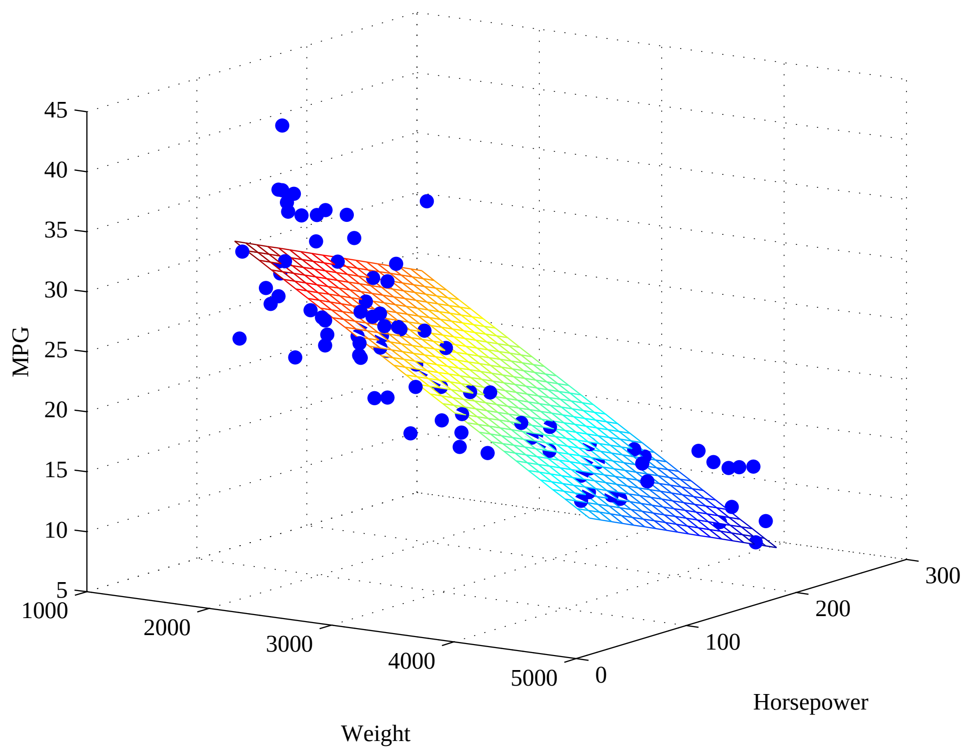
- Hence this gradient is zero for $\left[\begin{smallmatrix} b \\ \beta \end{smallmatrix}\right] = (XX^T)^{-1}Xy$
- $XX^T \in \mathbf{S}_+^n$. This works if $XX^T \in \mathbb{R}^{d+1}$ is **invertible**, that is $XX^T \in \mathbf{S}_{++}^n$.
- Remark:

$$XX^T = \begin{bmatrix} n & n\bar{x}_1 & n\bar{x}_2 & \cdots & n\bar{x}_d \\ n\bar{x}_1 & & & & \\ n\bar{x}_2 & & & & \\ \vdots & & \mathbf{X}\mathbf{X}^T & & \\ n\bar{x}_d & & & & \end{bmatrix} = \begin{bmatrix} n & n\mu^T \\ n\mu & \mathbf{X}\mathbf{X}^T \end{bmatrix}$$

where $\mathbf{X}$ is simply the $d \times n$ sample matrix without the constant 1.

Example in $\mathbb{R}^3$

- Sample of cars: x desribes weight and horsepower of a car.
- y is the miles-per-gallon : high is eco-friendly, low is bad.



- The hyperplane fits the data quite well, $\begin{bmatrix} b \\ \beta \end{bmatrix} \begin{bmatrix} 47.7694 \\ -0.0066 \\ -0.0420 \end{bmatrix} \begin{bmatrix} b \\ \beta \end{bmatrix}$.

Linear least-squares is not the ideal tool though...

- What happens when $d \gg n$? (XX^T) is **no longer invertible**...
  - high-dimensional data in genomics,
  - images analysis ($e.g.$lots of features)

- What happens when (XX^T) is **badly conditioned** ($\frac{\lambda_{\min}(XX^T)}{\lambda_{\max}(XX^T)} \approx 0$)?
  - if $\lambda_{\min}(XX^T) = 1e-10$, $\lambda_{\max}\left((XX^T)^{-1}\right) = 1e10!!$
  - Very bad numerical stability of the solution...

- When $d \gg n$, we might want to do **variable selection**,
  - $i.e.$pick a subset d' of the d variables which is relevant to predict $\mathbf{y}$.
  - $i.e.$favor vectors β such that $\|\beta\|_0 = \operatorname{card} \beta_i \neq 0$ is small.

Penalized Least-Squares

- For all these problems, there is an appropriate penalization:

$$(\hat{\beta}, \hat{b}) = \underset{\beta\in\mathbb{R}^d, b\in\mathbb{R}}{\operatorname{argmin}} \frac{1}{n}\sum_{i=1}^{n} \|\beta^T \mathbf{x}_i + b - \mathbf{y}_i\|^2 + \lambda \|(\beta, b)\|$$

  - we recover **least-square regression** when $\lambda = 0$;
  - **ridge regression** when $\lambda > 0$ and $\|(\beta, b)\| = \|(\beta, b)\|_2^2 = b^2 + \left(\sum_{i=1}^n \beta_i^2\right)^2$:

$$\left[\begin{smallmatrix} b \\ \beta \end{smallmatrix}\right] = \left(XX^T + \lambda \left[\begin{smallmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 \\ \vdots & 0 & \ddots & 0 \\ 0 & 0 & 0 & 1 \end{smallmatrix}\right]\right)^{-1} Xy$$

  - the **lasso** when $\lambda > 0$ and $\|(\beta, b)\| = \|(\beta, b)\|_1 = |b| + \sum_{i=1}^n |\beta_i|$;

What about the case where linearity does not work?

- Many examples show that life is not always linear... **kernels at the rescue**.

- Let us take a further look at $\beta = (XX^T)^{-1}Xy$.
- For any new point, $\beta^T\mathbf{x}$ plays the same role as $\mathbf{w}^T\mathbf{x}$ in the SVM.
- We consider a new point $\mathbf{x} \in \mathbb{R}^d$ with the constant 1, *i.e.* $\mathbf{x} \leftarrow \left[\begin{smallmatrix} 1 \\ \mathbf{x} \end{smallmatrix}\right]$.
- $[b, \beta^T]\mathbf{x} = \mathbf{x}^T(XX^T + \lambda I_d)^{-1}Xy$.

Kernel ridge regression

- A simple inversion trick states that $(XX^T + \lambda I_d)^{-1} X y = X(\lambda I_n + X^T X)^{-1} y$

- Hence $[b, \beta^T]\mathbf{x} = \mathbf{x}^T X(\lambda I_n + X^T X)^{-1} y = \begin{bmatrix} \mathbf{x}^T\mathbf{x}_1 \\ \mathbf{x}^T\mathbf{x}_2 \\ \vdots \\ \mathbf{x}^T\mathbf{x}_d \end{bmatrix}^T (\lambda I_n + [\, \mathbf{x}_i^T \mathbf{x}_j \,])^{-1} y$!

- Bottom line: we have shown how to compute a regression tool which only depends on dot-products.

- Dot-products can be replaced by **kernels**!

$$f(\mathbf{x}) = \begin{bmatrix} k(\mathbf{x},\mathbf{x}_1) \\ k(\mathbf{x},\mathbf{x}_2) \\ \vdots \\ k(\mathbf{x},\mathbf{x}_d) \end{bmatrix}^T (\lambda I_n + \left[k(\mathbf{x}_i, \mathbf{x}_j)\right])^{-1} y$$

Kernel methods

- **Many** other standard **linear** algorithms,
  - Principal Component Analysis,
  - Canonical Correlation Analysis,
  - Fisher Discriminant analysis,
  - $etc.$can be modified to **incorporate** kernel similarities.

Algorithms based on **kernels** are known as **kernel methods**.

