Kernel Methods

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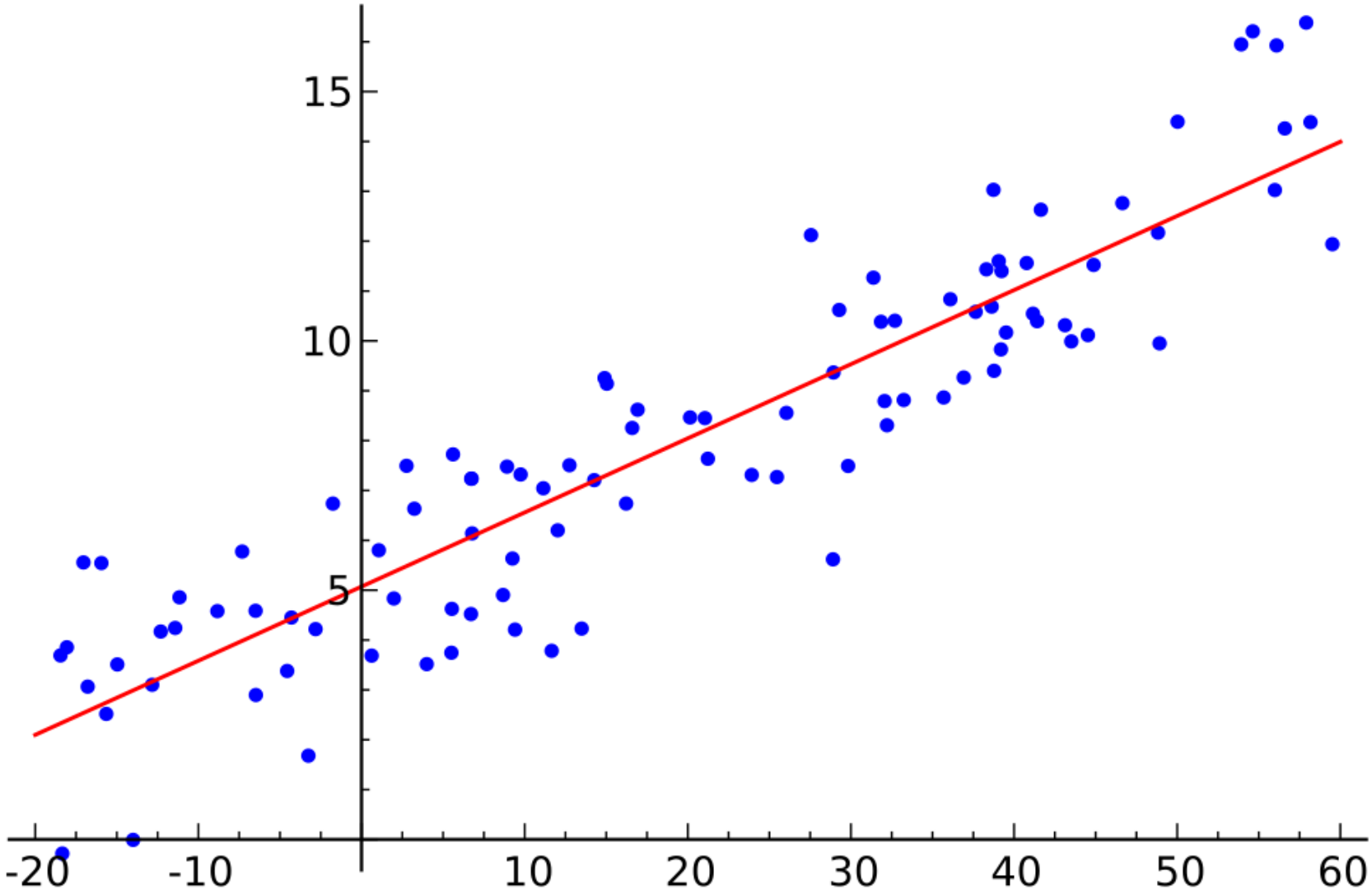
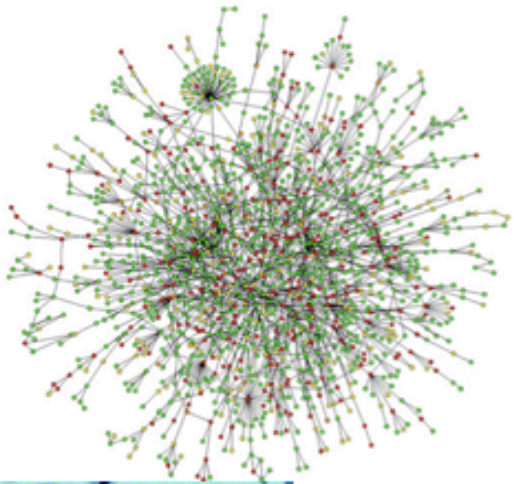
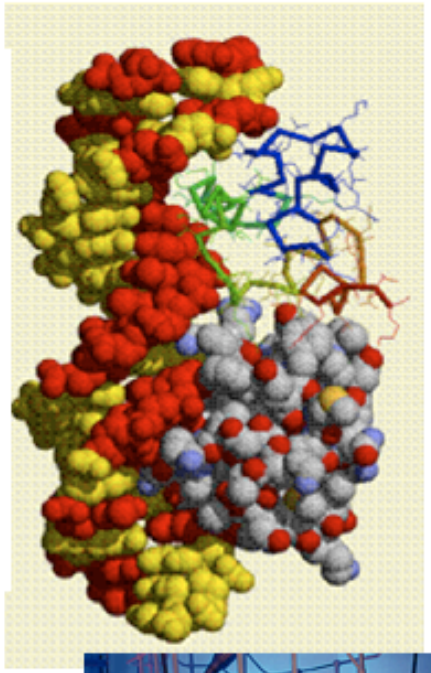
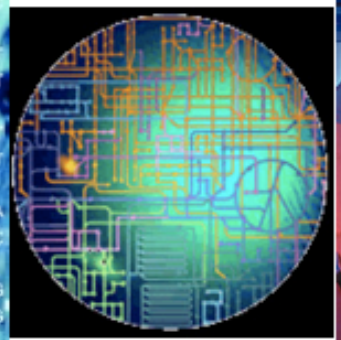
What we know how to solve



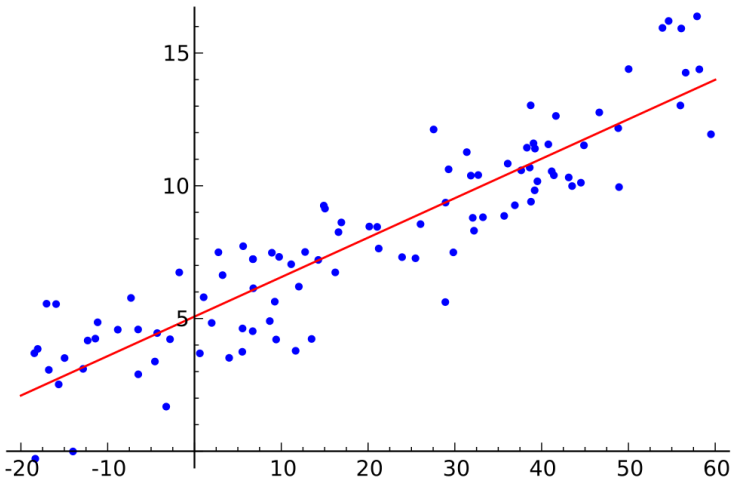
But real data are often more complicated...

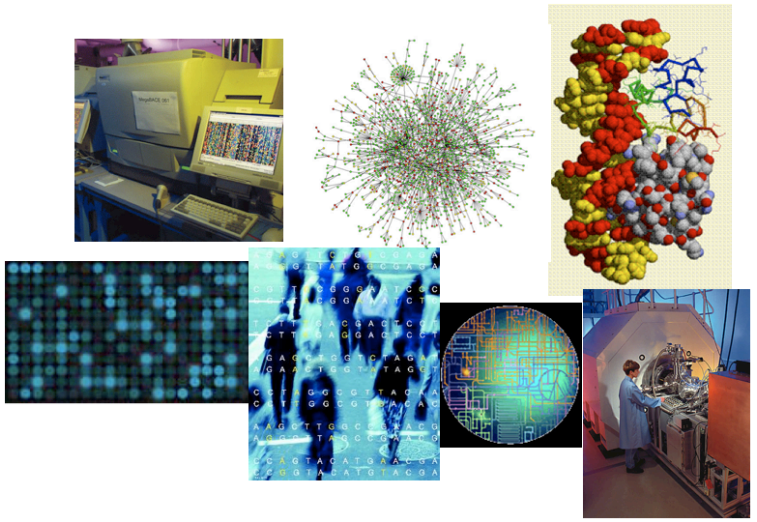






Main goal of this course





Extend well-understood, linear statistical learning techniques to real-world, complicated, structured, high-dimensional data (images, texts, time series, graphs, distributions, permutations...)

Organization of the course

Content

1. Present the basic theory of positive definite kernels, RKHS and kernel methods.
2. Develop a working knowledge of kernel engineering for specific data and applications

Practical

- Course homepage with slides, schedules, homework's etc...: `http://cbio.ensmp.fr/~jvert/teaching`
- Evaluation: Weekly homework

Outline

Outline

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Part 1

Kernels and RKHS

Overview

Motivations

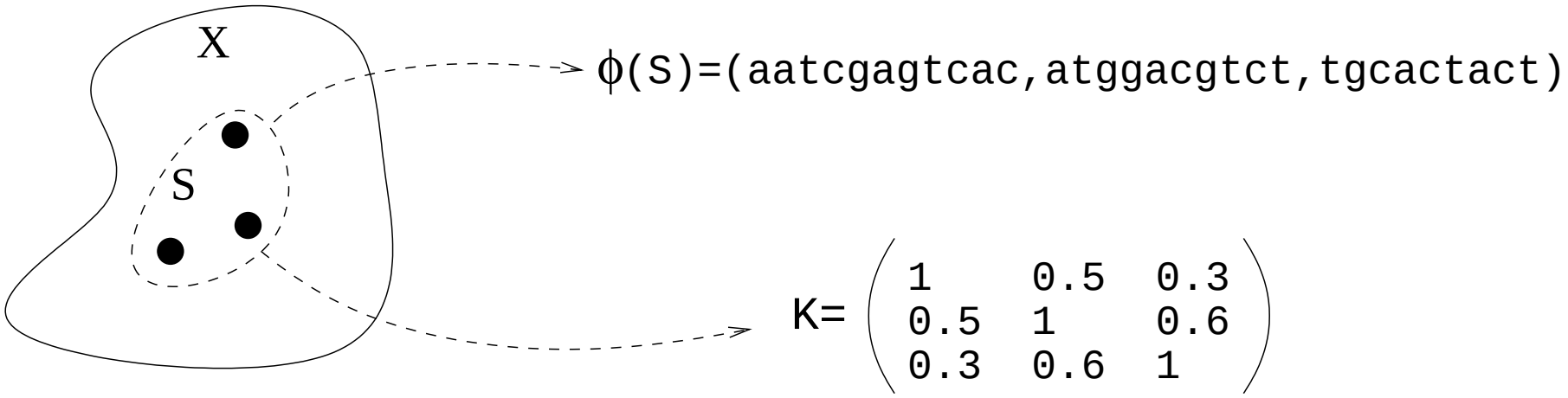
- Develop versatile algorithms to process and analyze data
- No hypothesis made regarding the type of data (vectors, strings, graphs, images, ...)

The approach

- Develop methods based on pairwise comparisons.
- By imposing constraints on the pairwise comparison function (positive definite kernels), we obtain a general framework for learning from data (optimization in RKHS).

Outline

Representation by pairwise comparisons



Idea

- Define a "comparison function": $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$.
- Represent a set of n data points $\mathcal{S} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ by the $n \times n$ matrix:

$$[K]_{ij} := K\left(\mathbf{x}_i, \mathbf{x}_j\right)$$

Representation by pairwise comparisons

Remarks

- Always a $n \times n$ matrix, whatever the nature of data: the same algorithm will work for any type of data (vectors, strings, ...).
- Total modularity between the choice of K and the choice of the algorithm.
- Poor scalability w.r.t to the dataset size (n^2)
- We will restrict ourselves to a particular class of pairwise comparison functions.

Positive Definite (p.d.) Kernels

Definition

A positive definite (p.d.) kernel 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 $(a_1, a_2, \ldots, a_N) \in \mathbb{R}^N$:

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

Similarity matrices of p.d. kernels

Remarks

- Equivalently, a kernel K is p.d. if and only if, for any $N \in \mathbb{N}$ and any set of points $(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \in \mathcal{X}^N$, the similarity matrix $[K]_{ij} := K\left(\mathbf{x}_i, \mathbf{x}_j\right)$ is positive semidefinite.
- Kernel methods are algorithm that take such matrices as input.

The simplest p.d. kernel

Lemma

Let $\mathcal{X} = \mathbb{R}^d$. The function $K : \mathcal{X}^2 \mapsto \mathbb{R}$ defined by:

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

is p.d. (it is often called the linear kernel).

Proof

- $\left\langle \mathbf{x}, \mathbf{x}' \right\rangle_{\mathbb{R}^d} = \left\langle \mathbf{x}', \mathbf{x} \right\rangle_{\mathbb{R}^d}$,
- $\sum_{i=1}^N \sum_{j=1}^N a_i a_j \left\langle \mathbf{x}_i, \mathbf{x}_j \right\rangle_{\mathbb{R}^d} = \| \sum_{i=1}^N a_i \mathbf{x}_i \|_{\mathbb{R}^d}^2 \geq 0$

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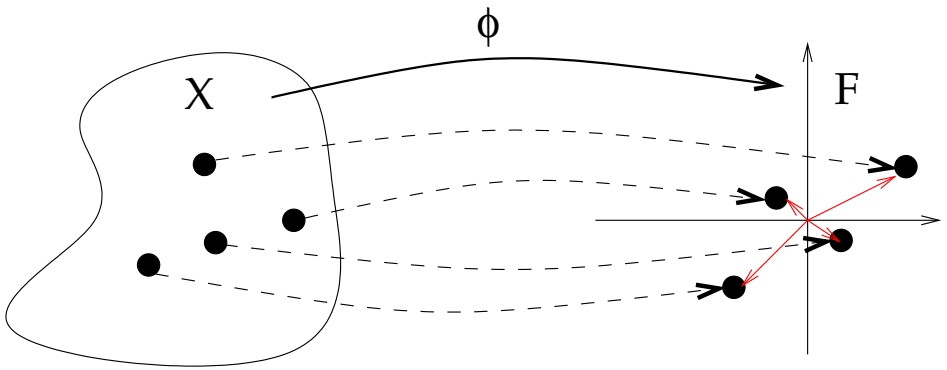
A more ambitious p.d. kernel



Lemma

Let $\mathcal{X}$ be any set, and $\Phi : \mathcal{X} \mapsto \mathbb{R}^d$. Then the function $K : \mathcal{X}^2 \mapsto \mathbb{R}$ defined as follows is p.d.:

$$\forall \left(\mathbf{x}, \mathbf{x}'\right) \in \mathcal{X}^2, \quad K\left(\mathbf{x}, \mathbf{x}'\right) = \left\langle \Phi\left(\mathbf{x}\right), \Phi\left(\mathbf{x}'\right) \right\rangle_{\mathbb{R}^d} .$$

Proof

- $\left\langle \Phi\left(\mathbf{x}\right), \Phi\left(\mathbf{x}'\right) \right\rangle_{\mathbb{R}^d} = \left\langle \Phi\left(\mathbf{x}'\right), \Phi\left(\mathbf{x}\right)_{\mathbb{R}^d} \right\rangle$,
- $\sum_{i=1}^N \sum_{j=1}^N a_i a_j \left\langle \Phi\left(\mathbf{x}_i\right), \Phi\left(\mathbf{x}_j\right) \right\rangle_{\mathbb{R}^d} = \| \sum_{i=1}^N a_i \Phi\left(\mathbf{x}_i\right) \|_{\mathbb{R}^d}^2 \geq 0$.

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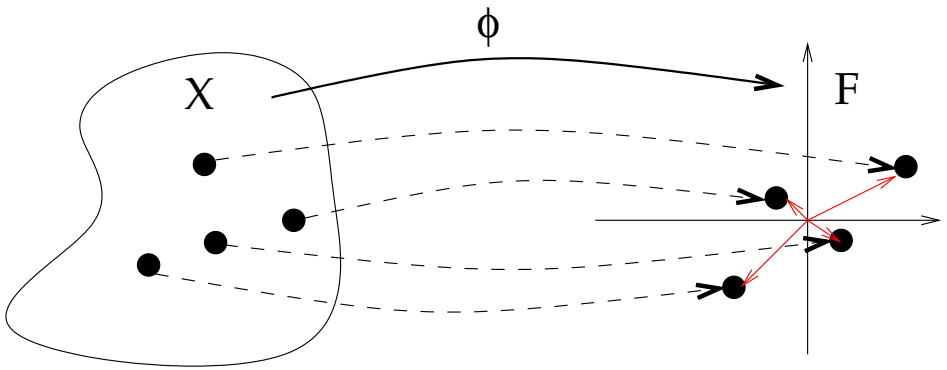

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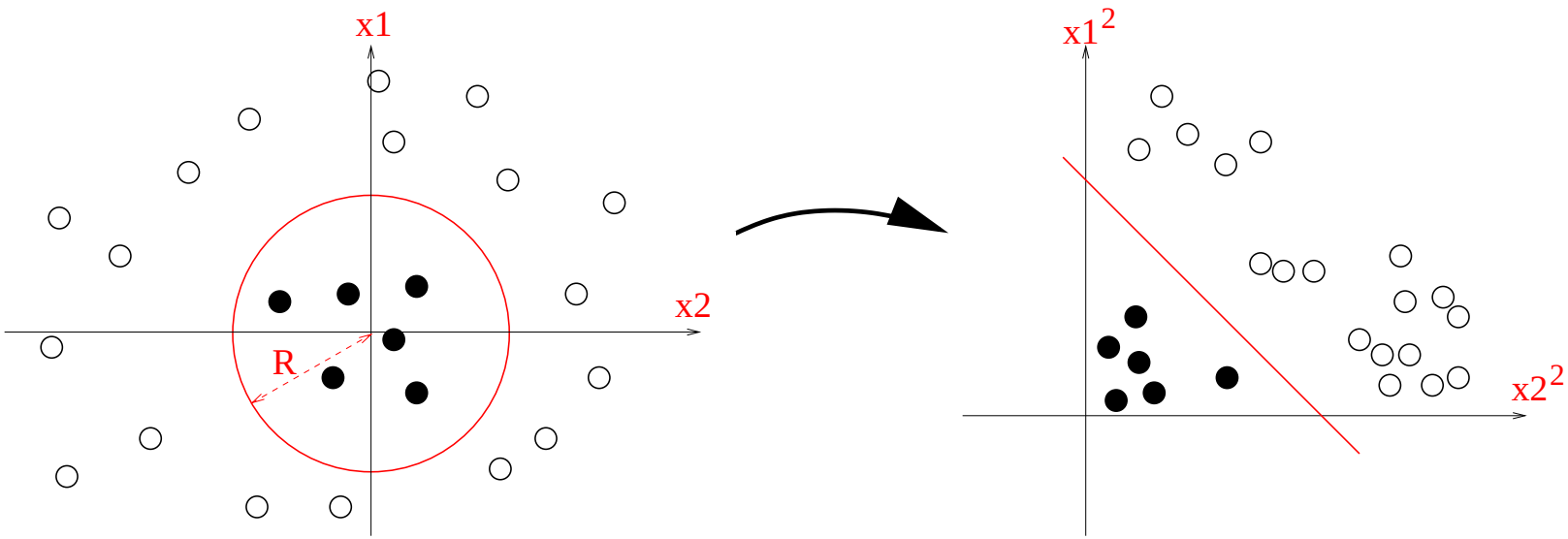
Example: polynomial kernel



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

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

Exercice: show that $\left(\vec{x}.\vec{x}'\right)^d$ is p.d. for any integer d.

Conversely: Kernels as Inner Products

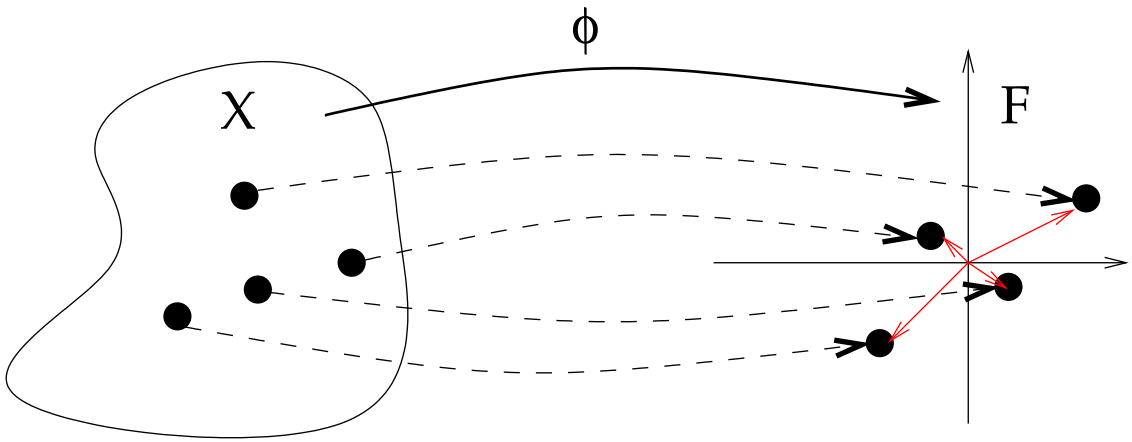
Theorem (Aronszajn, 1950)

K is a p.d. kernel on the set $\mathcal{X}$ if and only if there exists a Hilbert space $\mathcal{H}$ and a mapping

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

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

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



In case of ...

Definitions

- An inner product on an $\mathbb{R}$-vector space $\mathcal{H}$ is a mapping $(f, g) \mapsto \langle f, g \rangle_{\mathcal{H}}$ from $\mathcal{H}^2$ to $\mathbb{R}$ that is bilinear, symmetric and such that $\langle f, f \rangle > 0$ for all $f \in \mathcal{H} \backslash \{0\}$.
- A vector space endowed with an inner product is called pre-Hilbert. It is endowed with a norm defined by the inner product as $\| f \|_{\mathcal{H}} = \langle f, f \rangle_{\mathcal{H}}^{\frac{1}{2}}$.
- A Hilbert space is a pre-Hilbert space complete for the norm defined by the inner product.

Proof: finite case

Proof

- Suppose $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ is finite of size N.
- Any p.d. kernel $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is entirely defined by the $N \times N$ symmetric positive semidefinite matrix $[K]_{ij} := K\left(\mathbf{x}_i, \mathbf{x}_j\right)$.
- It can therefore be diagonalized on an orthonormal basis of eigenvectors $(u_1, u_2, \ldots, u_N)$, with non-negative eigenvalues $0 \leq \lambda_1 \leq \ldots \leq \lambda_N$, i.e.,

$$K\left(\mathbf{x}_i, \mathbf{x}_j\right) = \left[\sum_{l=1}^{N} \lambda_l u_l u_l^\top\right]_{ij} = \sum_{l=1}^{N} \lambda_l u_l(i) u_l(j) = \left\langle \Phi\left(\mathbf{x}_i\right), \Phi\left(\mathbf{x}_j\right)\right\rangle_{\mathbb{R}^N},$$

with

$$\Phi\left(\mathbf{x}_i\right) = \begin{pmatrix} \sqrt{\lambda_1} u_1(i) \\ \vdots \\ \sqrt{\lambda_N} u_N(i) \end{pmatrix}. \qquad \square$$

Proof: general case

- Mercer (1909) for $\mathcal{X} = [a, b] \subset \mathbb{R}$ (more generally $\mathcal{X}$ compact) and K continuous.
- Kolmogorov (1941) for $\mathcal{X}$ countable.
- Aronszajn (1944, 1950) for the general case.

Outline

RKHS Definition

Definition

Let $\mathcal{X}$ be a set and $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ be a class of functions forming a (real) Hilbert space with inner product $\langle ., . \rangle_{\mathcal{H}}$. The function $K : \mathcal{X}^2 \mapsto \mathbb{R}$ is called a reproducing kernel (r.k.) of $\mathcal{H}$ if

1. $\mathcal{H}$ contains all functions of the form

$$\forall \mathbf{x} \in \mathcal{X}, \quad K_{\mathbf{x}} : \mathbf{t} \mapsto K(\mathbf{x}, \mathbf{t}) .$$

2. For every $\mathbf{x} \in \mathcal{X}$ and $f \in \mathcal{H}$ the reproducing property holds:

$$f(\mathbf{x}) = \langle f, K_{\mathbf{x}} \rangle_{\mathcal{H}} .$$

If a r.k. exists, then $\mathcal{H}$ is called a reproducing kernel Hilbert space (RKHS).

An equivalent definition of RKHS

Theorem

The Hilbert space $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ is a RKHS if and only if for any $\mathbf{x} \in \mathcal{X}$, the mapping:

$$\begin{aligned} F : \quad \mathcal{H} &\to \mathbb{R} \\ f &\mapsto f(\mathbf{x}) \end{aligned}$$

is continuous.

Corollary

Convergence in a RKHS implies pointwise convergence, i.e., if $(f_n)_{n\in\mathbb{N}}$ converges to f in $\mathcal{H}$, then $(f_n(\mathbf{x}))_{n\in\mathbb{N}}$ converges to $f(\mathbf{x})$ for any $\mathbf{x} \in \mathcal{X}$.

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Proof

If $\mathcal{H}$ is a RKHS then $f \mapsto f(\mathbf{x})$ is continuous

If a r.k. K exists, then for any $(\mathbf{x}, f) \in \mathcal{X} \times \mathcal{H}$:

$$\begin{aligned} | f(\mathbf{x}) | &= | \langle f, K_{\mathbf{x}} \rangle_{\mathcal{H}} | \\ &\leq \| f \|_{\mathcal{H}} . \| K_{\mathbf{x}} \|_{\mathcal{H}} \text{ (Cauchy-Schwarz)} \\ &\leq \| f \|_{\mathcal{H}} . K(\mathbf{x}, \mathbf{x})^{\frac{1}{2}} \ , \end{aligned}$$

because $\| K_{\mathbf{x}} \|_{\mathcal{H}}^2 = \langle K_{\mathbf{x}}, K_{\mathbf{x}} \rangle_{\mathcal{H}} = K(\mathbf{x}, \mathbf{x})$. Therefore $f \in \mathcal{H} \mapsto f(\mathbf{x}) \in \mathbb{R}$ is a continuous linear mapping. $\square$

Proof (Converse)

If $f \mapsto f(\mathbf{x})$ is continuous then $\mathcal{H}$ is a RKHS

Conversely, let us assume that for any $\mathbf{x} \in \mathcal{X}$ the linear form $f \in \mathcal{H} \mapsto f(\mathbf{x})$ is continuous.
Then by Riesz representation theorem there (general property of Hilbert spaces) there exists a unique $g_{\mathbf{x}} \in \mathcal{H}$ such that:

$$f(\mathbf{x}) = \langle f, g_{\mathbf{x}} \rangle_{\mathcal{H}}$$

The function $K(\mathbf{x}, \mathbf{y}) = g_{\mathbf{x}}(\mathbf{y})$ is then a r.k. for $\mathcal{H}$. $\square$

Unicity of r.k. and RKHS

Theorem

- If $\mathcal{H}$ is a RKHS, then it has a unique r.k.
- Conversely, a function K can be the r.k. of at most one RKHS.

Consequence

This shows that we can talk of "the" kernel of a RKHS, or "the" RKHS of a kernel.

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Proof

If a r.k. exists then it is unique

Let K and K' be two r.k. of a RKHS $\mathcal{H}$. Then for any $\mathbf{x} \in \mathcal{X}$:

$$\begin{aligned} \| K_{\mathbf{x}} - K'_{\mathbf{x}} \|^2_{\mathcal{H}} &= \left\langle K_{\mathbf{x}} - K'_{\mathbf{x}}, K_{\mathbf{x}} - K'_{\mathbf{x}} \right\rangle_{\mathcal{H}} \\ &= \left\langle K_{\mathbf{x}} - K'_{\mathbf{x}}, K_{\mathbf{x}} \right\rangle_{\mathcal{H}} - \left\langle K_{\mathbf{x}} - K'_{\mathbf{x}}, K'_{\mathbf{x}} \right\rangle_{\mathcal{H}} \\ &= K_{\mathbf{x}}(\mathbf{x}) - K'_{\mathbf{x}}(\mathbf{x}) - K_{\mathbf{x}}(\mathbf{x}) + K'_{\mathbf{x}}(\mathbf{x}) \\ &= 0 \,. \end{aligned}$$

This shows that $K_{\mathbf{x}} = K'_{\mathbf{x}}$ as functions, i.e., $K_{\mathbf{x}}(\mathbf{y}) = K'_{\mathbf{x}}(\mathbf{y})$ for any $\mathbf{y} \in \mathcal{X}$. In other words, K=K'. $\square$

The RKHS of a r.k. K is unique

Left as exercice.

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An important result

Theorem

A function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is p.d. if and only if it is a r.k.

Proof

A r.k. is p.d.

1. A r.k. is symmetric because, for any $(\mathbf{x}, \mathbf{y}) \in \mathcal{X}^2$:

$$K(\mathbf{x}, \mathbf{y}) = \langle K_{\mathbf{x}}, K_{\mathbf{y}} \rangle_{\mathcal{H}} = \langle K_{\mathbf{y}}, K_{\mathbf{x}} \rangle_{\mathcal{H}} = K(\mathbf{y}, \mathbf{x}).$$

2. It is p.d. because for any $N \in \mathbb{N}$,$(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \in \mathcal{X}^N$, and $(a_1, a_2, \ldots, a_N) \in \mathbb{R}^N$:

$$\begin{aligned}
\sum_{i,j=1}^{N} a_i a_j K(\mathbf{x}_i, \mathbf{x}_j) &= \sum_{i,j=1}^{N} a_i a_j \left\langle K_{\mathbf{x}_i}, K_{\mathbf{x}_j} \right\rangle_{\mathcal{H}} \\
&= \| \sum_{i=1}^{N} a_i K_{\mathbf{x}_i} \|_{\mathcal{H}}^2 \\
&\geq 0. \quad \square
\end{aligned}$$

Proof

A p.d. kernel is a r.k. (1/4)

- Let $\mathcal{H}_0$ be the vector subspace of $\mathbb{R}^{\mathcal{X}}$ spanned by the functions $\{K_{\mathbf{x}}\}_{\mathbf{x}\in\mathcal{X}}$.
- For any $f, g \in \mathcal{H}_0$, given by:

$$f = \sum_{i=1}^{m} a_i K_{\mathbf{x}_i}, \quad g = \sum_{j=1}^{n} b_j K_{\mathbf{y}_j},$$

let:

$$\langle f, g \rangle_{\mathcal{H}_0} := \sum_{i,j} a_i b_j K\left(\mathbf{x}_i, \mathbf{y}_j\right).$$

A p.d. kernel is a r.k. (2/4)

- $\langle f, g \rangle_{\mathcal{H}_0}$ does not depend on the expansion of f and g because:

$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_{i=1}^{m} a_i g(\mathbf{x}_i) = \sum_{j=1}^{n} b_j f(\mathbf{y}_j) .$$

- This also shows that $\langle ., . \rangle_{\mathcal{H}_0}$ is a symmetric bilinear form.
- This also shows that for any $\mathbf{x} \in \mathcal{X}$ and $f \in \mathcal{H}_0$:

$$\langle f, K_{\mathbf{x}} \rangle_{\mathcal{H}_0} = f(\mathbf{x}) .$$

A p.d. kernel is a r.k. (3/4)

- K is assumed to be p.d., therefore:

$$\| f \|^2_{\mathcal{H}_0} = \sum_{i,j=1}^{m} a_i a_j K(\mathbf{x}_i, \mathbf{x}_j) \geq 0 .$$

  In particular Cauchy-Schwarz is valid with $\langle ., . \rangle_{\mathcal{H}_0}$.
- By Cauchy-Schwarz we deduce that $\forall \mathbf{x} \in \mathcal{X}$:

$$| f(\mathbf{x}) | = \left| \langle f, K_{\mathbf{x}} \rangle_{\mathcal{H}_0} \right| \leq \| f \|_{\mathcal{H}_0} . K(\mathbf{x}, \mathbf{x})^{\frac{1}{2}} ,$$

  therefore $\| f \|_{\mathcal{H}_0} = 0 \implies f = 0$.
- $\mathcal{H}_0$ is therefore a pre-Hilbert space endowed with the inner product $\langle ., . \rangle_{\mathcal{H}_0}$.

A p.d. kernel is a r.k. (4/4)

- For any Cauchy sequence $(f_n)_{n\geq 0}$ in $\left(\mathcal{H}_0, \langle ., . \rangle_{\mathcal{H}_0}\right)$, we note that:

$$\forall (\mathbf{x}, m, n) \in \mathcal{X} \times \mathbb{N}^2, \quad |f_m(\mathbf{x}) - f_n(\mathbf{x})| \leq \|f_m - f_n\|_{\mathcal{H}_0} . K(\mathbf{x}, \mathbf{x})^{\frac{1}{2}} .$$

  Therefore for any $\mathbf{x}$ the sequence $(f_n(\mathbf{x}))_{n\geq 0}$ is Cauchy in $\mathbb{R}$ and has therefore a limit.

- If we add to $\mathcal{H}_0$ the functions defined as the pointwise limits of Cauchy sequences, then the space becomes complete and is therefore a Hilbert space, with K as r.k. (up to a few technicalities, left as exercice). $\square$

Application: back to Aronzsajn's theorem

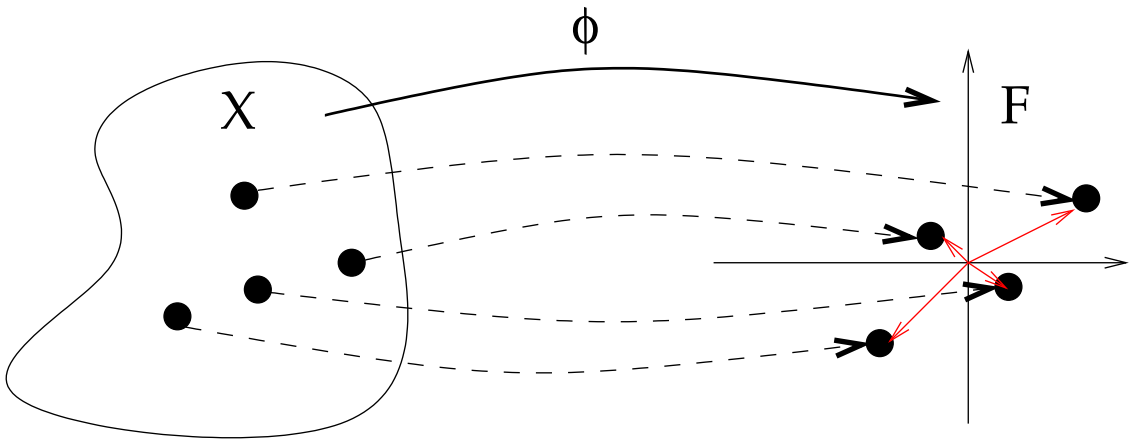
Theorem (Aronszajn, 1950)

K is a p.d. kernel on the set $\mathcal{X}$ if and only if there exists a Hilbert space $\mathcal{H}$ and a mapping

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

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

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



Proof of Aronzsajn's theorem

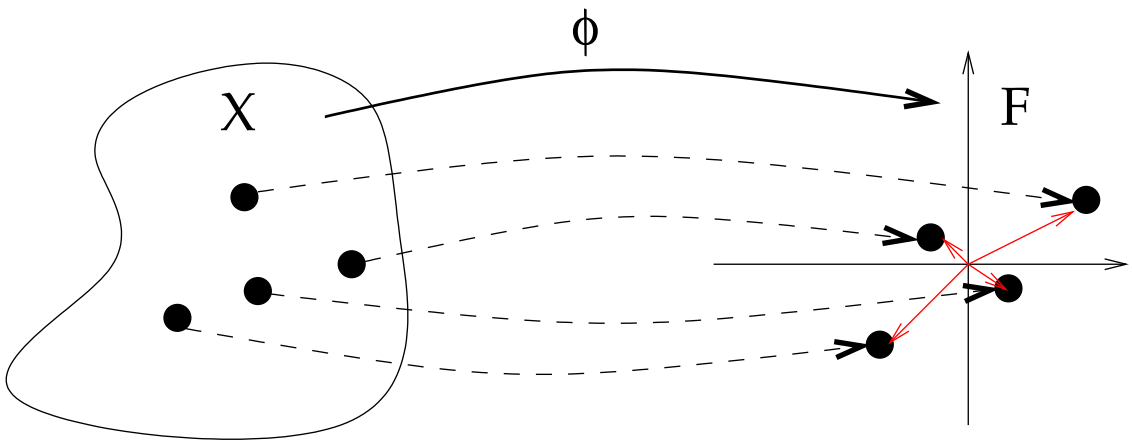
Proof

- If K is p.d. over a set $\mathcal{X}$ then it is the r.k. of a Hilbert space $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$.
- Let the mapping $\Phi : \mathcal{X} \to \mathcal{H}$ defined by:

$$\forall \mathbf{x} \in \mathcal{X}\,, \quad \Phi(\mathbf{x}) = K_{\mathbf{x}}\,.$$

- By the reproducing property we have:

$$\forall\,(\mathbf{x}, \mathbf{y}) \in \mathcal{X}^2, \quad \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}} = \langle K_{\mathbf{x}}, K_{\mathbf{y}} \rangle_{\mathcal{H}} = K\,(\mathbf{x}, \mathbf{y})\,. \qquad \square$$



Outline

The linear kernel

Take $\mathcal{X} = \mathbb{R}^d$ and the linear kernel:

$$K(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^d}$$

Theorem

The RKHS of the linear kernel is the set of linear functions of the form

$$f_w(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle_{\mathbb{R}^d} \quad \text{for} \quad \mathbf{w} \in \mathbb{R}^d ,$$

endowed with the norm

$$\| f \|_{\mathcal{H}} = \| w \|_2 .$$

Proof

- The RKHS of the linear kernel consists of functions:

$$\mathbf{x} \in \mathbb{R}^d \mapsto f(\mathbf{x}) = \sum_i a_i \langle \mathbf{x}_i, \mathbf{x} \rangle_{\mathbb{R}^d} = \langle \mathbf{w}, \mathbf{x} \rangle_{\mathbb{R}^d} \ ,$$

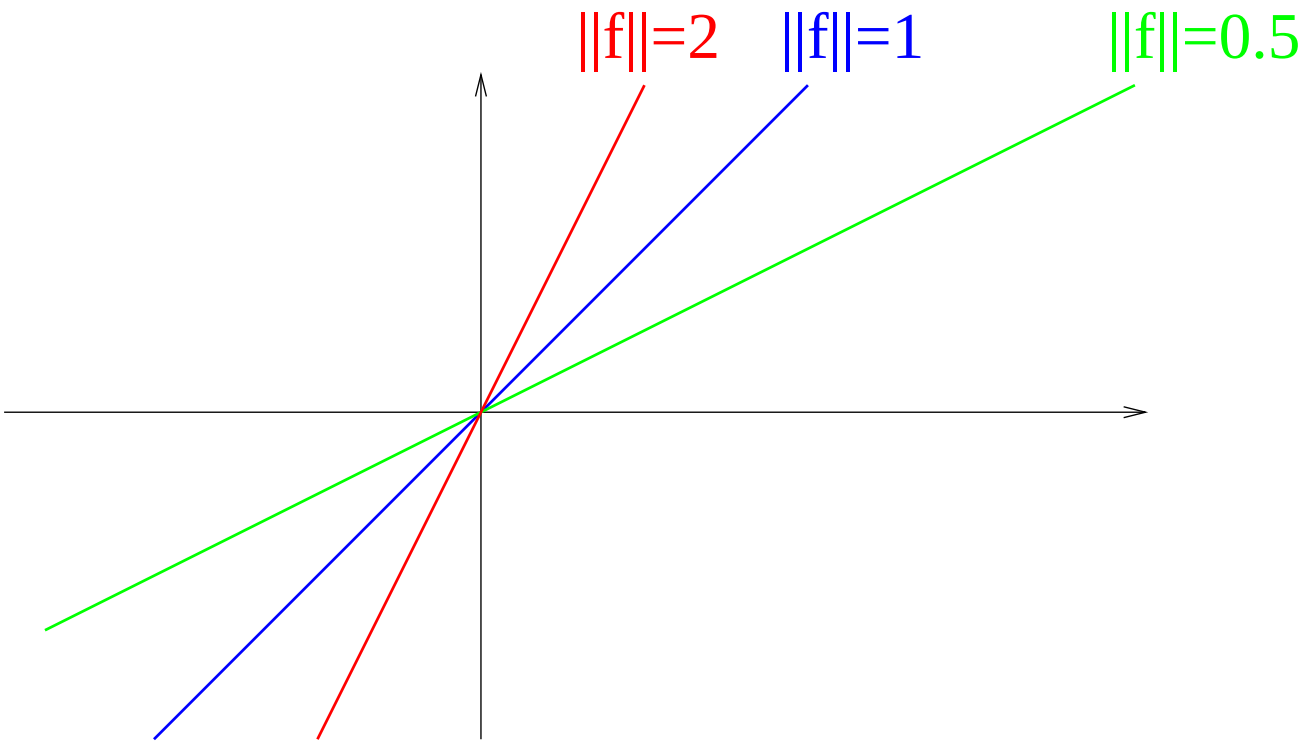
  with $\mathbf{w} = \sum_i a_i \mathbf{x}_i$.
- The RKHS is therefore the set of linear forms endowed with the following inner product:

$$\langle f, g \rangle_{\mathcal{H}_K} = \langle \mathbf{w}, \mathbf{v} \rangle_{\mathbb{R}^d} \ ,$$

  when $f(\mathbf{x}) = \mathbf{w}.\mathbf{x}$ and $g(\mathbf{x}) = \mathbf{v}.\mathbf{x}$.

RKHS of the linear kernel (cont.)

$$\begin{cases} K_{lin}(\mathbf{x}, \mathbf{x}') & = \mathbf{x}^\top \mathbf{x}' \ . \\ f(\mathbf{x}) & = w^\top x \ , \\ \| f \|_{\mathcal{H}} & = \| w \|_2 \ . \end{cases}$$



The polynomial kernel

We have already mentioned a generalization of the linear kernel: the polynomial kernel of degree p:

$$K_{poly}(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^d} + c)^p$$

Exercice: what is the RKHS of the polynomial kernel?

Combining kernels

Theorem

- If K_1 and K_2 are p.d. kernels, then:

$$K_1 + K_2,$$
$$K_1 K_2, \text{ and}$$
$$cK_1, \text{ for } c \geq 0,$$

  are also p.d. kernels
- If $(K_i)_{i \geq 1}$ is a sequence of p.d. kernels that converges pointwisely to a function K:

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

  then K is also a p.d. kernel.

Proof: left as exercice

Examples

Theorem

If K is a kernel, then e^K is a kernel too.

Proof:

$$e^{K(\mathbf{x},\mathbf{x}')} = \lim_{n \to +\infty} \sum_{i=0}^{n} \frac{K(\mathbf{x},\mathbf{x}')^i}{i!}$$

Quizz : which of the following are p.d. kernels?

- $\mathcal{X} = (-1, 1), \quad K(\mathbf{x}, \mathbf{x}') = \frac{1}{1-\mathbf{x}\mathbf{x}'}$
- $\mathcal{X} = \mathbb{N}, \quad K(\mathbf{x}, \mathbf{x}') = 2^{\mathbf{x}+\mathbf{x}'}$
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- $\mathcal{X} = \mathbb{R}_+, \quad K(\mathbf{x}, \mathbf{x}') = \min(\mathbf{x}, \mathbf{x}') / \max(\mathbf{x}, \mathbf{x}')$
- $\mathcal{X} = \mathbb{N}, \quad K(\mathbf{x}, \mathbf{x}') = GCD(\mathbf{x}, \mathbf{x}')$
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Quizz : which of the following are p.d. kernels?

- $\mathcal{X} = (-1, 1), \quad K(\mathbf{x}, \mathbf{x}') = \frac{1}{1-\mathbf{x}\mathbf{x}'}$
- $\mathcal{X} = \mathbb{N}, \quad K(\mathbf{x}, \mathbf{x}') = 2^{\mathbf{x}+\mathbf{x}'}$
- $\mathcal{X} = \mathbb{N}, \quad K(\mathbf{x}, \mathbf{x}') = 2^{\mathbf{x}\mathbf{x}'}$
- $\mathcal{X} = \mathbb{R}_+, \quad K(\mathbf{x}, \mathbf{x}') = \log(1 + \mathbf{x}\mathbf{x}')$
- $\mathcal{X} = \mathbb{R}, \quad K(\mathbf{x}, \mathbf{x}') = \exp\left(-|\mathbf{x} - \mathbf{x}'|^2\right)$
- $\mathcal{X} = \mathbb{R}, \quad K(\mathbf{x}, \mathbf{x}') = \cos(\mathbf{x} + \mathbf{x}')$
- $\mathcal{X} = \mathbb{R}, \quad K(\mathbf{x}, \mathbf{x}') = \cos(\mathbf{x} - \mathbf{x}')$
- $\mathcal{X} = \mathbb{R}_+, \quad K(\mathbf{x}, \mathbf{x}') = \min(\mathbf{x}, \mathbf{x}')$
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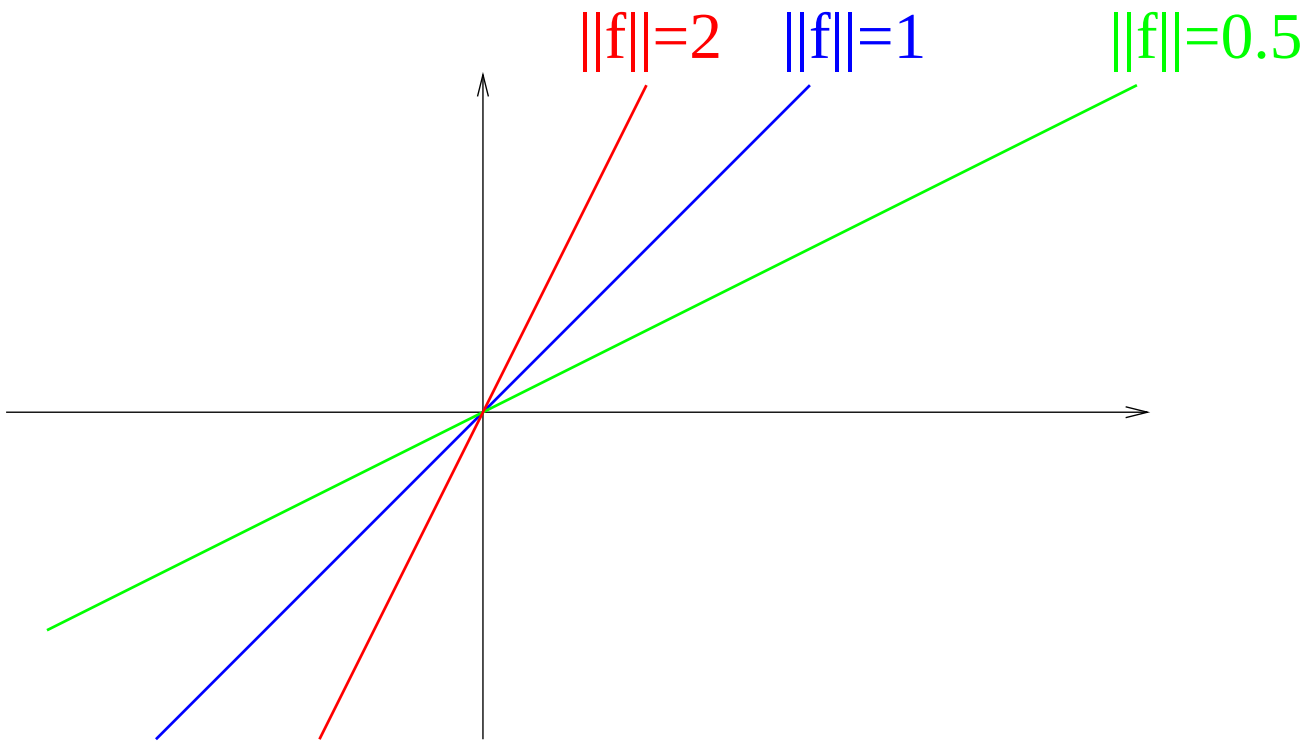
Outline

Remember the RKHS of the linear kernel

$$\begin{cases} K_{lin}(\mathbf{x}, \mathbf{x}') & = \mathbf{x}^\top \mathbf{x}' \ . \\ f(\mathbf{x}) & = w^\top x \ , \\ \| f \|_{\mathcal{H}} & = \| w \|_2 \ . \end{cases}$$



Smoothness functional

A simple inequality

- By Cauchy-Schwarz we have, for any function $f \in \mathcal{H}$ and any two points $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$:

$$\begin{aligned} \left| f(\mathbf{x}) - f(\mathbf{x}') \right| &= \left| \langle f, K_{\mathbf{x}} - K_{\mathbf{x}'} \rangle_{\mathcal{H}} \right| \\ &\leq \| f \|_{\mathcal{H}} \times \| K_{\mathbf{x}} - K_{\mathbf{x}'} \|_{\mathcal{H}} \\ &= \| f \|_{\mathcal{H}} \times d_K(\mathbf{x}, \mathbf{x}') \ . \end{aligned}$$

- The norm of a function in the RKHS controls how fast the function varies over $\mathcal{X}$ with respect to the geometry defined by the kernel (Lipschitz with constant $\| f \|_{\mathcal{H}}$).