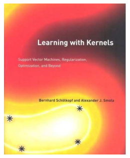
Kernel Methods

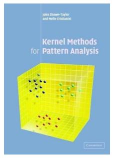
A reasonably large academic subfield

- Widespread popularity in machine learning now

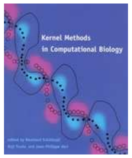
- Gained momentum in the late 90's with the support vector machine,
- Rooted in much older maths.
- Kernel methods are a pluridisciplinary field, publications appearing in
  - computer science (*nips, journ. of machine learning, ICML..*),
  - statistics and functional analysis (*annals of statistics..*),
  - optimization (*Mathematical Programming..*),
  - Different application subfields (*Neural Computation..*)

Kernel Methods

- Standard text-books:
  - Introduction [SS02] 

  - More about kernels [STC04] 

  - More learning theory [SC08] 

  - First chapters [STV04] 

  - “Mathematical” perspective [BTA03]. The real deal: [BCR84].
- Some short surveys,
  - journal papers [HHS08], [MMR+01]
  - a survey on my webpage (local copy, not arxiv): key to all citations!
- On the web:
  - Courses by J.-P. Vert, Francis Bach, Kenji Fukumizu, Stéphane Canu.

Some terminology

Etymology : from old english *cyrnel*, diminutive of corn (seed)

the word **kernel** appears in different different contexts...

- The *linux* kernel...
- Kernel of a linear operator of $\mathcal{X}$: $\ker(L) = \{x \in \mathcal{X} | L(x) = 0\}$.
- Kernel of a matrix in $\mathbb{R}^{d\times d}$, $i.e.$ its nullspace $\{\mathbf{x} \in \mathbb{R}^d | A\mathbf{x} = \mathbf{0}\}$.
- In set theory, for a function $f : \mathcal{X} \mapsto \mathcal{Y}$, $\ker(f) = \{(x, x') | \, f(x) = f(x')\}$.
- Kernel of an integral transform T, $Tf(u) = \int_{t_1}^{t_2} k(t,u) f(t) dt$
- Smoothing kernel, a function $k \geq 0, k(u) = k(-u), \int_{-\infty}^{\infty} k(u) du = 1$.
- $K(t,x,y) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{\|x-y\|^2}{4t}}$ solves heat equation $K(t,x,y) = \Delta_x K(t,x,y)$

sets, subspaces, **one-**variable, **two-**variables, **three-**variables function...

Moral of the story

No need to look for a common or primitive meaning

- Kernel is just a word mathematicians fancy (unfortunately!)
- People enjoy it because of its vague "core" meaning.
- Don't feel you have missed something if you do not see the connection between different *kernel* objects in mathematics. There might be none...
- Will mention some links during the lecture between different definitions.

What is a kernel

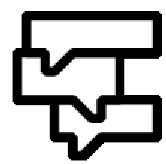
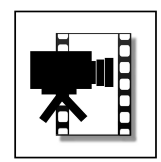
In the context of this lecture...

- A kernel k is a function

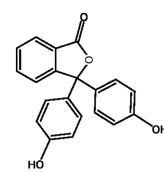
$$
\begin{array}{rccc}
k: & \mathcal{X} \times \mathcal{X} & \longmapsto & \mathbb{R} \\
 & (\mathbf{x}, \mathbf{y}) & \longrightarrow & k(\mathbf{x}, \mathbf{y})
\end{array}
$$

- 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).

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

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

$\boxed{\text{Important concepts and perspectives}}$

- The functional perspective: represent **points as functions**.
- The new or **alternative dot-product** perspective.
- **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 $\mathbf{x}$, the map

$$\mathbf{x} \longrightarrow k(\mathbf{x}, \cdot)$$

associates to $\mathbf{x}$ a function $k(\mathbf{x}, \cdot)$ from $\mathcal{X}$ to $\mathbb{R}$.

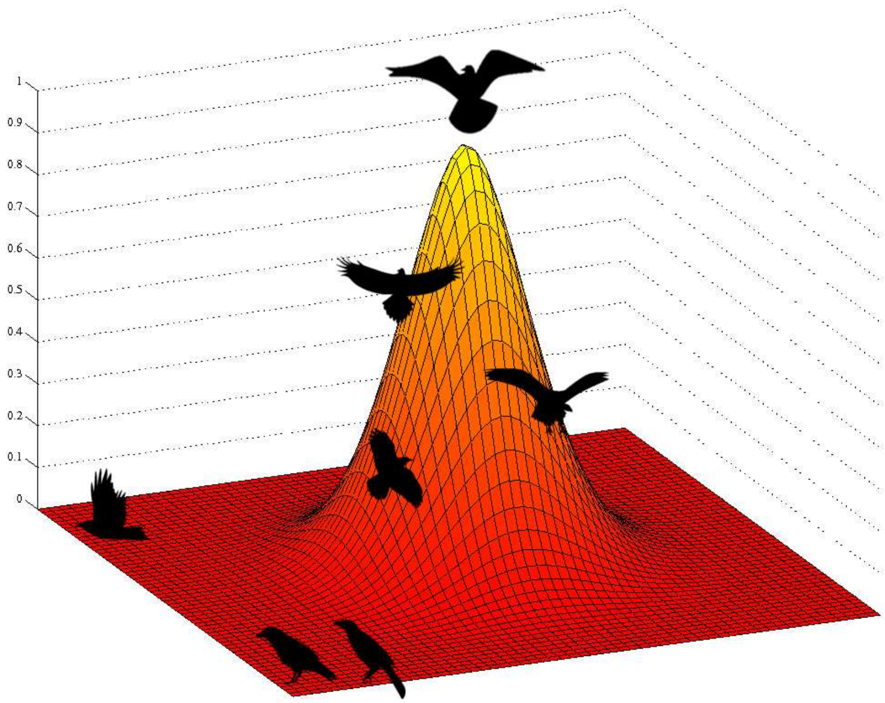
- Suppose we have a kernel k on bird images

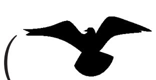
- Suppose for instance

$k\,($  $,$  $) = .32$

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

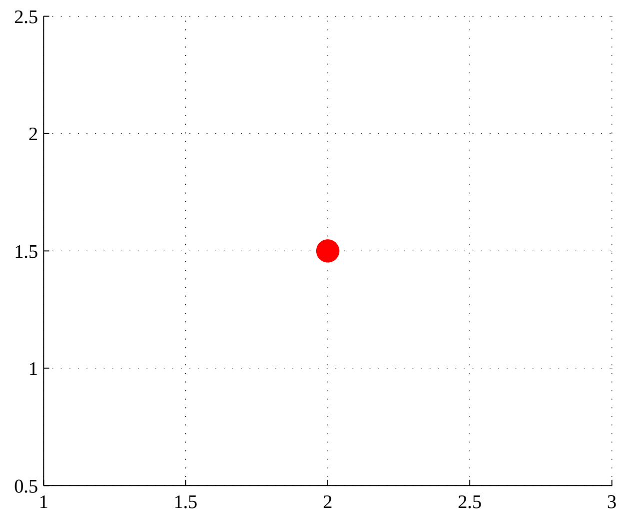
- We examine one image in particular: 
- With kernels, we get a **representation** of that bird as a real-valued function, defined on the space of birds, represented here as $\mathbb{R}^2$ for simplicity.



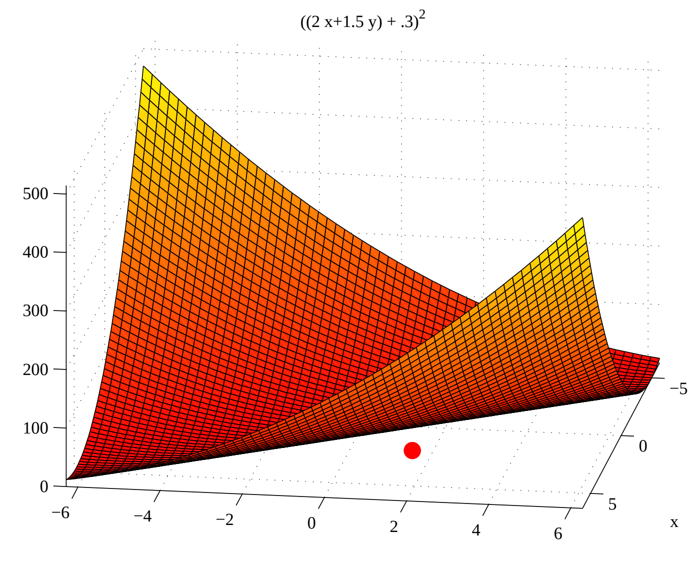
schematic plot of $k\,($  $, \cdot\ )$.