Important message

Small norm $\Longrightarrow$ slow variations.

Kernels and RKHS : Summary

- P.d. kernels can be thought of as inner product after embedding the data space $\mathcal{X}$ in some Hilbert space. As such a p.d. kernel defines a metric on $\mathcal{X}$.
- A realization of this embedding is the RKHS, valid without restriction on the space $\mathcal{X}$ nor on the kernel.
- The RKHS is a space of functions over $\mathcal{X}$. The norm of a function in the RKHS is related to its degree of smoothness w.r.t. the metric defined by the kernel on $\mathcal{X}$.
- We will now see some applications of kernels and RKHS in statistics, before coming back to the problem of choosing (and eventually designing) the kernel.

Part 2

Kernels Methods

Motivations

Two theoretical results underpin a family of powerful algorithms for data analysis using positive definite kernels, collectively known as kernel methods:

- The kernel trick, based on the representation of p.d. kernels as inner products,
- the representer theorem, based on some properties of the regularization functional defined by the RKHS norm.

Outline

Motivations

- Choosing a p.d. kernel K on a set $\mathcal{X}$ amounts to embedding the data in a Hilbert space: there exists a Hilbert space $\mathcal{H}$ and a mapping $\Phi : \mathcal{X} \mapsto \mathcal{H}$ such that, for all $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$,

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

- However this mapping might not be explicitly given, nor convenient to work with in practice (e.g., large or even infinite dimensions).
- A solution is to work implicitly in the feature space!

The kernel trick

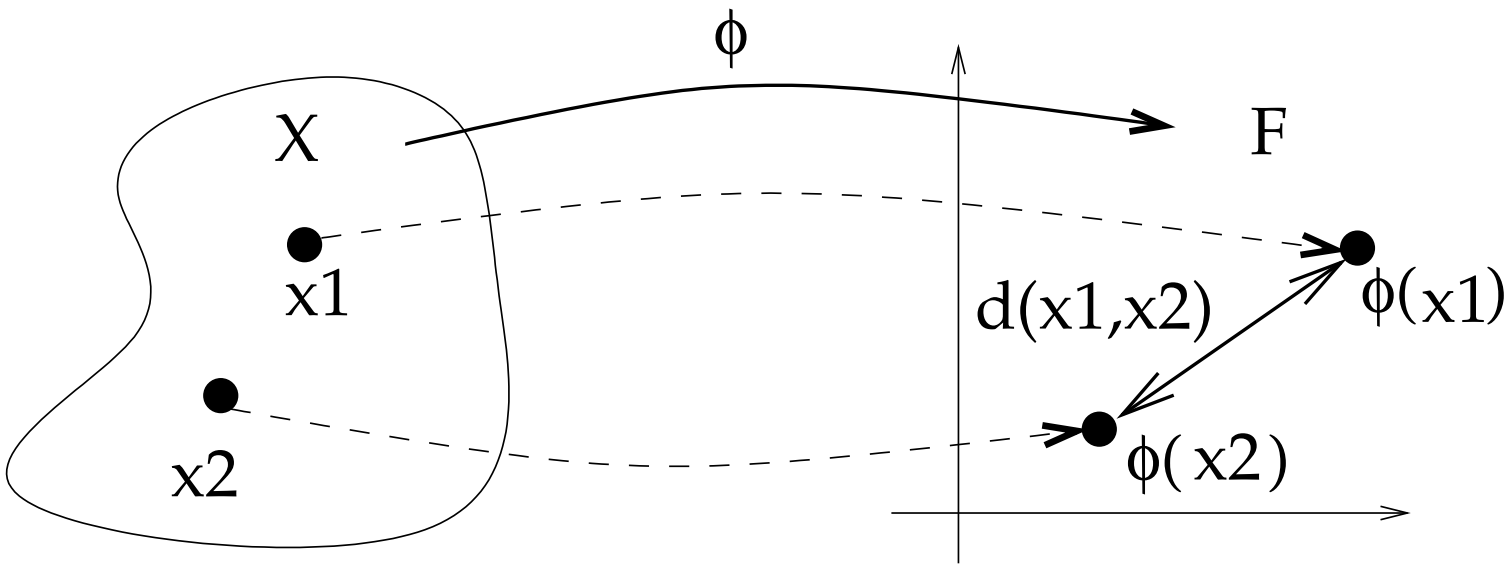
Kernel trick

Any algorithm to process finite-dimensional vectors that can be expressed only in terms of pairwise inner products can be applied to potentially infinite-dimensional vectors in the feature space of a p.d. kernel by replacing each inner product evaluation by a kernel evaluation.

Remark

- The proof of this proposition is trivial, because the kernel is exactly the inner product in the feature space.
- This trick has huge practical applications.
- Vectors in the feature space are only manipulated implicitly, through pairwise inner products.

Example 1: computing distances in the feature space



$$
\begin{aligned}
d_K(\mathbf{x}_1, \mathbf{x}_2)^2 &= \| \Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2) \|_{\mathcal{H}}^2 \\
&= \langle \Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2), \Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2) \rangle_{\mathcal{H}} \\
&= \langle \Phi(\mathbf{x}_1), \Phi(\mathbf{x}_1) \rangle_{\mathcal{H}} + \langle \Phi(\mathbf{x}_2), \Phi(\mathbf{x}_2) \rangle_{\mathcal{H}} - 2 \langle \Phi(\mathbf{x}_1), \Phi(\mathbf{x}_2) \rangle_{\mathcal{H}} \\
d_K(\mathbf{x}_1, \mathbf{x}_2)^2 &= K(\mathbf{x}_1, \mathbf{x}_1) + K(\mathbf{x}_2, \mathbf{x}_2) - 2K(\mathbf{x}_1, \mathbf{x}_2)
\end{aligned}
$$

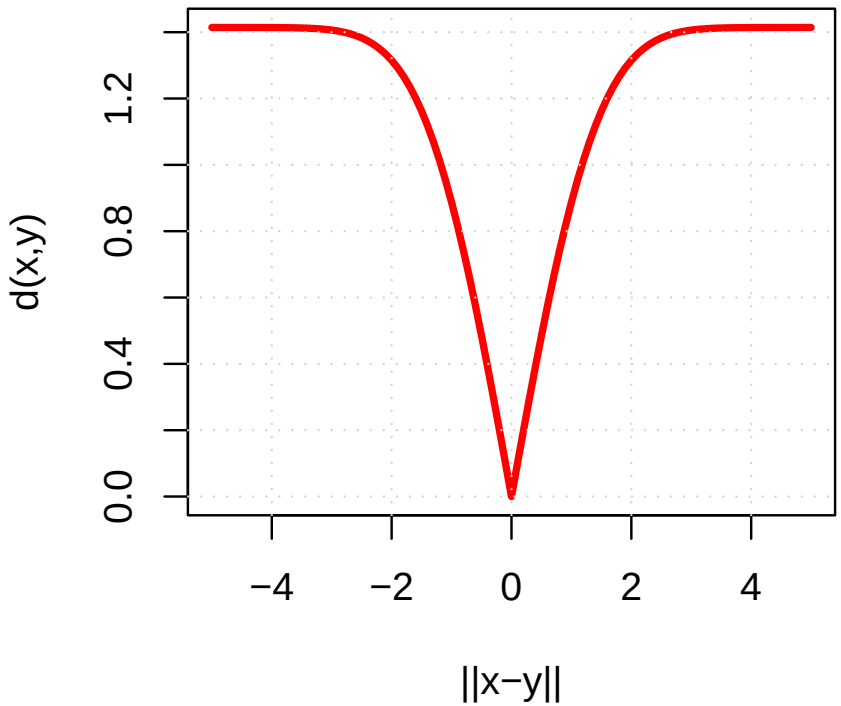
Distance for the Gaussian kernel

- The Gaussian kernel with bandwidth σ on $\mathbb{R}^d$ is:

$$K(\mathbf{x}, \mathbf{y}) = e^{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}},$$

- $K(\mathbf{x}, \mathbf{x}) = 1 = \|\Phi(\mathbf{x})\|^2_{\mathcal{H}}$, so all points are on the unit sphere in the feature space.
- The distance between the images of two points $\mathbf{x}$ and $\mathbf{y}$ in the feature space is given by:

$$d_K(\mathbf{x}, \mathbf{y}) = \sqrt{2\left[1 - e^{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}}\right]}$$



Example 2: distance between a point and a set

Problem

- Let $\mathcal{S} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)$ be a finite set of points in $\mathcal{X}$.
- How to define and compute the similarity between any point $\mathbf{x}$ in $\mathcal{X}$ and the set $\mathcal{S}$?

A solution

- Map all points to the feature space
- Summarize $\mathcal{S}$ by the barycenter of the points:

$$m := \frac{1}{n} \sum_{i=1}^{n} \Phi(\mathbf{x}_i) .$$

- Define the distance between $\mathbf{x}$ and $\mathcal{S}$ by:

$$d_K(\mathbf{x}, \mathcal{S}) := \| \Phi(\mathbf{x}) - m \|_{\mathcal{H}} .$$

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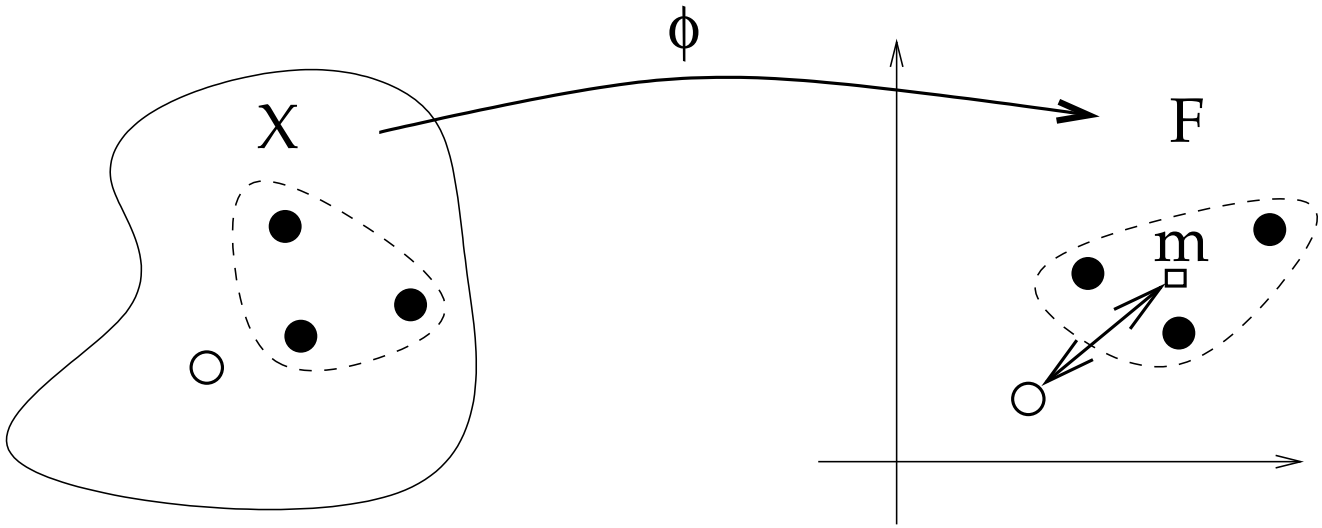
Computation



Kernel trick

$$d_K(\mathbf{x}, \mathcal{S}) = \| \Phi(\mathbf{x}) - \frac{1}{n} \sum_{i=1}^{n} \Phi(\mathbf{x}_i) \|_{\mathcal{H}}$$

$$= \sqrt{K(\mathbf{x}, \mathbf{x}) - \frac{2}{n} \sum_{i=1}^{n} K(\mathbf{x}, \mathbf{x}_i) + \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} K(\mathbf{x}_i, \mathbf{x}_j)}.$$

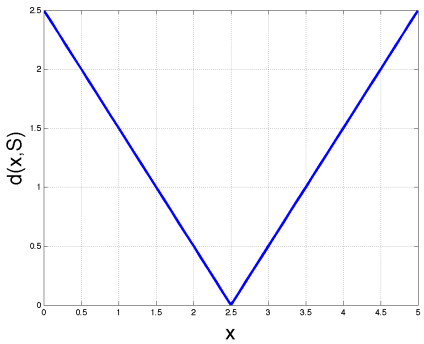
Remarks

Remarks

- The barycentre m only exists in the feature space in general: it does not necessarily have a pre-image $\mathbf{x}_m$ such that $\Phi(\mathbf{x}_m) = m$.
- The distance obtained is a Hilbert metric (e.g., Pythagoras theorem holds etc..)

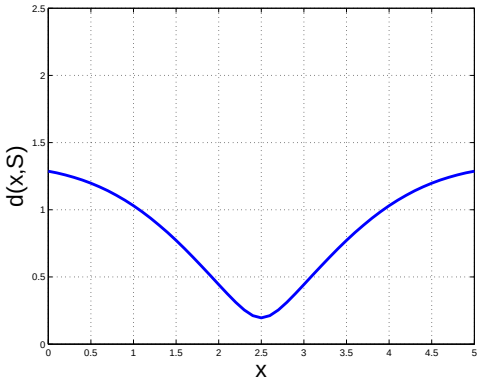
1D illustration

- $\mathcal{S} = \{2, 3\}$
- Plot $f(x) = d(x, \mathcal{S})$



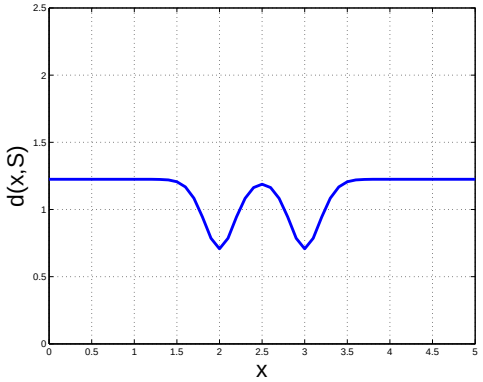
$$k(\mathbf{x}, \mathbf{y}) = \mathbf{x}\mathbf{y}.$$

(linear)



$$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}}.$$

with $\sigma = 1$.

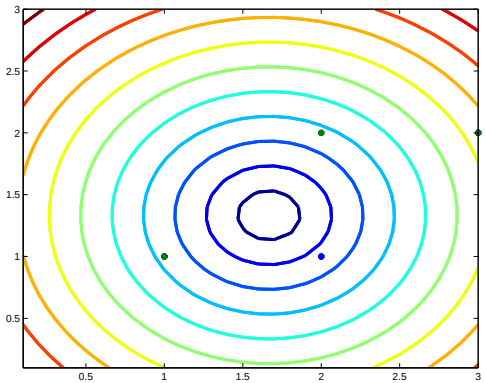


$$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}}.$$

with $\sigma = 0.2$.

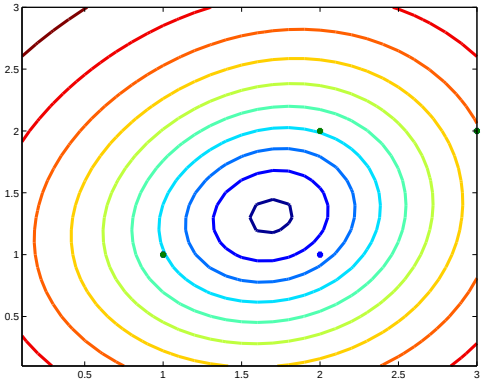
2D illustration

- $\mathcal{S} = \{(1,1)', (1,2)', (2,2)'\}$
- Plot $f(x) = d(x, \mathcal{S})$



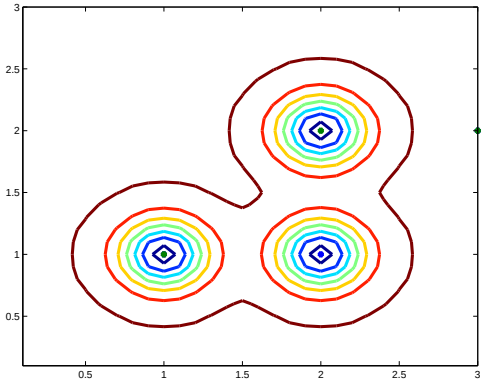
$k(\mathbf{x}, \mathbf{y}) = \mathbf{x}\mathbf{y}$.

(linear)



$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}}$.

with $\sigma = 1$.

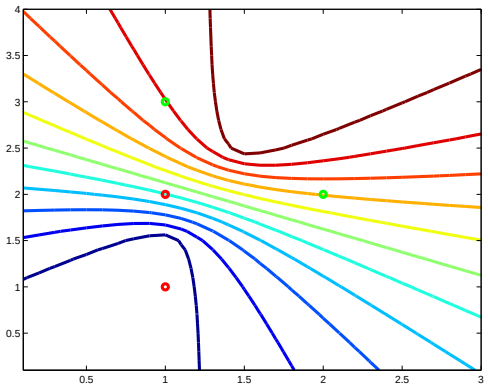


$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}}$.

with $\sigma = 0.2$.

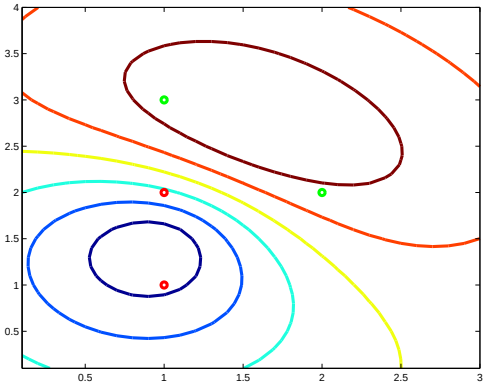
Application in discrimination

- $\mathcal{S}_1 = \{(1,1)', (1,2)'\}$ and $\mathcal{S}_2 = \{(1,3)', (2,2)'\}$
- Plot $f(x) = d(\mathbf{x}, \mathcal{S}_1)^2 - d(\mathbf{x}, \mathcal{S}_2)^2$



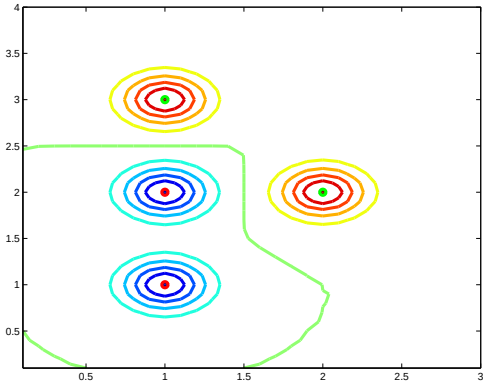
$k(\mathbf{x}, \mathbf{y}) = \mathbf{x}\mathbf{y}$.

(linear)



$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}}$.

with $\sigma = 1$.



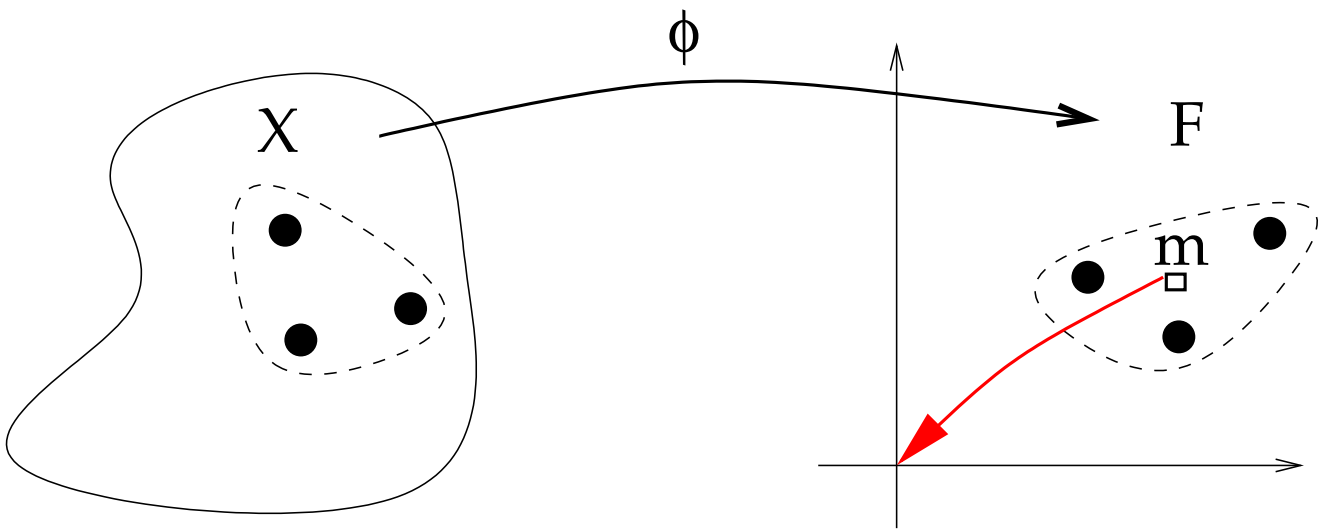
$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}}$.

with $\sigma = 0.2$.

Example 3: Centering data in the feature space

Problem

- Let $\mathcal{S} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)$ be a finite set of points in $\mathcal{X}$ endowed with a p.d. kernel K. Let G be their $n \times n$ Gram matrix: $G_{i,j} = K\left(\mathbf{x}_i, \mathbf{x}_j\right)$.
- Let $m = 1/n \sum_{i=1}^{n} \Phi\left(\mathbf{x}_i\right)$ their barycenter, and $u_i = \Phi\left(\mathbf{x}_i\right) - m$ for $i = 1, \ldots, n$ be centered data in $\mathcal{H}$.
- How to compute the centered Gram matrix $G^c_{i,j} = \left\langle u_i, u_j \right\rangle_{\mathcal{H}}$?



Kernel trick

- A direct computation gives, for $0 \leq i, j \leq n$:

$$\begin{aligned} G^c_{i,j} &= \left\langle \Phi(\mathbf{x}_i) - m, \Phi(\mathbf{x}_j) - m \right\rangle_{\mathcal{H}} \\ &= \left\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \right\rangle_{\mathcal{H}} - \left\langle m, \Phi(\mathbf{x}_i) + \Phi(\mathbf{x}_j) \right\rangle_{\mathcal{H}} + \langle m, m \rangle_{\mathcal{H}} \\ &= G_{i,j} - \frac{1}{n} \sum_{k=1}^{n} (G_{i,k} + G_{j,k}) + \frac{1}{n^2} \sum_{k,l=1}^{n} G_{k,l} \,. \end{aligned}$$

- This can be rewritten in matricial form:

$$G^c = G - UG - GU + UGU = (I - U) G (I - U) \,,$$

where $U_{i,j} = 1/n$ for $1 \leq i, j \leq n$.

Kernel trick Summary

Summary

- The kernel trick is a trivial statement with important applications.
- It can be used to obtain nonlinear versions of well-known linear algorithms, e.g., by replacing the classical inner product by a Gaussian kernel.
- It can be used to apply classical algorithms to non vectorial data (e.g., strings, graphs) by again replacing the classical inner product by a valid kernel for the data.
- It allows in some cases to embed the initial space to a larger feature space and involve points in the feature space with no pre-image (e.g., barycenter).

Outline

The Theorem

Representer Theorem

- Let $\mathcal{X}$ be a set endowed with a p.d. kernel K, $\mathcal{H}_K$ the corresponding RKHS, and $\mathcal{S} = \{\mathbf{x}_1, \cdots, \mathbf{x}_n\} \subset \mathcal{X}$ a finite set of points in $\mathcal{X}$.
- Let $\Psi : \mathbb{R}^{n+1} \to \mathbb{R}$ be a function of $n+1$ variables, strictly increasing with respect to the last variable.
- Then, any solution to the optimization problem:

$$\min_{f \in \mathcal{H}_K} \Psi\left(f(\mathbf{x}_1), \cdots, f(\mathbf{x}_n), \| f \|_{\mathcal{H}_K}\right), \tag{1}$$

admits a representation of the form:

$$\forall \mathbf{x} \in \mathcal{X}, \quad f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}). \tag{2}$$

Proof (1/2)

- Let $\xi(f, \mathcal{S})$ be the functional that is minimized in the statement of the representer theorem, and $\mathcal{H}_K^{\mathcal{S}}$ the linear span in $\mathcal{H}_K$ of the vectors K_{x_i}, i.e.,

$$\mathcal{H}_K^{\mathcal{S}} = \left\{ f \in \mathcal{H}_K : f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}), (\alpha_1, \cdots, \alpha_n) \in \mathbb{R}^n \right\}.$$

- $\mathcal{H}_K^{\mathcal{S}}$ finite-dimensional subspace, therefore any function $f \in \mathcal{H}_K$ can be uniquely decomposed as:

$$f = f_{\mathcal{S}} + f_{\perp},$$

with $f_{\mathcal{S}} \in \mathcal{H}_K^{\mathcal{S}}$ and $f_{\perp} \perp \mathcal{H}_K^{\mathcal{S}}$ (by orthogonal projection).

Proof (2/2)

- $\mathcal{H}_K$ being a RKHS it holds that:

$$\forall i = 1, \cdots, n, \quad f_\perp(\mathbf{x}_i) = \langle f_\perp, K(\mathbf{x}_i, .)\rangle_{\mathcal{H}_K} = 0\,,$$

because $K(\mathbf{x}_i, .) \in \mathcal{H}_K$, therefore:

$$\forall i = 1, \cdots, n, \quad f(\mathbf{x}_i) = f_{\mathcal{S}}(\mathbf{x}_i)\,.$$

- Pythagoras' theorem in $\mathcal{H}_K$ then shows that:

$$\| f \|^2_{\mathcal{H}_K} = \| f_{\mathcal{S}} \|^2_{\mathcal{H}_K} + \| f_\perp \|^2_{\mathcal{H}_K}\,.$$

- As a consequence, $\xi(f, \mathcal{S}) \geq \xi(f_{\mathcal{S}}, \mathcal{S})$, with equality if and only if $\| f_\perp \|_{\mathcal{H}_K} = 0$. The minimum of Ψ is therefore necessarily in $\mathcal{H}_K^{\mathcal{S}}$.

□

Remarks

Practical and theoretical consequences

Often the function Ψ has the form:

$$\Psi\left(f\left(\mathbf{x}_1\right), \cdots, f\left(\mathbf{x}_n\right), \| f \|_{\mathcal{H}_K}\right) = c\left(f\left(\mathbf{x}_1\right), \cdots, f\left(\mathbf{x}_n\right)\right) + \lambda \Omega\left(\| f \|_{\mathcal{H}_K}\right)$$

where $c(.)$ measures the "fit" of f to a given problem (regression, classification, dimension reduction, ...) and Ω is strictly increasing. This formulation has two important consequences:

- Theoretically, the minimization will enforce the norm $\| f \|_{\mathcal{H}_K}$ to be "small", which can be beneficial by ensuring a sufficient level of smoothness for the solution (regularization effect).
- Practically, we know by the representer theorem that the solution lives in a subspace of dimension n, which can lead to efficient algorithms although the RKHS itself can be of infinite dimension.

Remarks

Dual interpretations of kernel methods

Most kernel methods have two complementary interpretations:

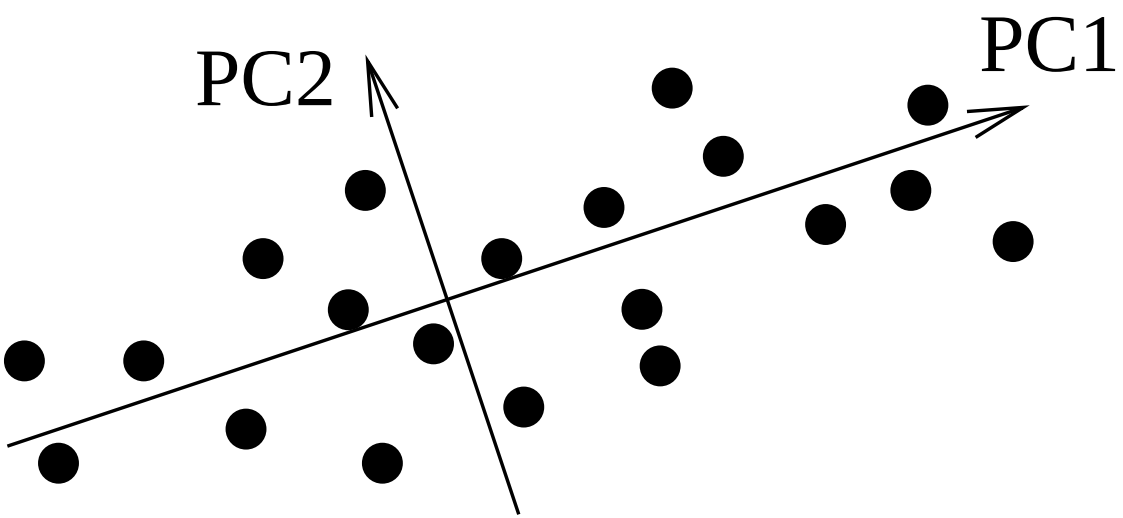
- A geometric interpretation in the feature space, thanks to the kernel trick. Even when the feature space is "large", most kernel methods work in the linear span of the embeddings of the points available.
- A functional interpretation, often as an optimization problem over (subsets of) the RKHS associated to the kernel.

Outline

Principal Component Analysis (PCA)

Classical setting

- Let $\mathcal{S} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ be a set of vectors ($\mathbf{x}_i \in \mathbb{R}^d$)
- PCA is a classical algorithm in multivariate statistics to define a set of orthogonal directions that capture the maximum variance
- Applications: low-dimensional representation of high-dimensional points, visualization



Principal Component Analysis (PCA)

Formalization

- Assume that the data are centered (otherwise center them as preprocessing), i.e.:

$$\sum_{i=1}^{n} \mathbf{x}_i = 0.$$

- The orthogonal projection onto a direction $\mathbf{w} \in \mathbb{R}^d$ is the function $h_{\mathbf{w}} : \mathcal{X} \to \mathbb{R}$ defined by:

$$h_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}^\top \frac{\mathbf{w}}{\| \mathbf{w} \|}.$$

Principal Component Analysis (PCA)

Formalization

- The empirical variance captured by $h_{\mathbf{w}}$ is:

$$\hat{var}\left(h_{\mathbf{w}}\right) := \frac{1}{n}\sum_{i=1}^{n} h_{\mathbf{w}}\left(\mathbf{x}_i\right)^2 = \frac{1}{n}\sum_{i=1}^{n} \frac{\left(\mathbf{x}_i^\top \mathbf{w}\right)^2}{\| \mathbf{w} \|^2}.$$

- The i-th principal direction w_i $(i = 1, \ldots, d)$ defined by:

$$\mathbf{w}_i = \underset{\mathbf{w} \perp \{\mathbf{w}_1, \ldots, \mathbf{w}_{i-1}\}}{\arg\max} \hat{var}\left(h_{\mathbf{w}}\right).$$

Principal Component Analysis (PCA)

Solution

- Let X be the $n \times d$ data matrix whose rows are the vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$. We can then write:

$$\hat{var}\left(h_{\mathbf{w}}\right) = \frac{1}{n} \sum_{i=1}^{n} \frac{\left(\mathbf{x}_i^\top \mathbf{w}\right)^2}{\| \mathbf{w} \|^2} = \frac{1}{n} \frac{\mathbf{w}^\top X^\top X \mathbf{w}}{\mathbf{w}^\top \mathbf{w}}.$$

- The solutions of:

$$\mathbf{w}_i = \underset{\mathbf{w} \perp \{\mathbf{w}_1, \ldots, \mathbf{w}_{i-1}\}}{\arg\max} \frac{1}{n} \frac{\mathbf{w}^\top X^\top X \mathbf{w}}{\mathbf{w}^\top \mathbf{w}}$$

  are the successive eigenvectors of $C = X^\top X$, ranked by decreasing eigenvalues.

Functional point of view

- Let $K(\mathbf{x}, \mathbf{y}) = \mathbf{x}^\top \mathbf{y}$ be the linear kernel.
- The associated RKHS $\mathcal{H}$ is the set of linear functions:

$$f_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}\,,$$

  endowed with the norm $\| f_{\mathbf{w}} \|_{\mathcal{H}} = \| \mathbf{w} \|_{\mathbb{R}^d}$.
- Therefore we can write:

$$\hat{var}(h_{\mathbf{w}}) = \frac{1}{n} \sum_{i=1}^{n} \frac{\left(\mathbf{x}_i^\top \mathbf{w}\right)^2}{\| \mathbf{w} \|^2} = \frac{1}{n \| f_{\mathbf{w}} \|^2} \sum_{i=1}^{n} f_{\mathbf{w}}(\mathbf{x}_i)^2.$$

- Moreover, $\mathbf{w} \perp \mathbf{w}' \Leftrightarrow f_{\mathbf{w}} \perp f_{\mathbf{w}'}$.

Functional point of view

- In other words, PCA solves, for $i = 1, \ldots, d$:

$$f_i = \underset{f \perp \{f_1, \ldots, f_{i-1}\}}{\arg\max} \frac{1}{n \| f \|^2} \sum_{i=1}^{n} f(\mathbf{x}_i)^2.$$

- We can apply the representer theorem (*exercice: check that is is also valid in a linear subspace*): for $i = 1, \ldots, d$, we have:

$$\forall \mathbf{x} \in \mathcal{X}, \quad f_i(\mathbf{x}) = \sum_{j=1}^{n} \alpha_{i,j} K(\mathbf{x}_j, \mathbf{x}),$$

with $\boldsymbol{\alpha}_i = (\alpha_{i,1}, \ldots, \alpha_{i,n})^\top \in \mathbb{R}^n$.

Functional point of view

- Therefore we have:

$$\| f_i \|_{\mathcal{H}}^2 = \sum_{k,l=1}^{d} \alpha_{i,k} \alpha_{i,l} k(\mathbf{x}_k, \mathbf{x}_l) = \boldsymbol{\alpha}_i^\top K \boldsymbol{\alpha}_i,$$

- Similarly:

$$\sum_{k=1}^{n} f_i(\mathbf{x}_k)^2 = \boldsymbol{\alpha}_i^\top K^2 \boldsymbol{\alpha}_i.$$

Functional point of view

PCA maximizes in α the function:

$$\alpha_i = \arg\max_{\alpha} \frac{\alpha^\top K^2 \alpha}{n \alpha^\top K \alpha},$$

under the constraints:

$$\alpha_i^\top K \alpha_j = 0 \quad \text{for } j = 1, \ldots, i-1 \,.$$

Solution

- Let $(e_1, \ldots, e_n)$ be an orthonormal basis of eigenvectors of K with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n \geq 0$.
- Let $\alpha_i = \sum_{j=1}^n \beta_{ij} e_j$, then

$$\frac{\alpha_i^\top K^2 \alpha_i}{n \alpha_i^\top K \alpha_i} = \frac{\sum_{j=1}^n \beta_{ij}^2 \lambda_j^2}{n \sum_{j=1}^n \beta_{ij}^2 \lambda_j},$$

which is maximized at $\alpha_1 = \beta_{11} e_1$, $\alpha_2 = \beta_{22} e_2$, etc...

Normalization

- For $\alpha_i = \beta_{ii} e_i$, we want:

$$1 = \| f_i \|^2_{\mathcal{H}} = \alpha_i^\top K \alpha_i = \beta_{ii}^2 \lambda_i \, .$$

- Therefore:

$$\alpha_i = \frac{1}{\sqrt{\lambda_i}} e_i .$$

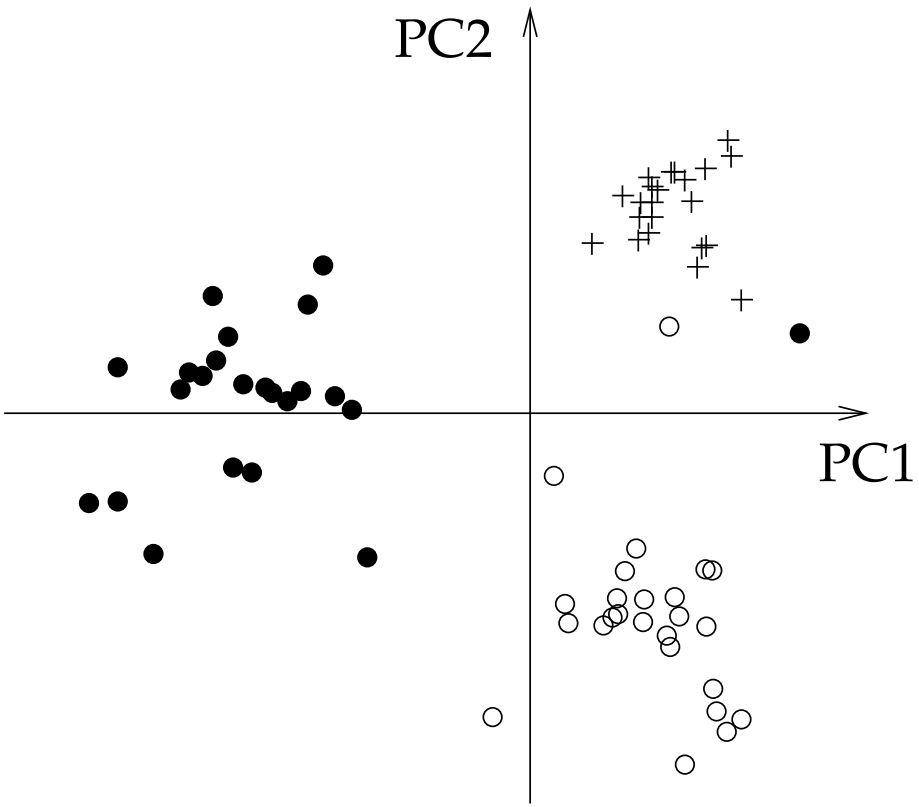
Kernel PCA: summary

1. Center the Gram matrix
2. Compute the first eigenvectors (e_i, λ_i)
3. Normalize the eigenvectors $\alpha_i = e_i / \sqrt{\lambda_i}$
4. The projections of the points onto the i-th eigenvector is given by $K\alpha_i$

Kernel PCA: remarks

- In this formulation, we must diagonalize the centered kernel Gram matrix, instead of the covariance matrix in the classical setting
- *Exercice: check that $X^\top X$ and $XX^\top$ have the same spectrum (up to 0 eigenvalues) and that the eigenvectors are related by a simple relationship.*
- This formulation remains valid for any p.d. kernel: this is kernel PCA
- Applications: nonlinear PCA with nonlinear kernels for vectors, PCA of non-vector objects (strings, graphs..) with specific kernels...

Example



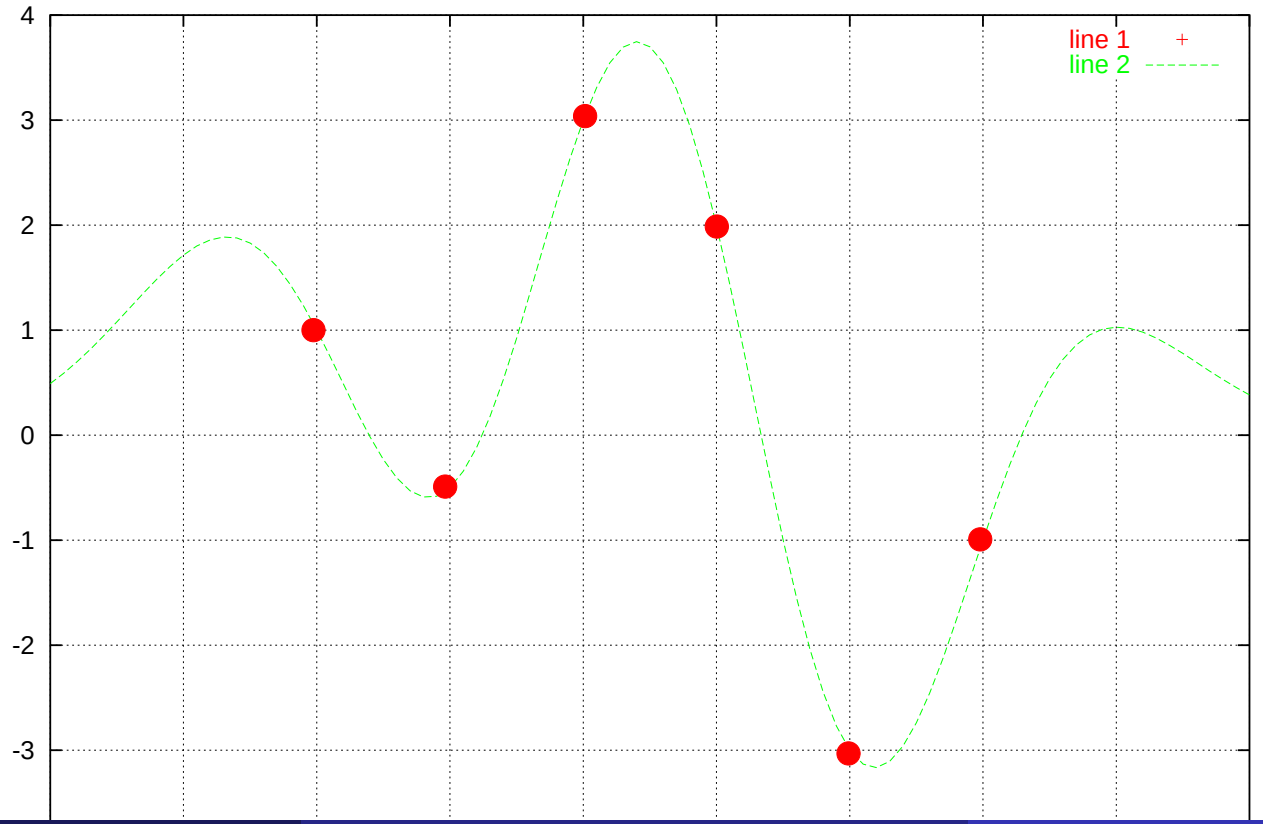
A set of 74 human tRNA sequences is analyzed using a kernel for sequences (the second-order marginalized kernel based on SCFG). This set of tRNAs contains three classes, called Ala-AGC (*white circles*), Asn-GTT (*black circles*) and Cys-GCA (*plus symbols*) (from Tsuda et al., 2003).

Outline

Regression

Setup

- Let $\mathcal{S} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \in \mathcal{X}^n$ be a set of points
- Let $\{y_1, \ldots, y_n\} \in \mathbb{R}^n$ be real numbers attached to the points
- Regression = find a function $f : \mathcal{X} \to \mathbb{R}$ to predict y by $f(\mathbf{x})$



Least-square regression

- Let us quantify the error if f predicts $f(\mathbf{x})$ instead of y by:

$$V(f(\mathbf{x}), y) = (y - f(\mathbf{x}))^2 .$$

- Fix a set of functions $\mathcal{H}$
- Least-square regression amounts to solve:

$$\hat{f} = \arg\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i))^2$$

- Issues: unstable (especially in large dimensions), overfitting if $\mathcal{H}$ is too "large"

Regularized least-square

- Let us take $\mathcal{H} = \mathcal{H}_k$, the RKHS associated to a p.d. kernel k on $\mathcal{X}$
- Let us regularize the functional to be minimized by:

$$\hat{f} = \arg\min_{f \in \mathcal{H}_k} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i))^2 + \lambda \| f \|^2_{\mathcal{H}_k}.$$

- *1st effect = prevent overfitting by penalizing the non-smooth functions*

Representation of the solution

- By the representer theorem, any solution of:

$$\hat{f} = \arg\min_{f \in \mathcal{H}_k} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i))^2 + \lambda \| f \|_{\mathcal{H}_k}^2 .$$

  can be expanded as:

$$\hat{f} = \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}) .$$

- *2nd effect = simplify the solution*

Dual formulation

- Let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^\top \in \mathbb{R}^n$,
- Let K be the $n \times n$ Gram matrix: $K_{i,j} = K\left(\mathbf{x}_i, \mathbf{x}_j\right)$.
- We can then write:

$$\left(\hat{f}\left(\mathbf{x}_1\right), \ldots, \hat{f}\left(\mathbf{x}_n\right)\right)^\top = K\boldsymbol{\alpha},$$

- The following holds as usual:

$$\| \hat{f} \|_{\mathcal{H}_k}^2 = \boldsymbol{\alpha}^\top K \boldsymbol{\alpha}.$$

Dual formulation

- The problem is therefore equivalent to:

$$\arg\min_{\boldsymbol{\alpha}\in\mathbb{R}^n} \frac{1}{n}\left(K\boldsymbol{\alpha}-y\right)^\top\left(K\boldsymbol{\alpha}-y\right)+\lambda\boldsymbol{\alpha}^\top K\boldsymbol{\alpha}.$$

- This is a convex and differentiable function of $\boldsymbol{\alpha}$. Its minimum can therefore be found by setting the gradient in $\boldsymbol{\alpha}$ to zero:

$$\begin{aligned} 0 &= \frac{2}{n}K\left(K\boldsymbol{\alpha}-y\right)+2\lambda K\boldsymbol{\alpha} \\ &= K\left[\left(K+\lambda n I\right)\boldsymbol{\alpha}-y\right] \end{aligned}$$

Dual formulation

- K being a symmetric matrix, it can be diagonalized in an orthonormal basis and $Ker(K) \perp Im(K)$.
- In this basis we see that $(K + \lambda nI)^{-1}$ leaves $Im(K)$ and $Ker(K)$ invariant.
- The problem is therefore equivalent to:

$$
\begin{aligned}
&(K + \lambda nI)\,\boldsymbol{\alpha} - y \in Ker(K) \\
\Leftrightarrow &\boldsymbol{\alpha} - (K + \lambda nI)^{-1}\, y \in Ker(K) \\
\Leftrightarrow &\boldsymbol{\alpha} = (K + \lambda nI)^{-1}\, y + \epsilon, \text{ with } K\epsilon = 0.
\end{aligned}
$$

Kernel ridge regression

- However, if $\boldsymbol{\alpha}' = \boldsymbol{\alpha} + \epsilon$ with $K\epsilon = 0$, then:

$$\| f - f' \|^2_{\mathcal{H}_K} = \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}'\right)^\top K \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}'\right) = 0,$$

  therefore $f = f'$.