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 $\mathbb{R}^2$.



$\longrightarrow$



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

Dot-product perspective

- Suppose $\mathcal{X} = \mathbb{R}^d$.
- The simplest kernel: $k(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{y}$.
- For a data sample $X = \{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\}$.
- In matrix form, $X = \begin{bmatrix} \vdots & \vdots & \cdots & \vdots \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \in \mathbb{R}^{d \times n}$.
- In standard linear algebra, the Gram matrix of X is

$$K = \left[\mathbf{x}_i^T \mathbf{x}_j\right]_{1 \le i,j \le n} = X^T X.$$

Dot-product perspective

- Consider a different kernel $k_G(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{\sigma^2}\right)$,

$$K_G = \left[k_G(\mathbf{x}_i, \mathbf{x}_j)\right]_{1 \leq i,j \leq n}.$$

- obviously $\mathbf{x}_i^T \mathbf{x}_j \neq k_G(\mathbf{x}_i, \mathbf{x}_j)$.
- is there a representation $\xi_i \in \mathbb{R}^{??}$ for each point such that $\xi_i^T \xi_j = k_G(\mathbf{x}_i, \mathbf{x}_j)$?
- Linear algebra to the rescue: $K = PDP^T$, $U = P\sqrt{D}P^T$, hence $K = U^T U$, providing $U = \begin{bmatrix} \vdots & \vdots & \cdots & \vdots \\ \xi_1 & \xi_2 & \cdots & \xi_n \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \in \mathbb{R}^{\boldsymbol{n} \times n}$.

Dot-product perspective

- In summary, we have defined n vectors such that

$$\left[k_G(\mathbf{x}_i, \mathbf{x}_j)\right] = \left[\xi_i^T \xi_j\right]$$

- Great: for each $\mathbf{x}_i$ we have a vector representation ξ_i.
- Problem:
  - this representation depends explicitly on the sample X.
  - For a new $\mathbf{x}_{n+1}$, difficult to find ξ_{n+1} such that $\xi_{n+1}^T \xi_j = k_G(\mathbf{x}_{n+1}, \mathbf{x}_j)$.
- **We will see that there exists a mapping ϕ**, such that
  - $\phi : \mathcal{X} \rightarrow \mathcal{H}$ where $\mathcal{H}$ is a dot-product space,
  - which gives a dot product representation for k,

$$k_G(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle.$$

for **all points** $(\mathbf{x}, \mathbf{y})$...

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 $\boldsymbol{\beta_0, \beta_1, \cdots, \beta_d}$.

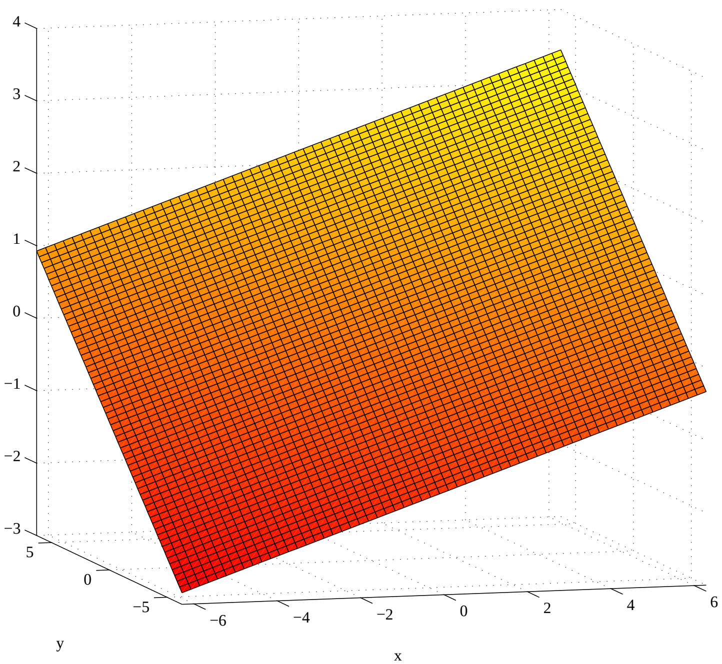
- Kernel methods yield candidate decision functions

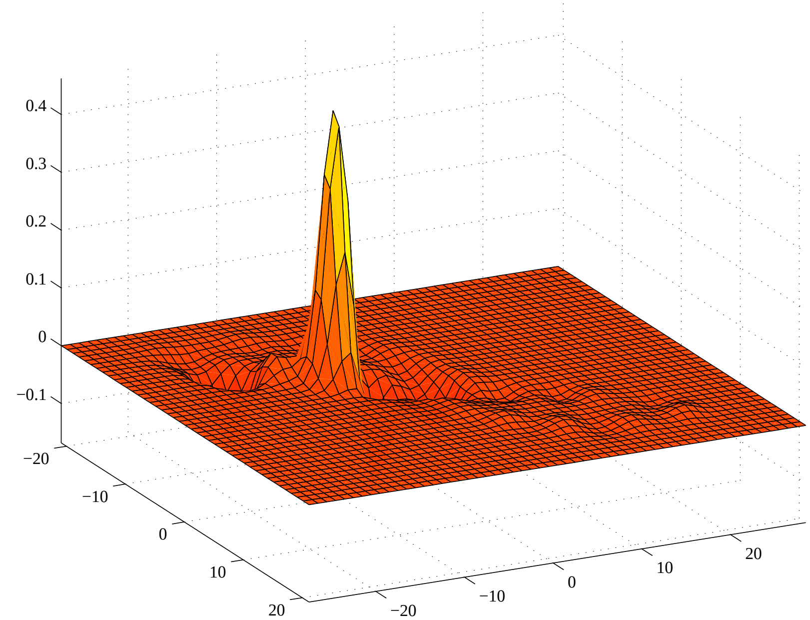
$$f(\mathbf{x}) = \sum_{j=1}^{\boldsymbol{n}} \boldsymbol{\alpha_j} k(\mathbf{x}_j, \mathbf{x}) + \boldsymbol{\alpha_0}.$$

  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" $\longrightarrow$ only one-layer of nonlinearity.

$$\boxed{\text{kernel methods use the data as a functional base to define decision functions}}$$

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 $\mathbf{x}$.
- Weights α are **optimized** with a kernel machine ($e.g.$ support vector machine)

intuitively, kernel methods provide decisions based on how *similar* a point $\mathbf{x}$ 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

$\boxed{\text{Two distinct approaches}}$

- 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 summary

- A feature based analysis of a data-driven problem:

$$\text{objects } o_1, \cdots, o_n \quad \longrightarrow \quad \text{feature vectors } X = \begin{bmatrix} \vdots & \vdots & \cdots & \vdots \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \in \mathbb{R}^{\boldsymbol{d} \times n}$$

- A similarity based analysis of a data driven problem:

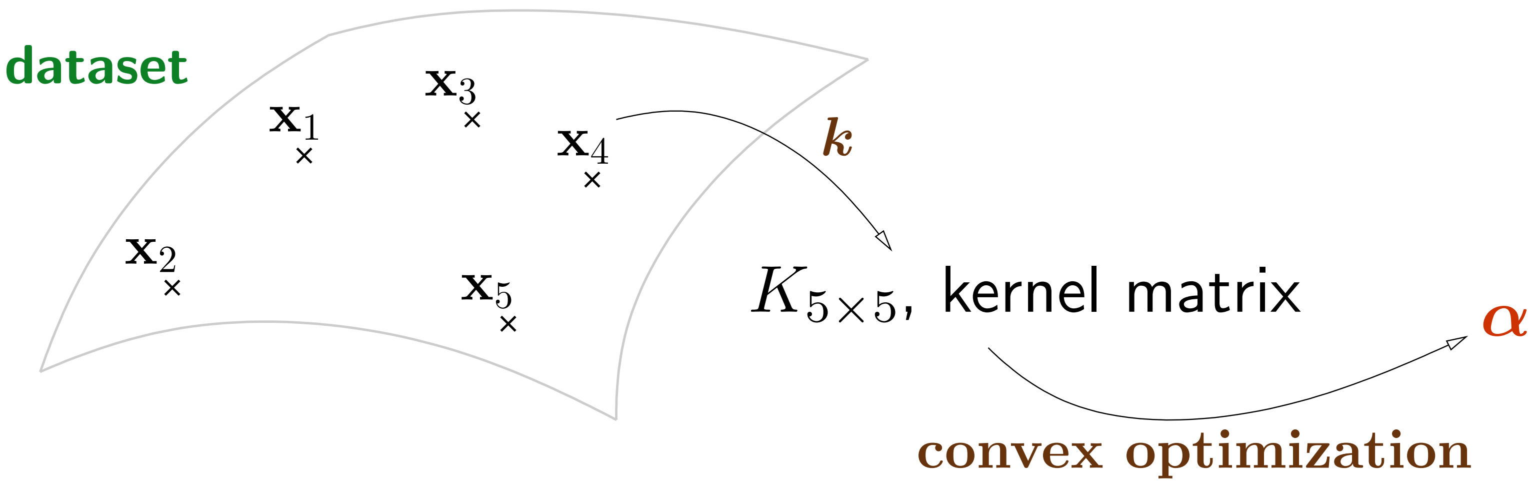
$$\text{objects } o_1, \cdots, o_n \quad \rightarrow \quad \text{Gram } K = \begin{bmatrix} k(o_1, o_1) & k(o_1, o_2) & \cdots & k(o_1, o_n) \\ k(o_2, o_1) & k(o_2, o_2) & \cdots & k(o_2, o_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(o_n, o_1) & k(o_n, o_2) & \cdots & k(o_n, o_n) \end{bmatrix} \in \mathbb{R}^{\boldsymbol{n} \times n}$$

- Some parallels (can define $K = X^T X$ or $X = \sqrt{K}$ or Cholesky) but...

Algorithms use either features *or* (kernel) similarities.

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.

Mathematical Considerations

different definitions and properties of the same mathematical object

An intuitive perspective: Feature maps

Theorem 1. *A function k on $\mathcal{X} \times \mathcal{X}$ is a positive definite kernel if and only if there exists a set T and a mapping ϕ from $\mathcal{X}$ to $l^2(T)$, the set of real sequences $\{u_t, t \in T\}$ such that $\sum_{t\in T} |u_t|^2 < \infty$, where*

$$\forall (\mathbf{x}, \mathbf{y}) \in \mathcal{X} \times \mathcal{X}, \; k(\mathbf{x}, \mathbf{y}) = \sum_{t \in T} \phi(\mathbf{x})_t \, \phi(\mathbf{y})_t = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle_{l^2(X)}$$

- A very popular perspective in the machine learning world.
- Equivalent to previous definitions, less stressed in the RHKS literature.

$$\mathbf{x} \longrightarrow \phi(\mathbf{x}) = \begin{bmatrix} \vdots \\ \vdots \\ \phi(\mathbf{x})_t \\ \vdots \\ \vdots \end{bmatrix}_{t \in T}$$

where the ϕ_t are a set of – possibly infinite but countable – features.

kernels $\rightarrow$ Gram matrices

- If $X = \{\mathbf{x}_i\}_{i \in I}$ in $\mathcal{X}$,
$$K_X = [k(\mathbf{x}_i, \mathbf{x}_j)]_{i,j \in I} \succeq 0.$$
- If one applies *any* transformation of K_X which keeps eigenvalues nonnegative,
$$\begin{array}{cccc} r: & \mathbf{S}_n & \longmapsto & \mathbf{S}_n \\ & K & \longrightarrow & r(K), \end{array}$$

  $r(K)$ is a valid positive definite matrix and hence a kernel on X.
- examples: $K + t(t > 0), K^2, e^K, etc.$
- in fact, if $K = P\Delta P^T$, any transformation that preserves the spectrum's non-negativity would be ok.
- Yet... this kernel is only valid on X, the sample, not the whole space $\mathcal{X}$.

$$\boxed{\text{Meaning somehow... Gram matrices} \not\rightarrow \text{kernels}}$$

positive definite kernels and distances

- Kernels are often called similarities.
- the **higher** $k(\mathbf{x},\mathbf{y})$, the more similar $\mathbf{x}$ and $\mathbf{y}$.
- With distances, the **lower** $d(\mathbf{x},\mathbf{y})$, the closer $\mathbf{x}$ and $\mathbf{y}$.

- Many distances exist in the literature. Can they be used to define kernels?

what is the link between kernels and distances?
high similarity $\stackrel{?}{=}$ **small distance**

- At least true for the Gaussian kernel $k(\mathbf{x},\mathbf{y}) = e^{-\|\mathbf{x}-\mathbf{y}\|^2/2\sigma^2}$...
- Important theorems taken from [BCR84].

Distances

Definition 1 (Distances, or metrics). *A* ***nonnegative-valued*** *function d on $\mathcal{X} \times \mathcal{X}$ is a distance if it satisfies, $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{X}$:*

(i) $d(\mathbf{x}, \mathbf{y}) \geq 0$, *and* $d(\mathbf{x}, \mathbf{y}) = 0$ *if and only if* $\mathbf{x} = \mathbf{y}$ *(non-degeneracy)*

(ii) $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$ *(symmetry),*

(iii) $d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z})$ *(triangle inequality)*

- Very simple example: if $\mathcal{X}$ is a Hilbert space, $\|\mathbf{x} - \mathbf{y}\|$ is a distance. It is usually called a... Hilbertian distance.
- By extension, any distance $d(\mathbf{x}, \mathbf{y})$ which can be written as $\|\phi(\mathbf{x}) - \phi(\mathbf{y})\|$ where ϕ maps $\mathcal{X}$ to any Hilbert space is called a **Hilbertian metric**.
- Useful. To build Gaussian kernel, Laplace kernels $k(\mathbf{x}, \mathbf{y}) = e^{-t\|\mathbf{x}-\mathbf{y}\|}$...
- Yet does not suffice:

the missing link: negative definite kernels

Definition 2 (Negative Definite Kernels)**.** *A symmetric function* $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ *is a negative definite (n.d.) kernel on* $\mathcal{X}$ *if*

$$\sum_{i,j=1}^{n} c_i c_j \, \psi\left(x_i, x_j\right) \leq 0 \tag{1}$$

holds for any $n \in \mathbb{N}, x_1, \ldots, x_n \in \mathcal{X}$ *and* $c_1 \ldots, c_n \in \mathbb{R}$ *such that* $\sum_{i=1}^{n} c_i = 0$.

- Example $\psi(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^2$.
    - prove by decomposing into $\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2 - 2\langle \mathbf{x}_i, \mathbf{x}_j \rangle$
- $\mathcal{N}(\mathcal{X})$ is also a closed convex cone.

important example: k is p.d. $\Rightarrow -k$ is n.d.
Converse completely false.

negative definite kernels & positive definite kernels

A first link between these two kernels:

Proposition 2. *Let* $x_0 \in \mathcal{X}$ *and let* $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ *be a symmetric kernel. Let*

$$\varphi(\mathbf{x}, \mathbf{y}) \stackrel{\text{def}}{=} \psi(\mathbf{x}, x_0) + \psi(\mathbf{y}, x_0) - \psi(\mathbf{x}, \mathbf{y}) - \psi(x_0, x_0).$$

Then k *is positive definite* $\Leftrightarrow$ ψ *is negative definite.*

- Example: $\|\mathbf{x} - x_0\|^2 + \|\mathbf{y} - x_0\|^2 - \|\mathbf{x} - \mathbf{y}\|^2$ is a p.d. kernel.

Proof.