- One solution to the initial problem is therefore:

$$\hat{f} = \sum_{i=1}^{n} \alpha_i K\left(\mathbf{x}_i, \mathbf{x}\right),$$

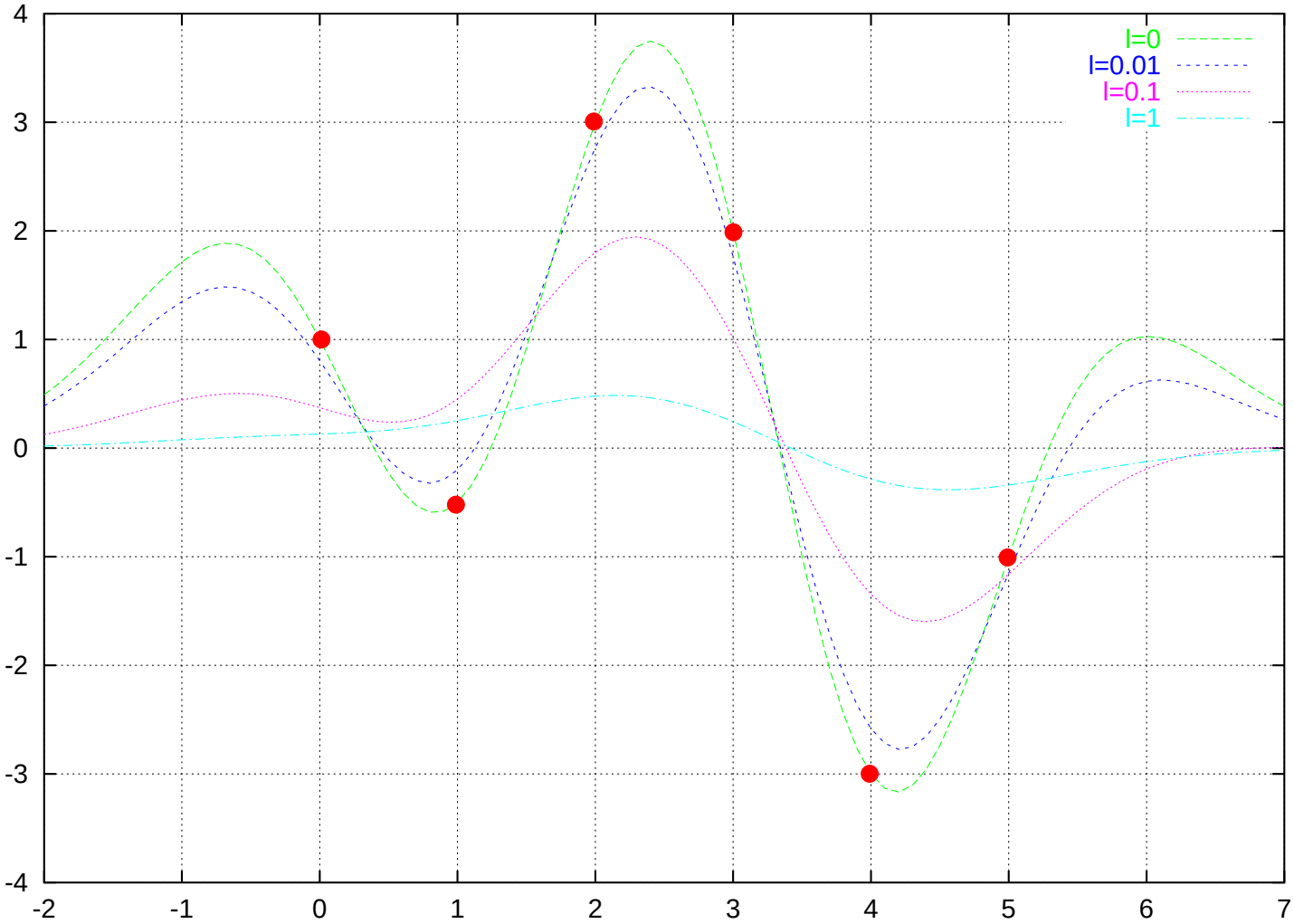
  with

$$\boldsymbol{\alpha} = \left(K + \lambda n I\right)^{-1} y.$$

Remarks

- The matrix $(K + n\lambda I)^{-1}$ is invertible when $\lambda > 0$.
- When $\lambda \to 0$, the method converges towards the solution of the classical unregularized least-square solution. When $\lambda \to \infty$, the solution converges to $f = 0$.
- In practice the symmetric matrix $K + n\lambda I$ is inverted with specific algorithms (e.g., Cholevsky decomposition).
- This method becomes difficult to use when the number of points becomes large.

Example



Kernel methods: Summary

- The kernel trick allows to extend many linear algorithms to non-linear settings and to general data (even non-vectorial).
- The representer theorem shows that that functional optimization over (subsets of) the RKHS is feasible in practice.
- We will see next a particularly successful applications of kernel methods, pattern recognition.

Part 3

Pattern recognition

Outline

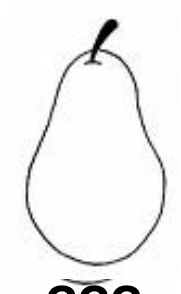
Pattern recognition


APPLE


APPLE


PEAR


PEAR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APPLE


PEAR


APPLE


APPLE


???

- Input variables $\mathbf{x} \in \mathcal{X}$
- Output $\mathbf{y} \in \{-1, 1\}$.
- Training set $\mathcal{S} = \{(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_n, \mathbf{y}_n)\}$.

Formalization

Risk

- P an (unknown) distribution on $\mathcal{X} \times \mathcal{Y}$.
- Observation: $\mathcal{S}_n = (X_i, Y_i)_{i=1,\ldots,n}$ i.i.d. random variables according to P.
- Loss function $l(f(\mathbf{x}), \mathbf{y}) \in \mathbb{R}$ small when $f(\mathbf{x})$ is a good predictor for y
- Risk: $R(f) = \mathbf{E} l(f(X), Y)$.
- Estimator $\hat{f}_n : \mathcal{X} \to \mathcal{Y}$.
- Goal: small risk $R\left(\hat{f}_n\right)$.

Large-margin classifiers

Margin

- For pattern recognition $\mathcal{Y} = \{-1, 1\}$
- Estimate a function $f : \mathcal{X} \to \mathbb{R}$.
- The margin of the function f for a pair $(\mathbf{x}, \mathbf{y})$ is:

$$\mathbf{y} f(\mathbf{x})$$

.

Large margin classifiers

- Focusing on large margins ensures that $f(\mathbf{x})$ has the same sign as $\mathbf{y}$ and a large absolute value (confidence).
- Suggests a loss function $l(f(\mathbf{x}), \mathbf{y}) = \phi(\mathbf{y} f(\mathbf{x}))$, where $\phi : \mathbb{R} \to \mathbb{R}$ is non-increasing.
- Goal: small ϕ-risk $R_\phi(f) = \mathbf{E}\phi(Yf(X))$

Empirical risk minimization (ERM)

ERM estimator

- The empirical ϕ-risk is:

$$R_\phi^n(f) = \frac{1}{n}\sum_{i=1}^n \phi\left(Y_i f\left(X_i\right)\right) .$$

- The ERM estimator on the functional class $\mathcal{F}$ is the solution (when it exists) of:

$$\hat{f}_n = \arg\min_{f\in\mathcal{F}} R_\phi^n(f) .$$

Class capacity

Motivations

- The ERM principle gives a good solution if $R_\phi^n\left(\hat{f}_n\right)$ is similar to $R_\phi(f)$.
- This can be ensured if $\mathcal{F}$ is not "too large".
- We need a measure of the "capacity" of $\mathcal{F}$.

Definition: Rademacher complexity

The Rademacher complexity of a class of functions $\mathcal{F}$ is:

$$\mathrm{Rad}_n(\mathcal{F}) = \mathbf{E}_{X,\sigma}\left[\sup_{f\in\mathcal{F}}\left|\frac{2}{n}\sum_{i=1}^n \sigma_i f(X_i)\right|\right],$$

where the expectation is over $(X_i)_{i=1,\dots,n}$ and the independent uniform $\{\pm 1\}$-valued (Rademacher) random variables $(\sigma_i)_{i=1,\dots,n}$.

Basic learning bounds

- Suppose ϕ is Lipschitz with constant L_ϕ:

$$\forall u, u' \in \mathbb{R}, \quad \left| \phi(u) - \phi(u') \right| \leq L_\phi \left| u - u' \right| .$$

- Then on average over the training set (and with high probability) the ϕ-risk of the ERM estimator is closed to the empirical one:

$$\mathbf{E}_{\mathcal{S}} \left[R_\phi \left(\hat{f}_n \right) - R_\phi^n \left(\hat{f}_n \right) \right] \leq 2 L_\phi \mathrm{Rad}_n \left(\mathcal{F} \right) .$$

- The ϕ-risk of the ERM estimator is also close to the smallest achievable on $\mathcal{F}$ (on average and with large probability):

$$\mathbf{E}_{\mathcal{S}} R_\phi \left(\hat{f}_n \right) \leq \inf_{f \in \mathcal{F}} R_\phi(f) + 4 L_\phi \mathrm{Rad}_n \left(\mathcal{F} \right) .$$

ERM in RKHS balls

Principle

- Suppose $\mathcal{X}$ is endowed with a p.d. kernel
- We consider the ball of radius B in the RKHS as function class for the ERM:

$$\mathcal{F}_B = \{f \in \mathcal{H} \,:\, \| f \|_{\mathcal{H}} \leq B\} \,.$$

Theorem (capacity control of RKHS balls)

$$\mathrm{Rad}_n(\mathcal{F}_B) \leq \frac{2B\sqrt{\mathbf{E}K(X,X)}}{\sqrt{n}} \,.$$

Proof (1/2)

$$
\begin{aligned}
\mathrm{Rad}_n\left(\mathcal{F}_B\right) &= \mathbf{E}_{X,\sigma}\left[\sup_{f\in\mathcal{F}_B}\left|\frac{2}{n}\sum_{i=1}^n \sigma_i f\left(X_i\right)\right|\right] \\
&= \mathbf{E}_{X,\sigma}\left[\sup_{f\in\mathcal{F}_B}\left|\left\langle f, \frac{2}{n}\sum_{i=1}^n \sigma_i K_{X_i}\right\rangle\right|\right] \qquad \text{(RKHS)} \\
&= \mathbf{E}_{X,\sigma}\left[B\| \frac{2}{n}\sum_{i=1}^n \sigma_i K_{X_i} \|_{\mathcal{H}}\right] \qquad \text{(Cauchy-Schwarz)} \\
&= \frac{2B}{n}\mathbf{E}_{X,\sigma}\left[\sqrt{\| \sum_{i=1}^n \sigma_i K_{X_i} \|_{\mathcal{H}}^2}\right] \\
&\leq \frac{2B}{n}\sqrt{\mathbf{E}_{X,\sigma}\left[\sum_{i,j=1}^n \sigma_i\sigma_j K\left(X_i, X_j\right)\right]} \qquad \text{(Jensen)}
\end{aligned}
$$

Proof (2/2)

But $\mathbf{E}_\sigma \left[\sigma_i \sigma_j\right]$ is 1 if $i = j$, 0 otherwise. Therefore:

$$\begin{aligned}
\mathrm{Rad}_n\left(\mathcal{F}_B\right) &\leq \frac{2B}{n} \sqrt{\mathbf{E}_X \left[\sum_{i,j=1}^{n} \mathbf{E}_\sigma \left[\sigma_i \sigma_j\right] K\left(X_i, X_j\right)\right]} \\
&\leq \frac{2B}{n} \sqrt{\mathbf{E}_X \sum_{i=1}^{n} K\left(X_i, X_i\right)} \\
&= \frac{2B\sqrt{\mathbf{E}_X K(X,X)}}{\sqrt{n}} . \quad \square
\end{aligned}$$

Basic learning bounds in RKHS balls

Corollary

- Suppose $K(X,X) \leq \kappa^2$ a.s. (e.g., Gaussian kernel and $\kappa = 1$).
- Let the minimum possibe ϕ-risk:

$$R_\phi^* = \inf_{f \text{ measurable}} R_\phi(f) \,.$$

- Then we directly get for the ERM estimator in $\mathcal{F}_B$:

$$\mathbf{E} R_\phi\left(\hat{f}_n\right) - R_\phi^* \leq \frac{8 L_\phi \kappa B}{\sqrt{n}} + \left[\inf_{f \in \mathcal{F}_B} R_\phi(f) - R_\phi^*\right] \,.$$

Choice of B by structural risk minimization

Remark

- The estimation error upper bound $8L_\phi \kappa B/\sqrt{n}$ increases (linearly) with B.
- The approximation error $\left[\inf_{f \in \mathcal{F}_B} R_\phi(f) - R_\phi^*\right]$ decreases with B.
- Ideally the choice of B should find a trade-off that minimizes the upper bound.
- This is achieved when

$$\frac{\partial \inf_{f \in \mathcal{F}_B} R_\phi(f)}{\partial B} = -\frac{8L_\phi \kappa}{\sqrt{n}} .$$

ERM in practice

Reformulation as penalized minimization

- We must solve the constrained minimization problem:

$$\begin{cases} \min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \phi\left(\mathbf{y}_i f\left(\mathbf{x}_i\right)\right) \\ \text{subject to } \| f \|_{\mathcal{H}} \leq B \,. \end{cases}$$

- This is a constrained optimization problem.

Outline

Optimization problems

Setting

- We consider an equality and inequality constrained optimization problem over a variable $x \in \mathcal{X}$:

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & h_i(x) = 0 \,, \quad i = 1, \dots, m \,, \\ & g_j(x) \leq 0 \,, \quad j = 1, \dots, r \,, \end{aligned}$$

  making no assumption of f, g and h.

- Let us denote by f^* the optimal value of the decision function under the constraints, i.e., $f^* = f(x^*)$ if the minimum is reached at a global minimum x^*.

Lagrangian and dual function

Lagrangian

The Lagrangian of this problem is the function $L : \mathcal{X} \times \mathbb{R}^m \times \mathbb{R}^r \to \mathbb{R}$ defined by:

$$L(x, \lambda, \mu) = f(x) + \sum_{i=1}^{m} \lambda_i h_i(x) + \sum_{j=1}^{r} \mu_j g_j(x) \, .$$

Lagrangian dual function

The Lagrange dual function $g : \mathbb{R}^m \times \mathbb{R}^r \to \mathbb{R}$ is:

$$\begin{aligned} q(\lambda, \mu) &= \inf_{x \in \mathcal{X}} L(x, \lambda, \mu) \\ &= \inf_{x \in \mathcal{X}} \left(f(x) + \sum_{i=1}^{m} \lambda_i h_i(x) + \sum_{j=1}^{r} \mu_j g_j(x) \right) \, . \end{aligned}$$

Properties of the dual function

- q is concave in (λ, μ), even if the original problem is not convex.
- The dual function yields lower bounds on the optimal value f^* of the original problem when μ is nonnegative:

$$q(\lambda, \mu) \leq f^* \ , \quad \forall \lambda \in \mathbb{R}^m, \forall \mu \in \mathbb{R}^r, \mu \geq 0 \ .$$

Proofs

- For each x, the function $(\lambda, \mu) \mapsto L(x, \lambda, \mu)$ is linear, and therefore both convex and concave in (λ, μ). The pointwise minimum of concave functions is concave, therefore q is concave.
- Let $\bar{x}$ be any feasible point, i.e., $h(\bar{x}) = 0$ and $g(\bar{x}) \leq 0$. Then we have, for any λ and $\mu \geq 0$:

$$\sum_{i=1}^{m} \lambda_i h_i(\bar{x}) + \sum_{i=1}^{r} \mu_i g_i(\bar{x}) \leq 0 \ ,$$

$$\implies \quad L(\bar{x}, \lambda, \mu) = f(\bar{x}) + \sum_{i=1}^{m} \lambda_i h_i(\bar{x}) + \sum_{i=1}^{r} \mu_i g_i(\bar{x}) \leq f(\bar{x}) \ ,$$

$$\implies \quad q(\lambda, \mu) = \inf_x L(x, \lambda, \mu) \leq L(\bar{x}, \lambda, \mu) \leq f(\bar{x}) \ , \quad \forall \bar{x} \ . \quad \square$$

Dual problem

Definition

For the (primal) problem:

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & h(x) = 0 \ , \quad g(x) \leq 0 \ , \end{aligned}$$

the Lagrange dual problem is:

$$\begin{aligned} \text{maximize} \quad & q(\lambda, \mu) \\ \text{subject to} \quad & \mu \geq 0 \ , \end{aligned}$$

where q is the (concave) Lagrange dual function and λ and μ are the Lagrange multipliers associated to the constraints $h(x) = 0$ and $g(x) \leq 0$.

Weak duality

- Let d^* the optimal value of the Lagrange dual problem. Each $q(\lambda, \mu)$ is an lower bound for f^* and by definition d^* is the best lower bound that is obtained. The following weak duality inequality therefore always hold:

$$d^* \leq f^* \ .$$

- This inequality holds when d^* or f^* are infinite. The difference $d^* - f^*$ is called the optimal duality gap of the original problem.

Strong duality

- We say that strong duality holds if the optimal duality gap is zero, i.e.:

$$d^* = f^* \ .$$

- If strong duality holds, then the best lower bound that can be obtained from the Lagrange dual function is tight
- Strong duality does not hold for general nonlinear problems.
- It usually holds for convex problems.
- Conditions that ensure strong duality for convex problems are called constraint qualification.

Slater's constraint qualification

Strong duality holds for a convex problem:

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & g_j(x) \leq 0 \;, \quad j = 1, \ldots, r \;, \\ & Ax = b \;, \end{aligned}$$

if it is strictly feasible, i.e., there exists at least one feasible point that satisfies:

$$g_j(x) < 0 \;, \quad j = 1, \ldots, r \;, \quad Ax = b \;.$$

Remarks

- Slater's conditions also ensure that the maximum d^* (if $> -\infty$) is attained, i.e., there exists a point (λ^*, μ^*) with

$$q(\lambda^*, \mu^*) = d^* = f^*$$

- They can be sharpened. For example, strict feasibility is not required for affine constraints.
- There exist many other types of constraint qualifications

Dual optimal pairs

Suppose that strong duality holds, x^* is primal optimal, (λ^*, μ^*) is dual optimal. Then we have:

$$\begin{aligned} f(x^*) &= q(\lambda^*, \mu^*) \\ &= \inf_{x \in \mathbb{R}^n} \left\{ f(x) + \sum_{i=1}^m \lambda_i^* h_i(x) + \sum_{j=1}^r \mu_j^* g_j(x) \right\} \\ &\leq f(x^*) + \sum_{i=1}^m \lambda_i^* h_i(x^*) + \sum_{j=1}^r \mu_j^* g_j(x^*) \\ &\leq f(x^*) \end{aligned}$$

Hence both inequalities are in fact equalities.

Complimentary slackness

The first equality shows that:

$$L(x^*, \lambda^*, \mu^*) = \inf_{x \in \mathbb{R}^n} L(x, \lambda^*, \mu^*) \ ,$$

showing that x^* minimizes the Lagrangian at (λ^*, μ^*). The second equality shows that:

$$\mu_j g_j(x^*) = 0 \ , \quad j = 1, \ldots, r \ .$$

This property is called complementary slackness:
the ith optimal Lagrange multiplier is zero unless the ith constraint is active at the optimum.

Outline

ERM in practice

Reformulation as penalized minimization

- We must solve the constrained minimization problem:

$$\begin{cases} \min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \phi\left(\mathbf{y}_i f\left(\mathbf{x}_i\right)\right) \\ \text{subject to } \| f \|_{\mathcal{H}} \leq B \,. \end{cases}$$

- To make this practical we assume that ϕ is convex.
- The problem is then a convex problem in f for which strong duality holds. In particular f solves the problem if and only if it solves for some dual parameter λ the unconstrained problem:

$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \phi\left(\mathbf{y}_i f\left(\mathbf{x}_i\right)\right) + \lambda \| f \|_{\mathcal{H}}^2 \right\} ,$$

and complimentary slackness holds ($\lambda = 0$ or $\| f \|_{\mathcal{H}} = B$).

Optimization in RKHS

- By the representer theorem, the solution of the unconstrained problem can be expanded as:

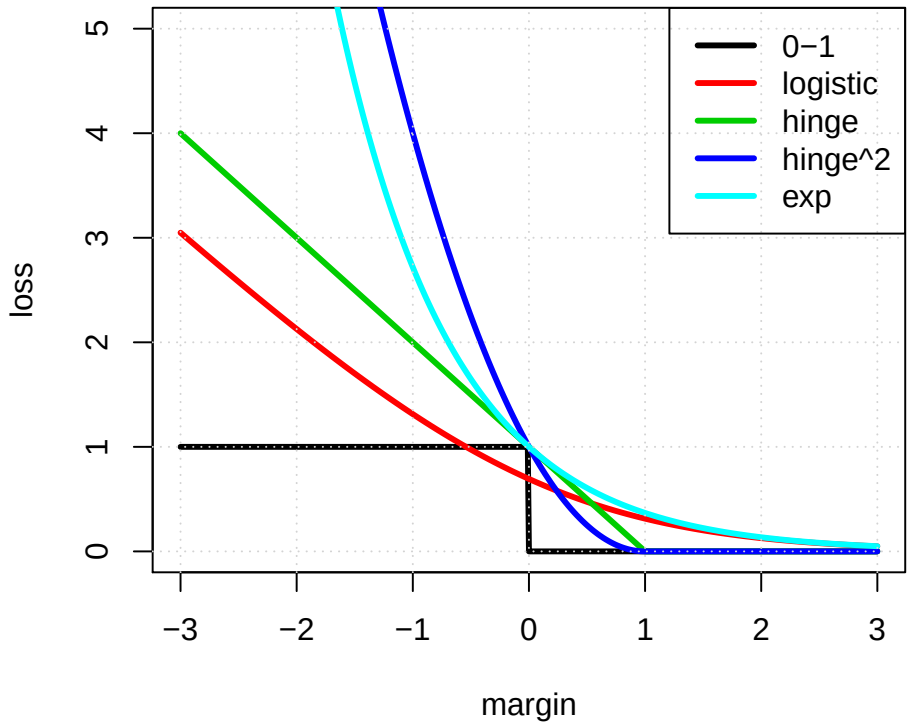
$$f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}) \ .$$

- Plugging into the original problem we obtain the following unconstrained and convex optimization problem in $\mathbb{R}^n$:

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^n} \left\{ \frac{1}{n} \sum_{i=1}^{n} \phi \left(\mathbf{y}_i \sum_{j=1}^{n} \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) \right) + \lambda \sum_{i,j=1}^{n} \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) \right\} \ .$$

- This can be implemented using general packages for convex optimization or specific algorithms (e.g., for SVM).

Loss function examples



Method	$\phi(u)$
Kernel logistic regression	$\log\left(1+e^{-u}\right)$
Support vector machine (1-SVM)	$\max\left(1-u,0\right)$
Support vector machine (2-SVM)	$\max\left(1-u,0\right)^2$
Boosting	e^{-u}

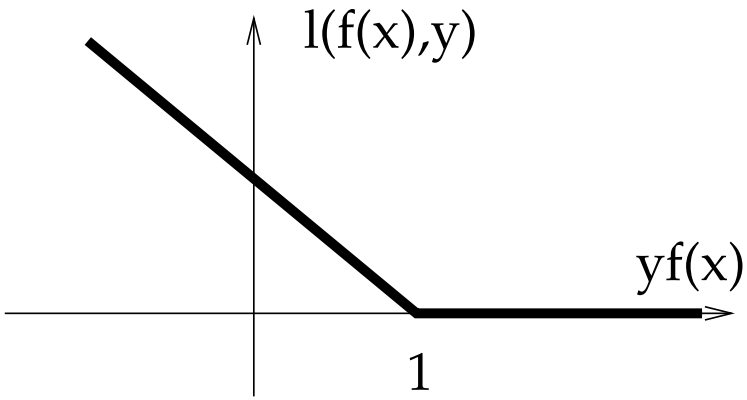
Outline

Motivations

Support vector machines (SVM)

- Historically the first "kernel method" for pattern recognition, still the most popular.
- Often stat-of-the-art in performance.
- One particular choice of loss function (hinge loss).
- Leads to a sparse solution, i.e., not all points are involved in the decomposition (compression).
- Particular algorithm for fast optimization (decomposition by chunking methods).

Definitions



- The loss function is the hinge loss:

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

- SVM solve the problem:

$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \phi_{\text{hinge}}\left(\mathbf{y}_i f\left(\mathbf{x}_i\right)\right) + \lambda \| f \|_{\mathcal{H}}^2 \right\} .$$

Problem reformulation (1/3)

Slack variables

- This is a convex optimization problem
- However the objective function in not differentiable, so we reformulate the problem with additional slack variables $\xi_1, \ldots, \xi_n \in \mathbb{R}$:

$$\min_{f \in \mathcal{H}, \boldsymbol{\xi} \in \mathbb{R}^n} \left\{ \frac{1}{n} \sum_{i=1}^{n} \xi_i + \lambda \| f \|_{\mathcal{H}}^2 \right\} ,$$

subject to:

$$\xi_i \geq \phi_{\text{hinge}} \left(\mathbf{y}_i f \left(\mathbf{x}_i \right) \right) .$$

Problem reformulation (2/3)

The objective function is now differentiable in f and ξ_i, and we can rewrite the constraints as a conjunction of linear constraints:

$$\min_{f \in \mathcal{H}, \boldsymbol{\xi} \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} \xi_i + \lambda \| f \|_{\mathcal{H}}^2 ,$$

subject to:

$$\begin{cases} \xi_i \geq 1 - \mathbf{y}_i f(\mathbf{x}_i), & \text{for } i = 1, \ldots, n, \\ \xi_i \geq 0, & \text{for } i = 1, \ldots, n. \end{cases}$$

Problem reformulation (3/3)

Finite-dimensional expansion

Replacing $\hat{f}$ by

$$\hat{f}(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}) \,,$$

the problem can be rewritten as an optimization problem in α and ξ:

$$\min_{\alpha \in \mathbb{R}^n, \xi \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} \xi_i + \lambda \alpha^\top K \alpha \,,$$

subject to:

$$\begin{cases} \mathbf{y}_i \sum_{j=1}^{n} \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) + \xi_i - 1 \geq 0 \,, & \text{for } i = 1, \ldots, n \,, \\ \xi_i \geq 0 \,, & \text{for } i = 1, \ldots, n \,. \end{cases}$$

Solving the problem

Remarks

- This is a classical quadratic program (minimization of a convex quadratic function with linear constraints) for which any out-of-the-box optimization package can be used.
- The dimension of the problem and the number of constraints, however, are $2n$ where n is the number of points. General-purpose QP solvers will have difficulties when n exceeds a few thousands.
- Solving the dual of this problem (also a QP) will be more convenient and lead to faster algorithms (due to the sparsity of the final solution).

Lagrangian

- Let us introduce the Lagrange multipliers $\boldsymbol{\mu} \in \mathbb{R}^n$ and $\boldsymbol{\nu} \in \mathbb{R}^n$.
- The Lagrangian of the problem is:

$$L(\boldsymbol{\alpha}, \boldsymbol{\xi}, \boldsymbol{\mu}, \boldsymbol{\nu}) = \frac{1}{n} \sum_{i=1}^{n} \xi_i + \lambda \boldsymbol{\alpha}^\top K \boldsymbol{\alpha}$$
$$- \sum_{i=1}^{n} \mu_i \left[\mathbf{y}_i \sum_{j=1}^{n} \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) + \xi_i - 1 \right] - \sum_{i=1}^{n} \nu_i \xi_i .$$

Minimizing $L(\alpha, \xi, \mu, \nu)$ w.r.t. α

- $L(\alpha, \xi, \mu, \nu)$ is a convex quadratic function in α. It is minimized when its gradient is null:

$$\nabla_{\alpha} L = 2\lambda K\alpha - KY\mu = K(2\lambda\alpha - Y\mu),$$

where Y is the diagonal matrix with entries $Y_{i,i} = \mathbf{y}_i$.

- Solving $\nabla_{\alpha} L = 0$ leads to

$$\alpha = \frac{Y\mu}{2\lambda} + \epsilon,$$

with $K\epsilon = 0$. But ϵ does not change f (same as kernel ridge regression), so we can choose for example $\epsilon = 0$ and:

$$\alpha_i^*(\mu, \nu) = \frac{\mathbf{y}_i \mu_i}{2\lambda}, \quad \text{for } i = 1, \ldots, n.$$

Minimizing $L(\alpha, \xi, \mu, \nu)$ w.r.t. ξ

- $L(\alpha, \xi, \mu, \nu)$ is a linear function in ξ.
- Its minimum is $-\infty$ except when $\nabla_\xi L = 0$, i.e.:

$$\frac{\partial L}{\partial \xi_i} = \frac{1}{n} - \mu_i - \nu_i = 0.$$

Dual function

- We therefore obtain the Lagrange dual function:

$$q(\mu, \nu) = \inf_{\alpha \in \mathbb{R}^n, \xi \in \mathbb{R}^n} L(\alpha, \xi, \mu, \nu)$$

$$= \begin{cases} \sum_{i=1}^n \mu_i - \frac{1}{4\lambda} \sum_{i,j=1}^n y_i y_j \mu_i \mu_j K(\mathbf{x}_i, \mathbf{x}_j) & \text{if } \mu_i + \nu_i = \frac{1}{n} \text{ for all } i, \\ -\infty & \text{otherwise.} \end{cases}$$

- The dual problem is:

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

Dual problem

- If $\mu_i > 1/n$ for some i, then there is no $\nu_i \geq 0$ such that $\mu_i + \nu_i = 1/n$, hence $q(\boldsymbol{\mu}, \boldsymbol{\nu}) = -\infty$.
- If $0 \leq \mu_i \leq 1/n$ for all i, then the dual function takes finite values that depend only on $\boldsymbol{\mu}$ by taking $\nu_i = 1/n - \mu_i$.
- The dual problem is therefore equivalent to:

$$\max_{0 \leq \boldsymbol{\mu} \leq 1/n} \sum_{i=1}^{n} \mu_i - \frac{1}{4\lambda} \sum_{i,j=1}^{n} \mathbf{y}_i \mathbf{y}_j \mu_i \mu_j K\left(\mathbf{x}_i, \mathbf{x}_j\right).$$

Back to the primal

- Once the dual problem is solved in $\boldsymbol{\mu}$ we get a solution of the primal problem by $\boldsymbol{\alpha} = Y\boldsymbol{\mu}/2\lambda$.
- We can therefore directly plug this into the dual problem to obtain the QP that $\boldsymbol{\alpha}$ must solve:

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^d} 2\sum_{i=1}^n \alpha_i \mathbf{y}_i - \sum_{i,j=1}^n \alpha_i \alpha_j K\left(\mathbf{x}_i, \mathbf{x}_j\right) = 2\boldsymbol{\alpha}^\top \mathbf{y} - \boldsymbol{\alpha}^\top K \boldsymbol{\alpha}\,,$$

subject to:

$$0 \leq y_i \alpha_i \leq \frac{1}{2\lambda n}, \quad \text{for } i = 1, \ldots, n\,.$$

Karush-Kuhn-Tucker (KKT) conditions

- The KKT optimality conditions are, for $i = 1, \ldots, n$:

$$\begin{cases} \mu_i \left[\mathbf{y}_i f\left(\mathbf{x}_i\right) + \xi_i - 1 \right] = 0, \\ \nu_i \xi_i = 0, \end{cases}$$

- In terms of α this can be rewritten as:

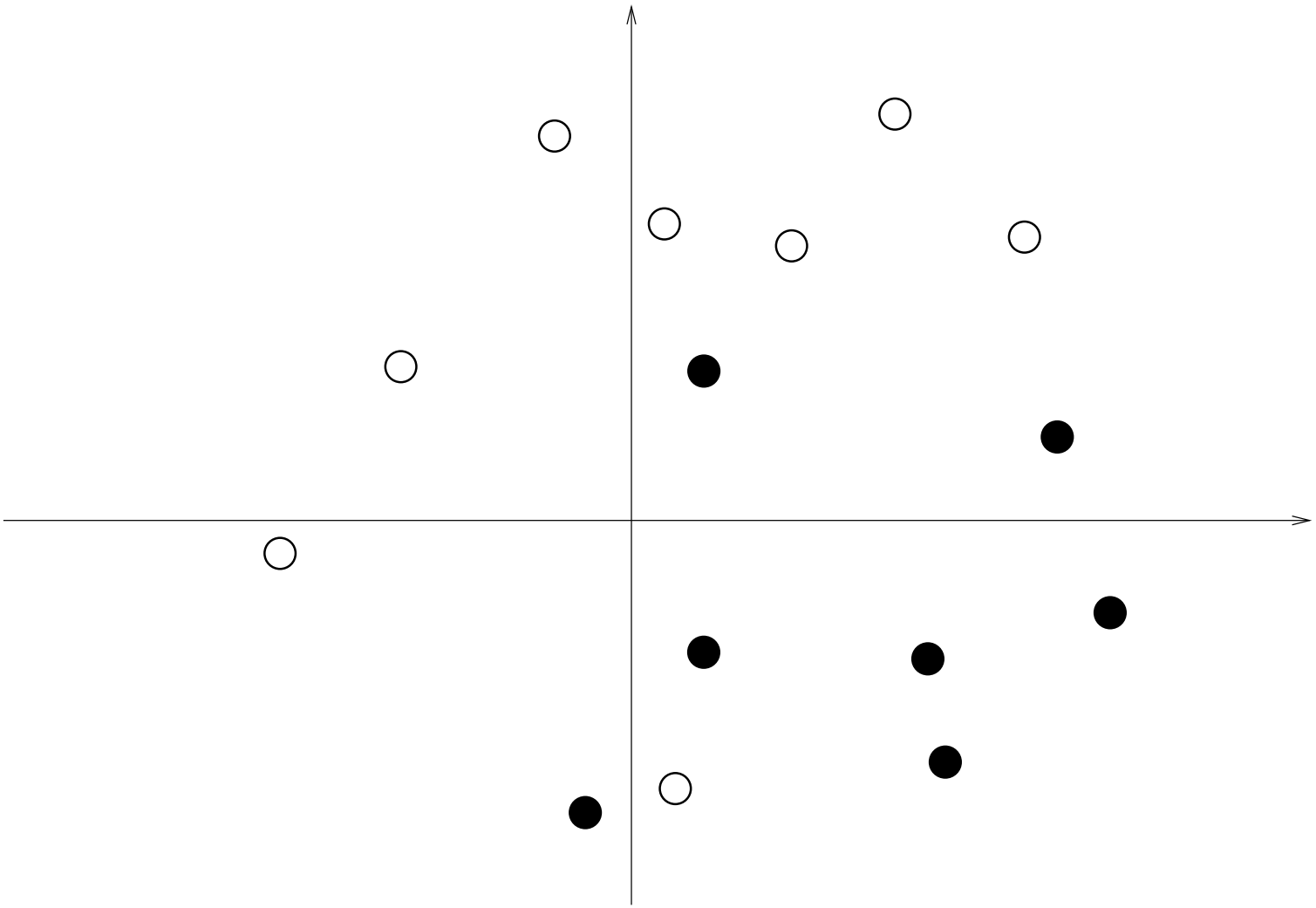
$$\begin{cases} \alpha_i \left[y_i f\left(\mathbf{x}_i\right) + \xi_i - 1 \right] = 0\,, \\ \left(\alpha_i - \frac{y_i}{2\lambda n} \right) \xi_i = 0\,. \end{cases}$$

Analysis of KKT conditions

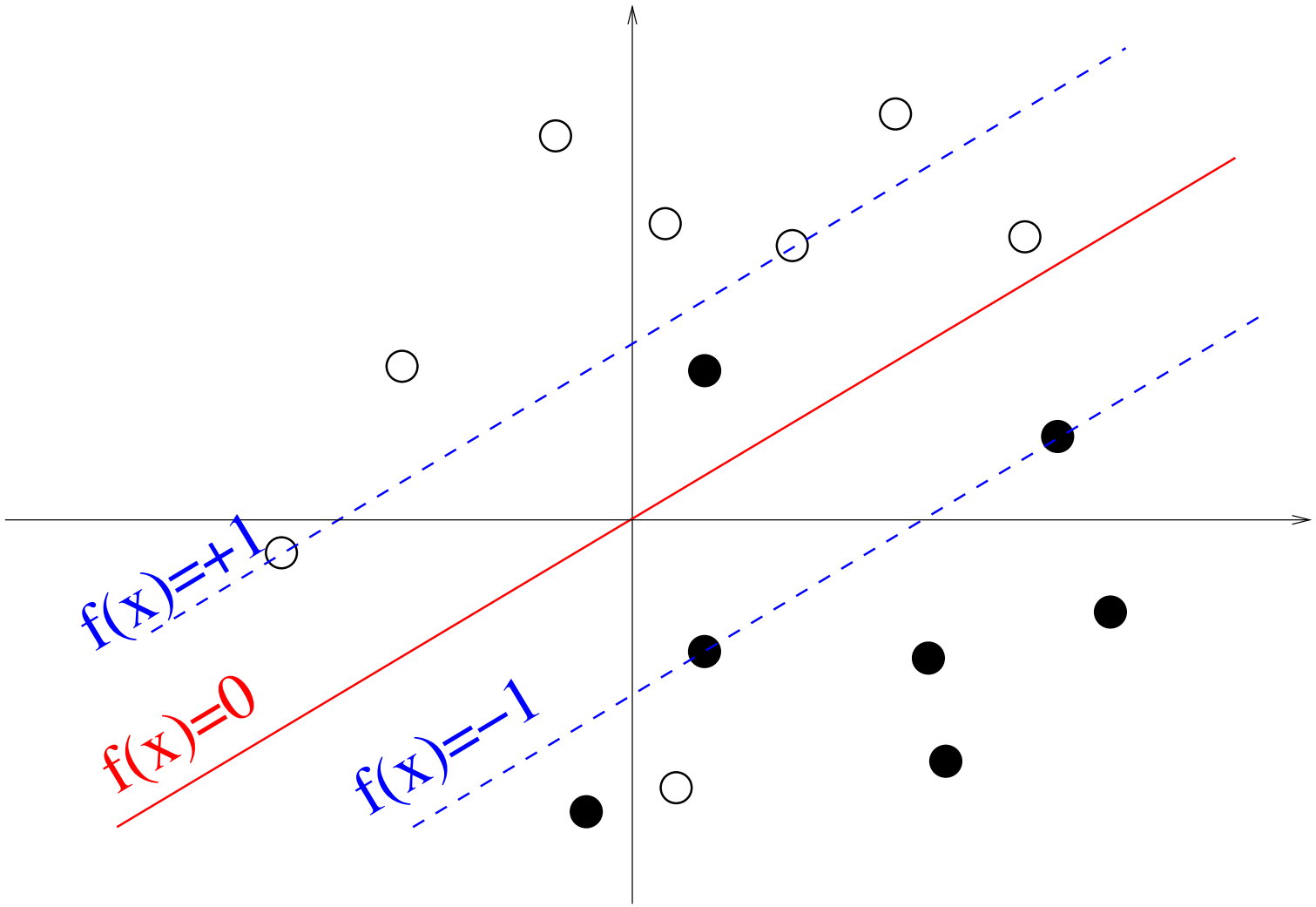
$$\begin{cases} \alpha_i \left[y_i f\left(\mathbf{x}_i\right) + \xi_i - 1 \right] = 0 \,, \\ \left(\alpha_i - \frac{y_i}{2\lambda n} \right) \xi_i = 0 \,. \end{cases}$$

- If $\alpha_i = 0$, then the second constraint is active: $\xi_i = 0$. This implies $y_i f\left(\mathbf{x}_i\right) \geq 1$.
- If $0 < \mathbf{y}_i \alpha_i < \frac{1}{2\lambda n}$, then both constraints are active: $\xi_i = 0$ et $y_i f\left(\mathbf{x}_i\right) + \xi_i - 1 = 0$. This implies $y_i f\left(\mathbf{x}_i\right) = 1$.
- If $\alpha_i = \frac{y_i}{2\lambda n}$, then the second constraint is not active ($\xi_i \geq 0$) while the first one is active: $y_i f\left(\mathbf{x}_i\right) + \xi_i = 1$. This implies $y_i f\left(\mathbf{x}_i\right) \leq 1$

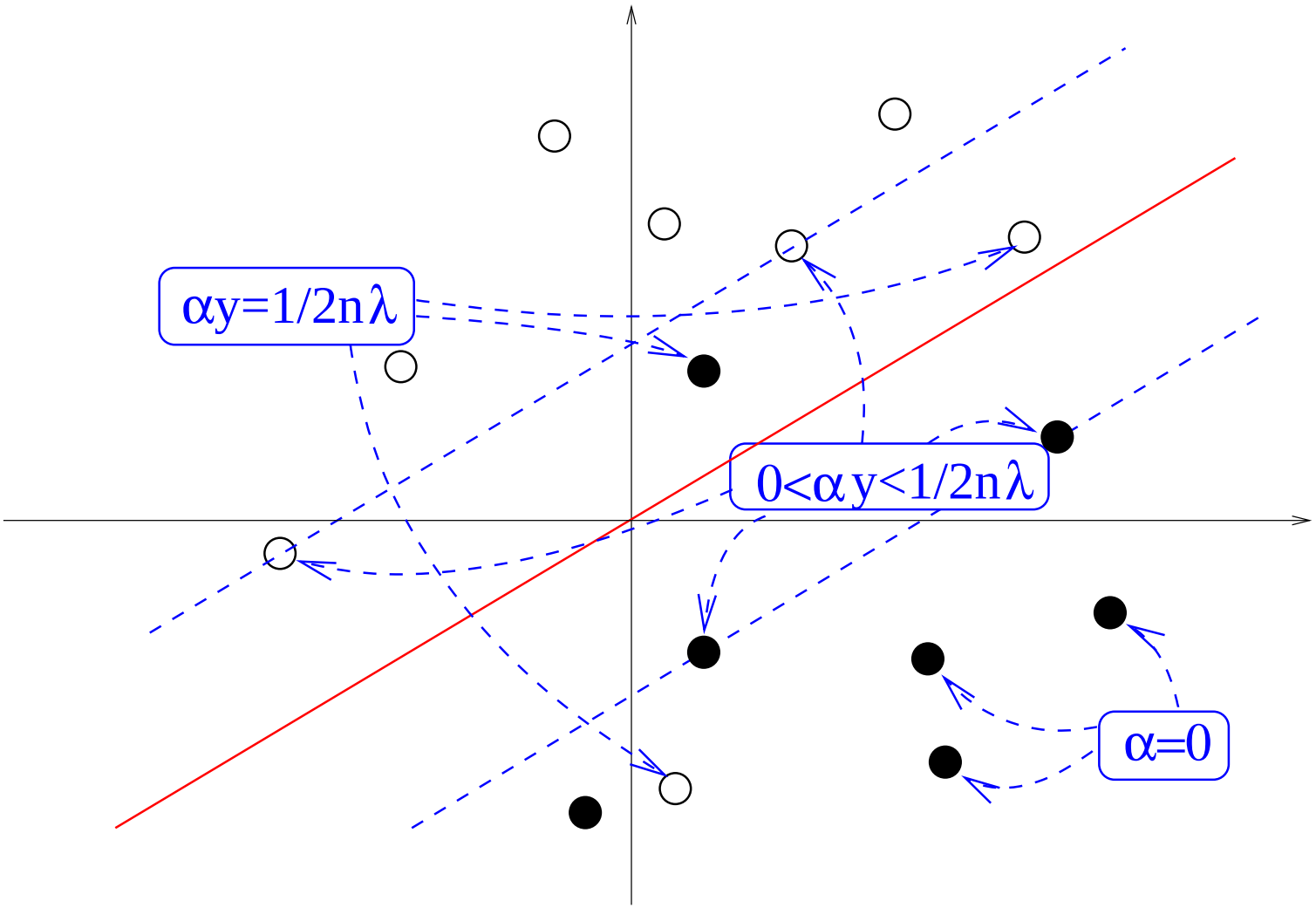
Geometric interpretation



Geometric interpretation



Geometric interpretation



Support vectors

Consequence of KKT conditions

- The training points with $\alpha_i \neq 0$ are called support vectors.
- Only support vectors are important for the classification of new points:

$$\forall \mathbf{x} \in \mathcal{X}, \quad f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}) = \sum_{i \in SV} \alpha_i K(\mathbf{x}_i, \mathbf{x}) \ ,$$

where SV is the set of support vectors.

Consequences

- The solution is sparse in α, leading to fast algorithms for training (use of decomposition methods).
- The classification of a new point only involves kernel evaluations with support vectors (fast).

Remark: C-SVM

- Often the SVM optimization problem is written in terms of a regularization parameter C instead of λ as follows:

$$\arg\min_{f\in\mathcal{H}} \frac{1}{2}\| f \|_{\mathcal{H}}^2 + C\sum_{i=1}^{n} V_{hinge}\left(f\left(\mathbf{x}_i\right), y_i\right).$$

- This is equivalent to our formulation with $C = \frac{1}{2n\lambda}$.
- The SVM optimization problem is then:

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^d} 2\sum_{i=1}^{n} \alpha_i \mathbf{y}_i - \sum_{i,j=1}^{n} \alpha_i\alpha_j K\left(\mathbf{x}_i, \mathbf{x}_j\right),$$

subject to:

$$0 \leq y_i\alpha_i \leq C, \quad \text{for } i = 1, \ldots, n.$$

- This formulation is often called C-SVM.

Remark: 2-SVM

- A variant of the SVM, sometimes called 2-SVM, is obtained by replacing the hinge loss by the square hinge loss:

$$\min_{f\in\mathcal{H}} \left\{ \frac{1}{n}\sum_{i=1}^{n} \phi_{\text{hinge}}\left(\mathbf{y}_i f\left(\mathbf{x}_i\right)\right)^2 + \lambda \| f \|_{\mathcal{H}}^2 \right\} .$$

- After some computation (left as exercice) we find that the dual problem of the 2-SVM is:

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^d} 2\boldsymbol{\alpha}^\top \mathbf{y} - \boldsymbol{\alpha}^\top \left(K + n\lambda I\right)\boldsymbol{\alpha} ,$$

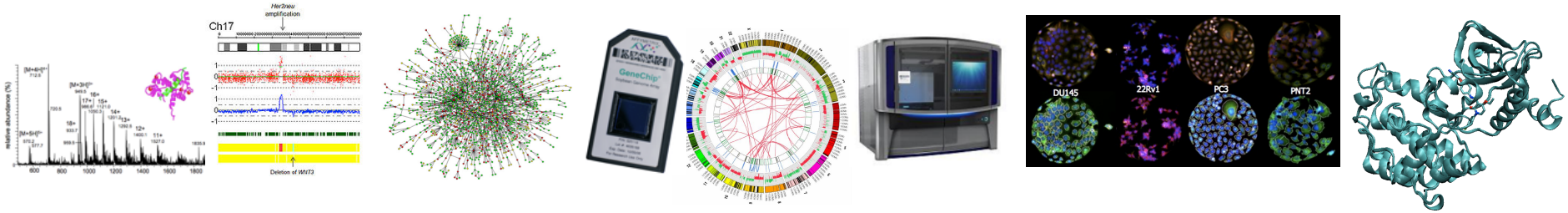
subject to:

$$0 \leq y_i \alpha_i, \qquad \text{for } i = 1, \ldots, n .$$

- This is therefore equivalent to the previous SVM with the kernel $K + n\lambda I$ and $C = +\infty$

Outline

Motivation



- We have seen how to make learning algorithms given a kernel K on some data space $\mathcal{X}$
- Often we may have several possible kernels:
  - by varying the kernel type or parameters on a given description of the data (eg, linear, polynomial, Gaussian kernels with different bandwidths...)
  - because we have different views of the same data, eg, a protein can be characterized by its sequence, its structure, its mass spectrometry profile...
- How to choose or integrate different kernels in a learning task?

Setting: learning with one kernel

- For any $f : \mathcal{X} \to \mathbb{R}$, let $f^n = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)) \in \mathbb{R}^n$
- Given a p.d. kernel $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, we learn with K by solving:

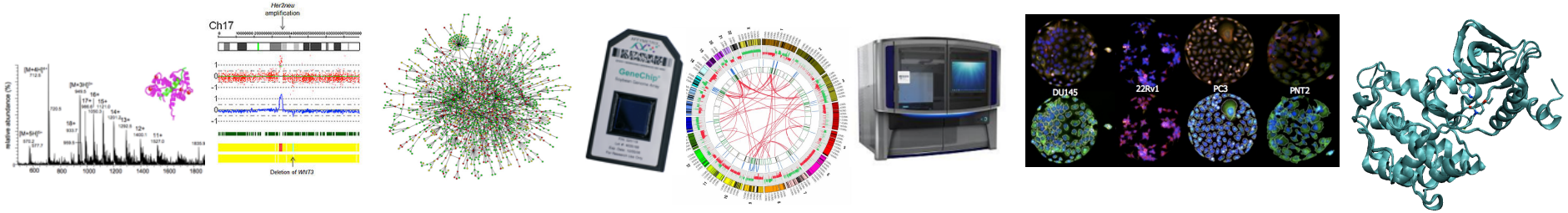
$$\min_{f \in \mathcal{H}_K} R(f^n) + \lambda \| f \|^2_{\mathcal{H}_K}, \tag{3}$$

where $\lambda > 0$ and $R : \mathbb{R}^n \to \mathbb{R}$ is an closed[1] and convex empirical risk:

- $R(u) = \frac{1}{n} \sum_{i=1}^n (u_i - y_i)^2$ for kernel ridge regression
- $R(u) = \frac{1}{n} \sum_{i=1}^n \max(1 - y_i u_i, 0)$ for SVM
- $R(u) = \frac{1}{n} \sum_{i=1}^n \log\left(1 + \exp\left(-y_i u_i\right)\right)$ for kernel logistic regression

[1] R is closed if, for each $A \in \mathbb{R}$, the sublevel set $\{u \in \mathbb{R}^n : R(u) \leq A\}$ is closed. For example, if R is continuous then it is closed.

Sum kernel



Definition

Let $K_1, \ldots, K_M$ be M kernels on $\mathcal{X}$. The sum kernel K_S is the kernel on $\mathcal{X}$ defined as

$$\forall \mathbf{x}, \mathbf{x}' \in \mathcal{X}\,, \quad K_S(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^{M} K_i(\mathbf{x}, \mathbf{x}')\,.$$

Sum kernel and vector concatenation

Theorem

For $i = 1, \ldots, M$, let $\Phi_i : \mathcal{X} \to \mathcal{H}_i$ be a feature map such that

$$K_i(\mathbf{x}, \mathbf{x}') = \left\langle \Phi_i(\mathbf{x}), \Phi_i(\mathbf{x}') \right\rangle_{\mathcal{H}_i} .$$

Then $K_S = \sum_{i=1}^{M} K_i$ can be written as:

$$K_S(\mathbf{x}, \mathbf{x}') = \left\langle \Phi_S(\mathbf{x}), \Phi_S(\mathbf{x}') \right\rangle_{\mathcal{H}_S} ,$$

where $\Phi_S : \mathcal{X} \to \mathcal{H}_S = \mathcal{H}_1 \oplus \ldots \oplus \mathcal{H}_M$ is the concatenation of the feature maps Φ_i:

$$\Phi_S(\mathbf{x}) = \left(\Phi_1(\mathbf{x}), \ldots, \Phi_M(\mathbf{x})\right)^\top .$$

Therefore, summing kernels amounts to concatenating their feature space representations, which is a quite natural way to integrate different features.

Proof

For $\Phi_S(\mathbf{x}) = (\Phi_1(\mathbf{x}), \ldots, \Phi_M(\mathbf{x}))^\top$, we easily compute:

$$\begin{aligned}
\left\langle \Phi_S(\mathbf{x}), \Phi_S(\mathbf{x}') \right\rangle_{\mathcal{H}_s} &= \sum_{i=1}^{M} \left\langle \Phi_i(\mathbf{x}), \Phi_i(\mathbf{x}') \right\rangle_{\mathcal{H}_i} \\
&= \sum_{i=1}^{M} K_i(\mathbf{x}, \mathbf{x}') \\
&= K_S(\mathbf{x}, \mathbf{x}') .
\end{aligned}$$

Example: data integration with the sum kernel

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Protein network inference from multiple genomic data: a supervised approach

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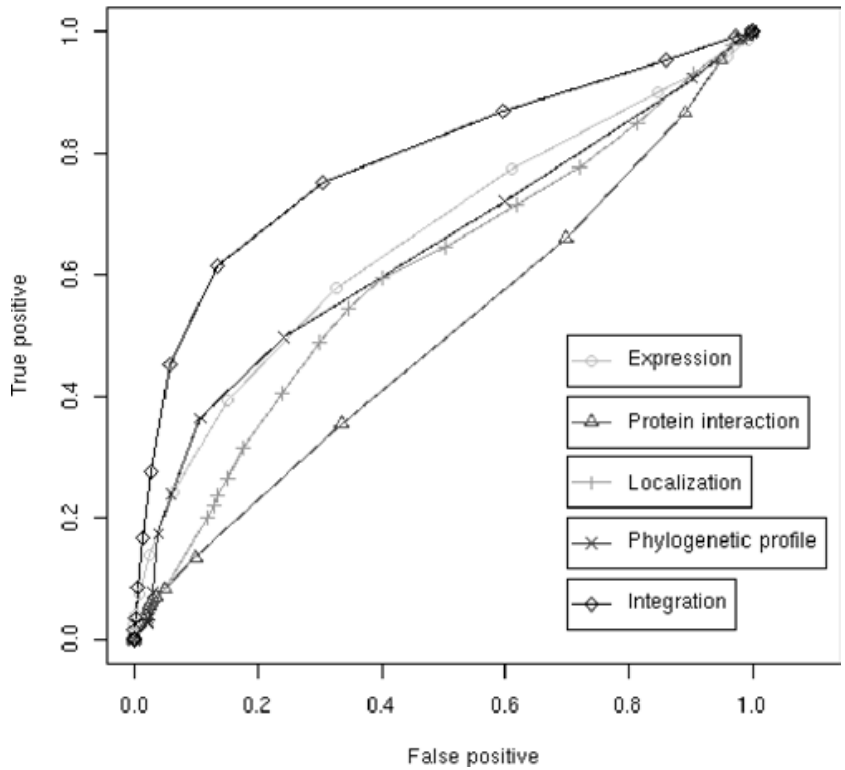


K_{exp} (Expression)
K_{ppi} (Protein interaction)
K_{loc} (Localization)
K_{phy} (Phylogenetic profile)
$K_{\text{exp}} + K_{\text{ppi}} + K_{\text{loc}} + K_{\text{phy}}$ (Integration)

The sum kernel: functional point of view

Theorem

The solution $f^* \in \mathcal{H}_{K_S}$ when we learn with $K_S = \sum_{i=1}^M K_i$ is equal to:

$$f^* = \sum_{i=1}^M f_i^* \,,$$

where $\left(f_1^*, \ldots, f_M^*\right) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1,\ldots,f_M} R\left(\sum_{i=1}^M f_i^n\right) + \lambda \sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}}^2 \,.$$

Generalization: The weighted sum kernel

Theorem

The solution f^* when we learn with $K_\eta = \sum_{i=1}^M \eta_i K_i$, with $\eta_1, \ldots, \eta_M \geq 0$, is equal to:

$$f^* = \sum_{i=1}^M f_i^* \,,$$

where $\left(f_1^*, \ldots, f_M^*\right) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \ldots, f_M} R\left(\sum_{i=1}^M f_i^n\right) + \lambda \sum_{i=1}^M \frac{\| f_i \|_{\mathcal{H}_{K_i}}^2}{\eta_i} \,.$$

Proof (1/4)

$$\min_{f_1,\ldots,f_M} R\left(\sum_{i=1}^M f_i^n\right) + \lambda \sum_{i=1}^M \frac{\| f_i \|^2_{\mathcal{H}_{K_i}}}{\eta_i} .$$

- R being convex, the problem is strictly convex and has a unique solution $\left(f_1^*, \ldots, f_M^*\right) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$.
- By the representer theorem, there exists $\alpha_1^*, \ldots, \alpha_M^* \in \mathbb{R}^n$ such that

$$f_i^*(\mathbf{x}) = \sum_{j=1}^n \alpha_{ij}^* K_i(\mathbf{x}_j, \mathbf{x}) .$$

- $\left(\alpha_1^*, \ldots, \alpha_M^*\right)$ is the solution of

$$\min_{\alpha_1,\ldots,\alpha_M \in \mathbb{R}^n} R\left(\sum_{i=1}^M K_i \alpha_i\right) + \lambda \sum_{i=1}^M \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} .$$

Proof (2/4)

- This is equivalent to

$$\min_{u,\alpha_1,\ldots,\alpha_M \in \mathbb{R}^n} R(u) + \lambda \sum_{i=1}^M \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} \quad \text{s.t.} \quad u = \sum_{i=1}^M K_i \alpha_i \,.$$

- This is equivalent to the saddle point problem:

$$\min_{u,\alpha_1,\ldots,\alpha_M \in \mathbb{R}^n} \max_{\gamma \in \mathbb{R}^n} R(u) + \lambda \sum_{i=1}^M \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} + 2\lambda \gamma^\top (u - \sum_{i=1}^M K_i \alpha_i) \,.$$

- By Slater's condition, strong duality holds, meaning we can invert min and max:

$$\max_{\gamma \in \mathbb{R}^n} \min_{u,\alpha_1,\ldots,\alpha_M \in \mathbb{R}^n} R(u) + \lambda \sum_{i=1}^M \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} + 2\lambda \gamma^\top (u - \sum_{i=1}^M K_i \alpha_i) \,.$$

Proof (3/4)

- Minimization in u:

$$\min_u R(u) + 2\lambda\gamma^\top u = -\max_u \left\{ -2\lambda\gamma^\top u - R(u) \right\} = -R^*(-2\lambda\gamma)\,,$$

where R^* is the Fenchel dual of R:

$$\forall v \in \mathbb{R}^n \quad R^*(v) = \sup_{u \in \mathbb{R}^n} u^\top v - R(u)\,.$$

- Minimization in α_i for $i = 1, \ldots, M$:

$$\min_{\alpha_i} \left\{ \lambda \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} - 2\lambda\gamma^\top K_i \alpha_i \right\} = -\lambda\eta_i\gamma^\top K_i\gamma\,,$$

where the minimum in α_i is reached for $\alpha_i^* = \eta_i\gamma$.

Proof (4/4)

- The dual problem is therefore

$$\max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top \left(\sum_{i=1}^M \eta_i K_i \right) \gamma \right\} .$$

- Note that if learn from a single kernel K_η, we get the same dual problem

$$\max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top K_\eta \gamma \right\} .$$

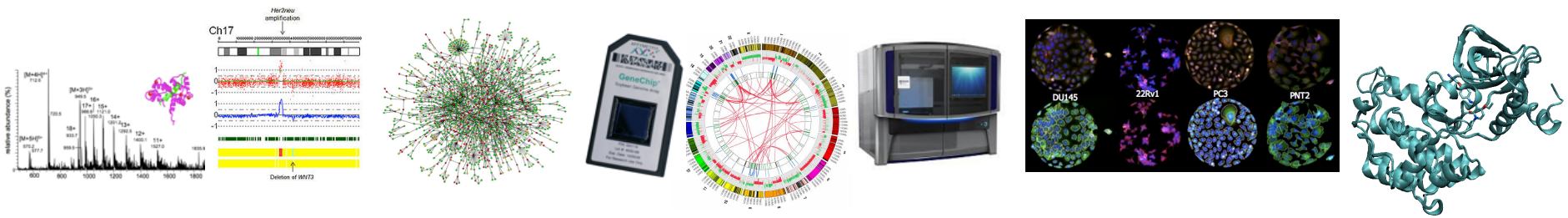
- If γ^* is a solution of the dual problem, then $\alpha_i^* = \eta_i \gamma^*$ leading to:

$$\forall \mathbf{x} \in \mathcal{X}\,, \quad f_i^*(\mathbf{x}) = \sum_{j=1}^n \alpha_{ij}^* K_i(\mathbf{x}_j, \mathbf{x}) = \sum_{j=1}^n \eta_i \gamma_j^* K_i(\mathbf{x}_j, \mathbf{x})$$

- Therefore, $f^* = \sum_{i=1}^M f_i^*$ satisfies

$$f^*(\mathbf{x}) = \sum_{i=1}^M \sum_{j=1}^n \eta_i \gamma_j^* K_i(\mathbf{x}_j, \mathbf{x}) = \sum_{j=1}^n \gamma_j^* K_\eta(\mathbf{x}_j, \mathbf{x}) \,. \quad \square$$

Learning the kernel



Motivation

- If we know how to weight each kernel, then we can learn with the weighted kernel

$$K_\eta = \sum_{i=1}^{M} \eta_i K_i$$

- However, usually we don't know...
- Perhaps we can optimize the weights η_i during learning?

An objective function for K

Theorem

For any p.d. kernel K on $\mathcal{X}$, let

$$J(K) = \min_{f \in \mathcal{H}_K} \left\{ R(f^n) + \lambda \| f \|^2_{\mathcal{H}_K} \right\} .$$

The function $K \mapsto J(K)$ is convex.

This suggests a principled way to "learn" a kernel: define a convex set of candidate kernels, and minimize $J(K)$ by convex optimization.

Proof

- We have shown by strong duality that

$$J(K) = \max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top K\gamma \right\} .$$

- For each γ fixed, this is an affine function of K, hence convex
- A supremum of convex functions is convex. □

MKL (Lanckriet et al., 2004)

- We consider the set of convex combinations

$$K_\eta = \sum_{i=1}^M \eta_i K_i \quad \text{with} \quad \eta \in \Sigma_M = \left\{ \eta_i \geq 0 \,, \sum_{i=1}^M \eta_i = 1 \right\}$$

- We optimize both η and f^* by solving:

$$\min_{\eta \in \Sigma_M} J(K_\eta) = \min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|^2_{\mathcal{H}_{K_\eta}} \right\}$$

- The problem is jointly convex in (η, α) and can be solved efficiently
- The output is both a set of weights η, and a predictor corresponding to the kernel method trained with kernel K_η.
- This method is usually called Multiple Kernel Learning (MKL).

Example: protein annotation

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A statistical framework for genomic data fusion

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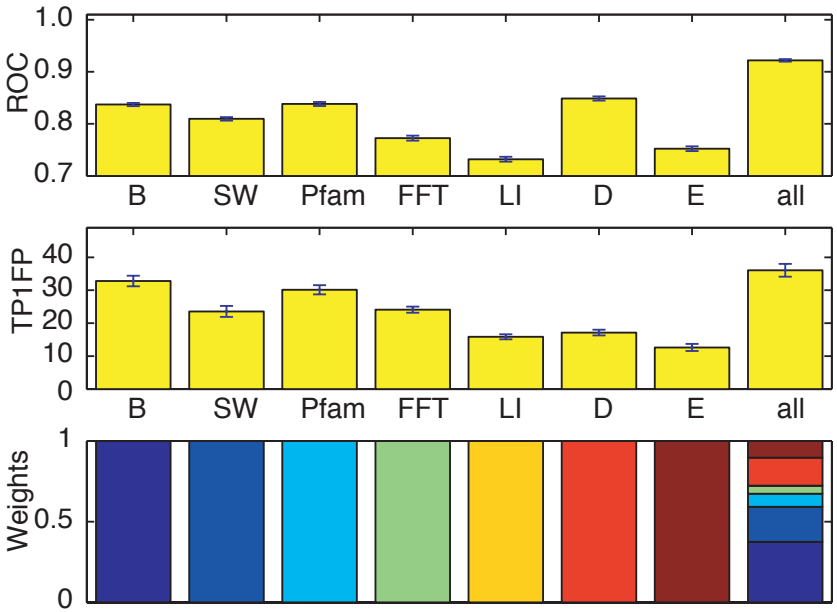
Kernel	Data	Similarity measure
K_{SW}	protein sequences	Smith-Waterman
K_{B}	protein sequences	BLAST
K_{Pfam}	protein sequences	Pfam HMM
K_{FFT}	hydropathy profile	FFT
K_{LI}	protein interactions	linear kernel
K_{D}	protein interactions	diffusion kernel
K_{E}	gene expression	radial basis kernel
K_{RND}	random numbers	linear kernel

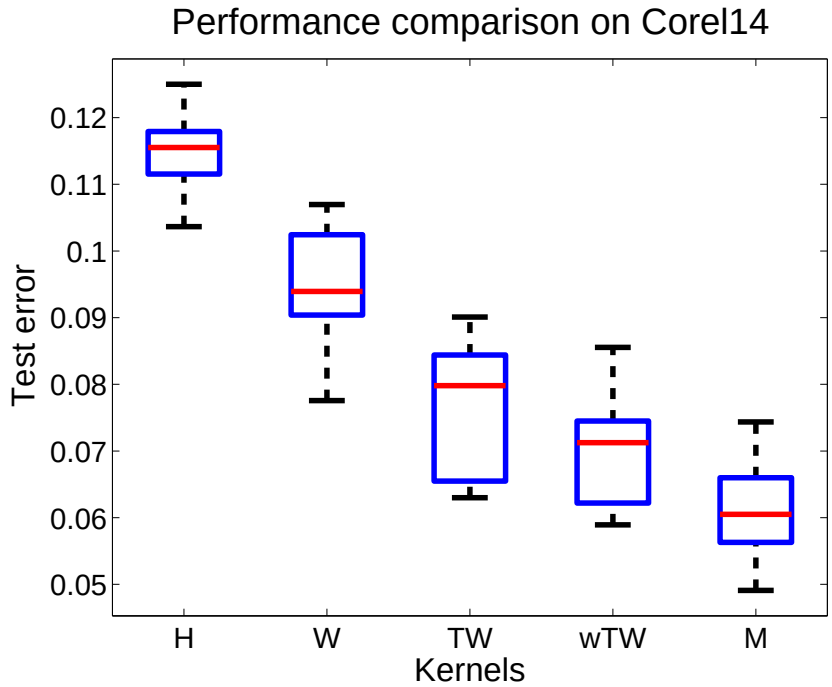


(B) Membrane proteins

Example: 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 by MKL (M).



MKL revisited (Bach et al., 2004)

$$K_\eta = \sum_{i=1}^M \eta_i K_i \quad \text{with} \quad \eta \in \Sigma_M = \left\{ \eta_i \geq 0 \,, \sum_{i=1}^M \eta_i = 1 \right\}$$

Theorem

The solution f^* of

$$\min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|^2_{\mathcal{H}_{K_\eta}} \right\}$$

is $f^* = \sum_{i=1}^M f_i^*$, where $\left(f_1^*, \ldots, f_M^*\right) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^M f_i^n \right) + \lambda \left(\sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}} \right)^2 \right\} .$$

Proof (1/2)

$$\min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|^2_{\mathcal{H}_{K_\eta}} \right\}$$

$$= \min_{\eta \in \Sigma_M} \min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^M f_i^n \right) + \lambda \sum_{i=1}^M \frac{\| f_i \|^2_{\mathcal{H}_{K_i}}}{\eta_i} \right\}$$

$$= \min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^M f_i^n \right) + \lambda \min_{\eta \in \Sigma_M} \left\{ \sum_{i=1}^M \frac{\| f_i \|^2_{\mathcal{H}_{K_i}}}{\eta_i} \right\} \right\}$$

$$= \min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^M f_i^n \right) + \lambda \left(\sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}} \right)^2 \right\},$$

Proof (2/2)

where the last equality results from:

$$\forall a \in \mathbb{R}_+^M, \quad \left(\sum_{i=1}^M a_i \right)^2 = \inf_{\eta \in \Sigma_M} \sum_{i=1}^M \frac{a_i^2}{\eta_i},$$

which is a direct consequence of the Cauchy-Schwarz inequality:

$$\sum_{i=1}^M a_i = \sum_{i=1}^M \frac{a_i}{\sqrt{\eta_i}} \times \sqrt{\eta_i} \leq \left(\sum_{i=1}^M \frac{a_i^2}{\eta_i} \right)^{\frac{1}{2}} \left(\sum_{i=1}^M \eta_i \right)^{\frac{1}{2}}.$$

Algorithm: simpleMKL (Rakotomamonjy et al., 2008)

- We want to minimize in $\eta \in \Sigma_M$:

$$\min_{\eta \in \Sigma_M} J(K_\eta) = \min_{\eta \in \Sigma_M} \max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda \gamma^\top K_\eta \gamma \right\} .$$

- For a fixed $\eta \in \Sigma_M$, we can compute $f(\eta) = J(K_\eta)$ by using a standard solver for a single kernel to find γ^*:

$$J(K_\eta) = -R^*(-2\lambda\gamma^*) - \lambda \gamma^{*\top} K_\eta \gamma^* .$$

- From γ^* we can also compute the gradient of $J(K_\eta)$ with respect to η:

$$\frac{\partial J(K_\eta)}{\partial \eta_i} = -\lambda \gamma^{*\top} K_i \gamma^* .$$

- $J(K_\eta)$ can then be minimized on Σ_M by a projected gradient or reduced gradient algorithm.

Sum kernel vs MKL

- Learning with the sum kernel (uniform combination) solves

$$\min_{f_1,\dots,f_M} \left\{ R\left(\sum_{i=1}^M f_i^n\right) + \lambda \sum_{i=1}^M \| f_i \|^2_{\mathcal{H}_{K_i}} \right\} .$$

- Learning with MKL (best convex combination) solves

$$\min_{f_1,\dots,f_M} \left\{ R\left(\sum_{i=1}^M f_i^n\right) + \lambda \left(\sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}}\right)^2 \right\} .$$

- Although MKL can be thought of as optimizing a convex combination of kernels, it is more correct to think of it as a penalized risk minimization estimator with the group lasso penalty:

$$\Omega(f) = \min_{f_1+\dots+f_M=f} \sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}} .$$

Example: ridge vs LASSO regression

- Take $\mathcal{X} = \mathbb{R}^d$, and for $\mathbf{x} = (x_1, \ldots, x_d)^\top$ consider the rank-1 kernels:

$$\forall i = 1, \ldots, d\,, \quad K_i\left(\mathbf{x}, \mathbf{x}'\right) = x_i x_i'\,.$$

- A function $f_i \in \mathcal{H}_{K_i}$ has the form $f_i\left(\mathbf{x}\right) = \beta_i x_i$, with $\| f_i \|_{\mathcal{H}_{K_i}} = | \beta_i |$
- The sum kernel is $K_S\left(\mathbf{x}, \mathbf{x}'\right) = \sum_{i=1}^d x_i x_i' = \mathbf{x}^\top \mathbf{x}$, a function $\mathcal{H}_{K_S}$ is of the form $f\left(\mathbf{x}\right) = \beta^\top \mathbf{x}$, with norm $\| f \|_{\mathcal{H}_{K_S}} = \| \beta \|_{\mathbb{R}^d}$.
- Learning with the sum kernel solves a ridge regression problem:

$$\min_{\beta \in \mathbb{R}^d} \left\{ R(X\beta) + \lambda \sum_{i=1}^d \beta_i^2 \right\}\,.$$

- Learning with MKL solves a LASSO regression problem:

$$\min_{\beta \in \mathbb{R}^d} \left\{ R(X\beta) + \lambda \left(\sum_{i=1}^d | \beta_i | \right)^2 \right\}\,.$$

Extensions (Micchelli et al., 2005)

$$\text{For } r > 0\,, \quad K_\eta = \sum_{i=1}^M \eta_i K_i \quad \text{with} \quad \eta \in \Sigma_M^r = \left\{ \eta_i \geq 0\,, \sum_{i=1}^M \eta_i^r = 1 \right\}$$

Theorem

The solution f^* of

$$\min_{\eta \in \Sigma_M^r} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|^2_{\mathcal{H}_{K_\eta}} \right\}$$

is $f^* = \sum_{i=1}^M f_i^*$, where $(f_1^*, \ldots, f_M^*) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^M f_i^n \right) + \lambda \left(\sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}}^{\frac{2r}{r+1}} \right)^{\frac{r+1}{r}} \right\}.$$

Kernel methods: Summary

- The kernel trick allows to extend many linear algorithms to non-linear settings and to general data (even non-vectorial).
- The representer theorem shows that that functional optimization over (subsets of) the RKHS is feasible in practice.
- The norm in the RKHS can be used as regularization for empirical risk minimization. This is theoretically justified and leads to efficient algorithms (often finite-dimensional convex problem).
- Various strategies exist for data integration with kernels, such as the sum kernel or MKL.

Part 4

Kernel examples

Introduction

- The kernel plays a critical role in the performance of kernel methods.
- Kernel is the place where prior knowledge about the problem can be inserted, in particular by controlling the norm of functions in the RKHS.
- In this part we provide some intuition about the link between kernels and smoothness functional through several examples.
- Subsequent parts will focus on the design of kernels for particular types of data.

Outline

Mercer kernels

Definition

A kernel K on a set $\mathcal{X}$ is called a Mercer kernel if:

1. $\mathcal{X}$ is a compact metric space (typically, a closed bounded subset of $\mathbb{R}^d$).
2. $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a continuous p.d. kernel (w.r.t. the Borel topology)

Motivations

- We can exhibit an explicit and intuitive feature space for a large class of p.d. kernels
- Historically, provided the first proof that a p.d. kernel is an inner product for non-finite sets $\mathcal{X}$ (Mercer, 1905).
- Can be thought of as the natural generalization of the factorization of positive semidefinite matrices over infinite spaces.

Sketch of the proof

1. The kernel matrix when $\mathcal{X}$ is finite becomes a linear operator when $\mathcal{X}$ is a metric space.
2. The matrix was positive semidefinite in the finite case, the linear operator is self-adjoint and positive in the metric case.
3. The spectral theorem states that any compact linear operator admits a complete orthonormal basis of eigenfunctions, with non-negative eigenvalues (just like positive semidefinite matrices can be diagonalized with nonnegative eigenvalues).
4. The kernel function can then be expanded over basis of eigenfunctions as:

$$K(\mathbf{x}, \mathbf{t}) = \sum_{k=1}^{\infty} \lambda_k \psi_k(\mathbf{x}) \psi_k(\mathbf{t}),$$

where $\lambda_i \geq 0$ are the non-negative eigenvalues.

In case of...

Definition

Let $\mathcal{H}$ be a Hilbert space

- A linear operator is a continuous linear mapping from $\mathcal{H}$ to itself.
- A linear operator L is called compact if, for any bounded sequence $\{f_n\}_{n=1}^{\infty}$, the sequence $\{Lf_n\}_{n=1}^{\infty}$ has a subsequence that converges.
- L is called self-adjoint if, for any $f, g \in \mathcal{H}$:

$$\langle f, Lg \rangle = \langle Lf, g \rangle .$$

- L is called positif if it is self-adjoint and, for any $f \in \mathcal{H}$:

$$\langle f, Lf \rangle \geq 0 .$$

An important lemma

The linear operator

- Let ν be any Borel measure on $\mathcal{X}$, and $L_2^\nu(\mathcal{X})$ the Hilbert space of square integrable functions on $\mathcal{X}$.
- For any function $K : \mathcal{X}^2 \mapsto \mathbb{R}$, let the transform:

$$\forall f \in L_2^\nu(\mathcal{X}), \quad (L_K f)(\mathbf{x}) = \int K(\mathbf{x}, \mathbf{t}) f(\mathbf{t}) \, d\nu(\mathbf{t}).$$

Lemma

If K is a Mercer kernel, then L_K is a compact and bounded linear operator over $L_2^\nu(\mathcal{X})$, self-adjoint and positif.

Proof (1/6)

L_K is a mapping from $L_2^\nu(\mathcal{X})$ to $L_2^\nu(\mathcal{X})$

For any $f \in L_2^\nu(\mathcal{X})$ and $(\mathbf{x}_1, \mathbf{x}_1) \in \mathcal{X}^2$:

$$
\begin{aligned}
|L_K f(\mathbf{x}_1) - L_K f(\mathbf{x}_2)| &= \left| \int (K(\mathbf{x}_1, \mathbf{t}) - K(\mathbf{x}_2, \mathbf{t})) f(\mathbf{t}) \, d\nu(\mathbf{t}) \right| \\
&\leq \| K(\mathbf{x}_1, \cdot) - K(\mathbf{x}_2, \cdot) \| \| f \| \\
&\qquad \text{(Cauchy-Schwarz)} \\
&\leq \sqrt{\nu(\mathcal{X})} \max_{\mathbf{t} \in \mathcal{X}} |K(\mathbf{x}_1, \mathbf{t}) - K(\mathbf{x}_2, \mathbf{t})| \, \| f \|.
\end{aligned}
$$

K being continuous and $\mathcal{X}$ compact, K is uniformly continuous, therefore $L_K f$ is continuous. In particular, $L_K f \in L_2^\nu(\mathcal{X})$ (with the slight abuse of notation $\mathcal{C}(\mathcal{X}) \subset L_2^\nu(\mathcal{X})$). $\square$

Proof (2/6)

L_K is linear and continuous

- Linearity is obvious (by definition of L_K and linearity of the integral).
- For continuity, we observe that for all $f \in L_2^\nu(\mathcal{X})$ and $\mathbf{x} \in \mathcal{X}$:

$$\begin{aligned} |(L_K f)(\mathbf{x})| &= \left| \int K(\mathbf{x}, \mathbf{t}) f(\mathbf{t}) \, d\nu(\mathbf{t}) \right| \\ &\leq \sqrt{\nu(\mathcal{X})} \max_{\mathbf{t} \in \mathcal{X}} |K(\mathbf{x}, \mathbf{t})| \, \|f\| \\ &\leq \sqrt{\nu(\mathcal{X})} C_K \|f\|. \end{aligned}$$

with $C_K = \max_{\mathbf{x},\mathbf{t} \in \mathcal{X}} |K(\mathbf{x}, \mathbf{t})|$. Therefore:

$$\|L_K f\| = \left(\int L_K f(\mathbf{t})^2 \, d\nu(\mathbf{t}) \right)^{\frac{1}{2}} \leq \nu(\mathcal{X}) C_K \|f\|. \quad \square$$

Proof (3/6)

Criterion for compacity

In order to prove the compacity of L_K we need the following criterion.
Let $C(\mathcal{X})$ denote the set of continuous functions on $\mathcal{X}$ endowed with infinite norm $\| f \|_\infty = max_{\mathbf{x} \in \mathcal{X}} | f(\mathbf{x}) |$.
A set of functions $G \subset C(\mathcal{X})$ is called equicontinuous if:

$$\forall \epsilon > 0, \exists \delta > 0, \forall (\mathbf{x}, \mathbf{y}) \in \mathcal{X}^2,$$
$$\| \mathbf{x} - \mathbf{y} \| < \delta \implies \forall g \in G, | g(\mathbf{x}) - g(\mathbf{y}) | < \epsilon.$$

Ascoli Theorem

A part $H \subset C(\mathcal{X})$ is relatively compact (i.e., its closure is compact) if and only if it is uniformly bounded and equicontinuous.

Proof (4/6)

L_K is compact

Let $(f_n)_{n\geq 0}$ be a bounded sequence of $L_2^\nu(\mathcal{X})$ ($\| f_n \| < M$ for all n). The sequence $(L_K f_n)_{n\geq 0}$ is a sequence of continuous functions, uniformly bounded because:

$$\| L_K f \|_\infty \leq \sqrt{\nu(\mathcal{X})} C_K \| f \| \leq \sqrt{\nu(\mathcal{X})} C_K M .$$

It is equicontinuous because:

$$| L_K f_n(\mathbf{x}_1) - L_K f_n(\mathbf{x}_2) | \leq \sqrt{\nu(\mathcal{X})} \max_{\mathbf{t}\in\mathcal{X}} | K(\mathbf{x}_1, \mathbf{t}) - K(\mathbf{x}_2, \mathbf{t}) | M .$$

By Ascoli theorem, we can extract a sequence uniformly convergent in $C(\mathcal{X})$, and therefore in $L_2^\nu(\mathcal{X})$. $\square$

Proof (5/6)

L_K is self-adjoint

K being symmetric, we have for all $f, g \in \mathcal{H}$:

$$\begin{aligned}
\langle f, Lg \rangle &= \int f(\mathbf{x}) (Lg)(\mathbf{x}) \nu(d\mathbf{x}) \\
&= \int \int f(\mathbf{x}) g(\mathbf{t}) K(\mathbf{x}, \mathbf{t}) \nu(d\mathbf{x}) \nu(d\mathbf{t}) \quad \text{(Fubini)} \\
&= \langle Lf, g \rangle .
\end{aligned}$$

Proof (6/6)

L_K is positif

We can approximate the integral by finite sums:

$$\begin{aligned}\langle f, Lf \rangle &= \int \int f(\mathbf{x}) f(\mathbf{t}) K(\mathbf{x}, \mathbf{t}) \nu(d\mathbf{x}) \nu(d\mathbf{t}) \\ &= \lim_{k \to \infty} \frac{\nu(\mathcal{X})}{k^2} \sum_{i,j=1}^{k} K(\mathbf{x}_i, \mathbf{x}_j) f(\mathbf{x}_i) f(\mathbf{x}_j) \\ &\geq 0 ,\end{aligned}$$

because K is positive definite. $\square$

Diagonalization of the operator

We need the following general result:

Spectral theorem

Let L be a compact linear operator on a Hilbert space $\mathcal{H}$. Then there exists in $\mathcal{H}$ a complete orthonormal system $(\psi_1, \psi_2, \ldots)$ of eigenvectors of L. The eigenvalues $(\lambda_1, \lambda_2, \ldots)$ are real if L is self-adjoint, and non-negative if L is positive.

Remark

This theorem can be applied to L_K. In that case the eigenfunctions ϕ_k associated to the eigenfunctions $\lambda_k \neq 0$ can be considered as continuous functions, because:

$$\psi_k = \frac{1}{\lambda_k} L\psi_K \,.$$

Main result

Mercer Theorem

Let $\mathcal{X}$ be a compact metric space, ν a Borel measure on $\mathcal{X}$, and K a continuous p.d. kernel. Let $(\lambda_1, \lambda_2, \ldots)$ denote the nonnegative eigenvalues of L_K and $(\psi_1, \psi_2, \ldots)$ the corresponding eigenfunctions. Then all ψ_k are continuous functions, and for any $\mathbf{x}, \mathbf{t} \in \mathcal{X}$:

$$K(\mathbf{x}, \mathbf{t}) = \sum_{k=1}^{\infty} \lambda_k \psi_k(\mathbf{x}) \psi_k(\mathbf{t}),$$

where the convergence is absolute for each $\mathbf{x}, \mathbf{t} \in \mathcal{X}$, and uniform on $\mathcal{X} \times \mathcal{X}$.

Mercer kernels as inner products

Corollary

The mapping

$$\begin{aligned} \Phi : \mathcal{X} &\mapsto l^2 \\ \mathbf{x} &\mapsto \left(\sqrt{\lambda_k} \psi_k (\mathbf{x}) \right)_{k \in \mathbb{N}} \end{aligned}$$

is well defined, continuous, and satisfies

$$K(\mathbf{x}, \mathbf{t}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{t}) \rangle_{l^2} \ .$$

Proof of the corollary

Proof

By Mercer theorem we see that for all $\mathbf{x} \in \mathcal{X}$, $\sum \lambda_k \psi_k^2(\mathbf{x})$ converges to $K(\mathbf{x}, \mathbf{x}) < \infty$, therefore $\Phi(\mathbf{x}) \in l^2$.
The continuity of Φ results from:

$$\begin{aligned} \| \Phi(\mathbf{x}) - \Phi(\mathbf{t}) \|_{l^2}^2 &= \sum_{k=1}^{\infty} \lambda_k \left(\psi_k(\mathbf{x}) - \psi_k(\mathbf{t}) \right)^2 \\ &= K(\mathbf{x}, \mathbf{x}) + K(\mathbf{t}, \mathbf{t}) - 2K(\mathbf{x}, \mathbf{t}) \end{aligned}$$

Summary

- This proof extends the proof valid when $\mathcal{X}$ is finite.
- This is a constructive proof, developed by Mercer (1905).
- Compacity and continuity are required.

RKHS of Mercer kernels

- Let $\mathcal{X}$ be a compact metric space, and K a Mercer kernel on $\mathcal{X}$ (symmetric, continuous and positive definite).
- We have expressed a decomposition of the kernel in terms of the eigenfunctions of the linear convolution operator.
- In some cases this provides an intuitive feature space.
- The kernel also has a RKHS, like any p.d. kernel.
- Can we get an intuition of the RKHS norm in terms of the eigenfunctions and eigenvalues of the convolution operator?

Reminder: expansion of Mercer kernel

Theorem

Denote by L_K the linear operator of $L_2^\nu(\mathcal{X})$ defined by:

$$\forall f \in L_2^\nu(\mathcal{X}), (L_K f)(\mathbf{x}) = \int K(\mathbf{x}, \mathbf{t}) f(\mathbf{t}) d\nu(\mathbf{t}).$$

Let $(\lambda_1, \lambda_2, \ldots)$ denote the eigenvalues of L_K in decreasing order, and $(\psi_1, \psi_2, \ldots)$ the corresponding eigenfunctions. Then it holds that for any $\mathbf{x}, \mathbf{y} \in \mathcal{X}$:

$$K(\mathbf{x}, \mathbf{y}) = \sum_{k=1}^{\infty} \lambda_k \psi_k(\mathbf{x}) \psi_k(\mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{l^2},$$

with $\Phi : \mathcal{X} \mapsto l^2$ defined par $\Phi(\mathbf{x}) = \left(\sqrt{\lambda_k}\psi_k(\mathbf{x})\right)_{k \in \mathbb{N}}$.

RKHS construction

Theorem

Assuming that all eigenvalues are positive, the RKHS is the Hilbert space:

$$H_K = \left\{ f \in L_2^\nu(\mathcal{X}) : f = \sum_{i=1}^{\infty} a_i \psi_i, \quad \text{with} \sum_{k=1}^{\infty} \frac{a_k^2}{\lambda_k} < \infty \right\}$$

endowed with the inner product:

$$\langle f, g \rangle_K = \sum_{k=1}^{\infty} \frac{a_k b_k}{\lambda_k}, \quad \text{for } f = \sum_k a_k \psi_k, g = \sum_k b_k \psi_k.$$

Remark

If some eigenvalues are equal to zero, then the result and the proof remain valid on the subspace spanned by the eigenfunctions with positive eigenvalues.

Proof (1/6)

Sketch

In order to show that H_K is the RKHS of the kernel K we need to show that:

1. it is a Hilbert space of functions from $\mathcal{X}$ to $\mathbb{R}$,
2. for any $\mathbf{x} \in \mathcal{X}$, $K_x \in H_K$,
3. for any $\mathbf{x} \in \mathcal{X}$ and $f \in H_K$, $f(\mathbf{x}) = \langle f, K_x \rangle_{H_K}$.

Proof (2/6)

H_K is a Hilbert space

Indeed the function:

$$
\begin{aligned}
L_K^{\frac{1}{2}} : & L_2^\nu(\mathcal{X}) \to H_K \\
& \sum_{i=1}^{\infty} a_i \psi_i \mapsto \sum_{i=1}^{\infty} a_i \sqrt{\lambda_i} \psi_i
\end{aligned}
$$

is an isomorphism, therefore H_K is a Hilbert space, like $L_2^\nu(\mathcal{X})$. $\square$

Proof (3/6)

H_K is a space of continuous functions

For any $f = \sum_{i=1}^{\infty} a_i \psi_i \in H_K$, and $\mathbf{x} \in \mathcal{X}$, we have (if $f(x)$ makes sense):

$$
\begin{aligned}
|f(\mathbf{x})| &= \left| \sum_{i=1}^{\infty} a_i \psi_i(\mathbf{x}) \right| = \left| \sum_{i=1}^{\infty} \frac{a_i}{\sqrt{\lambda_i}} \sqrt{\lambda_i} \psi_i(\mathbf{x}) \right| \\
&\leq \left(\sum_{i=1}^{\infty} \frac{a_i^2}{\lambda_i} \right)^{\frac{1}{2}} \cdot \left(\sum_{i=1}^{\infty} \lambda_i \psi_i(\mathbf{x})^2 \right)^{\frac{1}{2}} \\
&= \|f\|_{H_K} K(\mathbf{x}, \mathbf{x})^{\frac{1}{2}} \\
&= \|f\|_{H_K} \sqrt{C_K} \,.
\end{aligned}
$$

Therefore convergence in $\|.\|_{H_K}$ implies uniform convergence for functions.

Proof (4/6)

H_K is a space of continuous functions (cont.)

Let now $f_n = \sum_{i=1}^n a_i \psi_i \in H_K$. The functions ψ_i are continuous functions, therefore f_n is also continuous, for all n. The f_n's are convergent in H_K, therefore also in the (complete) space of continuous functions endowed with the uniform norm.
Let f_c the continuous limit function. Then $f_c \in L_2^\nu(\mathcal{X})$ and

$$\| f_n - f_c \|_{L_2^\nu(\mathcal{X})} \underset{n \to \infty}{\to} 0.$$

On the other hand,

$$\| f - f_n \|_{L_2^\nu(\mathcal{X})} \leq \lambda_1 \| f - f_n \|_{H_K} \underset{n \to \infty}{\to} 0,$$

therefore $f = f_c$. $\square$

Proof (5/6)

$K_x \in H_K$

For any $\mathbf{x} \in \mathcal{X}$ let, for all i, $a_i = \lambda_i \psi_i(\mathbf{x})$. We have:

$$\sum_{i=1}^{\infty} \frac{a_i^2}{\lambda_i} = \sum_{i=1}^{\infty} \lambda_i \psi_i(\mathbf{x})^2 = K(\mathbf{x}, \mathbf{x}) < \infty,$$

therefore $\phi_x := \sum_{i=1}^{\infty} a_i \psi_i \in H_K$. As seen earlier the convergence in H_K implies pointwise convergence, therefore for any $\mathbf{t} \in \mathcal{X}$:

$$\phi_x(\mathbf{t}) = \sum_{i=1}^{\infty} a_i \psi_i(\mathbf{t}) = \sum_{i=1}^{\infty} \lambda_i \psi_i(\mathbf{x}) \psi_i(\mathbf{t}) = K(\mathbf{x}, \mathbf{t}),$$

therefore $\phi_x = K_x \in H_K$. $\square$

Proof (6/6)

$f(\mathbf{x}) = \langle f, K_x \rangle_{H_K}$

Let $f = \sum_{i=1}^{\infty} a_i \psi_i \in H_K$, et $\mathbf{x} \in \mathcal{X}$. We have seen that:

$$K_x = \sum_{i=1}^{\infty} \lambda_i \psi_i(\mathbf{x}) \psi_i ,$$

therefore:

$$\langle f, K_x \rangle_{H_K} = \sum_{i=1}^{\infty} \frac{\lambda_i \psi_i(\mathbf{x}) a_i}{\lambda_i} = \sum_{i=1}^{\infty} a_i \psi_i(\mathbf{x}) = f(\mathbf{x}) ,$$

which concludes the proof. $\square$

Remarks

- Although H_K was built from the eigenfunctions of L_K, which depend on the choice of the measure $\nu(\mathbf{x})$, we know by unicity of the RKHS that H_K is independant of ν and L_K.
- Mercer theorem provides a concrete way to build the RKHS, by taking linear combinations of the eigenfunctions of L_K (with adequately chosen weights).
- The eigenfunctions $(\psi_i)_{i\in\mathbb{N}}$ form an orthogonal basis of the RKHS:

$$\langle \psi_i, \psi_j \rangle_{H_K} = 0 \quad \text{si } i \neq j, \quad \| \psi_i \|_{H_K} = \frac{1}{\sqrt{\lambda_i}}.$$

The RKHS is a well-defined ellipsoid with axes given by the eigenfunctions.

Outline

Motivations

- The RKHS norm is related to the smoothness of functions.
- Smoothness of a function is naturally quantified by Sobolev norms (in particular L_2 norms of derivatives).
- In this section we make a general link between RKHS and Green functions defined by differential operators.

A simple example

Explicit choice of smoothness

Let

$$\mathcal{H} = \left\{ f : [0,1] \mapsto \mathbb{R}, \text{absolutely continuous}, f' \in L^2([0,1]), f(0) = 0 \right\} .$$

endowed with the bilinear form:

$$\forall (f,g) \in \mathcal{F}^2 \, \langle f, g \rangle_{\mathcal{H}} = \int_0^1 f'(u) \, g'(u) \, du .$$

Note that $\langle f, f \rangle_{\mathcal{H}}$ measures the smoothness of f:

$$\langle f, f \rangle_{\mathcal{H}} = \int_0^1 f'(u)^2 \, du = \| f' \|^2_{L^2([0,1])} .$$

The RKHs point of view

Theorem

$\mathcal{H}$ is a RKHS with r.k. given by:

$$\forall (x, y) \in [0, 1]^2, \quad K(x, y) = \min(x, y).$$

Remark

Therefore, $\| f \|_{\mathcal{H}} = \| f' \|_{L^2}$: the RKHS norm is precisely the smoothness functional defined in the simple example.