- $\Rightarrow$ For $\mathbf{x}_1, \cdots, \mathbf{x}_n$, and $c_1, \cdots, c_n$ s.t. $\sum_{i=1}^n c_i = \mathbf{0}$,

$$\sum_{i,j=1}^{n} c_i c_j \varphi(\mathbf{x}_i, \mathbf{x}_j) = -\sum_{i,j=1}^{n} c_i c_j \psi(\mathbf{x}_i, \mathbf{x}_j) \geq 0.$$

- $\Leftarrow$ For $\mathbf{x}_1, \cdots, \mathbf{x}_n$ and $c_1, \cdots, c_n$, let $c_0 = -\sum_{i=1}^n$. Set $\mathbf{x}_0 = x_0$. Then

$$\begin{aligned}
0 &\geq \sum_{i,j=0}^{n} c_i c_j \psi(\mathbf{x}_i, \mathbf{x}_j) \\
&= \sum_{i,j=1}^{n} c_i c_j \psi(\mathbf{x}_i, \mathbf{x}_j) + \sum_{i=1}^{n} c_i c_0 \psi(\mathbf{x}_i, x_0) + \sum_{j=1}^{n} c_0 c_j \psi(x_0, \mathbf{x}_j) + c_0^2 \psi(x_0, x_0). \\
&= \sum_{i,j=1}^{n} \left[\psi(\mathbf{x}_i, x_0) + \psi(\mathbf{x}_j, x_0) - \psi(\mathbf{x}_i, \mathbf{y}_j) - \psi(x_0, x_0)\right] = \sum_{i,j=1}^{n} c_i c_j \varphi(\mathbf{x}_i, \mathbf{x}_j).
\end{aligned}$$

negative definite kernels & positive definite kernels

Proposition 3. *For a p.d. kernel $k \geq 0$ on $\mathcal{X} \times \mathcal{X}$, the following conditions are equivalent*

(i) $-\log k \in \mathcal{N}(\mathcal{X})$,

(ii) k^t *is positive definite for all* $t > 0$.

If k satisfies either, k is said to be ***infinitely divisible***,

Proof.

- $-\log k = \lim_{n\to\infty} n(1 - k^{\frac{1}{n}})$ which is the limit of a series of n.d. kernels if (ii) is true, hence $(ii) \Rightarrow (i)$.
- conversely, if $-\log k \in \mathcal{N}(\mathcal{X})$ we use Proposition 2. Writing $\psi = -\log k$ and choosing $x_0 \in \mathcal{X}$ we have

$$k^t = e^{-t\psi(\mathbf{x},\mathbf{y})} = e^{t\psi(x_0,x_0)} \boldsymbol{e^{t\varphi(\mathbf{x},\mathbf{y})}} \boldsymbol{e^{-t\psi(\mathbf{x},x_0)}} \boldsymbol{e^{-t\psi(\mathbf{y},x_0)}} \in \mathcal{P}(\mathcal{X})$$

negative definite kernels: $(\text{Hilbertian distance})^2$ + ...

Proposition 4. *Let $\psi : \mathcal{X} \times \mathcal{X}$ be a n.d. kernel. Then there is a Hilbert space H and a mapping ϕ from X to H such that*

$$\psi(\mathbf{x}, \mathbf{y}) = \|\phi(\mathbf{x}) - \phi(\mathbf{y})\|^2 + f(\mathbf{x}) + f(\mathbf{y}), \tag{2}$$

where $f : \mathcal{X} \to \mathbb{R}$. If $\psi(x, x) = 0$ for all $\mathbf{x} \in \mathcal{X}$ then f can be chosen as zero. If the set $\{(\mathbf{x}, \mathbf{y}) |\, \psi(\mathbf{x}, \mathbf{y}) = 0\}$ is exactly $\{(\mathbf{x}, \mathbf{x}), \mathbf{x} \in \mathcal{X}\}$ then $\sqrt{\psi}$ is a Hilbertian distance.

Proof. Fix x_0 and define

$$\varphi(\mathbf{x}, \mathbf{y}) \stackrel{\text{def}}{=} \frac{\mathbf{1}}{\mathbf{2}} \left[\psi(\mathbf{x}, x_0) + \psi(\mathbf{y}, x_0) - \psi(\mathbf{x}, \mathbf{y}) - \psi(x_0, x_0)\right].$$

By Proposition 2 φ is p.d. hence there is a RKHS and mapping ϕ such that $\varphi(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle$. Hence

$$\begin{aligned} \|\phi(\mathbf{x}) - \phi(\mathbf{y})\|^2 &= \varphi(\mathbf{x}, \mathbf{x}) + \varphi(\mathbf{y}, \mathbf{y}) - 2\varphi(\mathbf{x}, \mathbf{y}) \\ &= \psi(\mathbf{x}, \mathbf{y}) - \frac{\psi(\mathbf{x}, \mathbf{x}) + \psi(\mathbf{y}, \mathbf{y})}{2}. \end{aligned}$$

distances & negative definite kernels

- whenever a n.d. kernel ψ
  - vanishes on the *diagonal*, $i.e.$ on $\{(x,x), x \in \mathcal{X}\}$,
  - is 0 only on the diagonal, to ensure non-degeneracy,

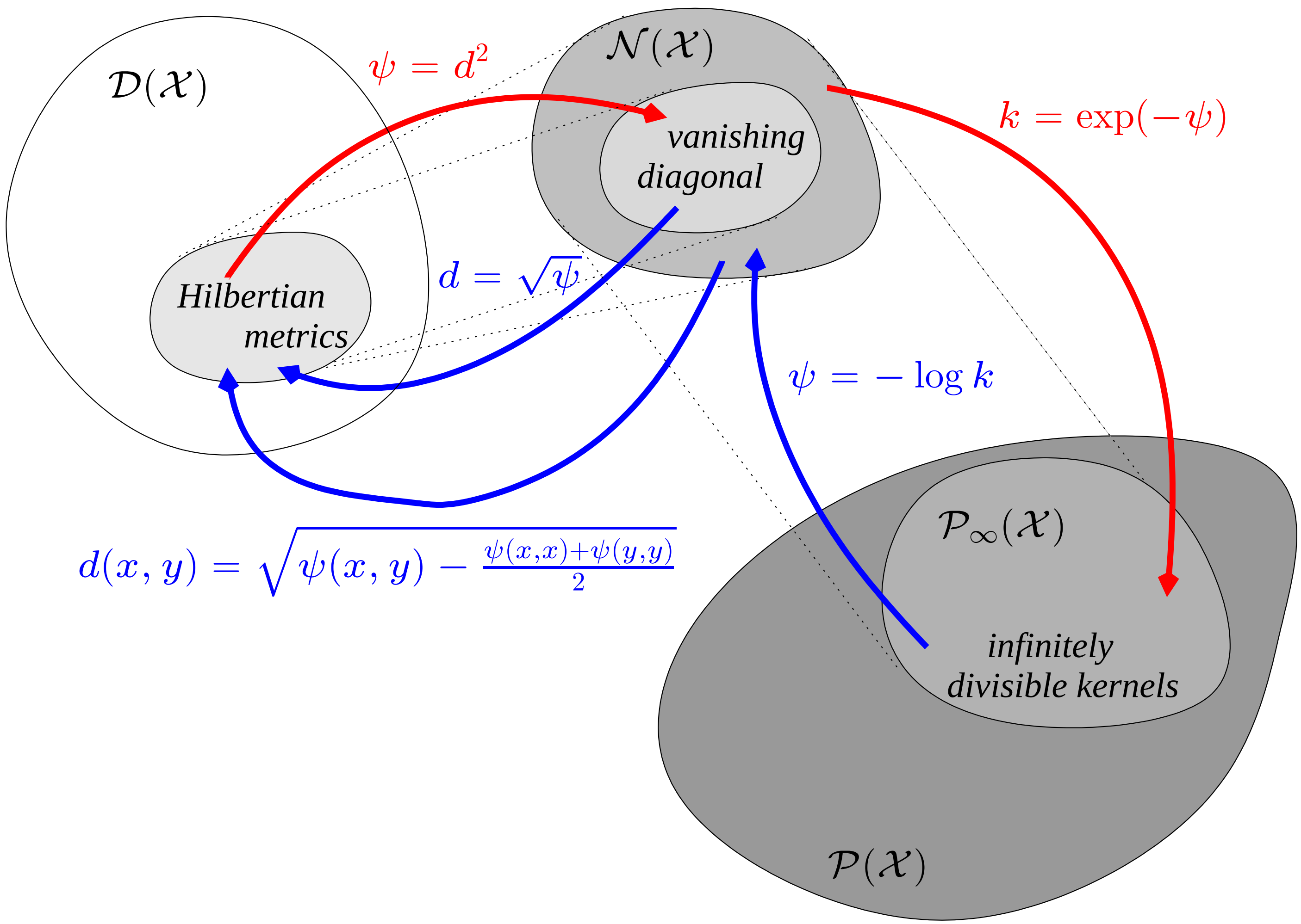
$\rightarrow \sqrt{\psi}$ is a Hilbertian distance for $\mathcal{X}$.