Proof (1/3)

Sketch

We need to show that

- $\mathcal{H}$ is a Hilbert space
- $\forall x \in [0,1]$, $K_x \in \mathcal{H}$,
- $\forall (x, f) \in [0,1] \times \mathcal{H}, \langle f, K_x \rangle_{\mathcal{H}} = f(x)$.

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Proof (2/3)

$\mathcal{H}$ is a pre-Hilbert space

- f absolutely continuous implies differentiable almost everywhere, and

$$\forall x \in [0,1], \quad f(x) = f(0) + \int_0^x f'(u)du\,.$$

- For any $f \in \mathcal{H}$, $f(0) = 0$ implies by Cauchy-Schwarz:

$$|\,f\,(x)\,| = \left| \int_0^x f'(u)du \right| \leq \sqrt{x} \left(\int_0^1 f'(u)^2 du \right)^{\frac{1}{2}} = \sqrt{x} \| f \|_{\mathcal{H}}\,.$$

Therefore, $\| f \|_{\mathcal{H}} = 0 \implies f = 0$, showing that $\langle ., . \rangle_{\mathcal{H}}$ is an inner product. $\mathcal{H}$ is thus a pre-Hilbert space.

Proof (2/3)

$\mathcal{H}$ is a Hilbert space

- To show that $\mathcal{H}$ is complete, let $(f_n)_{n\in\mathbb{N}}$ a Cauchy sequence in $\mathcal{H}$
- $(f_n')_{n\in\mathbb{N}}$ is a Cauchy sequence in $L^2[0,1]$, thus converges to $g \in L^2[0,1]$
- By the previous inequality, $(f_n(x))_{n\in\mathbb{N}}$ is a Cauchy sequence and thus converges to a real number $f(x)$, for any $x \in [0,1]$. Moreover:

$$f(x) = \lim_n f_n(x) = \lim_n \int_0^x f_n'(u)du = \int_0^x g(u)du\,,$$

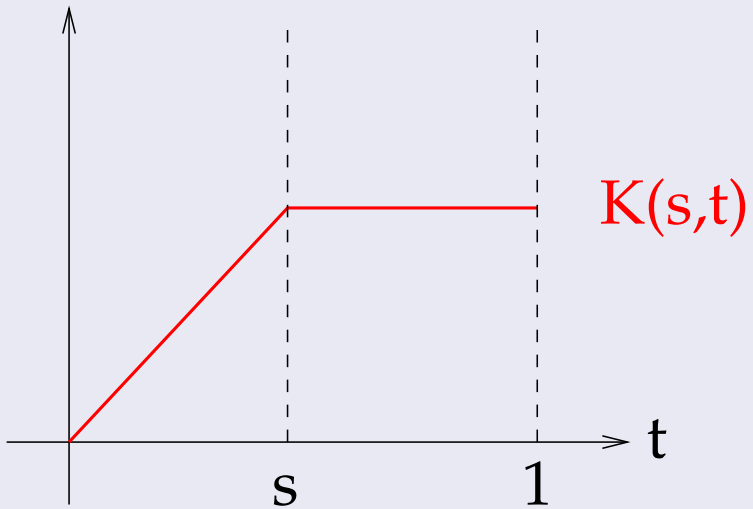
  showing that f is absolutely continuous and $f' = g$ almost everywhere; in particular, $f' \in L^2[0,1]$.
- Finally, $f(0) = \lim_n f_n(0) = 0$, therefore $f \in \mathcal{H}$ and

$$\lim_n \| f_n - f \|_{\mathcal{H}} = \| f' - g_n \|_{L^2[0,1]} = 0\,.$$

Proof (2/3)

$\forall x \in [0,1], K_x \in \mathcal{H}$

Let $K_x(y) = K(x,y) = \min(x,y)$ sur $[0,1]^2$:



K_x is differentiable except at s, has a square integrable derivative, and $K_x(0) = 0$, therefore $K_x \in \mathcal{H}$ for all $x \in [0,1]$. $\square$

Proof (3/3)

For all $x, f, \langle f, K_x \rangle_{\mathcal{H}} = f(x)$

For any $x \in [0,1]$ and $f \in \mathcal{H}$ we have:

$$\langle f, K_x \rangle_{\mathcal{H}} = \int_0^1 f'(u) K_x'(u) du = \int_0^x f'(u) du = f(x),$$

which shows that K is the r.k. associated to $\mathcal{H}$. $\square$

Generalization

Theorem

Let $\mathcal{X} = \mathbb{R}^d$ and D a differential operator on a class of functions $\mathcal{H}$ such that, endowed with the inner product:

$$\forall (f, g) \in \mathcal{H}^2, \quad \langle f, g \rangle_{\mathcal{H}} = \langle Df, Dg \rangle_{L^2(\mathcal{X})} ,$$

it is a Hilbert space.
Then $\mathcal{H}$ is a RKHS that admits as r.k. the Green function of the operator $D^* D$, where D^* denotes the adjoint operator of D.

In case of...

Green functions

Let the differential equation on $\mathcal{H}$:

$$f = Dg\,,$$

where g is unknown. In order to solve it we can look for g of the form:

$$g(x) = \int_{\mathcal{X}} k(x,y)\, f(y)\, dy$$

for some function $k : \mathcal{X}^2 \mapsto \mathbb{R}$. k must then satisfy, for all $x \in \mathcal{X}$,

$$f(x) = Dg(x) = \langle Dk_x, f \rangle_{L^2(\mathcal{X})}\,.$$

k is called the Green function of the operator D.

Proof

Let $\mathcal{H}$ be a Hilbert space endowed with the inner product:

$$\langle f, g \rangle_{\mathcal{X}} = \langle Df, Dg \rangle_{L^2(\mathcal{X})} \ ,$$

and K be the Green function of the operator D^*D. For all $x \in \mathcal{X}$, $K_x \in \mathcal{H}$ because:

$$\langle DK_x, DK_x \rangle_{L^2(\mathcal{X})} = \langle D^*DK_x, K_x \rangle_{L^2(\mathcal{X})} = K_x(x) < \infty \, .$$

Moreover, for all $f \in \mathcal{H}$ and $x \in \mathcal{X}$, we have:

$$f(x) = \langle D^*DK_x, f \rangle_{L^2(\mathcal{X})} = \langle DK_x, Df \rangle_{L^2(\mathcal{X})} = \langle K_x, f \rangle_{\mathcal{H}} \ ,$$

which shows that $\mathcal{H}$ is a RKHS with K as r.k. $\square$

Outline

Motivation

- Let us suppose that $\mathcal{X}$ is not compact, for example $\mathcal{X} = \mathbb{R}^d$.
- In that case, the eigenvalues of:

$$\int_{\mathcal{X}} K(\mathbf{x}, \mathbf{t}) \psi(\mathbf{t}) = \lambda \psi(\mathbf{t})$$

  are not necessarily countable, Mercer theorem does not hold.
- Fourier transforms provide a convenient extension for translation invariant kernels, i.e., kernels of the form $K(\mathbf{x}, \mathbf{y}) = \kappa(\mathbf{x} - \mathbf{y})$.
- Harmonic analysis also bring kernels well beyond vector spaces (e.g., groups and semigroups), a topic that we will barely touch upon in this course.

In case of...

Definition

Let $f \in L^1\left(\mathbb{R}^d\right)$. The Fourier transform of f, denoted $\hat{f}$ or $\mathcal{F}[f]$, the function defined for all $\omega \in \mathbb{R}^d$ by:

$$\hat{f}(\omega) = \int_{\mathbb{R}^d} e^{-ix.\omega} f(x)\, dx\,.$$

In case of...

Properties

- $\hat{f}$ is complex-valued, continuous, tends to 0 at infinity and $\| \hat{f} \|_{L^\infty} \leq \| f \|_{L^1}$.
- If $\hat{f} \in L^1\left(\mathbb{R}^d\right)$, then the inverse Fourier formula holds:

$$\forall x \in \mathbb{R}^d, \quad f(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{ix.\omega} \hat{f}(\omega) \, d\omega.$$

- If $f \in L^1\left(\mathbb{R}^d\right)$ is square integrable, then Parseval's formula holds:

$$\int_{\mathbb{R}^d} |f(x)|^2 \, dx = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left| \hat{f}(\omega) \right|^2 d\omega \, .$$

Translation invariant kernels

Definition

A kernel $K : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}$ is called translation invariant (t.i.) if it only depends on the difference between its argument, i.e.:

$$\forall (x, y) \in \mathbb{R}^{2d}, \quad K(x, y) = \kappa(x - y).$$

Intuition

If K is t.i. and $\kappa \in L^1\left(\mathbb{R}^d\right)$, then

$$\begin{aligned} \kappa(x - y) &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{i(x-y).\omega} \hat{\kappa}(\omega) \, d\omega \\ &= \int_{\mathbb{R}^d} \frac{\hat{\kappa}(\omega)}{(2\pi)^d} e^{i\omega(x)} e^{i\omega(-y)} d\omega . \end{aligned}$$

RKHS of translation invariant kernels

Theorem

Let K be a translation invariant p.d. kernel, such that κ is integrable on $\mathbb{R}^d$ as well as its Fourier transform $\hat{\kappa}$. The subset $\mathcal{H}_K$ of $L_2\left(\mathbb{R}^d\right)$ that consists of integrable and continuous functions f such that:

$$\| f \|_K^2 := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\left| \hat{f}(\omega) \right|^2}{\hat{\kappa}(\omega)} d\omega < +\infty \,,$$

endowed with the inner product:

$$\langle f, g \rangle := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\hat{f}(\omega) \hat{g}(\omega)^*}{\hat{\kappa}(\omega)} d\omega$$

is a RKHS with K as r.k.

Proof

For $x \in \mathbb{R}^d$, $K_x(y) = K(x,y) = \kappa(x-y)$ therefore:

$$\hat{K}_x(\omega) = \int e^{-i\omega.u} \kappa(u-x) du = e^{-i\omega.x} \hat{\kappa}(\omega)\,.$$

This leads to $K_x \in \mathcal{H}$, because:

$$\int_{\mathbb{R}^d} \frac{\left|\hat{K}_x(\omega)\right|^2}{\hat{\kappa}(\omega)} \leq \int_{\mathbb{R}^d} |\,\hat{\kappa}(\omega)\,| < \infty,$$

Moreover, if $f \in \mathcal{H}$ and $x \in \mathbb{R}^d$, we have:

$$\langle f, K_x \rangle_{\mathcal{H}} = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\hat{K}_x(\omega)\hat{f}\,(\omega)^*}{\hat{\kappa}(\omega)} d\omega = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \hat{f}\,(\omega)^*\, e^{-i\omega.x} = f(x) \qquad \square$$

Application: characterization of p.d. t.i. kernels

Theorem (Bochner)

A real-valued continuous function $\kappa(x - y)$ on $\mathbb{R}^d$ is positive definite if and only if it is the Fourier-Stieltjes transform of a symmetric, positive, and finite Borel measure.

Example

Gaussian kernel

$$K(x,y) = e^{-\frac{(x-y)^2}{2\sigma^2}}$$

corresponds to:

$$\hat{\kappa}(\omega) = e^{-\frac{\sigma^2\omega^2}{2}}$$

and

$$\mathcal{H} = \left\{ f : \int \left| \hat{f}(\omega) \right|^2 e^{\frac{\sigma^2\omega^2}{2}} d\omega < \infty \right\}.$$

In particular, all functions in $\mathcal{H}$ are infinitely differentiable with all derivatives in L^2.

Example

Laplace kernel

$$K(x,y) = \frac{1}{2} e^{-\gamma|x-y|}$$

corresponds to:

$$\hat{\kappa}(\omega) = \frac{\gamma}{\gamma^2 + \omega^2}$$

and

$$\mathcal{H} = \left\{ f : \int \left| \hat{f}(\omega) \right|^2 \frac{\left(\gamma^2 + \omega^2\right)}{\gamma} d\omega < \infty \right\},$$

the set of functions L^2 differentiable with derivatives in L^2 (Sobolev norm).

Example

Low-frequency filter

$$K(x,y) = \frac{\sin(\Omega(x-y))}{\pi(x-y)}$$

corresponds to:

$$\hat{\kappa}(\omega) = U(\omega+\Omega) - U(\omega-\Omega)$$

and

$$\mathcal{H} = \left\{ f : \int_{|\omega|>\Omega} \left| \hat{f}(\omega) \right|^2 d\omega = 0 \right\},$$

the set of functions whose spectrum is included in $[-\Omega, \Omega]$.

Generalization to semigroups (cf Berg et al., 1983)

Definition

- A semigroup $(S, \circ)$ is a nonempty set S equipped with an associative composition $\circ$ and a neutral element e.
- A semigroup with involution $(S, \circ, *)$ is a semigroup $(S, \circ)$ together with a mapping $* : S \to S$ called involution satisfying:
  1. $(s \circ t)^* = t^* \circ s^*$, for $s, t \in S$.
  2. $(s^*)^* = s$ for $s \in S$.

Examples

- Any group $(G, \circ)$ is a semigroup with involution when we define $s^* = s^{-1}$.
- Any abelian semigroup $(S, +)$ is a semigroup with involution when we define $s^* = s$, the identical involution.

Positive definite functions on semigroups

Definition

Let $(S, \circ, *)$ be a semigroup with involution. A function $\phi : S \to \mathbb{R}$ is called positive definite if the function:

$$\forall s, t \in S, \quad K(s,t) = \phi(s^* \circ t)$$

is a p.d. kernel on S.

Example: translation invariant kernels

$\left(\mathbb{R}^d, +, -\right)$ is an abelian group with involution. A function $\phi : \mathbb{R}^d \to \mathbb{R}$ is p.d. if the function

$$K(x,y) = \phi(x-y)$$

is p.d. on $\mathbb{R}^d$ (translation invariant kernels).

Semicharacters

Definition

A funtion $\rho : S \to \mathbb{C}$ on an abelian semigroup with involution $(S, +, *)$ is called a semicharacter if

1. $\rho(0) = 1$,
2. $\rho(s + t) = \rho(s)\rho(t)$ for $s, t \in S$,
3. $\rho(s^*) = \overline{\rho(s)}$ for $s \in S$.

The set of semicharacters on S is denoted by S^*.

Remarks

- If $*$ is the identity, a semicharacter is automatically real-valued.
- If $(S, +)$ is an abelian group and $s^* = -s$, a semicharacter has its values in the circle group $\{z \in \mathbb{C} \,|\, |z| = 1\}$ and is a group character.

Semicharacters are p.d.

Lemma

Every semicharacter is p.d., in the sense that:

- $K(s,t) = \overline{K(t,s)}$,
- $\sum_{i,j=1}^{n} a_i \overline{a_j} K(x_i, x_j) \geq 0$.

Proof

Direct from definition, e.g.,

$$\sum_{i,j=1}^{n} a_i \overline{a_j} \rho\left(x_i + x_j^*\right) = \sum_{i,j=1}^{n} a_i \overline{a_j} \rho\left(x_i\right) \overline{\rho\left(x_j\right)} \geq 0\,.$$

Examples

- $\phi(t) = e^{\beta t}$ on $(\mathbb{R}, +, Id)$.
- $\phi(t) = e^{i\omega t}$ on $(\mathbb{R}, +, -)$.

Integral representation of p.d. functions

Definition

- An function $\alpha : S \to \mathbb{R}$ on a semigroup with involution is called an absolute value if (i) $\alpha(e) = 1$, (ii)$\alpha(s \circ t) \leq \alpha(s)\alpha(t)$, and (iii) $\alpha(s^*) = \alpha(s)$.
- A function $f : S \to \mathbb{R}$ is called exponentially bounded if there exists an absolute value α and a constant $C > 0$ s.t. $|f(s)| \leq C\alpha(s)$ for $s \in S$.

Theorem

Let $(S, +, *)$ an abelian semigroup with involution. A function $\phi : S \to \mathbb{R}$ is p.d. and exponentially bounded (resp. bounded) if and only if it has a representation of the form:

$$\phi(s) = \int_{S^*} \rho(s) d\mu(\rho) \,.$$

where μ is a Radon measure with compact support on S^* (resp. on $\hat{S}$, the set of bounded semicharacters).

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Proof

Sketch (details in Berg et al., 1983, Theorem 4.2.5)

- For an absolute value α, the set P_1^α of α-bounded p.d. functions that satisfy $\phi(0) = 1$ is a compact convex set whose extreme points are precisely the α-bounded semicharacters.
- If ϕ is p.d. and exponentially bounded then there exists an absolute value α such that $\phi(0)^{-1}\phi \in P_1^\alpha$.
- By the Krein-Milman theorem there exits a Radon probability measure on P_1^α having $\phi(0)^{-1}\phi$ as barycentre.

Remarks

- The result is not true without the assumption of exponentially bounded semicharacters.
- In the case of abelian groups with $s^* = -s$ this reduces to Bochner's theorem for discrete abelian groups, cf. Rudin (1962).

Example 1: $(R_+, +, Id)$

Semicharacters

- $S = (\mathbb{R}_+, +, Id)$ is an abelian semigroup.
- P.d. functions are nonnegative, because $\phi(x) = \phi\left(\sqrt{x}\right)^2$.
- The set of bounded semicharacters is exactly the set of functions:

$$s \in \mathbb{R}_+ \mapsto \rho_a(s) = e^{-as},$$

  for $a \in [0, +\infty]$ (left as exercice).
- Non-bounded semicharacters are more difficult to characterize; in fact there exist nonmeasurable solutions of the equation $h(x+y) = h(x)h(y)$.

Example 1: $(R_+, +, Id)$ (cont.)

P.d. functions

- By the integral representation theorem for bounded semi-characters we obtain that a function $\phi : \mathbb{R}_+ \to \mathbb{R}$ is p.d. and bounded if and only if it has the form:

$$\phi(s) = \int_0^\infty e^{-as} d\mu(a) + b\rho_\infty(s)$$

  where $\mu \in \mathcal{M}_+^b(\mathbb{R}_+)$ and $b \geq 0$.
- The first term is the Laplace transform of μ. ϕ is p.d., bounded and continuous iff it is the Laplace transform of a measure in $\mathcal{M}_+^b(\mathbb{R})$.

Example 2: Semigroup kernels for finite measures (1/6)

Setting

- We assume that data to be processed are "bags-of-points", i.e., sets of points (with repeats) of a space $\mathcal{U}$.
- Example : a finite-length string as a set of k-mers.
- How to define a p.d. kernel between any two bags that only depends on the union of the bags?
- See details and proofs in Cuturi et al. (2005).

Example 2: Semigroup kernels for finite measures (2/6)

Semigroup of bounded measures

- We can represent any bag-of-point $\mathbf{x}$ as a finite measure on $\mathcal{U}$:

$$\mathbf{x} = \sum_i a_i \delta_{x_i} \,,$$

  where a_i is the number of occurrences on $\mathbf{x}_i$ in the bag.
- The measure that represents the union of two bags is the sum of the measures that represent each individual bag.
- This suggests to look at the semigroup $\left(\mathcal{M}_+^b(\mathcal{U}), +, Id\right)$ of bounded Radon measures on $\mathcal{U}$ and to search for p.d. functions ϕ on this semigroup.

Example 2: Semigroup kernels for finite measures (3/6)

Semicharacters

- For any Borel measurable function $f : \mathcal{U} \to \mathbb{R}$ the function $\rho_f : \mathcal{M}_+^b(\mathcal{U}) \to \mathbb{R}$ defined by:

$$\rho_f(\mu) = e^{\mu[f]}$$

  is a semicharacter on $\left(\mathcal{M}_+^b(\mathcal{U}), +\right)$.
- Conversely, ρ is continuous semicharacter (for the topology of weak convergence) if and only if there exists a continuous function $f : \mathcal{U} \to \mathbb{R}$ such that $\rho = \rho_f$.
- No such characterization for non-continuous characters, even bounded.

Example 2: Semigroup kernels for finite measures (4/6)

Corollary

Let $\mathcal{U}$ be a Hausdorff space. For any Radon measure $\mu \in \mathcal{M}_+^c\left(C\left(\mathcal{U}\right)\right)$ with compact support on the Hausdorff space of continuous real-valued functions on $\mathcal{U}$ endowed with the topology of pointwise convergence, the following function K is a continuous p.d. kernel on $\mathcal{M}_+^b\left(\mathcal{U}\right)$ (endowed with the topology of weak convergence):

$$K(\mu,\nu) = \int_{C(\mathcal{X})} e^{\mu[f]+\nu[f]} d\mu(f)\,.$$

Remarks

The converse is not true: there exist continuous p.d. kernels that do not have this integral representation (it might include non-continuous semicharacters)

Example 2: Semigroup kernels for finite measures (5/6)

Example : entropy kernel

- Let $\mathcal{X}$ be the set of probability densities (w.r.t. some reference measure) on $\mathcal{U}$ with finite entropy:

$$h(\mathbf{x}) = -\int_{\mathcal{U}} \mathbf{x} \ln \mathbf{x} \, .$$

- Then the following entropy kernel is a p.d. kernel on $\mathcal{X}$ for all $\beta > 0$:

$$K\left(\mathbf{x}, \mathbf{x}'\right) = e^{-\beta h\left(\frac{\mathbf{x}+\mathbf{x}}{2}\right)} \, .$$

- Remark: only valid for densities (e.g., for a kernel density estimator from a bag-of-parts)

Example 2: Semigroup kernels for finite measures (6/6)

Examples : inverse generalized variance kernel

- Let $\mathcal{U} = \mathbb{R}^d$ and $\mathcal{M}_+^V(\mathcal{U})$ be the set of finite measure μ with second order moment and non-singular variance

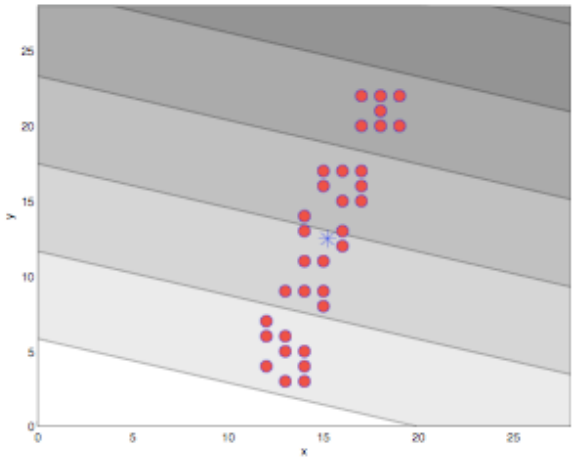
$$\Sigma(\mu) = \mu\left[xx^\top\right] - \mu[x]\,\mu[x]^\top \ .$$

- Then the following function is a p.d. kernel on $\mathcal{M}_+^V(\mathcal{U})$, called the inverse generalized variance kernel:

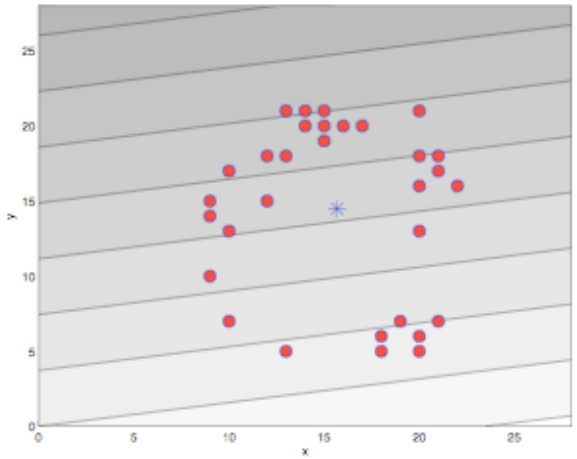
$$K\left(\mu, \mu'\right) = \frac{1}{\det \Sigma\left(\frac{\mu+\mu'}{2}\right)} \ .$$

- Generalization possible with regularization and kernel trick.

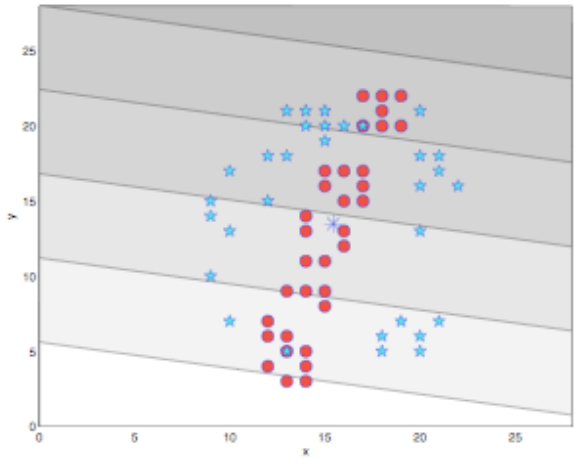
Application of semigroup kernel



$$\Sigma_{1,1} = 0.0552$$
$$\Sigma_{2,2} = 0.0013$$



$$\Sigma'_{1,1} = 0.0441$$
$$\Sigma'_{2,2} = 0.0237$$



$$\Sigma''_{1,1} = 0.0497$$
$$\Sigma''_{2,2} = 0.0139$$

Weighted linear PCA of two different measures, with the first PC shown. Variances captured by the first and second PC are shown. The generalized variance kernel is the inverse of the product of the two values.

Kernelization of the IGV kernel

Motivations

- Gaussian distributions may be poor models.
- The method fails in large dimension

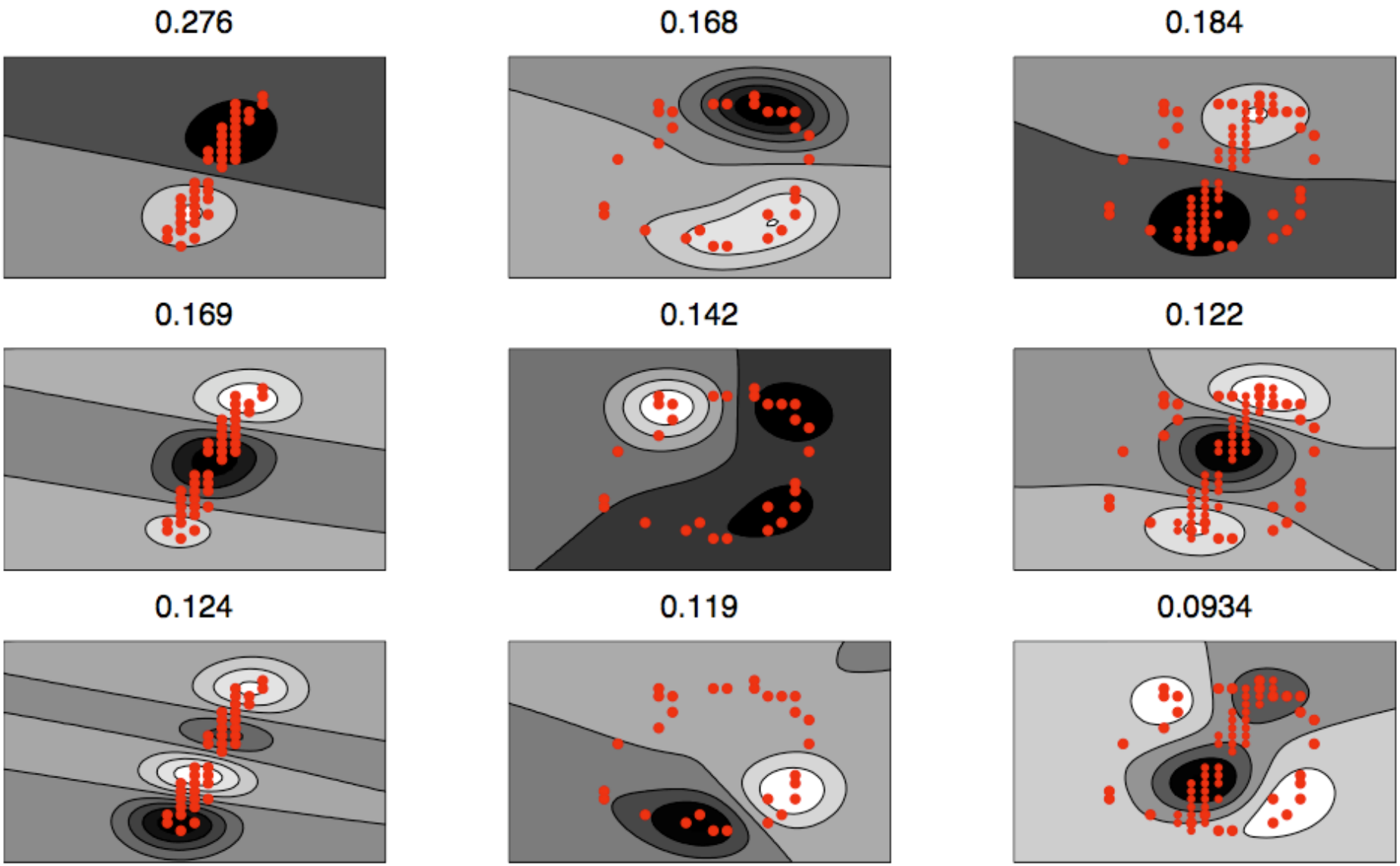
Solution

1. Regularization:

$$K_\lambda\left(\mu, \mu'\right) = \frac{1}{\det\left(\Sigma\left(\frac{\mu+\mu'}{2}\right) + \lambda I_d\right)}.$$

2. Kernel trick: the non-zero eigenvalues of $UU^\top$ and $U^\top U$ are the same $\Longrightarrow$ replace the covariance matrix by the centered Gram matrix (technical details in Cuturi et al., 2005).

Illustration of kernel IGV kernel



Semigroup kernel remarks

Motivations

- A very general formalism to exploit an algebric structure of the data.
- Kernel IVG kernel has given good results for character recognition from a subsampled image.
- The main motivation is more generally to develop kernels for complex objects from which simple "patches" can be extracted.
- The extension to nonabelian groups (e.g., permutation in the symmetric group) might find natural applications.

Kernel examples: Summary

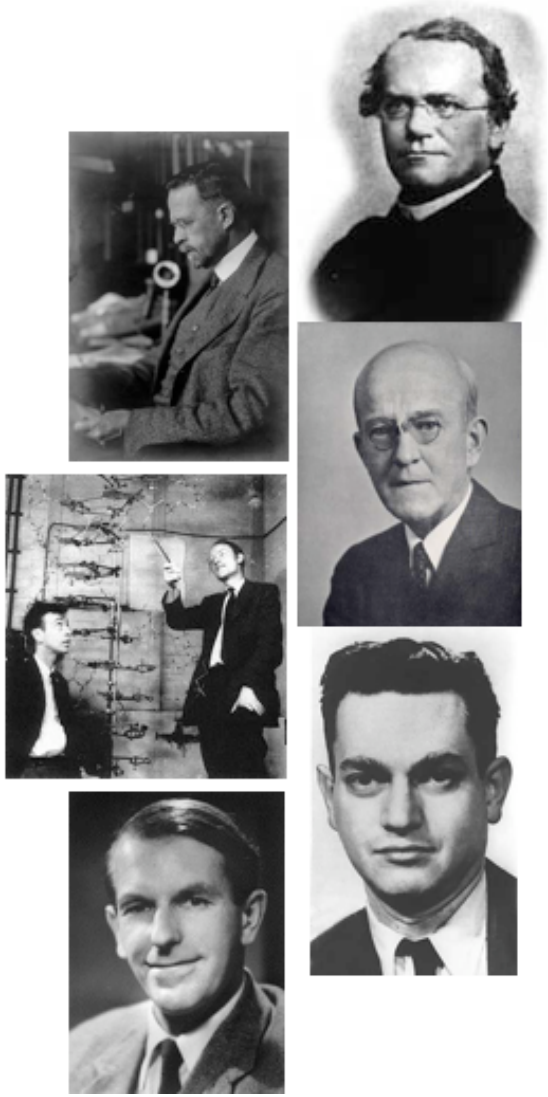
- Many notions of smoothness can be translated as RKHS norms for particular kernels (eigenvalues convolution operator, Sobolev norms and Green operators, Fourier transforms...).
- There is no "uniformly best kernel", but rather a large toolbox of methods and tricks to encode prior knowledge and exploit the nature or structure of the data.
- In the following sections we focus on particular data and applications to illustrate the process of kernel design.

Part 5

Kernels for Biological Sequences

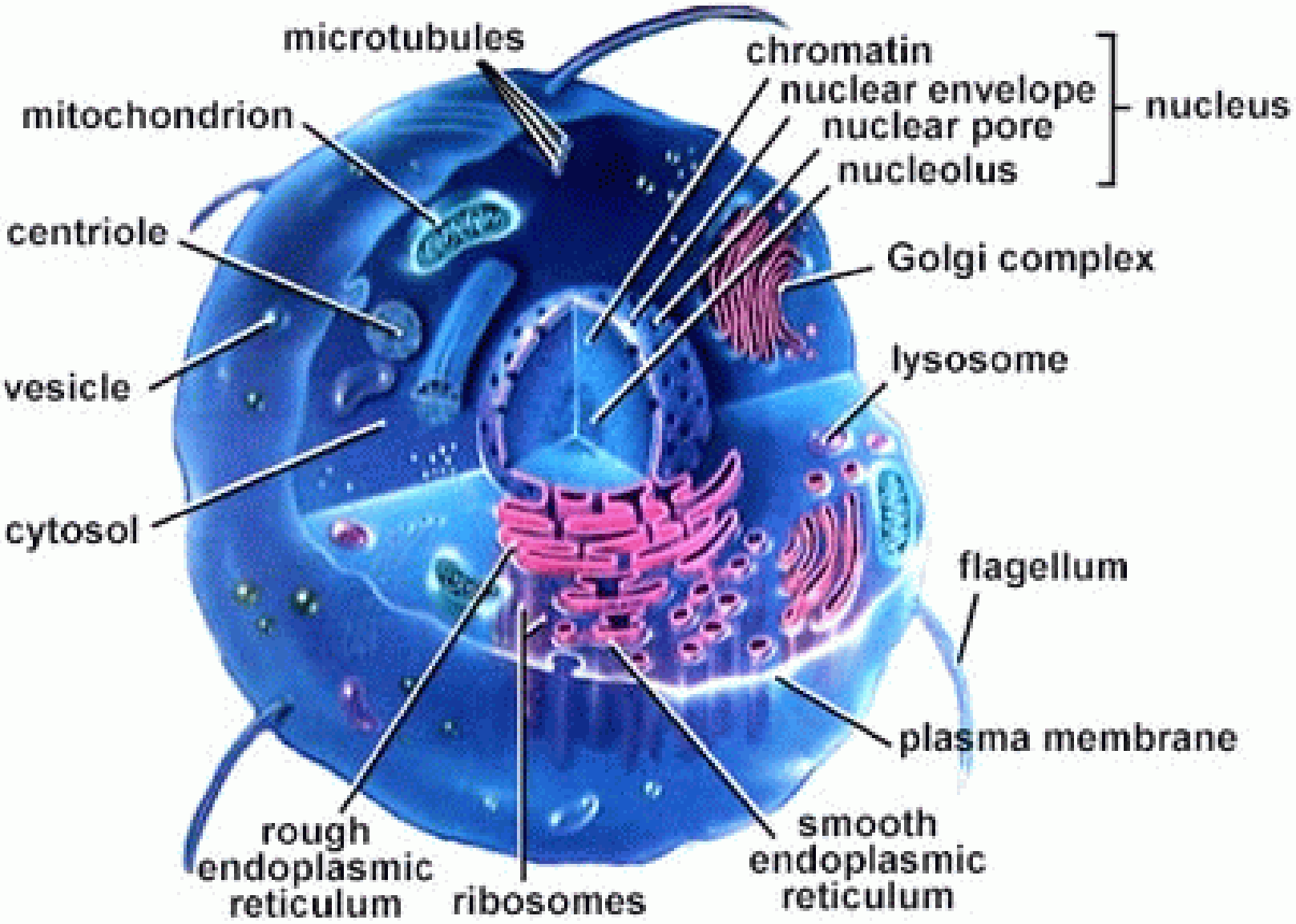
Outline

Short history of genomics

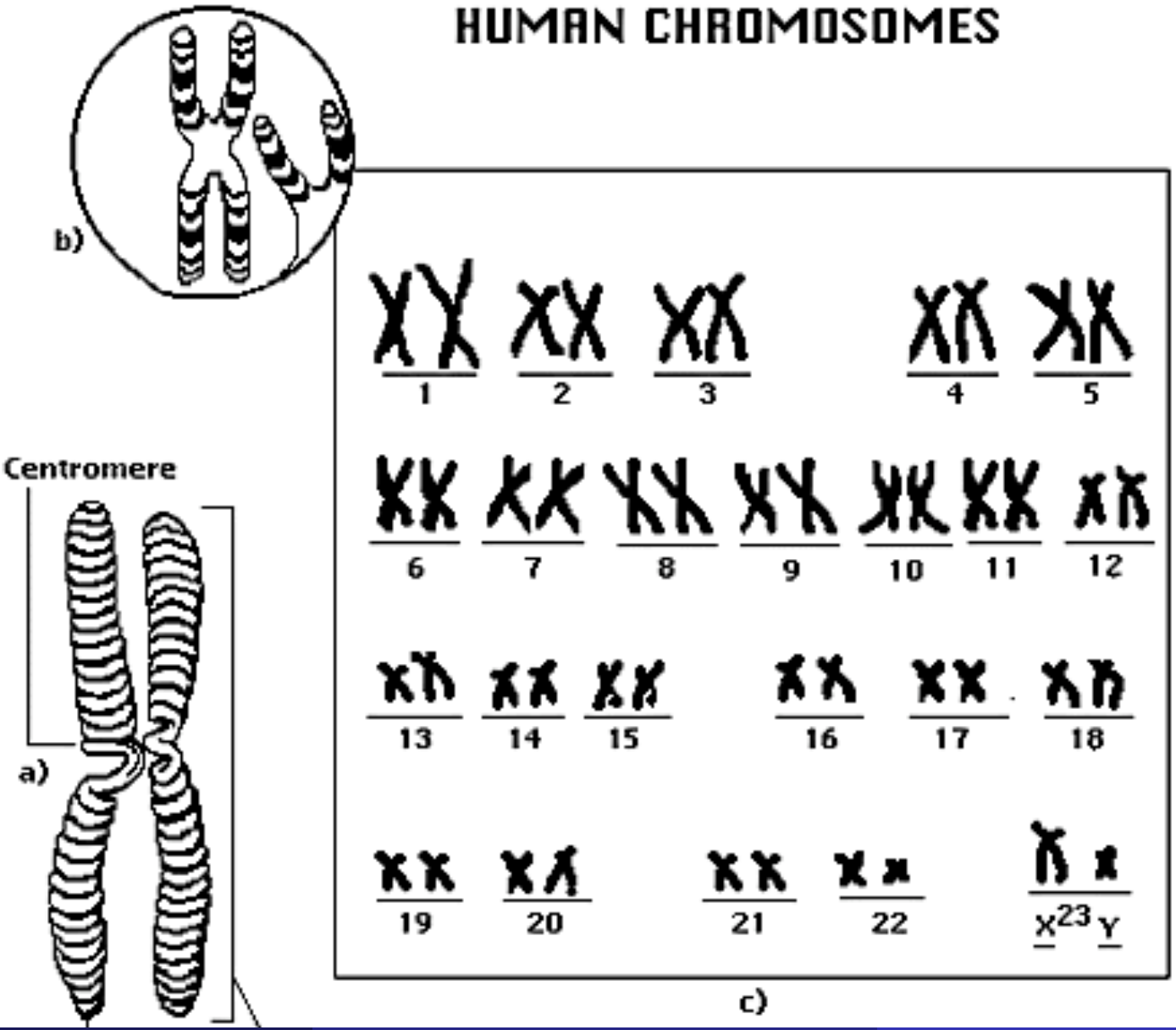


1866 : Laws of heredity (Mendel)
1909 : Morgan and the drosophilists
1944 : DNA supports heredity (Avery)
1953 : Structure of DNA (Crick and Watson)
1966 : Genetic code (Nirenberg)
1960-70 : Genetic engineering
1977 : Method for sequencing (Sanger)
1982 : Creation of Genbank
1990 : Human genome project launched
2003 : Human genome project completed

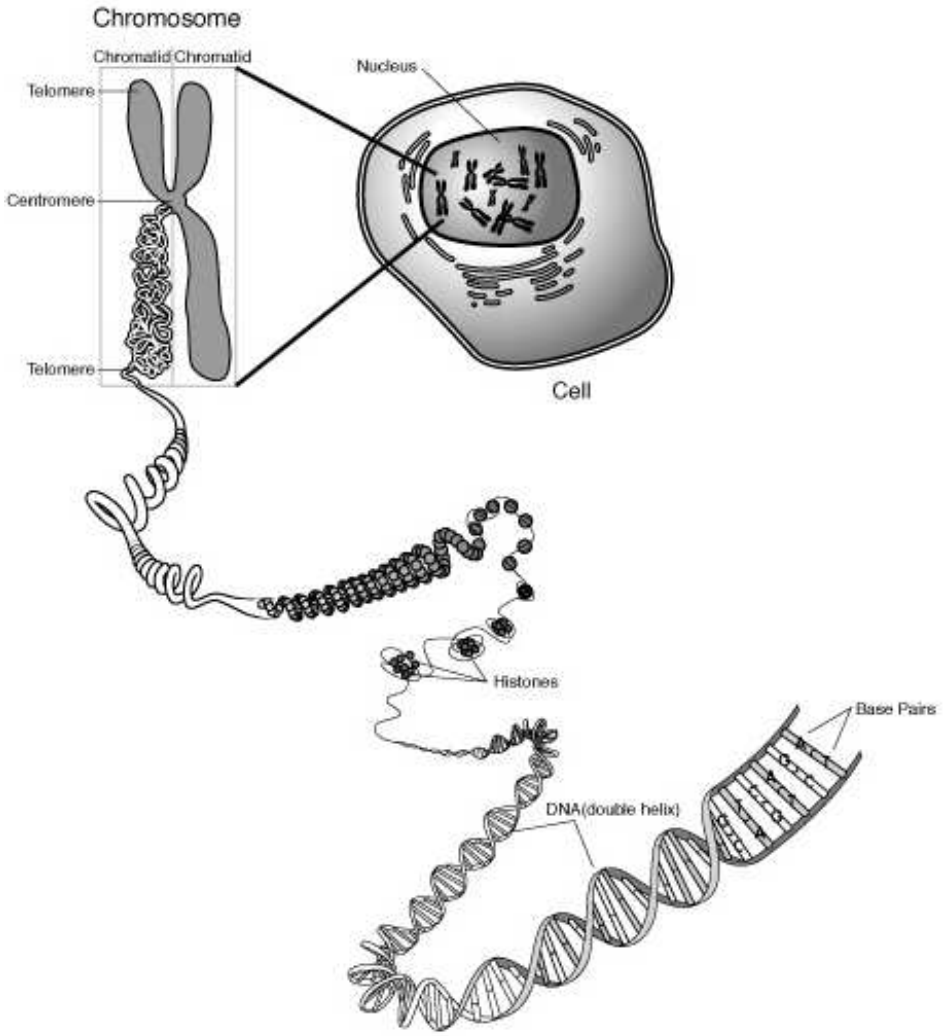
A cell


microtubules
mitochondrion
centriole
vesicle
cytosol
chromatin
nuclear envelope
nuclear pore
nucleolus
nucleus
Golgi complex
lysosome
flagellum
plasma membrane
rough endoplasmic reticulum
ribosomes
smooth endoplasmic reticulum