- **More generally**, for a n.d. kernel ψ,

$$\sqrt{\psi(\mathbf{x},\mathbf{y}) - \frac{\psi(\mathbf{x},\mathbf{x})}{2} - \frac{\psi(\mathbf{y},\mathbf{y})}{2}}$$ is a (pseudo)**metric** for $\mathcal{X}$.

- On the contrary, to each distance does not always correspond a n.d. kernel (Monge-Kantorovich distance, edit-distance $etc.$.)

In summary...



- Set of distances on $\mathcal{X}$ is $\mathcal{D}(\mathcal{X})$, Negative definite kernels $\mathcal{N}(\mathcal{X})$, positive and infinitely divisible positive kernels $\mathcal{P}(\mathcal{X})$ and $\mathcal{P}_\infty(\mathcal{X})$ respectively.

Some final remarks on $\mathcal{N}(\mathcal{X})$ and $\mathcal{P}(\mathcal{X})$

- $\mathcal{N}(\mathcal{X})$ is a cone. Additionally,
  - if $\psi \in \mathcal{N}(\mathcal{X}), \forall c \in \mathbb{R}$, $\psi + c \in \mathcal{N}(\mathcal{X})$.
  - if $\psi(x,x) \geq 0$ for all $x \in \mathcal{X}$, $\psi^\alpha \in \mathcal{N}(\mathcal{X})$ for $0 < \alpha < 1$ since

$$\psi^\alpha = \frac{\alpha}{\Gamma(1-\alpha)} \int_0^\infty t^{-\alpha-1}(1 - e^{-t\psi})dt$$

    and $\log(1+\psi) \in \mathcal{N}(\mathcal{X})$ since

$$\log(1+\psi) = \int_0^\infty (1 - e^{-t\psi}) \frac{e^{-t}}{t} dt.$$

  - if $\psi > 0$, then $\log(\psi) \in \mathcal{N}(\mathcal{X})$ since

$$\log(\psi) = \lim_{c \to \infty} \log\left(\psi + \frac{1}{c}\right) = \lim_{c \to \infty} \log\left(1 + c\psi\right) - \log c$$

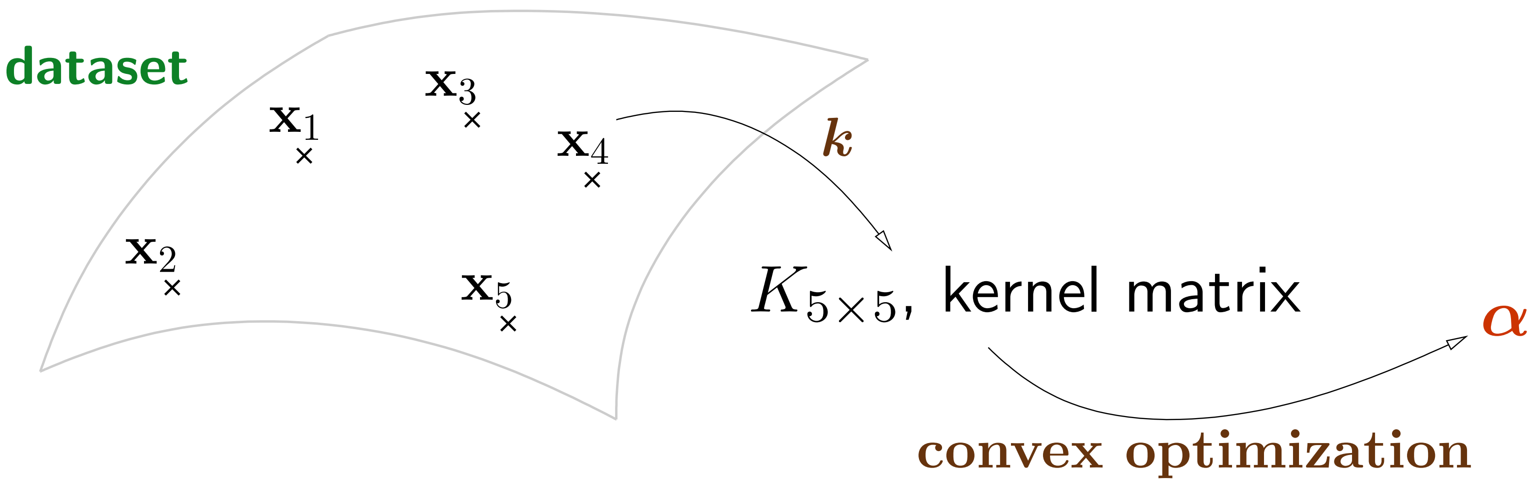
Some final remarks on $\mathcal{D}(\mathcal{X}), \mathcal{N}(\mathcal{X}), \mathcal{P}(\mathcal{X})$

- $\mathcal{P}(\mathcal{X})$ is a cone. Additionally,
  - The pointwise product $k_1 k_2$ of two p.d. kernels if a p.d. kernel
  - $k^n \in \mathcal{P}(\mathcal{X})$ for $n \in \mathbb{N}$. $(k+c)^n$ too...as well as $\exp(k) \in \mathcal{P}(\mathcal{X})$:
    - $\exp(k) = \sum_{i=0}^{\infty} \frac{k^i}{i!}$, a limit of p.d. kernels.
    - $\exp(k) = \exp(-(-k))$ where $-k \in \mathcal{N}(\mathcal{X})$.
- The sum of two infinitely divisible kernels is not necessarily infinitely divisible.
  - $-\log k_1$ and $-\log k_2$ might be in $\mathcal{N}(\mathcal{X})$, but $-\log(k_1 + k_2)$?...

Defining kernels

Intuitively an important issue...

Remember that kernel methods drop all previous information



to proceed exclusively with K.

if the kernel K is poorly informative, the optimization cannot be very useful...
it is therefore **crucial** that the kernel quantifies **noteworthy similarities**.

Kernels on vectors

(relatively) easy case: **we are only given feature vectors**, with **no access** to the original data.

- Reminder (copy paste of previous slide!): for a family of kernels $k_1, \cdots, k_n, \cdots$
  - The sum $\sum_{i=1}^{n} \lambda_i k_i$ is p.d., given $\lambda_1, \ldots, \lambda_n \geq 0$
  - The product $k_1^{a_1} \cdots k_n^{a_n}$ is p.d., given $a_1, \ldots, a_n \in \mathbb{N}$
  - $\lim_{n \to \infty} k_n$ is p.d. (if the limit exists!).
- Using these properties we can prove the p.d. of
  - the polynomial kernel $k_p(x, y) = (\langle \mathbf{x}, \mathbf{y} \rangle + b)^d, \quad b > 0, d \in \mathbb{N}$,
  - the Gaussian kernel $k_\sigma(x, y) = e^{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}}$ which can be rewritten as

$$k_\sigma(x, y) = \left[e^{-\frac{\|\mathbf{x}\|^2}{2\sigma^2}} e^{-\frac{\|\mathbf{y}\|^2}{2\sigma^2}} \right] \cdot \left[\sum_{i=0}^{\infty} \frac{\langle \mathbf{x}, \mathbf{y} \rangle^i}{i!} \right]$$

Kernels on vectors

- the Laplace kernels, using some n.d. kernel weaponry,

$$k_\lambda(x,y) = e^{-\lambda\|\mathbf{x}-\mathbf{y}\|^{\boldsymbol{a}}}, \quad 0 < \lambda,\, 0 < \boldsymbol{a} \leq 2$$

- the all-subset Gaussian kernel in $\mathbb{R}^d$,

$$k(x,y) = \prod_{i=1}^{d}\left(1 + ae^{-b(x_i-y_i)^2}\right) = \sum_{I\subset\{1,\cdots,d\}} a^{\#(I)}e^{-b\|\mathbf{x}_I-\mathbf{y}_I\|^2}.$$

- A variation on the Gaussian kernel: Mahalanobis kernel,

$$k_\Sigma(x,y) = e^{-(\mathbf{x}-\mathbf{y})^T\Sigma^{-1}(\mathbf{x}-\mathbf{y})},$$

  idea: correct for discrepancies between the magnitudes and correlations of different variables.
- Usually Σ is the empirical covariance matrix of a sample of points.

Kernels on vectors

- These kernels can be seen as *meta*-kernels which can use any feature representation.
- Example: Gaussian kernel of Gaussian kernel feature maps,

$$k_{G^2}(\mathbf{x},\mathbf{y}) = k_G\left(e^{-\frac{\|\mathbf{x}-\cdot\|^2}{2\sigma^2}}, e^{-\frac{\|\mathbf{y}-\cdot\|^2}{2\sigma^2}}\right) = e^{-\frac{2-e^{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}}}{2\lambda^2}}.$$

- Not sure this is very useful though!

- Indeed, the real challenge is not to define funky kernels,

$$\boxed{\text{the challenge is to tune the parameters } b, d, \sigma, \Sigma.}$$

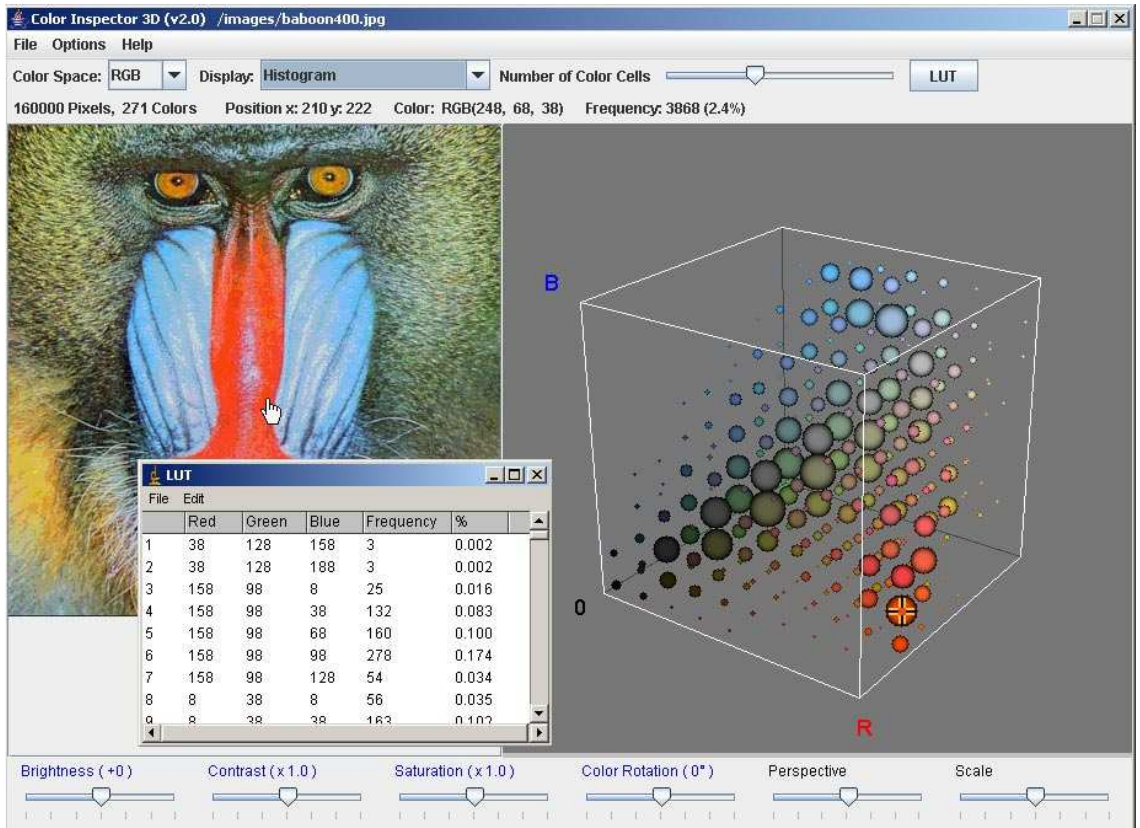
Kernels on structured objects

- Structured objects?
  - texts, webpages, documents
  - sounds, speech, music,
  - images, video segments, movies,
  - 3d structures, sequences, trees, graphs
- Structured objects means
  - objects with **a tricky structure**,
  - which cannot be simply embedded in a vector space of small dimensionality,
  - without obvious algebraic properties,

$$\boxed{\text{structured object} = \text{that which cannot be represented in a (small) Euclidian space}}$$

Vectors in $\mathbb{R}^n_+$ and Histograms

- A powerful and popular feature representation for structured objects: **histograms of smaller building-blocks of the object**:



- histograms are simple instances of **probability measures**,
  - nonnegative coordinates, sum up to 1.

Standard metrics for Histograms

Information geometry, introduced yesterday, studies distances between densities.

- Reference : [AN01]
- An abridged bestiary of **negative definite distances** on the probability simplex:

$$\psi_{JD}(\theta,\theta') = h\left(\frac{\theta+\theta'}{2}\right) - \frac{h(\theta)+h(\theta')}{2},$$

$$\psi_{\chi^2}(\theta,\theta') = \sum_i \frac{(\theta_i-\theta'_i)^2}{\theta_i+\theta'_i}, \quad \psi_{TV}(\theta,\theta') = \sum_i |\theta_i-\theta'_i|,$$

$$\psi_{H_2}(\theta,\theta') = \sum_i |\sqrt{\theta_i}-\sqrt{\theta'_i}|^2, \quad \psi_{H_1}(\theta,\theta') = \sum_i |\sqrt{\theta_i}-\sqrt{\theta'_i}|.$$

- Recover kernels through

$$k(\theta,\theta') = e^{-t\psi}, \quad t>0$$

Information Diffusion Kernel [LL05,ZLC05]

- Solve the heat equation on the multinomial manifold, using the Fisher metric
- Approximate the solution with

$$k_{\Sigma_d}(\theta,\theta') = e^{-\frac{1}{t}\arccos^2(\sqrt{\theta}\cdot\sqrt{\theta'})},$$

- $\arccos^2$ is the **squared** **geodesic distance** between θ and θ' as elements from the unit sphere ($\theta_i \to \sqrt{\theta_i}$).
- In [ZLC05]: the use of

$$k_{\Sigma_d}(\theta,\theta') = e^{-\frac{1}{t}\arccos(\sqrt{\theta}\cdot\sqrt{\theta'})},$$

  is advocated.
- the geodesic distance is a n.d. kernel on the *whole sphere* ($\arccos^2$ is not).

Transportation Metrics for Histograms

Beyond information geometry, the family of **transportation distances**.

- Suppose $\mathbf{r} = (r_1, \cdots, r_d)$ and $\mathbf{c} = (c_1, \cdots, c_d)$ are two histograms in $\mathbb{R}_+^n$.
- Define the set of transportations

$$U(\mathbf{r}, \mathbf{c}) = \{F \in \mathbb{R}_+^{d \times d} \,|\, F\mathbf{1} = \mathbf{r}, F^T\mathbf{1} = \mathbf{c}\}.$$

- Transportation distances between $\mathbf{r}$ and $\mathbf{c}$:

$$d_{\text{cost}}(\mathbf{r}\mathbf{c}) = \min_{F \in U(\mathbf{r}, \mathbf{c})} \text{cost}(F).$$

Monge-Kantorovich: $\text{cost}(F) = \langle F, D \rangle$ where D is a n.d. matrix.