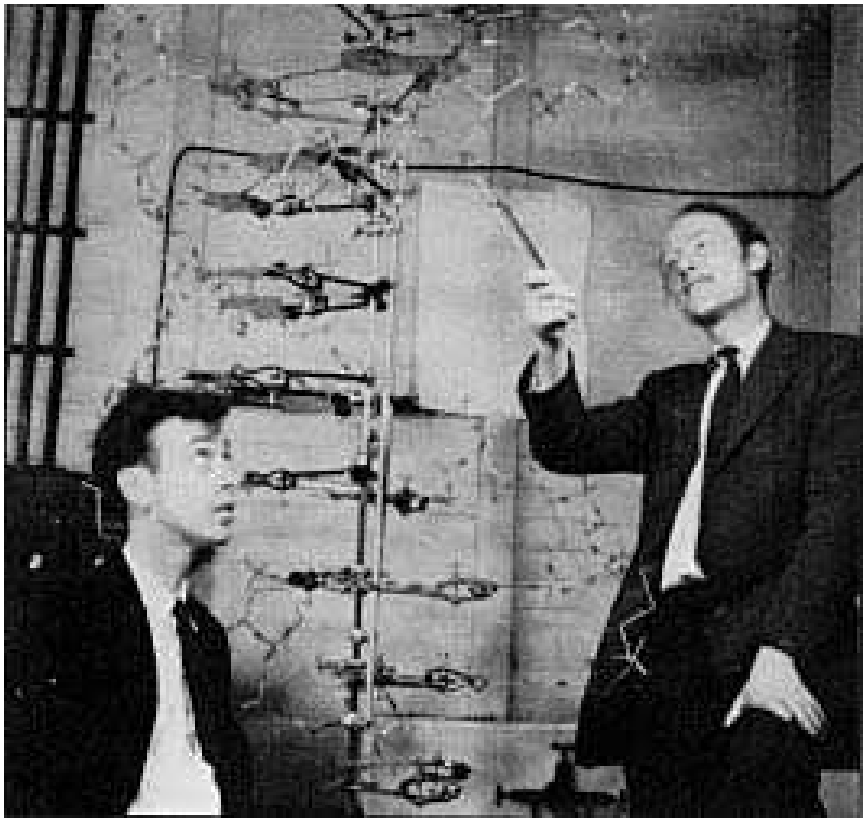
Chromosomes



Chromosomes and DNA

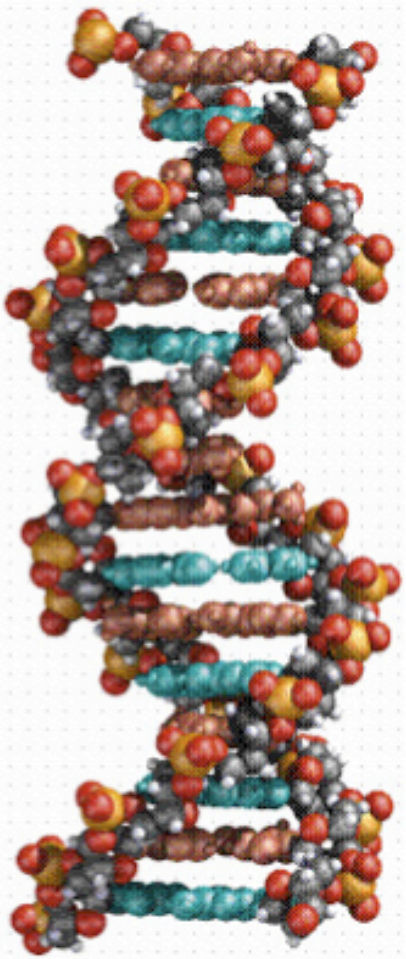


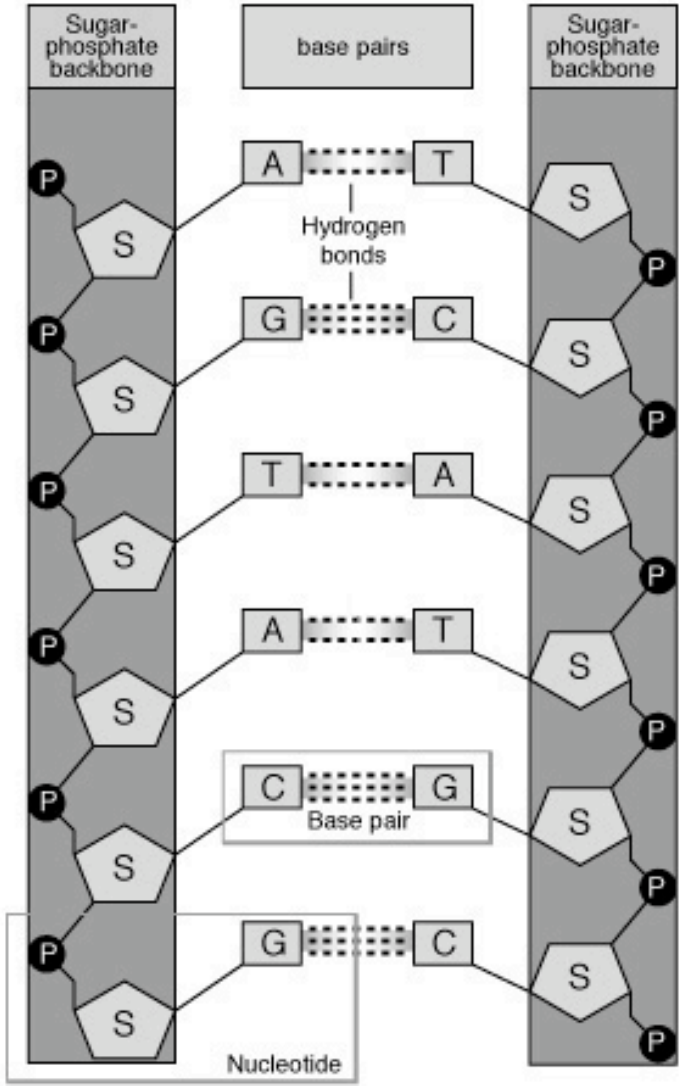
Structure of DNA



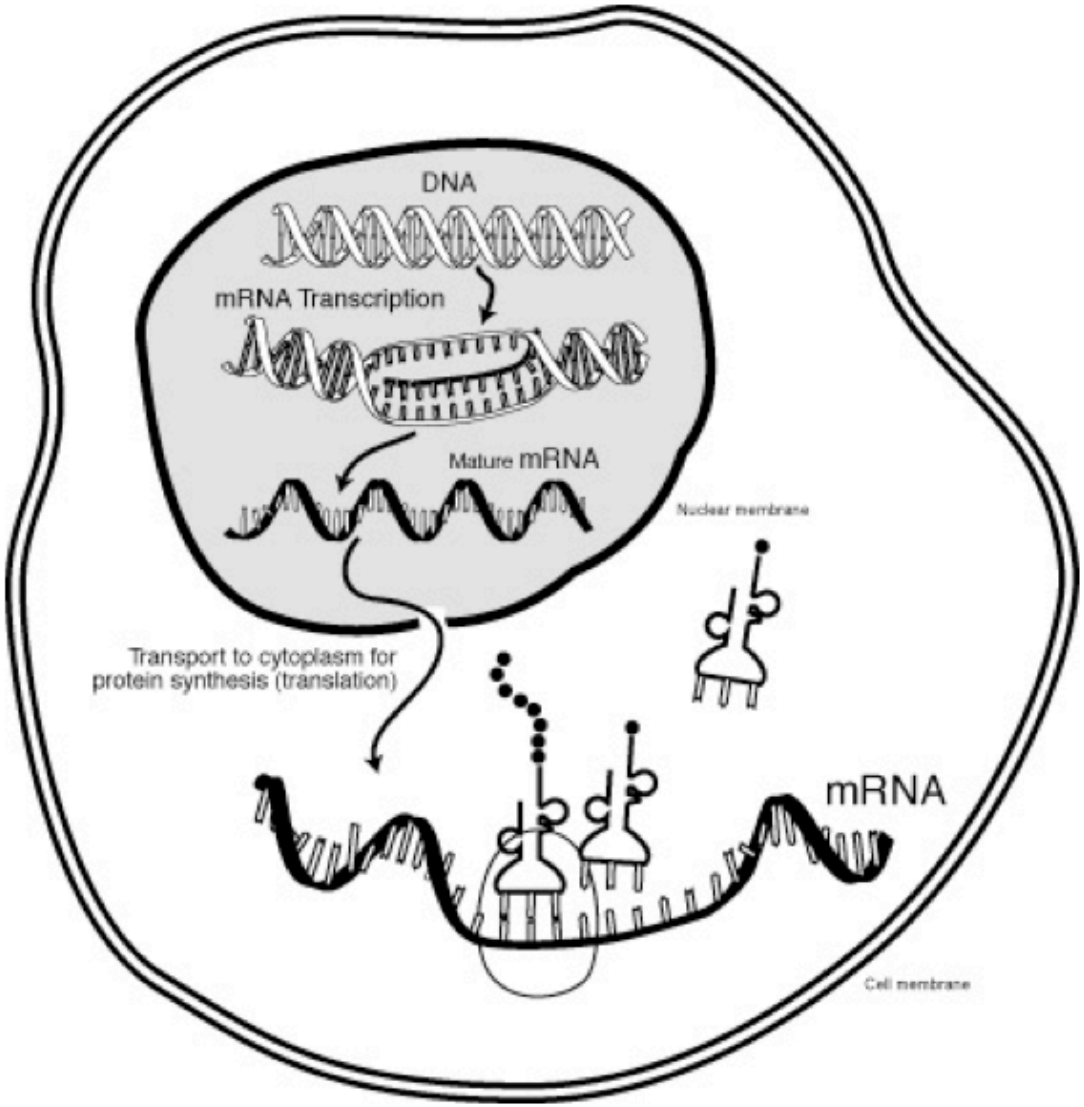
"We wish to suggest a structure for the salt of desoxyribose nucleic acid (D.N.A.). This structure have novel features which are of considerable biological interest" (Watson and Crick, 1953)

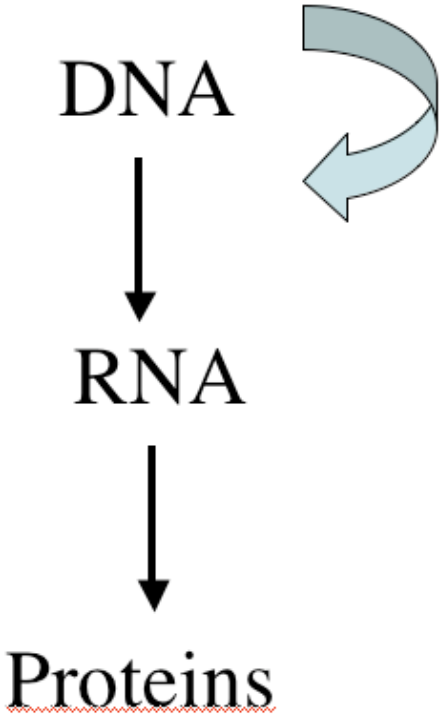
The double helix



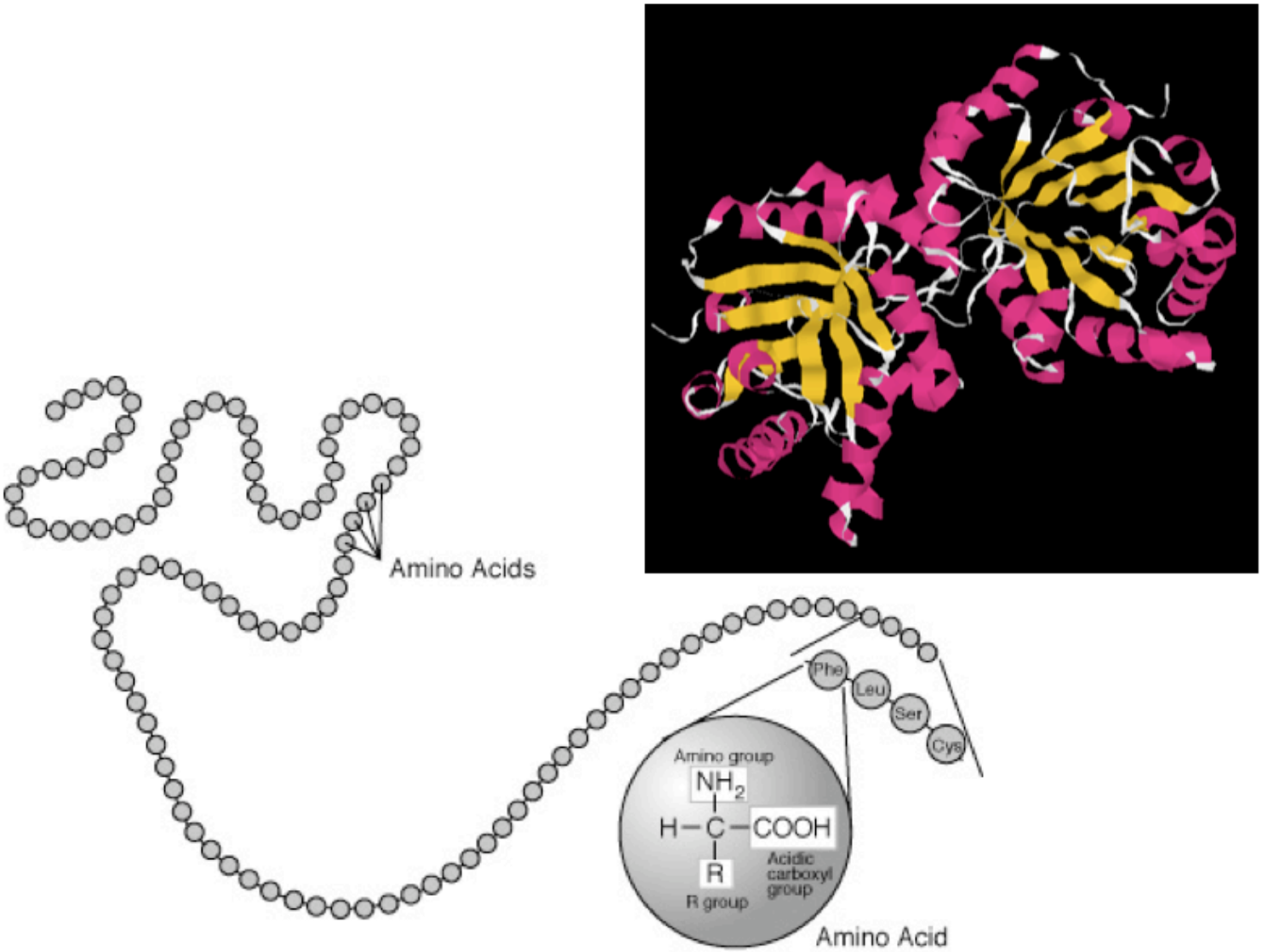


Central dogma

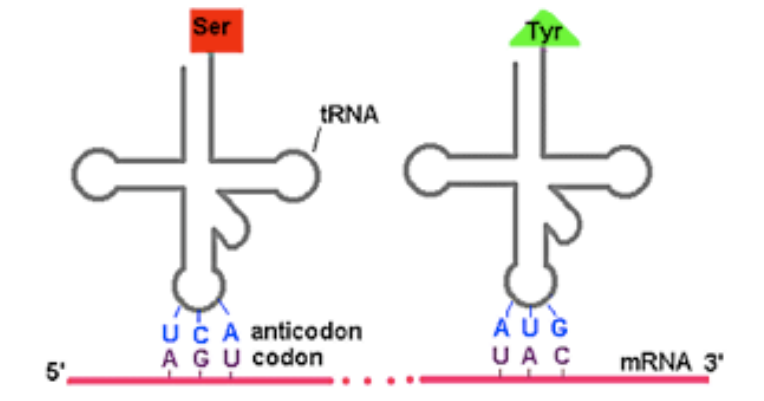




Proteins


Amino Acids
Phe
Leu
Ser
Cys
Amino group
NH_2
H—C—COOH
R
Acidic carboxyl group
R group
Amino Acid

Genetic code



2nd base in codon

1st base in codon	U	C	A	G	3rd base in codon
U	Phe	Ser	Tyr	Cys	U
	Phe	Ser	Tyr	Cys	C
	Leu	Ser	STOP	STOP	A
	Leu	Ser	STOP	Trp	G
C	Leu	Pro	His	Arg	U
	Leu	Pro	His	Arg	C
	Leu	Pro	Gln	Arg	A
	Leu	Pro	Gln	Arg	G
A	Ile	Thr	Asn	Ser	U
	Ile	Thr	Asn	Ser	C
	Ile	Thr	Lys	Arg	A
	Met	Thr	Lys	Arg	G
G	Val	Ala	Asp	Gly	U
	Val	Ala	Asp	Gly	C
	Val	Ala	Glu	Gly	A
	Val	Ala	Glu	Gly	G

The Genetic Code

DNA = 4 letters (ATCG)

↓

RNA = 4 letters (AUCG)

↓

Protein = 20 letters (amino acids)

1 amino acid

=

3 nucleotides

Human genome project

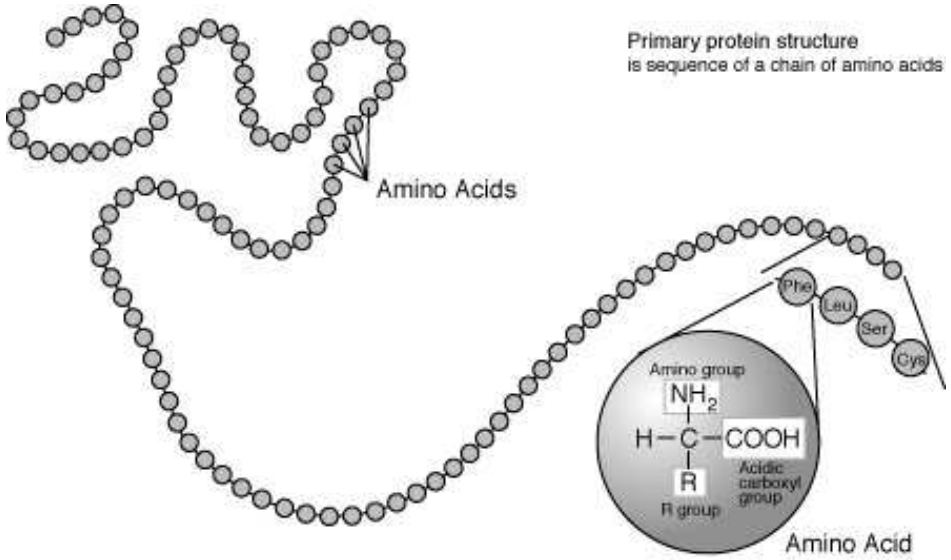
- Goal : sequence the 3,000,000,000 bases of the human genome
- Consortium with 20 labs, 6 countries
- Cost : about 3,000,000,000 USD

2003: End of genomics era

Findings

- About 25,000 genes only (representing 1.2% of the genome)
- Automatic gene finding with graphical models
- 97% of the genome is considered “junk DNA”
- Superposition of a variety of signals (many to be discovered)

Protein sequence



A : Alanine	V : Valine	L : Leucine
F : Phenylalanine	P : Proline	M : Methionine
E : Glutamic acid	K : Lysine	R : Arginine
T : Threonine	C : Cysteine	N : Asparagine
H : Histidine	Y : Tyrosine	W : Tryptophane
I : Isoleucine	S : Serine	Q : Glutamine
D : Aspartic acid	G : Glycine	

Challenges with protein sequences

- A protein sequences can be seen as a variable-length sequence over the 20-letter alphabet of amino-acids, e.g., insuline: `FVNQHLCGSHLVEALYLVCGERGFFYTPKA`
- These sequences are produced at a fast rate (result of the sequencing programs)
- Need for algorithms to compare, classify, analyze these sequences
- Applications: classification into functional or structural classes, prediction of cellular localization and interactions, ...

Example: supervised sequence classification

Data (training)

- Secreted proteins:

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

- Non-secreted proteins:

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

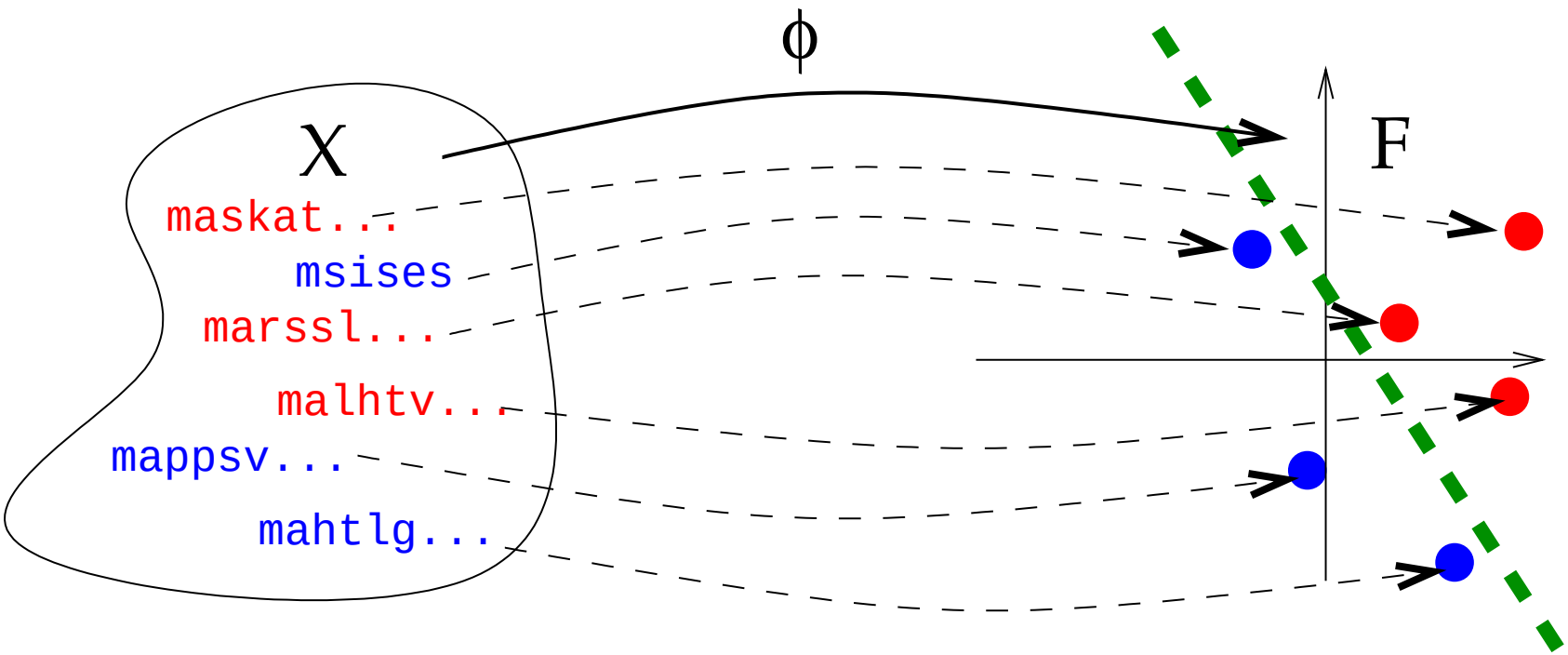
Goal

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

Supervised classification with vector embedding

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...)



Kernels for protein sequences

- Kernel methods have been widely investigated since Jaakkola et al.'s seminal paper (1998).
- What is a good kernel?
  - it should be mathematically valid (symmetric, p.d. or c.p.d.)
  - fast to compute
  - adapted to the problem (give good performances)

Kernel engineering for protein sequences

- Define a (possibly high-dimensional) feature space of interest
  - Physico-chemical kernels
  - Spectrum, mismatch, substring kernels
  - Pairwise, motif kernels
- Derive a kernel from a generative model
  - Fisher kernel
  - Mutual information kernel
  - Marginalized kernel
- Derive a kernel from a similarity measure
  - Local alignment kernel

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Outline

Vector embedding for strings

The idea

Represent each sequence $\mathbf{x}$ by a fixed-length numerical vector $\Phi(\mathbf{x}) \in \mathbb{R}^n$. How to perform this embedding?

Physico-chemical kernel

Extract relevant features, such as:

- length of the sequence
- time series analysis of numerical physico-chemical properties of amino-acids along the sequence (e.g., polarity, hydrophobicity), using for example:
  - Fourier transforms (Wang et al., 2004)
  - Autocorrelation functions (Zhang et al., 2003)

$$r_j = \frac{1}{n-j} \sum_{i=1}^{n-j} h_i h_{i+j}$$

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Substring indexation

The approach

Alternatively, 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)

Example: spectrum kernel (1/2)

Kernel definition

- The 3-spectrum of

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

is:

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

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

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

Example: 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.

Example 2: Substring kernel (1/11)

Definition

- For $1 \leq k \leq n \in \mathbb{N}$, we denote by $\mathcal{I}(k, n)$ the set of sequences of indices $\mathbf{i} = (i_1, \ldots, i_k)$, with $1 \leq i_1 < i_2 < \ldots < i_k \leq n$.
- For a string $\mathbf{x} = x_1 \ldots x_n \in \mathcal{X}$ of length n, for a sequence of indices $\mathbf{i} \in \mathcal{I}(k, n)$, we define a substring as:

$$\mathbf{x}(\mathbf{i}) := x_{i_1} x_{i_2} \ldots x_{i_k} .$$

- The length of the substring is:

$$l(\mathbf{i}) = i_k - i_1 + 1.$$

Example 2: Substring kernel (2/11)

Example

ABRACADABRA

- $\mathbf{i} = (3, 4, 7, 8, 10)$
- $\mathbf{x}(\mathbf{i}) =$RADAR
- $l(\mathbf{i}) = 10 - 3 + 1 = 8$

Example 2: Substring kernel (3/11)

The kernel

- Let $k \in \mathbb{N}$ and $\lambda \in \mathbb{R}^+$ fixed. For all $\mathbf{u} \in \mathcal{A}^k$, let $\Phi_{\mathbf{u}} : \mathcal{X} \to \mathbb{R}$ be defined by:

$$\forall \mathbf{x} \in \mathcal{X}, \quad \Phi_{\mathbf{u}}(\mathbf{x}) = \sum_{\mathbf{i} \in \mathcal{I}(k, |\mathbf{x}|):\ \mathbf{x}(\mathbf{i}) = \mathbf{u}} \lambda^{l(\mathbf{i})} .$$

- The substring kernel is the p.d. kernel defined by:

$$\forall (\mathbf{x}, \mathbf{x}') \in \mathcal{X}^2, \quad K_{k,\lambda}(\mathbf{x}, \mathbf{x}') = \sum_{\mathbf{u} \in \mathcal{A}^k} \Phi_{\mathbf{u}}(\mathbf{x}) \Phi_{\mathbf{u}}(\mathbf{x}') .$$

Example 2: Substring kernel (4/11)

Example

u	ca	ct	at	ba	bt	cr	ar	br
Φ_u(cat)	λ^2	λ^3	λ^2	0	0	0	0	0
Φ_u(car)	λ^2	0	0	0	0	λ^3	λ^2	0
Φ_u(bat)	0	0	λ^2	λ^2	λ^3	0	0	0
Φ_u(bar)	0	0	0	λ^2	0	0	λ^2	λ^3

$$\begin{cases} K\,(\text{cat,cat}) = K\,(\text{car,car}) = 2\lambda^4 + \lambda^6 \\ K\,(\text{cat,car}) = \lambda^4 \\ K\,(\text{cat,bar}) = 0 \end{cases}$$

Example 2: Substring kernel (5/11)

Kernel computation

- We need to compute, for any pair $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$, the kernel:

$$K_{n,\lambda}(\mathbf{x}, \mathbf{x}') = \sum_{\mathbf{u} \in \mathcal{A}^k} \Phi_{\mathbf{u}}(\mathbf{x}) \Phi_{\mathbf{u}}(\mathbf{x}')$$
$$= \sum_{\mathbf{u} \in \mathcal{A}^k} \sum_{\mathbf{i}: \mathbf{x}(\mathbf{i}) = \mathbf{u}} \sum_{\mathbf{i}': \mathbf{x}'(\mathbf{i}') = \mathbf{u}} \lambda^{l(\mathbf{i}) + l(\mathbf{i}')} .$$

- Enumerating the substrings is too slow (of order $|\mathbf{x}|^k$).

Example 2: Substring kernel (6/11)

Kernel computation (cont.)

- For $\mathbf{u} \in \mathcal{A}^k$ remember that:

$$\Phi_{\mathbf{u}}(\mathbf{x}) = \sum_{\mathbf{i}:\mathbf{x}(\mathbf{i})=\mathbf{u}} \lambda^{i_n - i_1 + 1} .$$

- Let now:

$$\Psi_{\mathbf{u}}(\mathbf{x}) = \sum_{\mathbf{i}:\mathbf{x}(\mathbf{i})=\mathbf{u}} \lambda^{|\mathbf{x}| - i_1 + 1} .$$

Example 2: Substring kernel (7/11)

Kernel computation (cont.)

Let us note $\mathbf{x}(1,j) = x_1 \ldots x_j$. A simple rewriting shows that, if we note $a \in \mathcal{A}$ the last letter of $\mathbf{u}$ ($\mathbf{u} = \mathbf{v}a$):

$$\Phi_{\mathbf{v}a}(\mathbf{x}) = \sum_{j \in [1,|\mathbf{x}|]: x_j = a} \Psi_{\mathbf{v}}(\mathbf{x}(1,j-1))\,\lambda\,,$$

and

$$\Psi_{\mathbf{v}a}(\mathbf{x}) = \sum_{j \in [1,|\mathbf{x}|]: x_j = a} \Psi_{\mathbf{v}}(\mathbf{x}(1,j-1))\,\lambda^{|\mathbf{x}|-j+1}\,.$$

Example 2: Substring kernel (8/11)

Kernel computation (cont.)

Moreover we observe that if the string is of the form $\mathbf{x}a$ (i.e., the last letter is $a \in \mathcal{A}$), then:

- If the last letter of $\mathbf{u}$ is not a:

$$\begin{cases} \Phi_{\mathbf{u}}(\mathbf{x}a) & = \Phi_{\mathbf{u}}(\mathbf{x}) \,, \\ \Psi_{\mathbf{u}}(\mathbf{x}a) & = \lambda \Psi_{\mathbf{u}}(\mathbf{x}) \,. \end{cases}$$

- If the last letter of $\mathbf{u}$ is a (i.e., $\mathbf{u} = \mathbf{v}a$ with $\mathbf{v} \in \mathcal{A}^{n-1}$):

$$\begin{cases} \Phi_{\mathbf{v}a}(\mathbf{x}a) & = \Phi_{\mathbf{v}a}(\mathbf{x}) + \lambda \Psi_{\mathbf{v}}(\mathbf{x}) \,, \\ \Psi_{\mathbf{v}a}(\mathbf{x}a) & = \lambda \Psi_{\mathbf{v}a}(\mathbf{x}) + \lambda \Psi_{\mathbf{v}}(\mathbf{x}) \,. \end{cases}$$

Example 2: Substring kernel (9/11)

Kernel computation (cont.)

Let us now show how the function:

$$B_n(\mathbf{x}, \mathbf{x}') := \sum_{\mathbf{u} \in \mathcal{A}^n} \Psi_{\mathbf{u}}(\mathbf{x}) \Psi_{\mathbf{u}}(\mathbf{x}')$$

and the kernel:

$$K_n(\mathbf{x}, \mathbf{x}') := \sum_{\mathbf{u} \in \mathcal{A}^n} \Phi_{\mathbf{u}}(\mathbf{x}) \Phi_{\mathbf{u}}(\mathbf{x}')$$

can be computed recursively. We note that:

$$\begin{cases} B_0(\mathbf{x}, \mathbf{x}') = K_0(\mathbf{x}, \mathbf{x}') = 0 & \text{for all } \mathbf{x}, \mathbf{x}' \\ B_k(\mathbf{x}, \mathbf{x}') = K_k(\mathbf{x}, \mathbf{x}') = 0 & \text{if } \min(|\mathbf{x}|, |\mathbf{x}'|) < k \end{cases}$$

Example 2: Substring kernel (10/11)

Recursive computation of B_n

$$
\begin{aligned}
&B_n\left(\mathbf{x}a, \mathbf{x}'\right) \\
&= \sum_{\mathbf{u}\in\mathcal{A}^n} \Psi_{\mathbf{u}}\left(\mathbf{x}a\right)\Psi_{\mathbf{u}}\left(\mathbf{x}'\right) \\
&= \lambda \sum_{\mathbf{u}\in\mathcal{A}^n} \Psi_{\mathbf{u}}\left(\mathbf{x}\right)\Psi_{\mathbf{u}}\left(\mathbf{x}'\right) + \lambda \sum_{\mathbf{v}\in\mathcal{A}^{n-1}} \Psi_{\mathbf{v}}\left(\mathbf{x}\right)\Psi_{\mathbf{v}a}\left(\mathbf{x}'\right) \\
&= \lambda B_n\left(\mathbf{x}, \mathbf{x}'\right) + \\
&\quad \lambda \sum_{\mathbf{v}\in\mathcal{A}^{n-1}} \Psi_{\mathbf{v}}\left(\mathbf{x}\right) \left(\sum_{j\in[1,|\,\mathbf{x}'\,|]:x'_j=a} \Psi_{\mathbf{v}}\left(\mathbf{x}'\left(1, j-1\right)\right) \lambda^{|\,\mathbf{x}'\,|-j+1} \right) \\
&= \lambda B_n\left(\mathbf{x}, \mathbf{x}'\right) + \sum_{j\in[1,|\,\mathbf{x}'\,|]:x'_j=a} B_{n-1}\left(\mathbf{x}, \mathbf{x}'\left(1, j-1\right)\right) \lambda^{|\,\mathbf{x}'\,|-j+2}
\end{aligned}
$$

Example 2: Substring kernel (10/11)

Recursive computation of K_n

$$
\begin{aligned}
&K_n\left(\mathbf{x}a, \mathbf{x}'\right) \\
&= \sum_{\mathbf{u}\in\mathcal{A}^n} \Phi_{\mathbf{u}}\left(\mathbf{x}a\right)\Phi_{\mathbf{u}}\left(\mathbf{x}'\right) \\
&= \sum_{\mathbf{u}\in\mathcal{A}^n} \Phi_{\mathbf{u}}\left(\mathbf{x}\right)\Phi_{\mathbf{u}}\left(\mathbf{x}'\right) + \lambda \sum_{\mathbf{v}\in\mathcal{A}^{n-1}} \Psi_{\mathbf{v}}\left(\mathbf{x}\right)\Phi_{\mathbf{v}a}\left(\mathbf{x}'\right) \\
&= K_n\left(\mathbf{x}, \mathbf{x}'\right) + \\
&\quad \lambda \sum_{\mathbf{v}\in\mathcal{A}^{n-1}} \Psi_{\mathbf{v}}\left(\mathbf{x}\right) \left(\sum_{j\in[1,|\,\mathbf{x}'\,|]:x'_j=a} \Psi_{\mathbf{v}}\left(\mathbf{x}'\left(1,j-1\right)\right)\lambda \right) \\
&= \lambda K_n\left(\mathbf{x}, \mathbf{x}'\right) + \lambda^2 \sum_{j\in[1,|\,\mathbf{x}'\,|]:x'_j=a} B_{n-1}\left(\mathbf{x}, \mathbf{x}'\left(1,j-1\right)\right)
\end{aligned}
$$

Summary: Substring indexation

- Implementation in $O(|\mathbf{x}| + |\mathbf{x}'|)$ in memory and time for the spectrum and mismatch kernels (with suffix trees)
- Implementation in $O(|\mathbf{x}| \times |\mathbf{x}'|)$ in memory and time for the substring kernels
- The feature space has high dimension ($|\mathcal{A}|^k$), so learning requires regularized methods (such as SVM)

Dictionary-based indexation

The approach

- Chose a dictionary of sequences $\mathcal{D} = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$
- Chose a measure of similarity $s(\mathbf{x}, \mathbf{x}')$
- Define the mapping $\Phi_{\mathcal{D}}(\mathbf{x}) = (s(\mathbf{x}, \mathbf{x}_i))_{\mathbf{x}_i \in \mathcal{D}}$

Examples

This includes:

- Motif kernels (Logan et al., 2001): the dictionary is a library of motifs, the similarity function is a matching function
- Pairwise kernel (Liao & Noble, 2003): the dictionary is the training set, the similarity is a classical measure of similarity between sequences.

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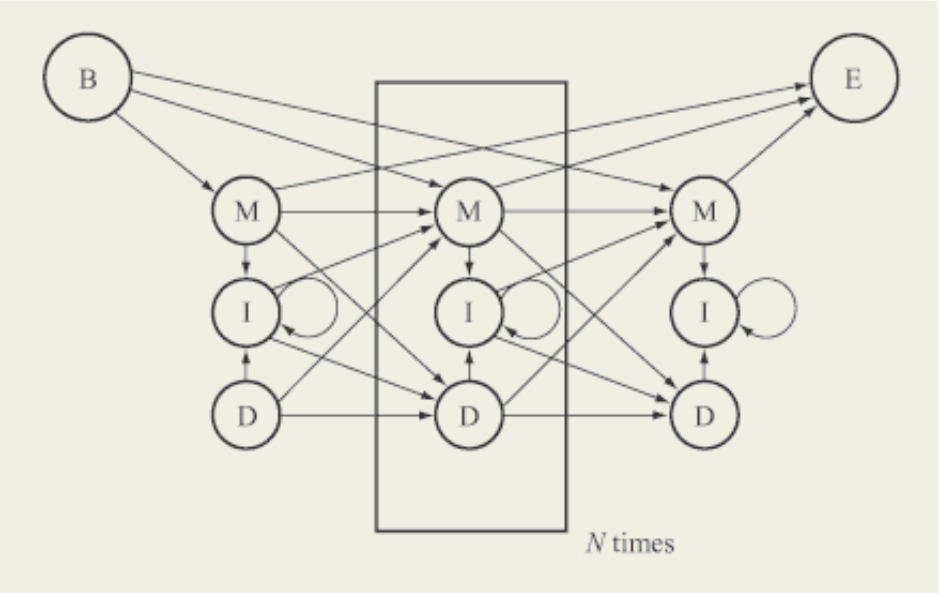
Outline

Probabilistic models for sequences

Probabilistic modeling of biological sequences is older than kernel designs. Important models include HMM for protein sequences, SCFG for RNA sequences.



Parametric model

A model is a family of distribution

$$\{P_\theta, \theta \in \Theta \subset \mathbb{R}^m\} \subset \mathcal{M}_1^+(\mathcal{X})$$

Fisher kernel

Definition

- Fix a parameter $\theta_0 \in \Theta$ (e.g., by maximum likelihood over a training set of sequences)
- For each sequence $\mathbf{x}$, compute the Fisher score vector:

$$\Phi_{\theta_0}(\mathbf{x}) = \nabla_\theta \log P_\theta(\mathbf{x})|_{\theta=\theta_0} \ .$$

- Form the kernel (Jaakkola et al., 2000):

$$K\left(\mathbf{x}, \mathbf{x}'\right) = \Phi_{\theta_0}(\mathbf{x})^\top I(\theta_0)^{-1} \Phi_{\theta_0}(\mathbf{x}') \ ,$$

where $I(\theta_0) = E_{\theta_0}\left[\Phi_{\theta_0}(\mathbf{x})\Phi_{\theta_0}(\mathbf{x})^\top\right]$ is the Fisher information matrix.

Fisher kernel properties

- The Fisher score describes how each parameter contributes to the process of generating a particular example
- The Fisher kernel is invariant under change of parametrization of the model
- A kernel classifier employing the Fisher kernel derived from a model that contains the label as a latent variable is, asymptotically, at least as good a classifier as the MAP labelling based on the model (Jaakkola and Haussler, 1999).
- A variant of the Fisher kernel (called the Tangent of Posterior kernel) can also improve over the direct posterior classification by helping to correct the effect of estimation errors in the parameter (Tsuda et al., 2002).

Fisher kernel in practice

- $\Phi_{\theta_0}(\mathbf{x})$ can be computed explicitly for many models (e.g., HMMs)
- $I(\theta_0)$ is often replaced by the identity matrix
- Several different models (i.e., different θ_0) can be trained and combined
- Feature vectors are explicitly computed

Mutual information kernels

Definition

- Chose a prior $w(d\theta)$ on the measurable set Θ
- Form the kernel (Seeger, 2002):

$$K\left(\mathbf{x},\mathbf{x}'\right)=\int_{\theta\in\Theta}P_\theta(\mathbf{x})P_\theta(\mathbf{x}')w(d\theta)\ .$$

- No explicit computation of a finite-dimensional feature vector
- $K\left(\mathbf{x},\mathbf{x}'\right)=<\phi\left(\mathbf{x}\right),\phi\left(\mathbf{x}'\right)>_{L_2(w)}$ with

$$\phi\left(\mathbf{x}\right)=\left(P_\theta\left(\mathbf{x}\right)\right)_{\theta\in\Theta}\ .$$

Example: coin toss

- Let $P_\theta(X = 1) = \theta$ and $P_\theta(X = 0) = 1 - \theta$ a model for random coin toss, with $\theta \in [0, 1]$.
- Let $d\theta$ be the Lebesgue measure on $[0, 1]$
- The mutual information kernel between $\mathbf{x} = 001$ and $\mathbf{x}' = 1010$ is:

$$\begin{cases} P_\theta(\mathbf{x}) &= \theta(1-\theta)^2 \ , \\ P_\theta(\mathbf{x}') &= \theta^2(1-\theta)^2 \ , \end{cases}$$

$$K(\mathbf{x}, \mathbf{x}') = \int_0^1 \theta^3 (1-\theta)^4 \, d\theta = \frac{3!4!}{8!} = \frac{1}{280} \ .$$

Context-tree model

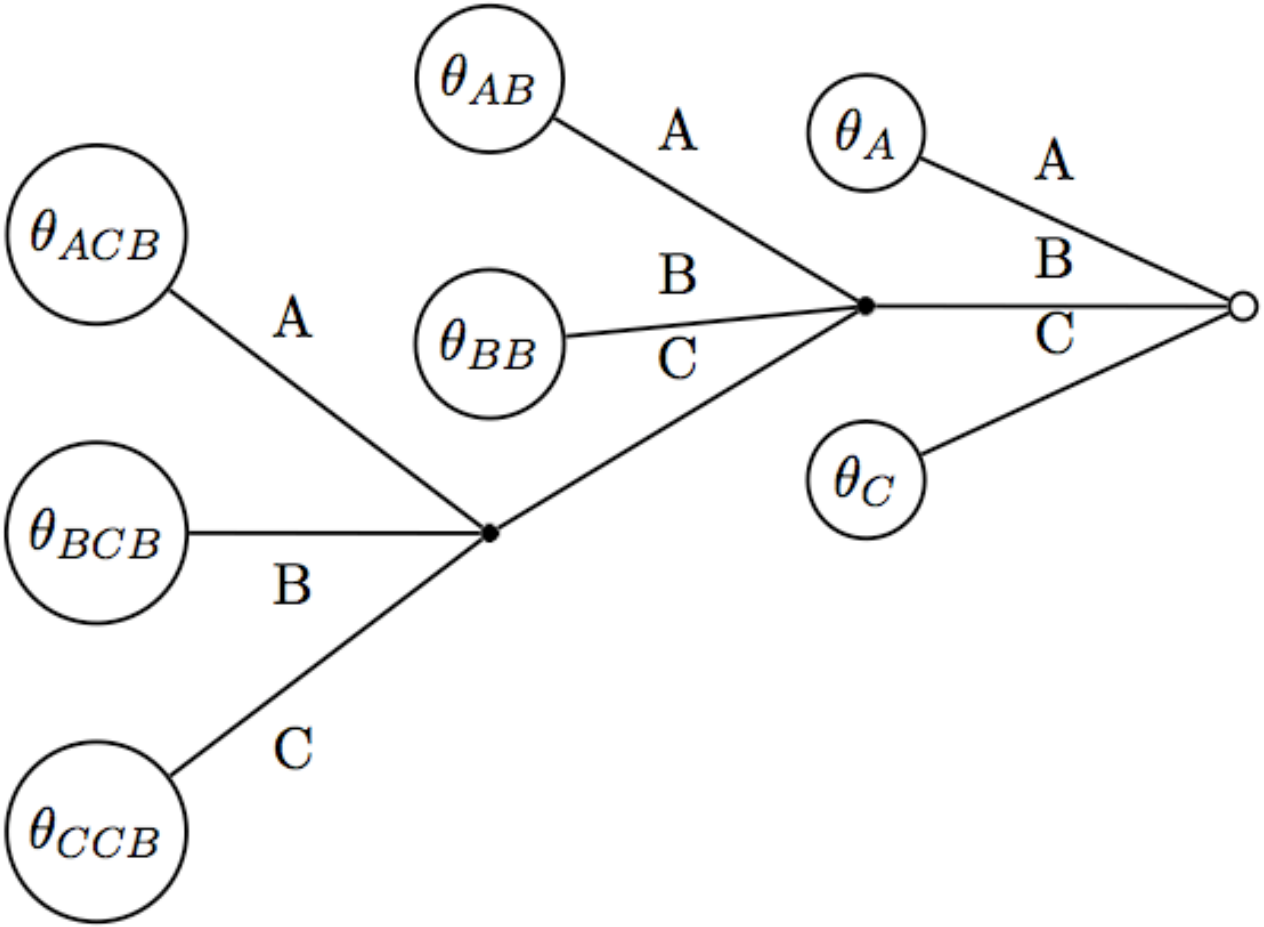
Definition

A context-tree model is a variable-memory Markov chain:

$$P_{\mathcal{D},\theta}(\mathbf{x}) = P_{\mathcal{D},\theta}(x_1 \dots x_D) \prod_{i=D+1}^{n} P_{\mathcal{D},\theta}(x_i \mid x_{i-D} \dots x_{i-1})$$

- $\mathcal{D}$ is a suffix tree
- $\theta \in \Sigma^{\mathcal{D}}$ is a set of conditional probabilities (multinomials)

Context-tree model: example



$$P(AABACBACC) = P(AAB)\theta_{AB}(A)\theta_A(C)\theta_C(B)\theta_{ACB}(A)\theta_A(C)\theta_C(A) \ .$$

The context-tree kernel

Theorem (Cuturi et al., 2005)

- *For particular choices of priors, the context-tree kernel:*

$$K(\mathbf{x}, \mathbf{x}') = \sum_{\mathcal{D}} \int_{\theta \in \Sigma^{\mathcal{D}}} P_{\mathcal{D},\theta}(\mathbf{x}) P_{\mathcal{D},\theta}(\mathbf{x}') w(d\theta|\mathcal{D}) \pi(\mathcal{D})$$

  can be computed in $O(|\mathbf{x}| + |\mathbf{x}'|)$ with a variant of the Context-Tree Weighting algorithm.

- *This is a valid mutual information kernel.*
- *The similarity is related to information-theoretical measure of mutual information between strings.*

Marginalized kernels

Definition

- For any observed data $\mathbf{x} \in \mathcal{X}$, let a latent variable $\mathbf{y} \in \mathcal{Y}$ be associated probabilistically through a conditional probability $P_{\mathbf{x}}(d\mathbf{y})$.
- Let $K_{\mathcal{Z}}$ be a kernel for the complete data $\mathbf{z} = (\mathbf{x}, \mathbf{y})$
- Then the following kernel is a valid kernel on $\mathcal{X}$, called a marginalized kernel (Tsuda et al., 2002):

$$K_{\mathcal{X}}(\mathbf{x}, \mathbf{x}') := E_{P_{\mathbf{x}}(d\mathbf{y}) \times P_{\mathbf{x}'}(d\mathbf{y}')} K_{\mathcal{Z}}(\mathbf{z}, \mathbf{z}')$$
$$= \int \int K_{\mathcal{Z}}((\mathbf{x}, \mathbf{y}), (\mathbf{x}', \mathbf{y}')) P_{\mathbf{x}}(d\mathbf{y}) P_{\mathbf{x}'}(d\mathbf{y}') \ .$$

Marginalized kernels: proof of positive definiteness

- $K_{\mathcal{Z}}$ is p.d. on $\mathcal{Z}$. Therefore there exists a Hilbert space $\mathcal{H}$ and $\Phi_{\mathcal{Z}} : \mathcal{Z} \to \mathcal{H}$ such that:

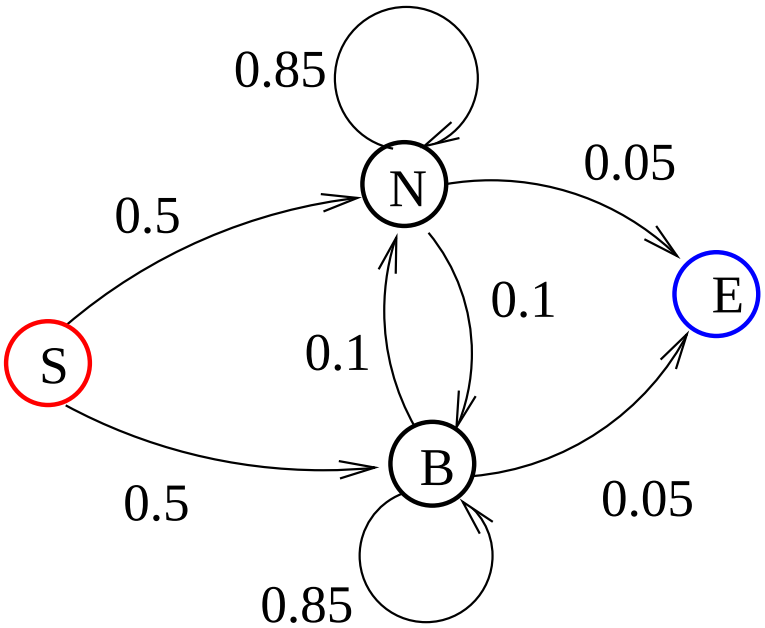
$$K_{\mathcal{Z}}\left(\mathbf{z}, \mathbf{z}'\right) = \left\langle \Phi_{\mathcal{Z}}\left(\mathbf{z}\right), \Phi_{\mathcal{Z}}\left(\mathbf{z}'\right) \right\rangle_{\mathcal{H}} .$$

- Marginalizing therefore gives:

$$\begin{aligned} K_{\mathcal{X}}\left(\mathbf{x}, \mathbf{x}'\right) &= E_{P_{\mathbf{x}}(d\mathbf{y}) \times P_{\mathbf{x}'}(d\mathbf{y}')} K_{\mathcal{Z}}\left(\mathbf{z}, \mathbf{z}'\right) \\ &= E_{P_{\mathbf{x}}(d\mathbf{y}) \times P_{\mathbf{x}'}(d\mathbf{y}')} \left\langle \Phi_{\mathcal{Z}}\left(\mathbf{z}\right), \Phi_{\mathcal{Z}}\left(\mathbf{z}'\right) \right\rangle_{\mathcal{H}} \\ &= \left\langle E_{P_{\mathbf{x}}(d\mathbf{y})} \Phi_{\mathcal{Z}}\left(\mathbf{z}\right), E_{P_{\mathbf{x}}(d\mathbf{y}')} \Phi_{\mathcal{Z}}\left(\mathbf{z}'\right) \right\rangle_{\mathcal{H}} , \end{aligned}$$

therefore $K_{\mathcal{X}}$ is p.d. on $\mathcal{X}$. $\square$

Example: HMM for normal/biased coin toss



- Normal (N) and biased (B) coins (not observed)

- Observed output are 0/1 with probabilities:

$$\begin{cases} \pi(0|N) = 1 - \pi(1|N) = 0.5, \\ \pi(0|B) = 1 - \pi(1|B) = 0.8. \end{cases}$$

- Example of realization (complete data):

NNNNNBBBBBBBBBNNNNNNNNNNNNBBBBBB

100101110111101001011001111011

1-spectrum kernel on complete data

- If both $\mathbf{x} \in \mathcal{A}^*$ and $\mathbf{y} \in \mathcal{S}^*$ were observed, we might rather use the 1-spectrum kernel on the complete data $\mathbf{z} = (\mathbf{x}, \mathbf{y})$:

$$K_{\mathcal{Z}}\left(\mathbf{z}, \mathbf{z}'\right) = \sum_{(a,s) \in \mathcal{A} \times \mathcal{S}} n_{a,s}\left(\mathbf{z}\right) n_{a,s}\left(\mathbf{z}\right),$$

  where $n_{a,s}\left(\mathbf{x}, \mathbf{y}\right)$ for $a = 0, 1$ and $s = N, B$ is the number of occurrences of s in $\mathbf{y}$ which emit a in $\mathbf{x}$.

- Example:

$$\begin{aligned} \mathbf{z} &= 1001011101111010010111001111011, \\ \mathbf{z}' &= 0011010110011111011010111101100101, \end{aligned}$$

$$\begin{aligned} K_{\mathcal{Z}}\left(\mathbf{z}, \mathbf{z}'\right) &= n_0\left(\mathbf{z}\right) n_0\left(\mathbf{z}'\right) + n_0\left(\mathbf{z}\right) n_0\left(\mathbf{z}'\right) + n_1\left(\mathbf{z}\right) n_1\left(\mathbf{z}'\right) + n_1\left(\mathbf{z}\right) n_1\left(\mathbf{z}\right. \\ &= 7 \times 15 + 9 \times 12 + 13 \times 6 + 2 \times 1 = 293. \end{aligned}$$

1-spectrum marginalized kernel on observed data

- The marginalized kernel for observed data is:

$$K_{\mathcal{X}}\left(\mathbf{x},\mathbf{x}'\right) = \sum_{\mathbf{y},\mathbf{y}'\in\mathcal{S}^*} K_{\mathcal{Z}}\left(\left(\mathbf{x},\mathbf{y}\right),\left(\mathbf{x},\mathbf{y}\right)\right) P\left(\mathbf{y}|\mathbf{x}\right) P\left(\mathbf{y}'|\mathbf{x}'\right)$$
$$= \sum_{(a,s)\in\mathcal{A}\times\mathcal{S}} \Phi_{a,s}\left(\mathbf{x}\right)\Phi_{a,s}\left(\mathbf{x}'\right),$$

with

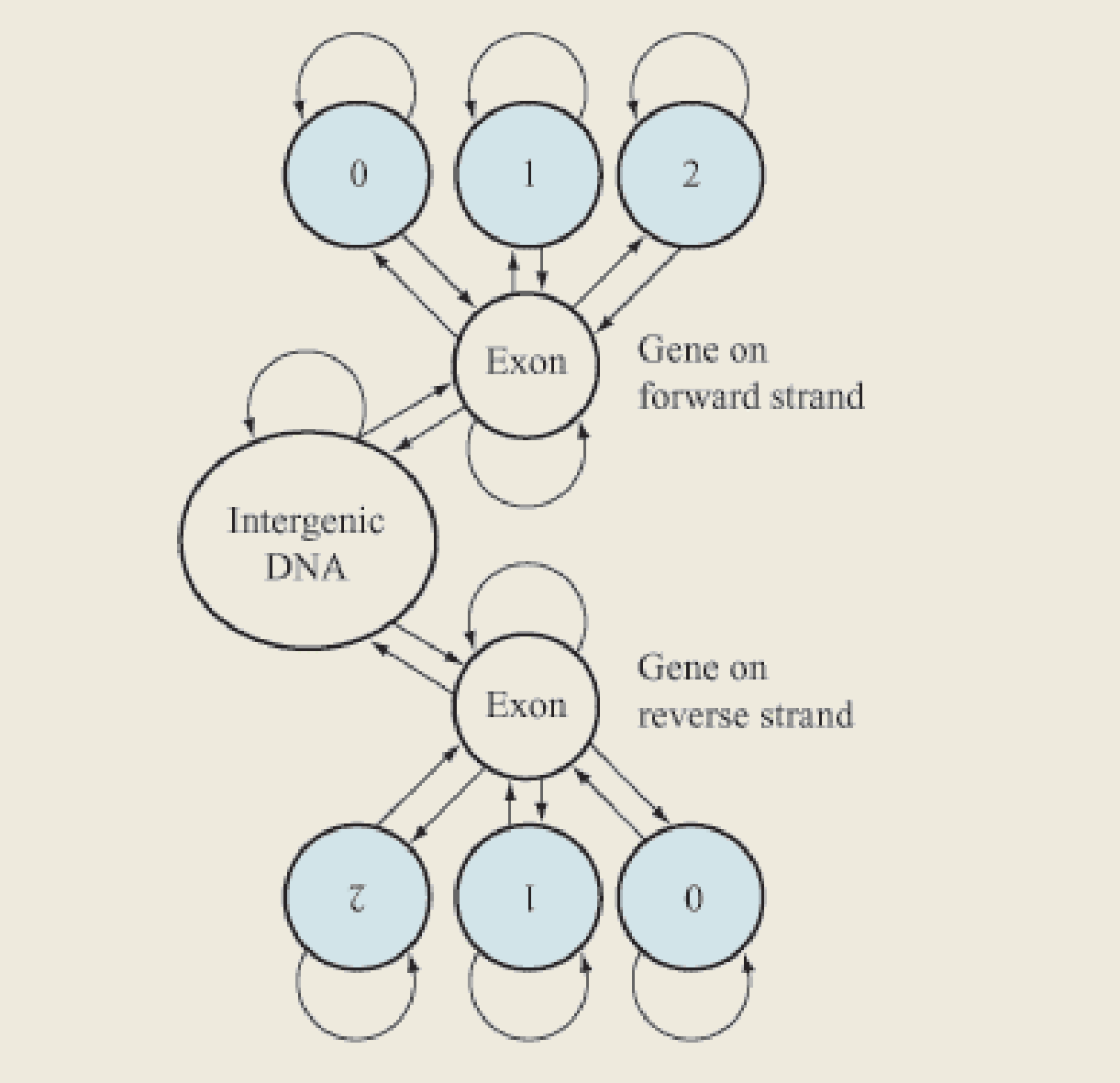
$$\Phi_{a,s}\left(\mathbf{x}\right) = \sum_{\mathbf{y}\in\mathcal{S}^*} P\left(\mathbf{y}|\mathbf{x}\right) n_{a,s}\left(\mathbf{x},\mathbf{y}\right)$$

Computation of the 1-spectrum marginalized kernel

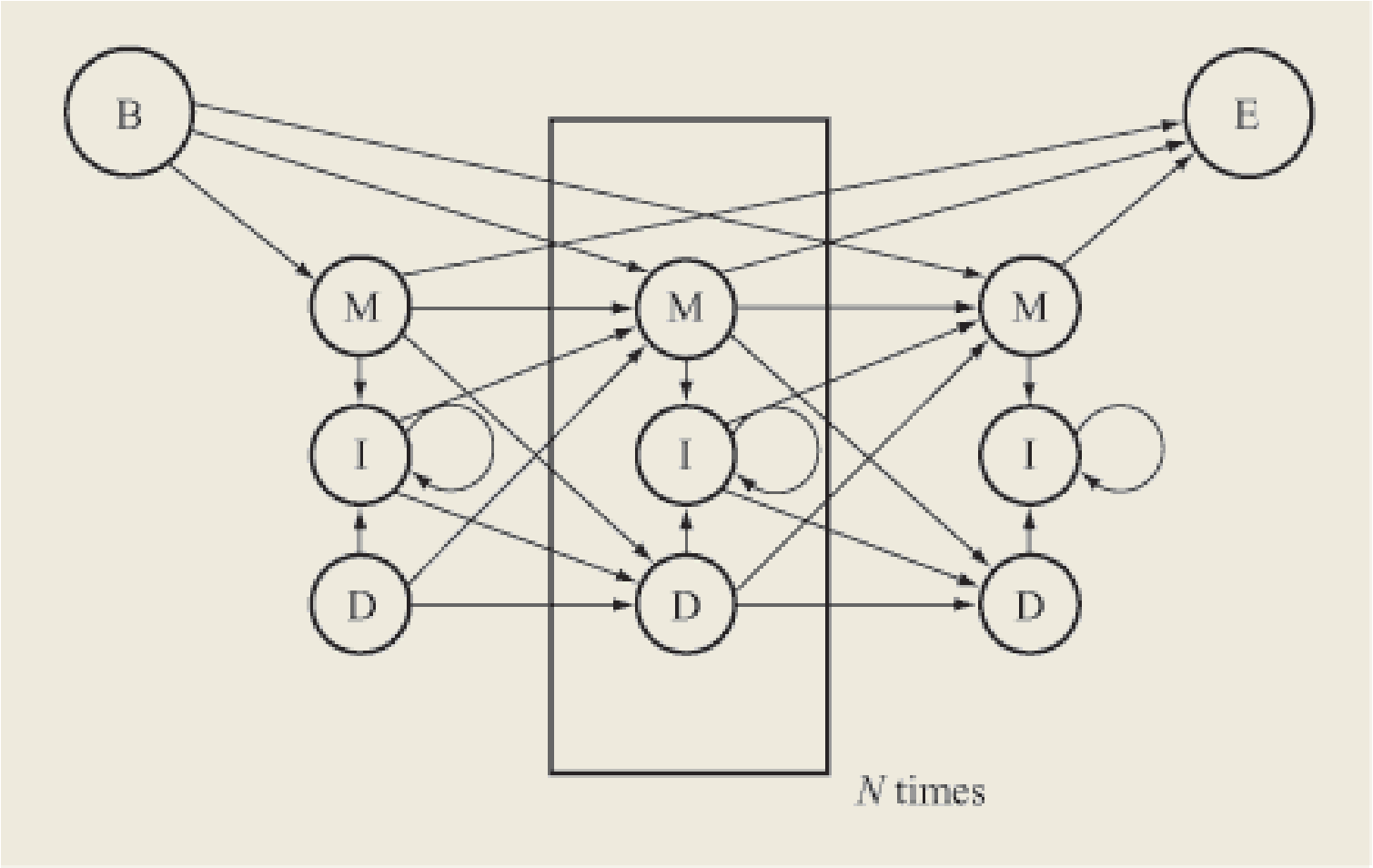
$$
\begin{aligned}
\Phi_{a,s}(\mathbf{x}) &= \sum_{\mathbf{y}\in\mathcal{S}^*} P(\mathbf{y}|\mathbf{x})\, n_{a,s}(\mathbf{x},\mathbf{y}) \\
&= \sum_{\mathbf{y}\in\mathcal{S}^*} P(\mathbf{y}|\mathbf{x}) \left\{ \sum_{i=1}^{n} \delta(x_i, a)\, \delta(y_i, s) \right\} \\
&= \sum_{i=1}^{n} \delta(x_i, a) \left\{ \sum_{\mathbf{y}\in\mathcal{S}^*} P(\mathbf{y}|\mathbf{x})\, \delta(y_i, s) \right\} \\
&= \sum_{i=1}^{n} \delta(x_i, a)\, P(y_i = s|\mathbf{x})\,.
\end{aligned}
$$

and $P(y_i = s|\mathbf{x})$ can be computed efficiently by forward-backward algorithm!

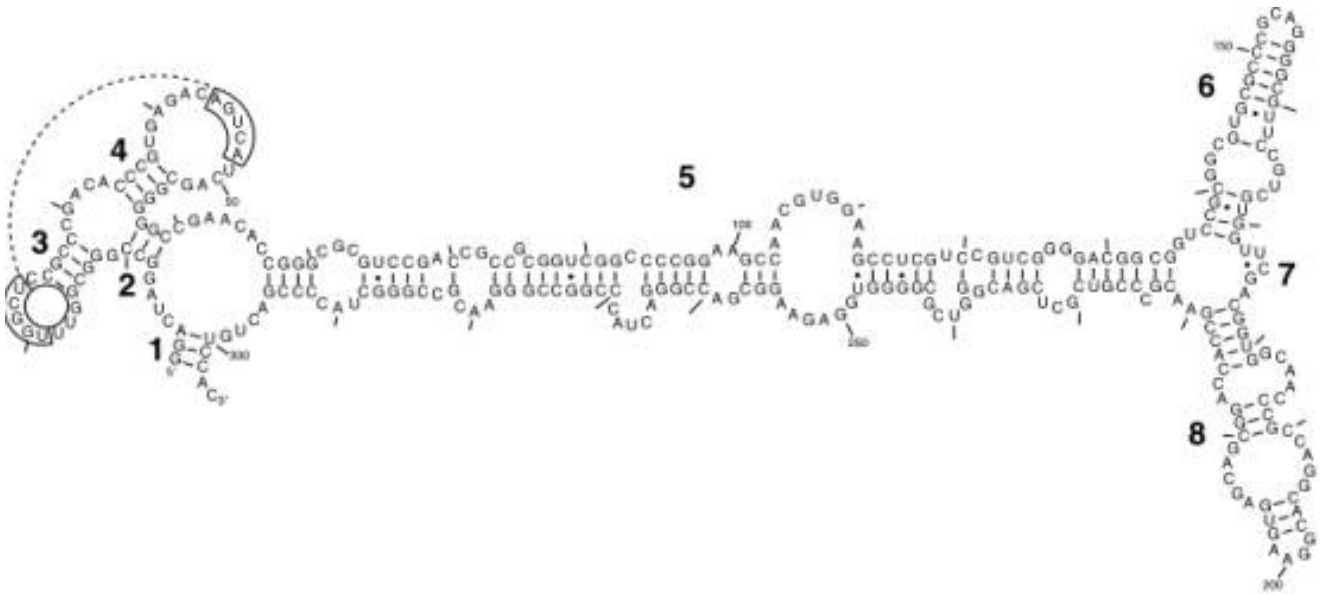
HMM example (DNA)



HMM example (protein)



SCFG for RNA sequences



SFCG rules

- $S \to SS$
- $S \to aSa$
- $S \to aS$
- $S \to a$

Marginalized kernel (Kin et al., 2002)

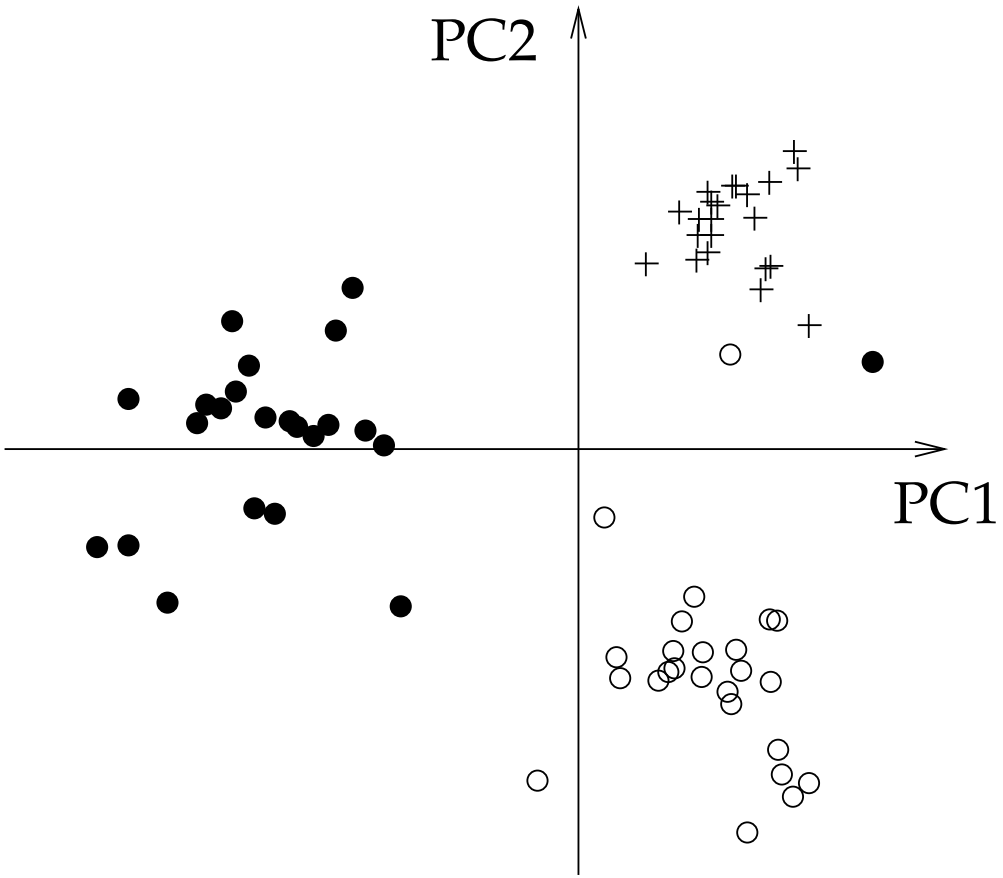
- Feature: number of occurrences of each (base,state) combination
- Marginalization using classical inside/outside algorithm

Marginalized kernels in practice

Examples

- Spectrum kernel on the hidden states of a HMM for protein sequences (Tsuda et al., 2002)
- Kernels for RNA sequences based on SCFG (Kin et al., 2002)
- Kernels for graphs based on random walks on graphs (Kashima et al., 2004)
- Kernels for multiple alignments based on phylogenetic models (Vert et al., 2006)

Marginalized kernels: example



A set of 74 human tRNA sequences is analyzed using a kernel for sequences (the second-order marginalized kernel based on SCFG). This set of tRNAs contains three classes, called Ala-AGC (*white circles*), Asn-GTT (*black circles*) and Cys-GCA (*plus symbols*) (from Tsuda et al., 2002).

Outline

Sequence alignment

Motivation

How to compare 2 sequences?

$$\mathbf{x}_1 = \texttt{CGGSLIAMMWFGV}$$
$$\mathbf{x}_2 = \texttt{CLIVMMNRLMWFGV}$$

Find a good alignment:

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

Alignment score

In order to quantify the relevance of an alignment π, define:

- a substitution matrix $S \in \mathbb{R}^{\mathcal{A} \times \mathcal{A}}$
- a gap penalty function $g : \mathbb{N} \to \mathbb{R}$

Any alignment is then scored as follows

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

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

Local alignment kernel

Smith-Waterman score (Smith and Waterman, 1981)

- The widely-used Smith-Waterman local alignment score is defined by:

$$SW_{S,g}(\mathbf{x},\mathbf{y}) := \max_{\pi \in \Pi(\mathbf{x},\mathbf{y})} s_{S,g}(\pi).$$

- It is symmetric, but not positive definite...

LA kernel (Saigo et al., 2004)

The local alignment kernel:

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

is symmetric positive definite.

Local alignment kernel

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is symmetric positive definite.

LA kernel is p.d.: proof (1/11)

Lemma

- If K_1 and K_2 are p.d. kernels, then:

$$K_1 + K_2,$$
$$K_1 K_2, \text{ and}$$
$$cK_1, \text{ for } c \geq 0,$$

  are also p.d. kernels
- If $(K_i)_{i \geq 1}$ is a sequence of p.d. kernels that converges pointwisely to a function K:

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

  then K is also a p.d. kernel.

LA kernel is p.d.: proof (2/11)

Proof of lemma

Let A and B be $n \times n$ positive semidefinite matrices. By diagonalization of A:

$$A_{i,j} = \sum_{p=1}^{n} f_p(i) f_p(j)$$

for some vectors $f_1, \ldots, f_n$. Then, for any $\alpha \in \mathbb{R}^n$:

$$\sum_{i,j=1}^{n} \alpha_i \alpha_j A_{i,j} B_{i,j} = \sum_{p=1}^{n} \sum_{i,j=1}^{n} \alpha_i f_p(i) \alpha_j f_p(j) B_{i,j} \geq 0.$$

The matrix $C_{i,j} = A_{i,j} B_{i,j}$ is therefore p.d. Other properties are obvious from definition. $\square$

LA kernel is p.d.: proof (3/11)

Lemma (direct sum and product of kernels)

Let $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2$. Let K_1 be a p.d. kernel on $\mathcal{X}_1$, and K_2 be a p.d. kernel on $\mathcal{X}_2$. Then the following functions are p.d. kernels on $\mathcal{X}$:

- the direct sum,

$$K\left((\mathbf{x}_1, \mathbf{x}_2), (\mathbf{y}_1, \mathbf{y}_2)\right) = K_1\left(\mathbf{x}_1, \mathbf{y}_1\right) + K_2\left(\mathbf{x}_2, \mathbf{y}_2\right),$$

- The direct product:

$$K\left((\mathbf{x}_1, \mathbf{x}_2), (\mathbf{y}_1, \mathbf{y}_2)\right) = K_1\left(\mathbf{x}_1, \mathbf{y}_1\right) K_2\left(\mathbf{x}_2, \mathbf{y}_2\right).$$

LA kernel is p.d.: proof (4/11)

Proof of lemma

If K_1 is a p.d. kernel, let $\Phi_1 : \mathcal{X}_1 \mapsto \mathcal{H}$ be such that:

$$K_1(\mathbf{x}_1, \mathbf{y}_1) = \langle \Phi_1(\mathbf{x}_1), \Phi_1(\mathbf{y}_1) \rangle_{\mathcal{H}}.$$

Let $\Phi : \mathcal{X}_1 \times \mathcal{X}_2 \to \mathcal{H}$ be defined by:

$$\Phi((\mathbf{x}_1, \mathbf{x}_2)) = \Phi_1(\mathbf{x}_1).$$

Then for $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$ and $\mathbf{y} = (\mathbf{y}_1, \mathbf{y}_2) \in \mathcal{X}$, we get

$$\langle \Phi((\mathbf{x}_1, \mathbf{x}_2)), \Phi((\mathbf{y}_1, \mathbf{y}_2)) \rangle_{\mathcal{H}} = K_1(\mathbf{x}_1, \mathbf{x}_2),$$

which shows that $K(\mathbf{x}, \mathbf{y}) := K_1(\mathbf{x}_1, \mathbf{y}_1)$ is p.d. on $\mathcal{X}_1 \times \mathcal{X}_2$. The lemma follows from the properties of sums and products of p.d. kernels. $\square$

LA kernel is p.d.: proof (5/11)

Lemma: kernel for sets

Let K be a p.d. kernel on $\mathcal{X}$, and let $\mathcal{P}(\mathcal{X})$ be the set of finite subsets of $\mathcal{X}$. Then the function K_P on $\mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{X})$ defined by:

$$\forall A, B \in \mathcal{P}(\mathcal{X}), \quad K_P(A, B) := \sum_{\mathbf{x} \in A} \sum_{\mathbf{y} \in B} K(\mathbf{x}, \mathbf{y})$$

is a p.d. kernel on $\mathcal{P}(\mathcal{X})$.

LA kernel is p.d.: proof (6/11)

Proof of lemma

Let $\Phi : \mathcal{X} \mapsto \mathcal{H}$ be such that

$$K(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}}.$$

Then, for $A, B \in \mathcal{P}(\mathcal{X})$, we get:

$$\begin{aligned} K_P(A, B) &= \sum_{\mathbf{x} \in A} \sum_{\mathbf{y} \in B} \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}} \\ &= \left\langle \sum_{\mathbf{x} \in A} \Phi(\mathbf{x}), \sum_{\mathbf{y} \in B} \Phi(\mathbf{y}) \right\rangle_{\mathcal{H}} \\ &= \langle \Phi_P(A), \Phi_P(B) \rangle_{\mathcal{H}}, \end{aligned}$$

with $\Phi_P(A) := \sum_{\mathbf{x} \in A} \Phi(\mathbf{x})$. $\square$

LA kernel is p.d.: proof (7/11)

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 (8/11)

Proof of lemma

Let $\mathcal{X}$ be the set of finite-length strings. For $\mathbf{x} \in \mathcal{X}$, let

$$R(\mathbf{x}) = \{(\mathbf{x}_1, \mathbf{x}_2) \in \mathcal{X} \times \mathcal{X} : \mathbf{x} = \mathbf{x}_1 \mathbf{x}_2\} \subset \mathcal{X} \times \mathcal{X} \,.$$

We can then write

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

which is a p.d. kernel by the previous lemmas. $\square$

LA kernel is p.d.: proof (9/11)

3 basic string kernels

- 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:

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

LA kernel is p.d.: proof (10/11)

Remark

- $S : \mathcal{A}^2 \to \mathbb{R}$ is the similarity function between letters used in the alignment score. $K_a^{(\beta)}$ is only p.d. when the matrix:

$$\left(\exp\left(\beta s(a,b)\right)\right)_{(a,b)\in\mathcal{A}^2}$$

  is positive semidefinite (this is true for all β when s is conditionally p.d..
- g is the gap penalty function used in alignment score. The gap kernel is always p.d. (with no restriction on g) because it can be written as:

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

LA kernel is p.d.: proof (11/11)

Lemma

The local alignment kernel is a (limit) of convolution kernel:

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

As such it is p.d..

Proof (sketch)

- By induction on n (simple but long to write).
- See details in Vert et al. (2004).

LA kernel computation

- We assume an affine gap penalty:

$$\begin{cases} g(0) & = 0, \\ g(n) & = d + e(n-1) \text{ si } n \geq 1, \end{cases}$$

- The LA kernel can then be computed by dynamic programming by:

$$K_{LA}^{(\beta)}(\mathbf{x}, \mathbf{y}) = 1 + X_2(|\mathbf{x}|, |\mathbf{y}|) + Y_2(|\mathbf{x}|, |\mathbf{y}|) + M(|\mathbf{x}|, |\mathbf{y}|),$$

where $M(i,j), X(i,j), Y(i,j), X_2(i,j)$, and $Y_2(i,j)$ for $0 \leq i \leq |\mathbf{x}|$, and $0 \leq j \leq |\mathbf{y}|$ are defined recursively.

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

Initialization

$$\begin{cases} M(i,0) = M(0,j) = 0, \\ X(i,0) = X(0,j) = 0, \\ Y(i,0) = Y(0,j) = 0, \\ X_2(i,0) = X_2(0,j) = 0, \\ Y_2(i,0) = Y_2(0,j) = 0, \end{cases}$$

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

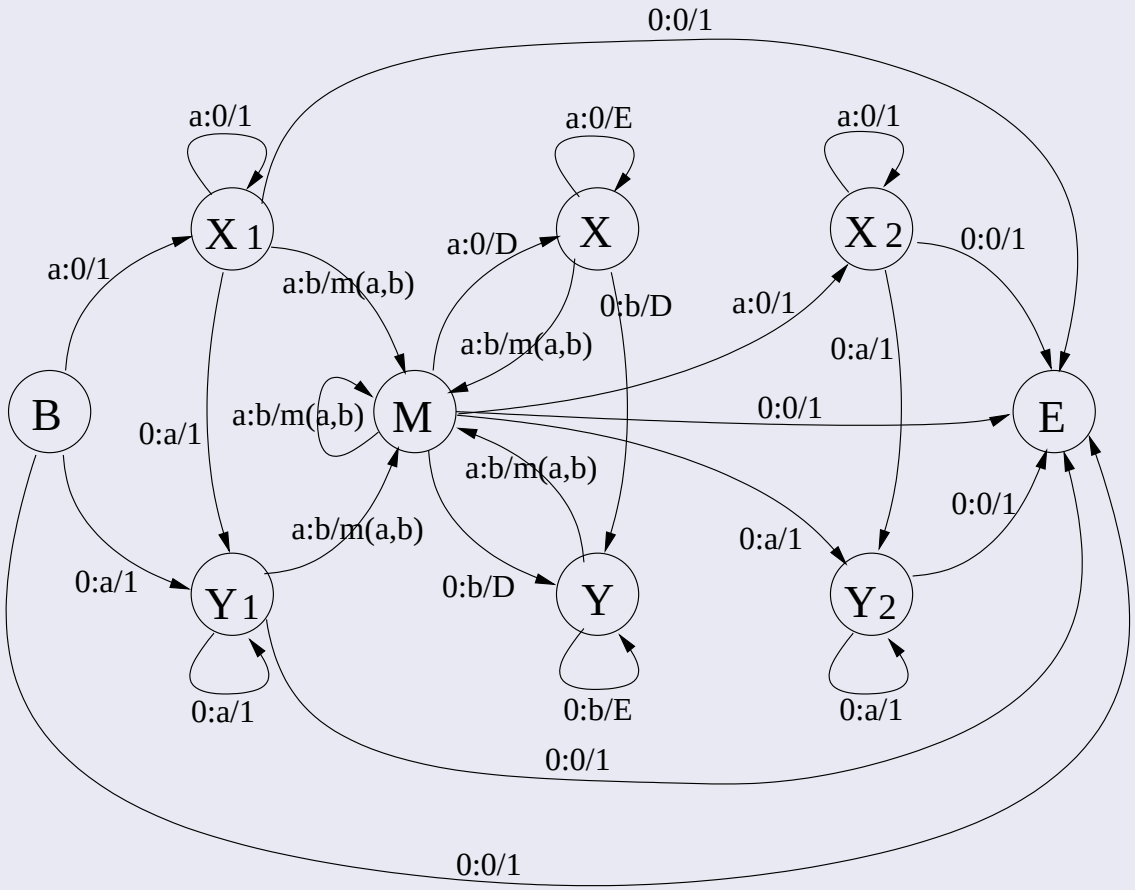
Recursion

For $i = 1, \ldots, |\mathbf{x}|$ and $j = 1, \ldots, |\mathbf{y}|$:

$$
\begin{cases}
M(i,j) & = \exp(\beta S(x_i, y_j)) \Big[1 + X(i-1, j-1) \\
& \qquad + Y(i-1, j-1) + M(i-1, j-1) \Big], \\
X(i,j) & = \exp(\beta d) M(i-1, j) + \exp(\beta e) X(i-1, j), \\
Y(i,j) & = \exp(\beta d) \left[M(i, j-1) + X(i, j-1) \right] \\
& \qquad + \exp(\beta e) Y(i, j-1), \\
X_2(i,j) & = M(i-1, j) + X_2(i-1, j), \\
Y_2(i,j) & = M(i, j-1) + X_2(i, j-1) + Y_2(i, j-1).
\end{cases}
$$

LA kernel in practice

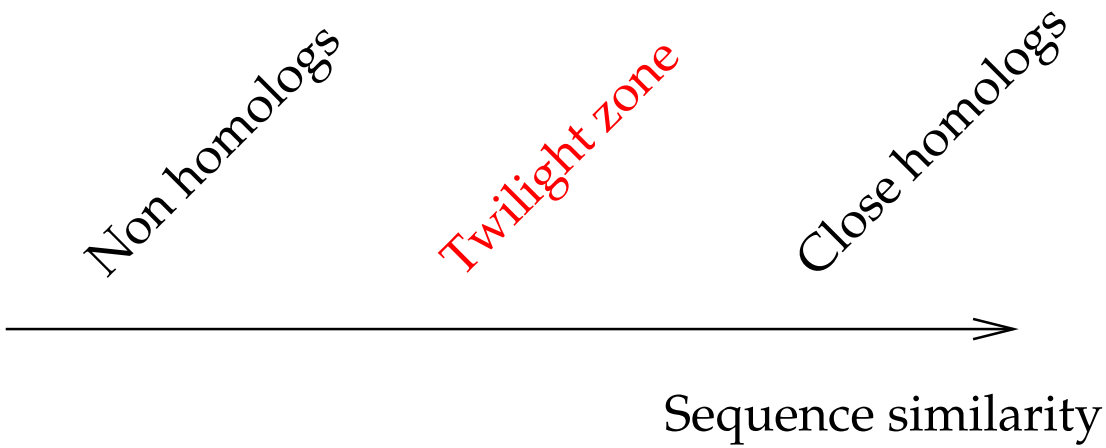
- Implementation by a finite-state transducer in $O(|\mathbf{x}| \times |\mathbf{x}'|)$



- In practice, values are too large (exponential scale) so taking its logarithm is a safer choice (but not p.d. anymore!)

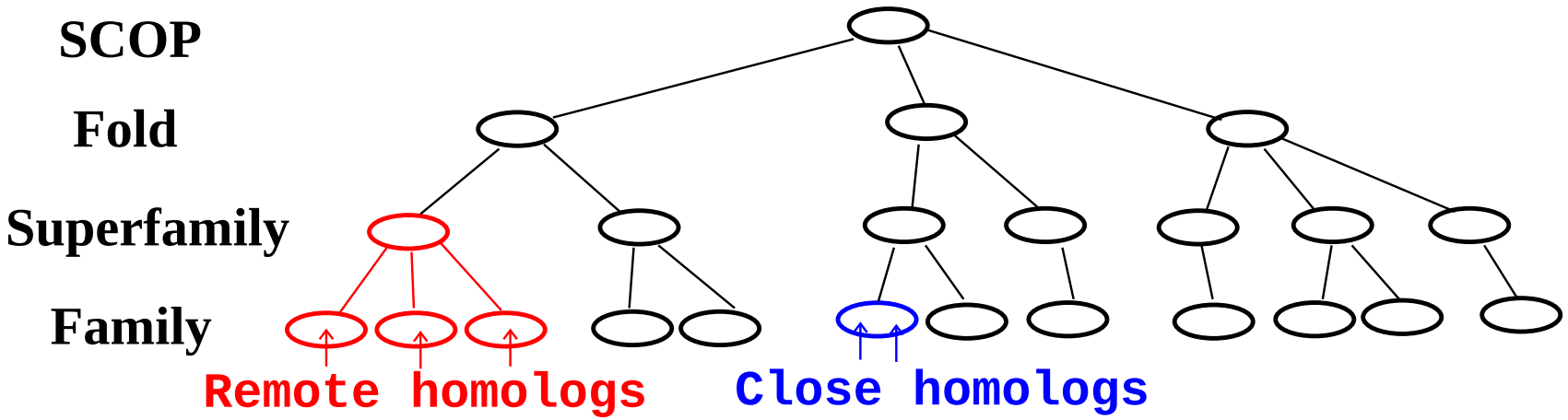
Outline

Remote homology



- Homologs have common ancestors
- Structures and functions are more conserved than sequences
- Remote homologs can not be detected by direct sequence comparison

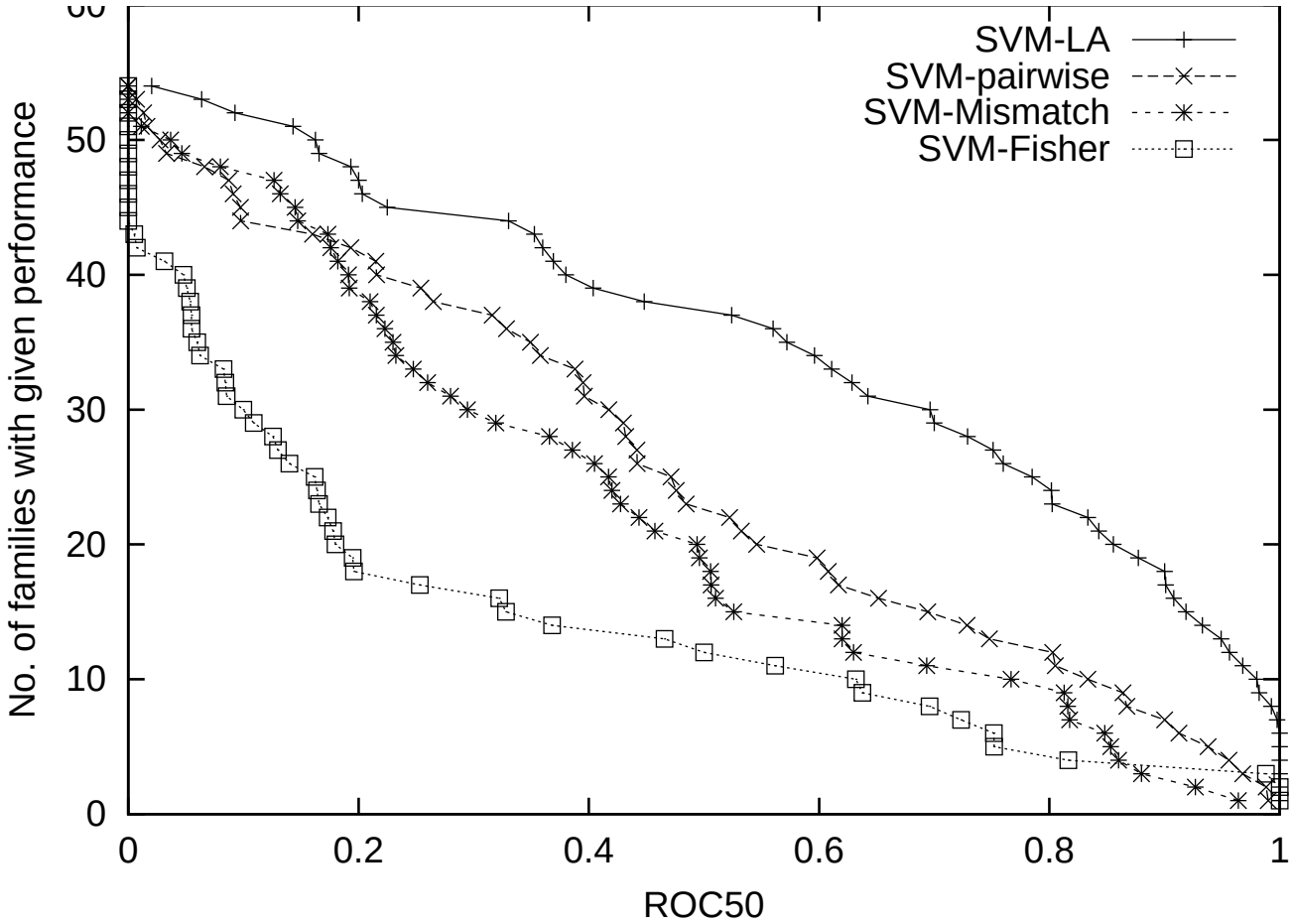
SCOP database



A benchmark experiment

- Goal: recognize directly the superfamily
- Training: for a sequence of interest, positive examples come from the same superfamily, but different families. Negative from other superfamilies.
- Test: predict the superfamily.

Difference in performance



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

String kernels: Summary

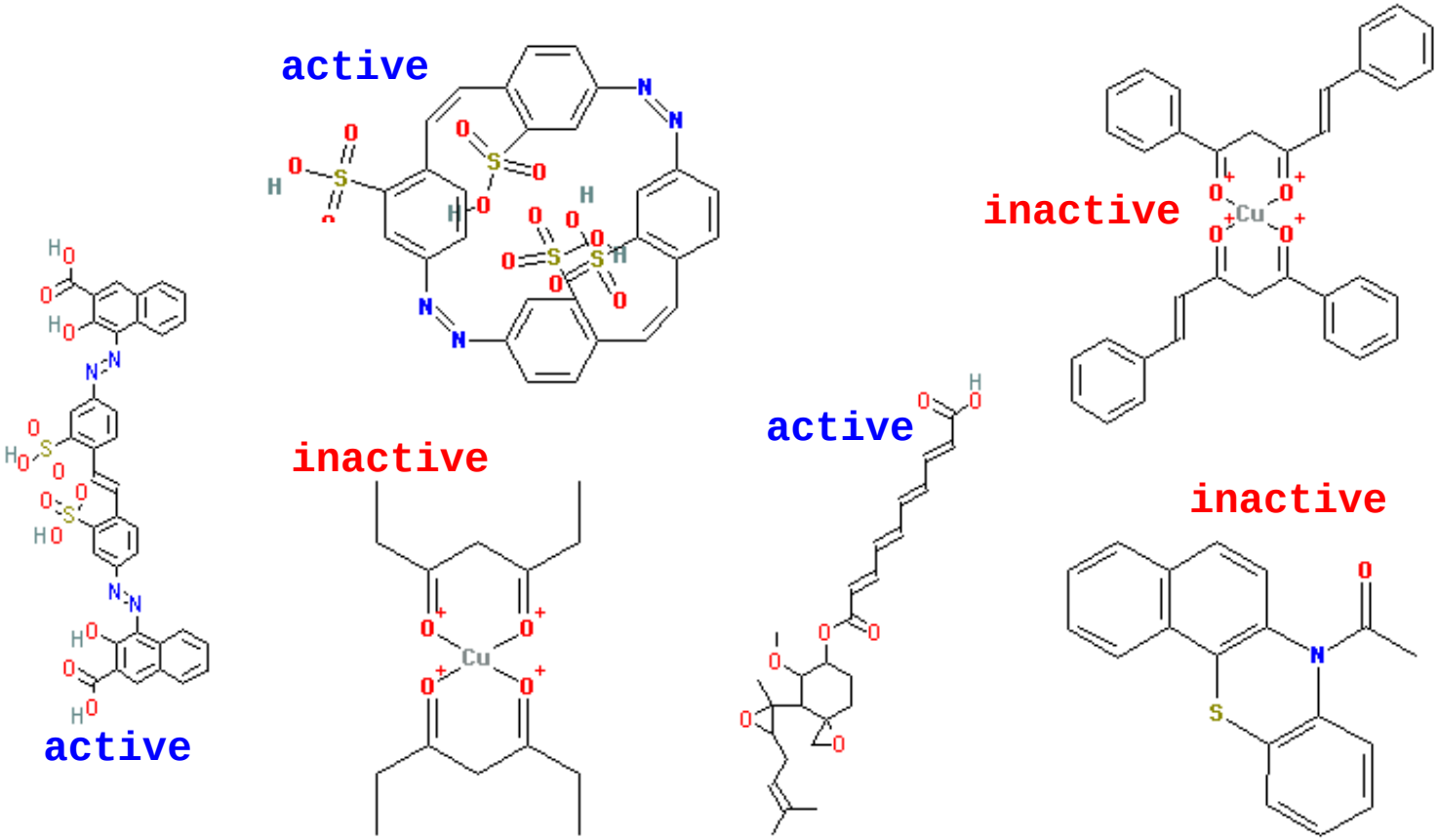
- A variety of principles for string kernel design have been proposed.
- Good kernel design is important for each data and each task. Performance is not the only criterion.
- Still an art, although principled ways have started to emerge.
- Fast implementation with string algorithms is often possible.
- Their application goes well beyond computational biology.

Part 3

Kernels for graphs

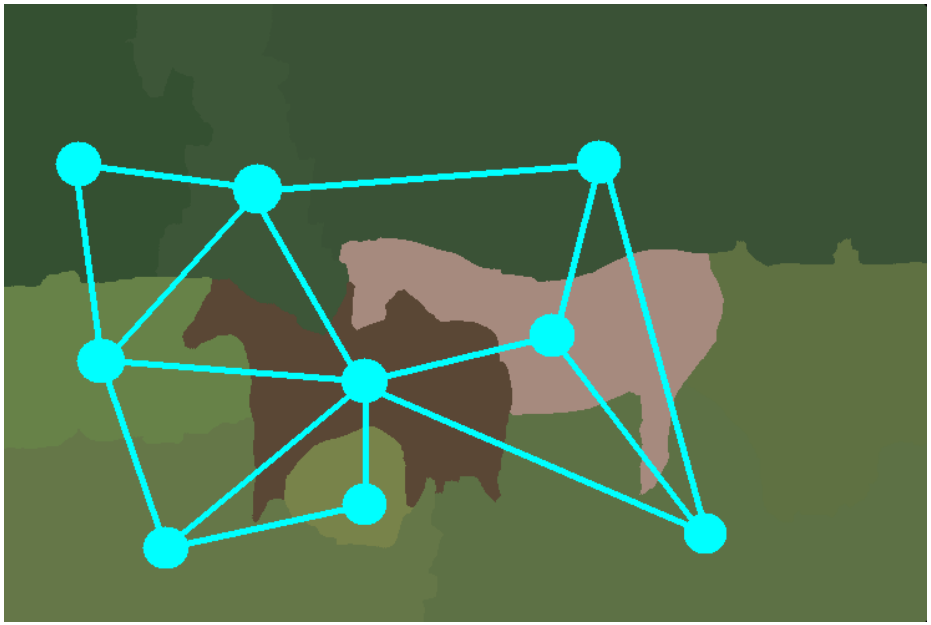
Outline

Virtual screening for drug discovery



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

Image retrieval and classification



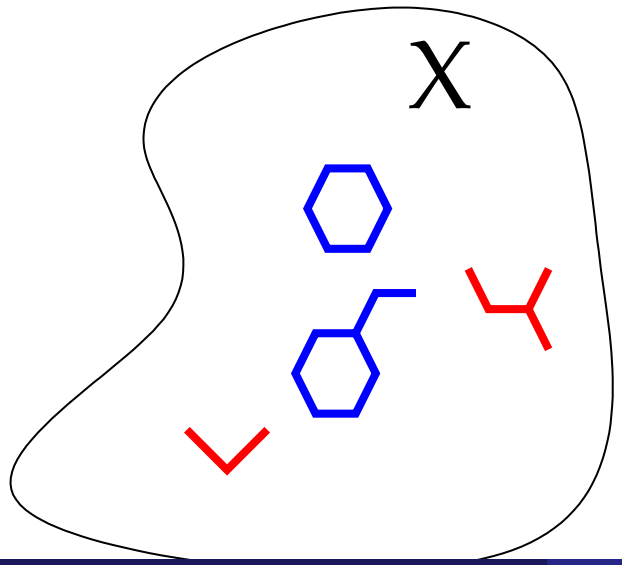
From Harchaoui and Bach (2007).