- d_{cost} is **not** n.d. in the general case.
- Alternatives:

$$k_{\text{cost}}(\mathbf{r}\mathbf{c}) = \int_{F \in U(\mathbf{r}, \mathbf{c})} e^{-\text{cost}(F)}.$$

- works when $\text{cost} = 0$: the volume of $U(\mathbf{r}, \mathbf{c})$ is a p.d. kernel of $\mathbf{r}$ and $\mathbf{c}$. [Cut07]

Statistical Modeling and Kernels

Histograms cannot always summarize efficiently the structures of $\mathcal{X}$

- Statistical models of complex objects provide richer explanations:
  - Hidden Markov Models for sequences and time-series,
  - VAR, VARMA, ARIMA *etc.* models for time-series,
  - Branching processes for trees and graphs
  - Random Markov Fields for images *etc.*
- $\{\mathbf{x}_1, \cdots, \mathbf{x}_n\}$ are interpreted as i.i.d realizations of one or many densities on $\mathcal{X}$.
- These densities belong to a model $\boldsymbol{\{p_\theta, \theta \in \Theta \subset \mathbb{R}^d\}}$

Can we use **generative** (statistical) **models** in **discriminative** (kernel and metric based) **methods**?

Fisher Kernel

- The Fisher kernel [JH99] between two elements $\mathbf{x}, \mathbf{y}$ of $\mathcal{X}$ is

$$k_{\hat\theta}(\mathbf{x},\mathbf{y}) = \left(\frac{\partial \ln \boldsymbol{p_\theta}(\mathbf{x})}{\partial \theta}\Big|_{\hat{\boldsymbol\theta}}\right)^T \boldsymbol{J}_{\hat{\boldsymbol\theta}}^{-1} \left(\frac{\partial \ln \boldsymbol{p_\theta}(\mathbf{y})}{\partial \theta}\Big|_{\hat{\boldsymbol\theta}}\right),$$

  - $\hat{\boldsymbol\theta}$ has been selected using sample data ($e.g.$ MLE),
  - $\boldsymbol{J}_{\hat{\boldsymbol\theta}}^{-1}$ is the Fisher information matrix computed in $\hat\theta$.

- The statistical model $\boldsymbol{\{p_\theta, \theta \in \Theta\}}$ provides:

  - finite dimensional *features* through the **score vectors**,
  - A ***Mahalanobis metric*** associated with these vectors through $J_{\hat\theta}$.

- Alternative formulation:

$$k_{\hat\theta}(x,y) = e^{-\frac{1}{\sigma^2}\left(\nabla_{\hat\theta}\ln p_\theta(\mathbf{x}) - \nabla_{\hat\theta}\ln p_\theta(\mathbf{y})\right)^T J_{\hat\theta}^{-1}\left(\nabla_{\hat\theta}\ln p_\theta(\mathbf{x}) - \nabla_{\hat\theta}\ln p_\theta(\mathbf{y})\right)}.$$

with the meta-kernel idea.

Fisher Kernel Extended [TKR+02,SG02]

- Minor extensions, useful for binary classification:
- Estimate $\hat{\theta}_1$ and $\hat{\theta}_2$ for each class respectively,
- consider the score vector of the likelihood ratio

$$\phi_{\hat{\theta}_1,\hat{\theta}_2} : \mathbf{x} \mapsto \left(\left.\frac{\partial \ln \frac{p_{\theta_1}(\mathbf{x})}{p_{\theta_2}(\mathbf{x})}}{\partial \vartheta}\right|_{\hat{\vartheta}=(\hat{\theta}_1,\hat{\theta}_2)} \right),$$

  where $\vartheta = (\theta_1, \theta_2)$ is in Θ^2.

- Use this logratio's score vector to propose instead the kernel

$$(x, y) \mapsto \phi_{\hat{\theta}_1,\hat{\theta}_2}(\mathbf{x})^T \phi_{\hat{\theta}_1,\hat{\theta}_2}(\mathbf{y}).$$

Mutual Information Kernel: densities as feature extractors

- More **bayesian** flavor $\rightarrow$ drops maximum-likelihood estimation of θ. [See02]
- Instead, use **prior knowledge** on $\boldsymbol{\{p_\theta, \theta \in \Theta\}}$ through a **density** ω on Θ
- Mutual information kernel k_ω:

$$k_\omega(\mathbf{x}, \mathbf{y}) = \int_\Theta p_\theta(\mathbf{x}) p_\theta(\mathbf{y})\, \omega(d\theta).$$

- The feature maps $0 \leq p_\theta(\mathbf{x}) \leq 1$ and $0 \leq p_\theta(\mathbf{y}) \leq 1$.

k_ω is big whenever many **common** densities p_θ score high probabilities for **both** $\mathbf{x}$ and $\mathbf{y}$

- Explicit computations sometimes possible, **namely conjugate priors**.
- Example: context-tree kernel for strings.

Mutual Information Kernel & Fisher Kernels

The Fisher kernel is a maximum *a posteriori* approximation of the MI kernel.

- What? How? by setting the prior ω to the multivariate Gaussian density

$$\mathcal{N}(\hat{\theta}, J_{\hat{\theta}}^{-1}),$$

  an approximation known as Laplace's method,

- Writing

$$\Phi(x) = \nabla_{\hat{\theta}} \ln p_\theta(x) = \frac{\partial \ln p_\theta(x)}{\partial \theta}\Big|_{\hat{\theta}}$$

  we get

$$\log p_\theta(x) \approx \log p_{\hat{\theta}}(x) + \Phi(x)(\theta - \hat{\theta}).$$

Mutual Information Kernel & Fisher Kernels

- Using $\mathcal{N}(\hat{\theta}, J_{\hat{\theta}}^{-1})$ for ω yields

$$\begin{aligned} k(x,y) &= \int_\Theta p_\theta(\mathbf{x}) p_\theta(\mathbf{y})\, \omega(d\theta), \\ &\approx C \int_\Theta e^{\log p_{\hat{\theta}}(x) + \Phi(x)^T(\theta-\hat{\theta})} e^{\log p_{\hat{\theta}}(y) + \Phi(y)^T(\theta-\hat{\theta})} \;\; e^{-(\theta-\hat{\theta})^T J_{\hat{\theta}}(\theta-\hat{\theta})} d\theta \\ &= C p_{\hat{\theta}}(x) p_{\hat{\theta}}(y) \int_\Theta e^{(\Phi(x)+\Phi(y))^T(\theta-\hat{\theta}) + (\theta-\hat{\theta})^T J_{\hat{\theta}}(\theta-\hat{\theta})} d\theta \\ &= C' p_{\hat{\theta}}(x) p_{\hat{\theta}}(y) e^{\frac{1}{2}(\Phi(x)+\Phi(y))^T J_{\hat{\theta}}^{-1}(\Phi(x)+\Phi(y))} \end{aligned} \tag{1}$$

- the kernel
$$\tilde{k}(x,y) = \frac{k(x,y)}{\sqrt{k(x,x)k(y,y)}}$$
is equal to the Fisher kernel in exponential form.

Marginalized kernels - Graphs and Sequences

- Similar ideas: leverage **latent variable models.** [TKA02,KTI03]
- For **location** or **time-based** data,
  - the probability of emission of a token x_i is conditioned by
  - an **unobserved** latent variable $s_i \in \mathcal{S}$, where $\mathcal{S}$ is a finite space of possible states.
- for observed sequences $\mathbf{x} = (x_1, \cdots, x_n), \mathbf{y} = (y_1, \cdots, y_n)$, sum over all possible state sequences the **weighted** product of **these probabilities**:

$$k(x, y) = \sum_{s \in \mathcal{S}} \sum_{s' \in \mathcal{S}} \boldsymbol{p(s|x)\, p(s'|y)\, \kappa\left((x, s), (y, s')\right)}$$

- closed form computations exist for graphs & sequences.

Kernels on MLE parameters

- Use model directly to extract a single representation from observed points:

$$x \mapsto \hat{\theta}_x, \quad y \mapsto \hat{\theta}_y,$$

  through MLE for instance.

- compare $\mathbf{x}$ and $\mathbf{y}$ through a kernel k_Θ on Θ,

$$k(x, y) = k_\Theta(\hat{\theta}_{\mathbf{x}}, \hat{\theta}_{\mathbf{y}}).$$

- Bhattacharrya affinities:

$$k_\beta(\mathbf{x}, \mathbf{y}) = \int_{\mathcal{X}} p_{\hat{\theta}_{\mathbf{x}}}(z)^\beta p_{\hat{\theta}_{\mathbf{y}}}(z)^\beta dz$$

  for $\beta > 0$.