Our approach

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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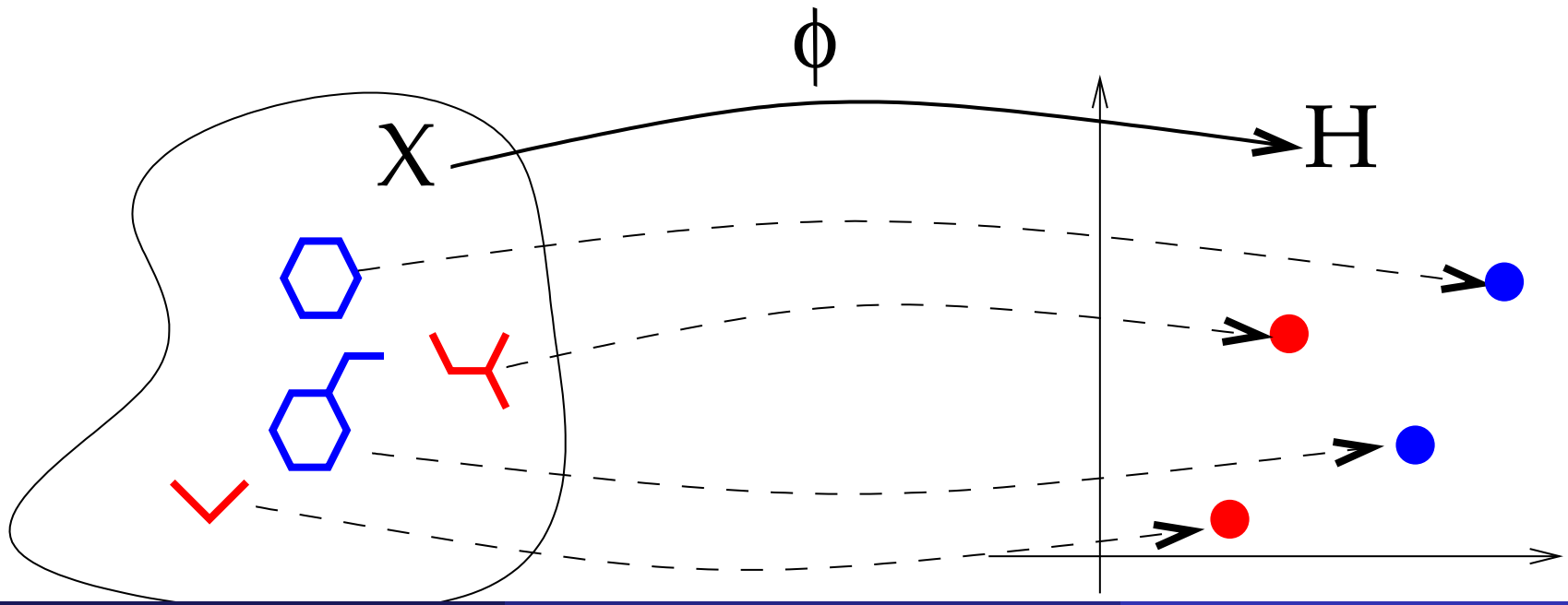

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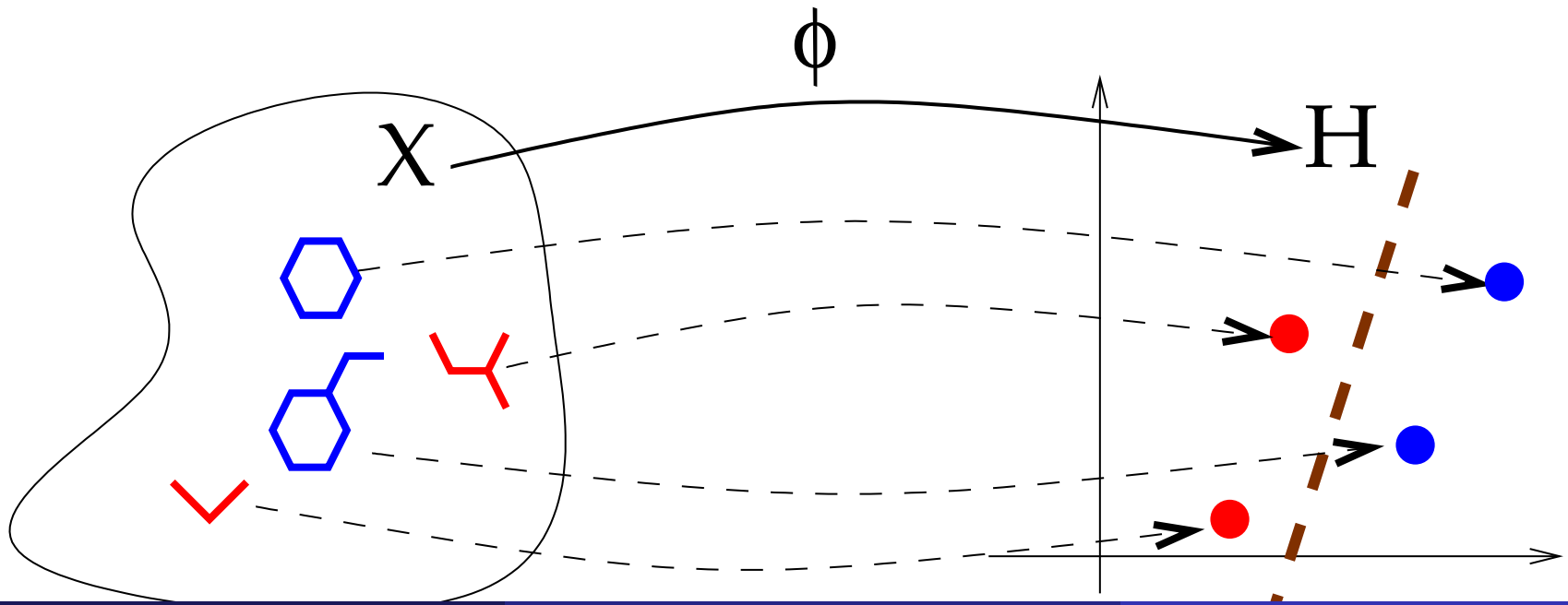
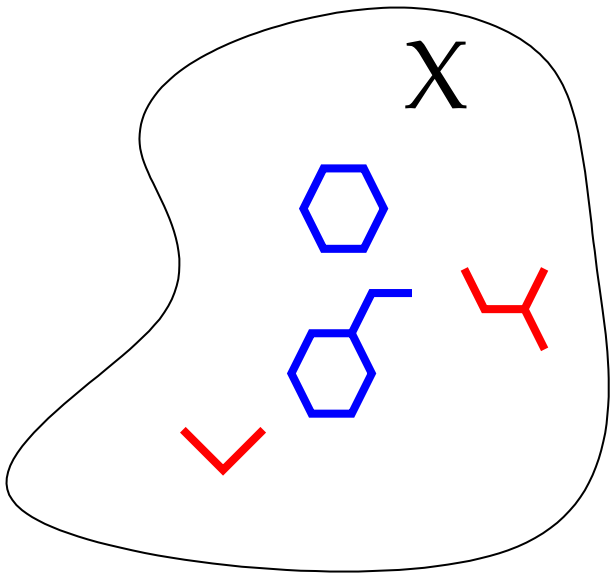


Outline

The approach

1. Represent explicitly each graph x by a vector of fixed dimension $\Phi(x) \in \mathbb{R}^p$.
2. Use an algorithm for regression or pattern recognition in $\mathbb{R}^p$.



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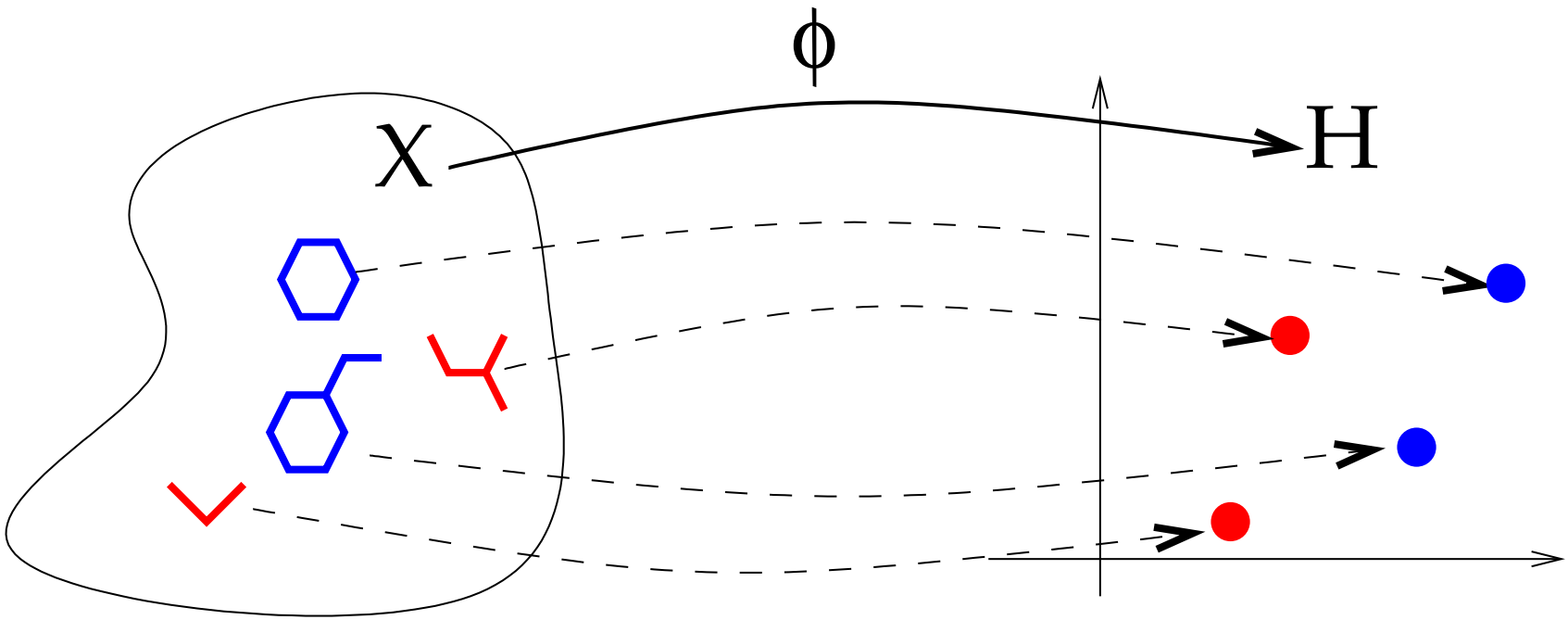

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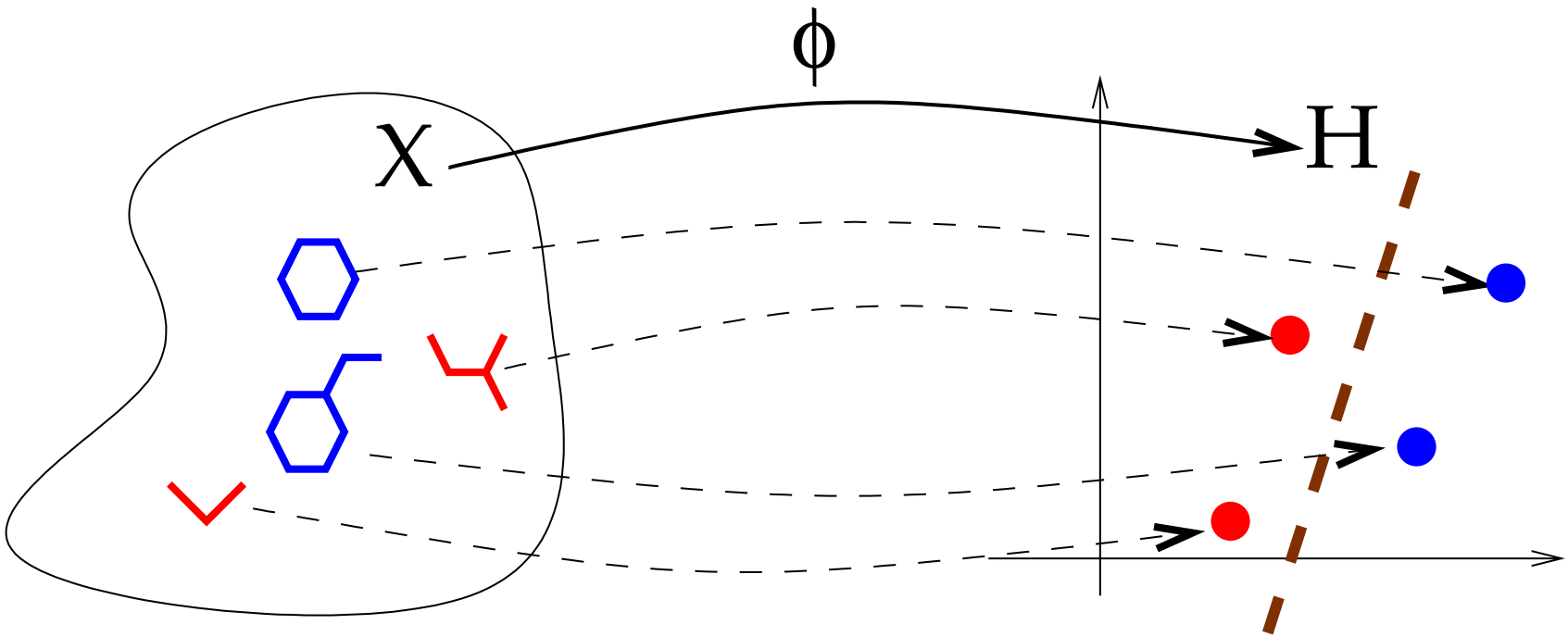
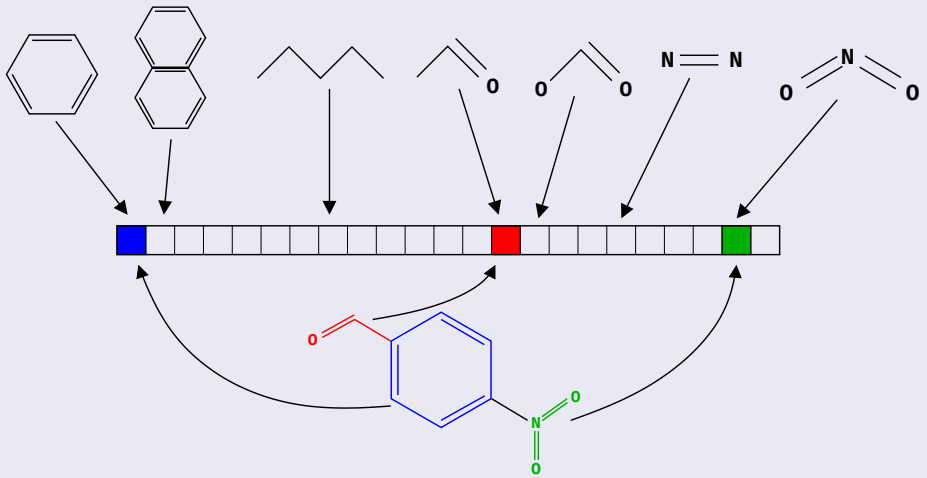


Example

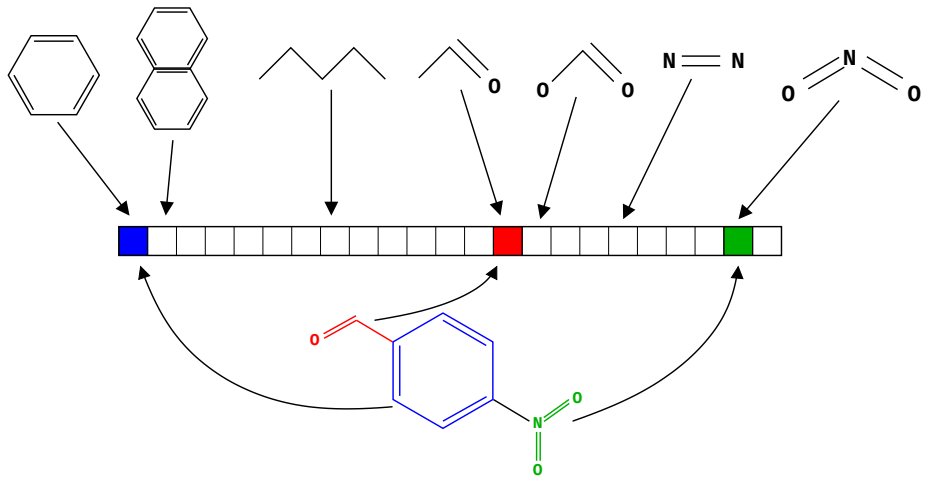
2D structural keys in chemoinformatics

- Index a molecule by a binary fingerprint defined by a limited set of pre-defined stuctures



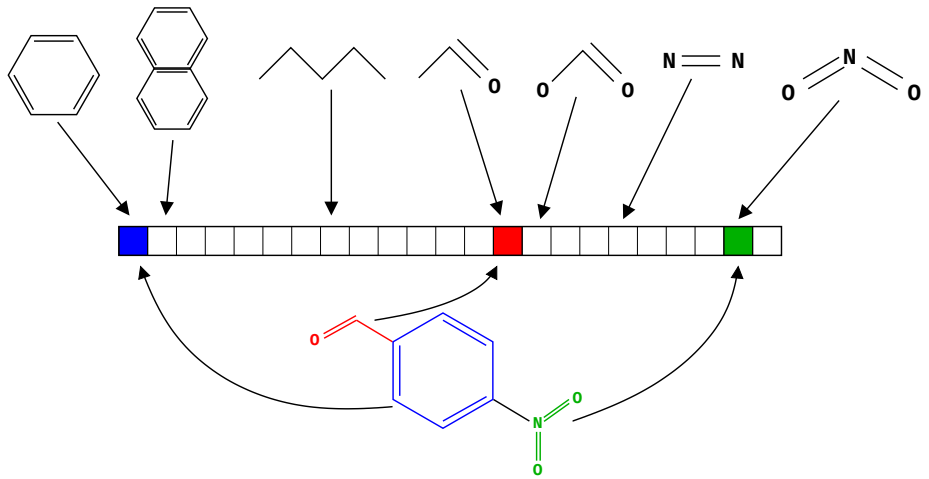
- Use a machine learning algorithms such as SVM, NN, PLS, decision tree, ...

Challenge: which descriptors (patterns)?



- Expressiveness: they should retain as much information as possible from the graph
- Computation : they should be fast to compute
- Large dimension of the vector representation: memory storage, speed, statistical issues

Indexing by substructures

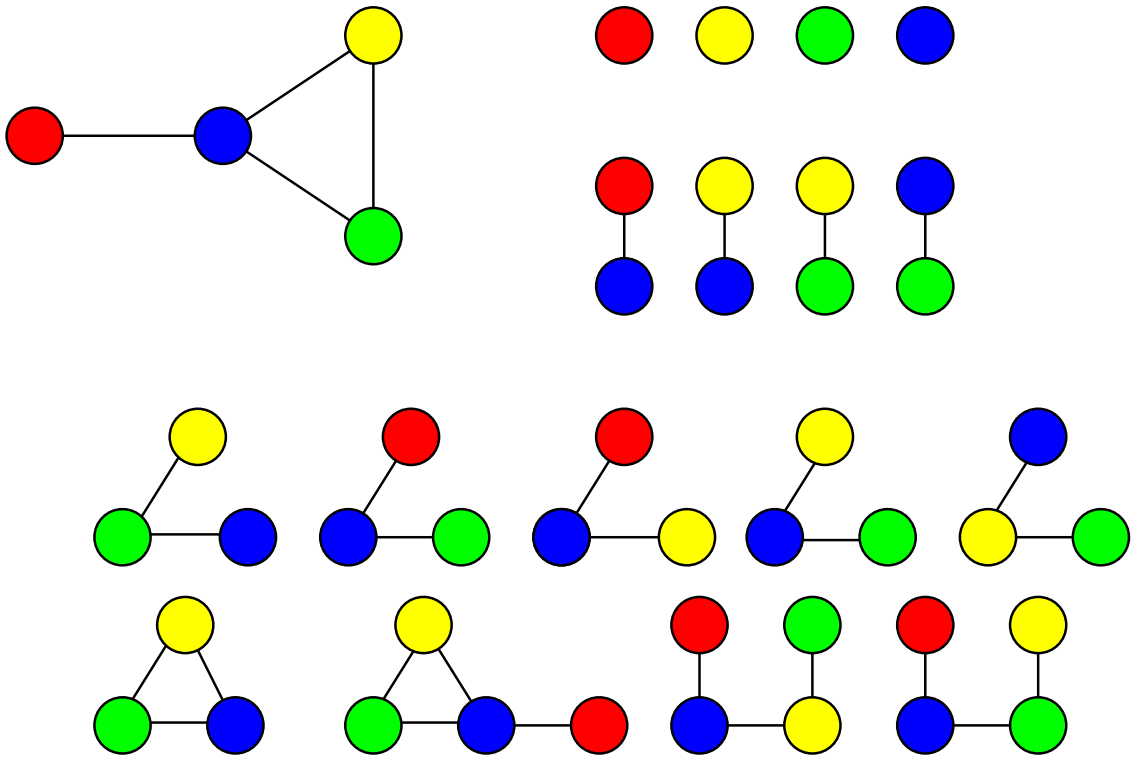


- Often we believe that the presence substructures are important predictive patterns
- Hence it makes sense to represent a graph by features that indicate the presence (or the number of occurrences) of particular substructures
- However, detecting the presence of particular substructures may be computationally challenging...

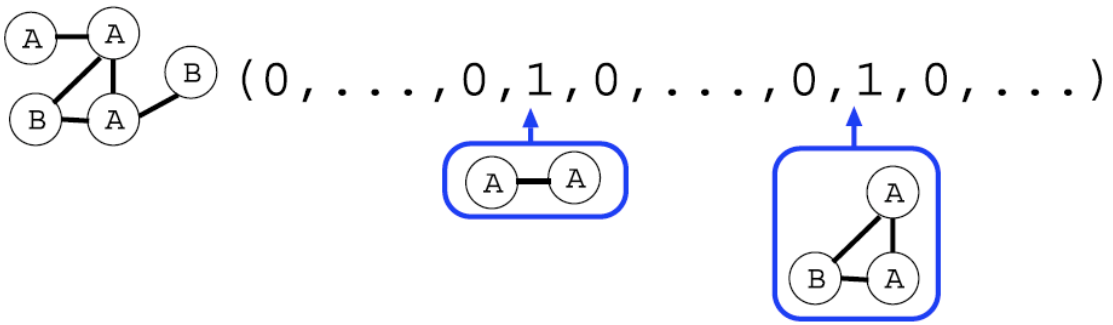
Subgraphs

Definition

A subgraph of a graph (V, E) is a connected graph (V', E') with $V' \subset V$ and $E' \subset E$.



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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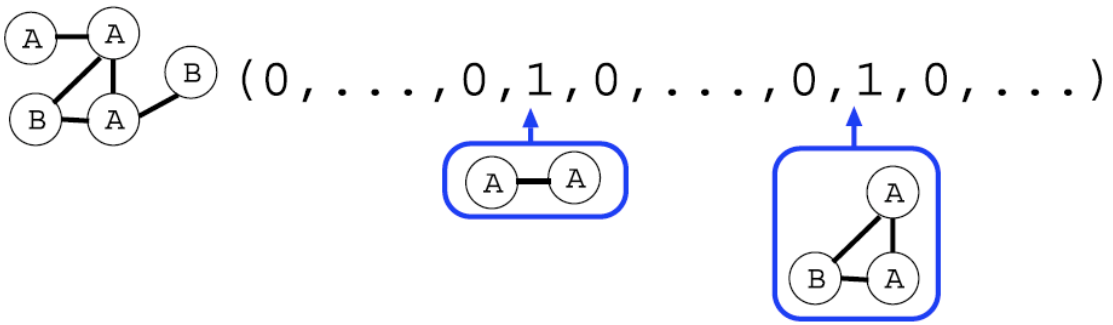

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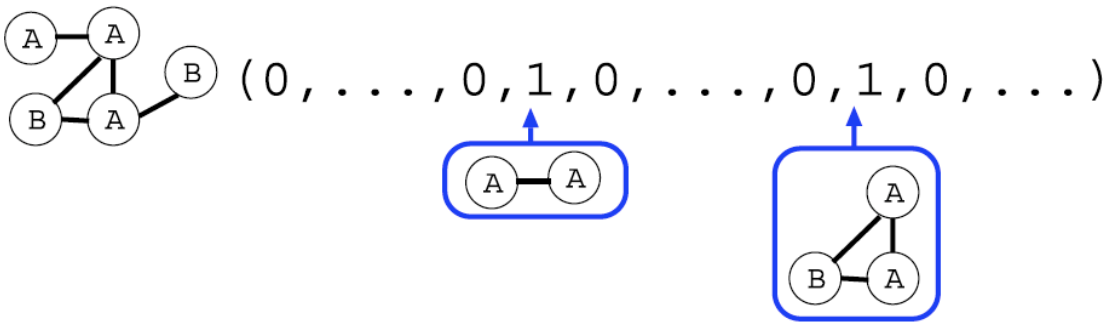

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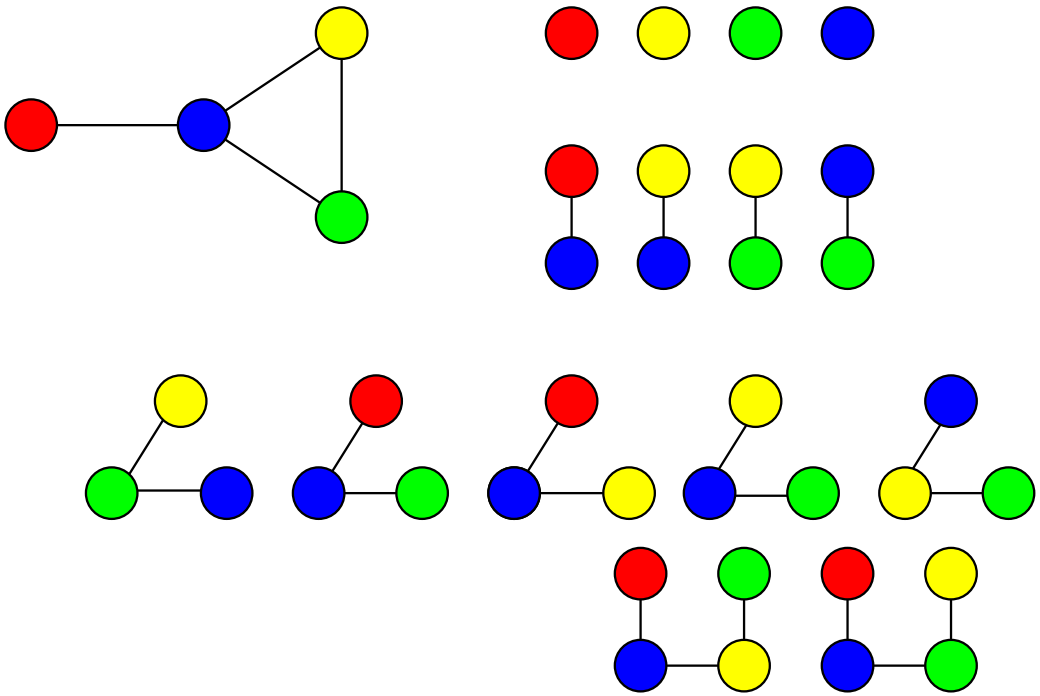
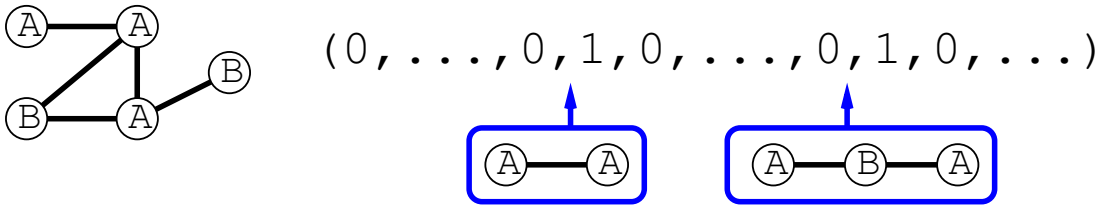
Paths

Definition

- A path of a graph (V, E) is sequence of distinct vertices $v_1, \ldots, v_n \in V$ $(i \neq j \implies v_i \neq v_j)$ such that $(v_i, v_{i+1}) \in E$ for $i = 1, \ldots, n-1$.
- Equivalently the paths are the linear subgraphs.



Indexing by all paths?



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Same as for subgraphs. □

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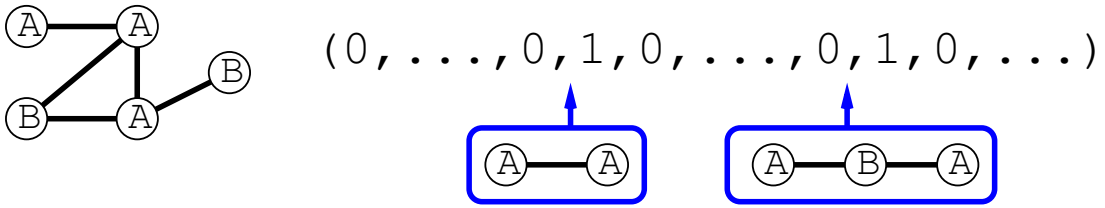

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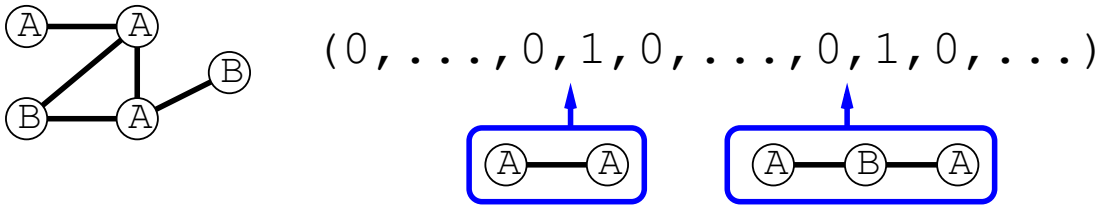

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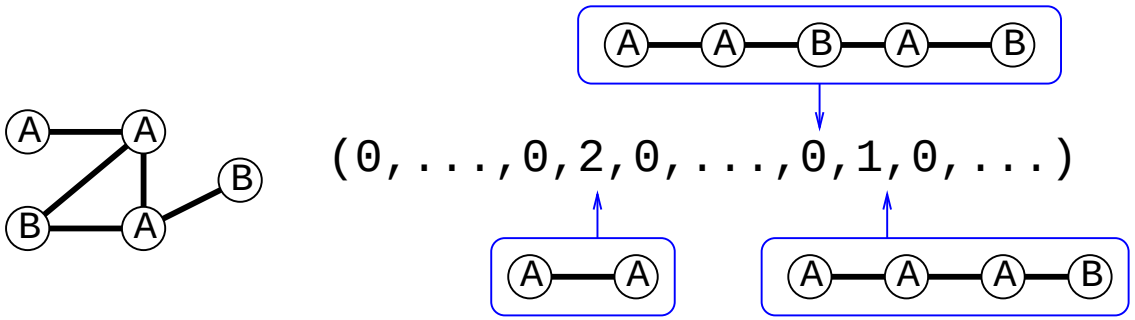
Indexing by what?

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.

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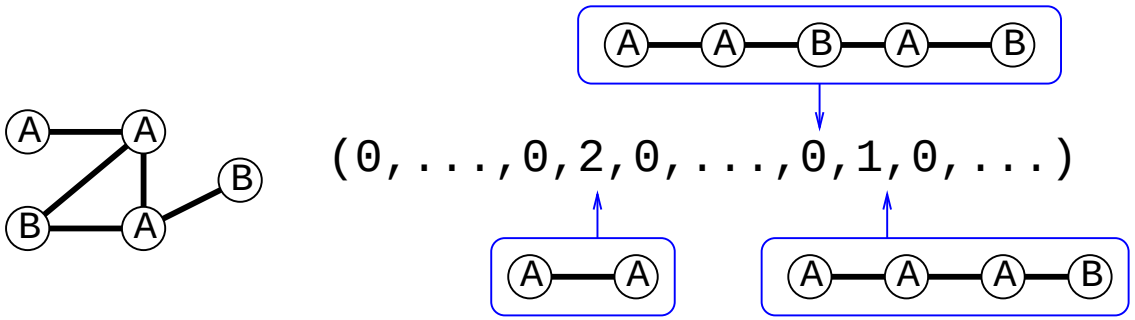

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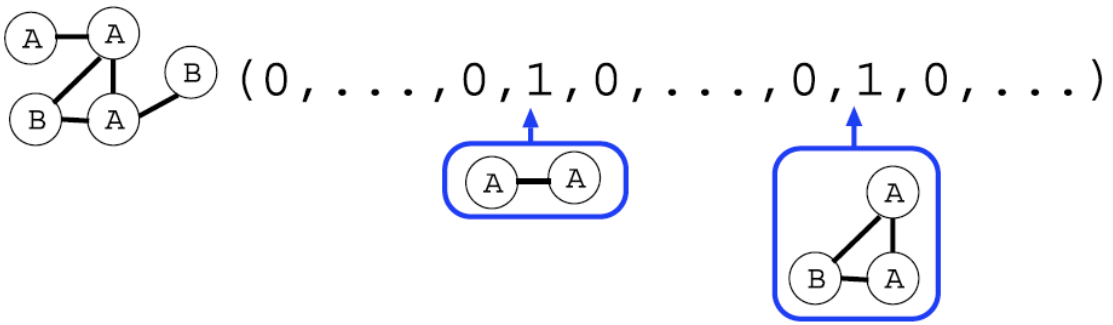

Properties (Shervashidze et al., 2009)

- 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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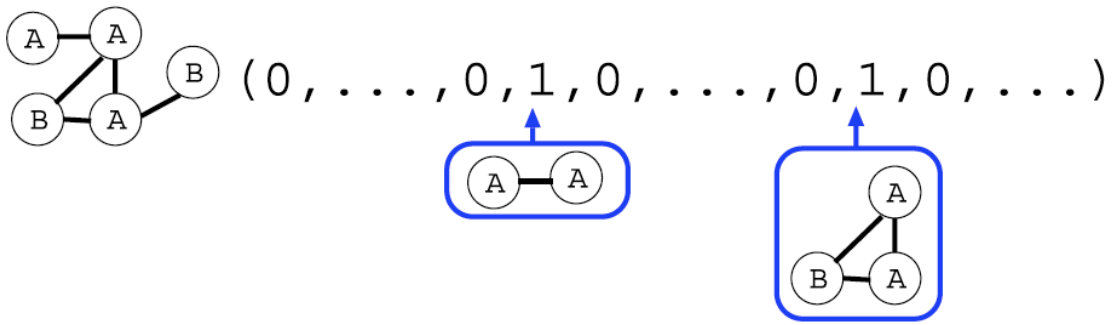

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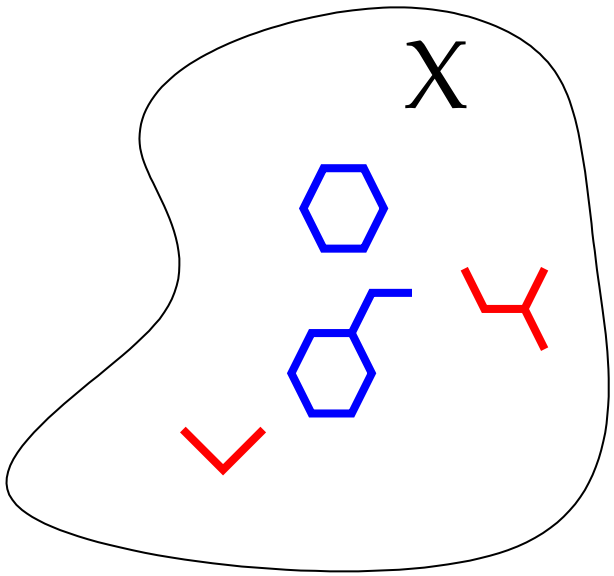
Summary

- Explicit computation of substructure occurrences can be computationnally prohibitive (subgraph, paths)
- Several ideas to reduce the set of substructures considered
- In practice, NP-hardness may not be so prohibitive (e.g., graphs with small degrees), the strategy followed should depend on the data considered.

Outline

The idea

1. Represent implicitly each graph x by a vector $\Phi(x) \in \mathcal{H}$ through the kernel
$$K(x, x') = \Phi(x)^\top \Phi(x') \, .$$
2. Use a kernel method for classification in $\mathcal{H}$.



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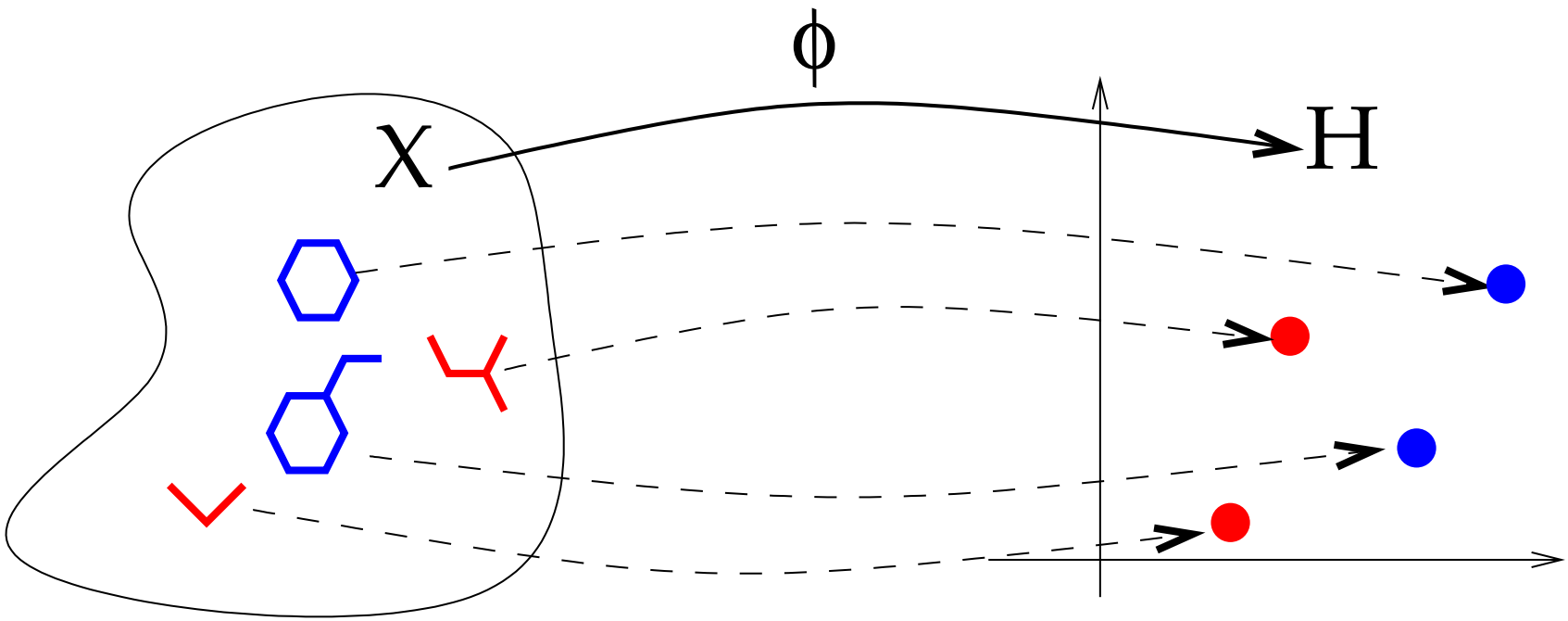

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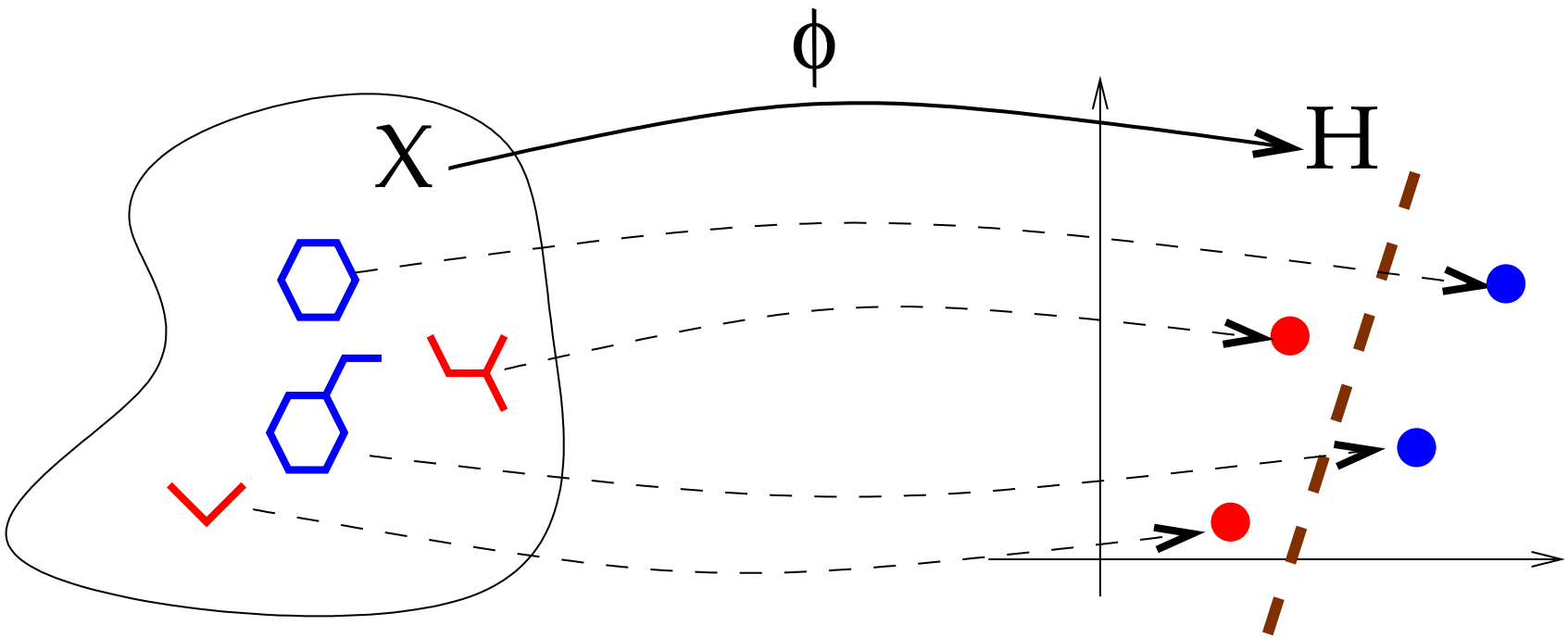

Expressiveness vs Complexity

Definition: Complete graph kernels

A graph kernel is complete if it separates non-isomorphic graphs, i.e.:

$$\forall G_1, G_2 \in \mathcal{X}, \quad d_K(G_1, G_2) = 0 \implies G_1 \simeq G_2 \,.$$

Equivalently, $\Phi(G_1) \neq \Phi(G_1)$ if G_1 and G_2 are not isomorphic.

Expressiveness vs Complexity trade-off

- If a graph kernel is not complete, then there is no hope to learn all possible functions over $\mathcal{X}$: the kernel is not expressive enough.
- On the other hand, kernel computation must be tractable, i.e., no more than polynomial (with small degree) for practical applications.
- Can we define tractable and expressive graph kernels?

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Complexity of complete kernels

Proposition (Gärtner et al., 2003)

Computing any complete graph kernel is at least as hard as the graph isomorphism problem.

Proof

- For any kernel K the complexity of computing d_K is the same as the complexity of computing K, because:

$$d_K(G_1, G_2)^2 = K(G_1, G_1) + K(G_2, G_2) - 2K(G_1, G_2)\,.$$

- If K is a complete graph kernel, then computing d_K solves the graph isomorphism problem ($d_K(G_1, G_2) = 0$ iff $G_1 \simeq G_2$). □

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Subgraph kernel

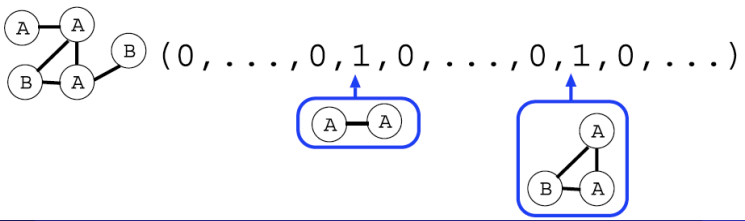
Definition

- Let $(\lambda_G)_{G \in \mathcal{X}}$ a set or nonnegative real-valued weights
- For any graph $G \in \mathcal{X}$, let

$$\forall H \in \mathcal{X}, \quad \Phi_H(G) = \left| \left\{ G' \text{ is a subgraph of } G \,:\, G' \simeq H \right\} \right| .$$

- The subgraph kernel between any two graphs G_1 and $G_2 \in \mathcal{X}$ is defined by:

$$K_{subgraph}(G_1, G_2) = \sum_{H \in \mathcal{X}} \lambda_H \Phi_H(G_1) \Phi_H(G_2) .$$



Subgraph kernel complexity

Proposition (Gärtner et al., 2003)

Computing the subgraph kernel is NP-hard.

Proof (1/2)

- Let P_n be the path graph with n vertices.
- Subgraphs of P_n are path graphs:

$$\Phi(P_n) = n e_{P_1} + (n-1) e_{P_2} + \ldots + e_{P_n} .$$

- The vectors $\Phi(P_1), \ldots, \Phi(P_n)$ are linearly independent, therefore:

$$e_{P_n} = \sum_{i=1}^{n} \alpha_i \Phi(P_i) ,$$

where the coefficients α_i can be found in polynomial time (solving a $n \times n$ triangular system).

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Subgraph kernel complexity

Proposition (Gärtner et al., 2003)

Computing the subgraph kernel is NP-hard.

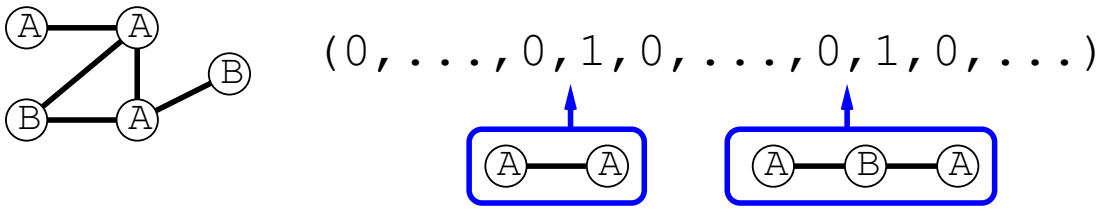
Proof (2/2)

- If G is a graph with n vertices, then it has a path that visits each node exactly once (Hamiltonian path) if and only if $\Phi(G)^\top e_n > 0$, i.e.,

$$\Phi(G)^\top \left(\sum_{i=1}^{n} \alpha_i \Phi(P_i) \right) = \sum_{i=1}^{n} \alpha_i K_{subgraph}(G, P_i) > 0 \,.$$

- The decision problem whether a graph has a Hamiltonian path is NP-complete. $\square$

Path kernel



Definition

The path kernel is the subgraph kernel restricted to paths, i.e.,

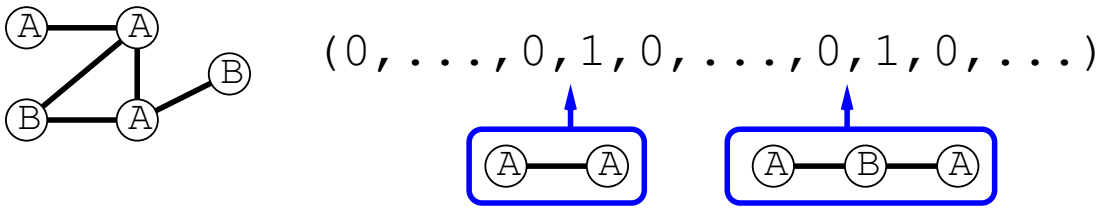
$$K_{path}(G_1, G_2) = \sum_{H \in \mathcal{P}} \lambda_H \Phi_H(G_1) \Phi_H(G_2) \,,$$

where $\mathcal{P} \subset \mathcal{X}$ is the set of path graphs.

Proposition (Gärtner et al., 2003)

Computing the path kernel is NP-hard.

Path kernel



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Proposition (Gärtner et al., 2003)

Computing the path kernel is NP-hard.

Summary

Expressiveness vs Complexity trade-off

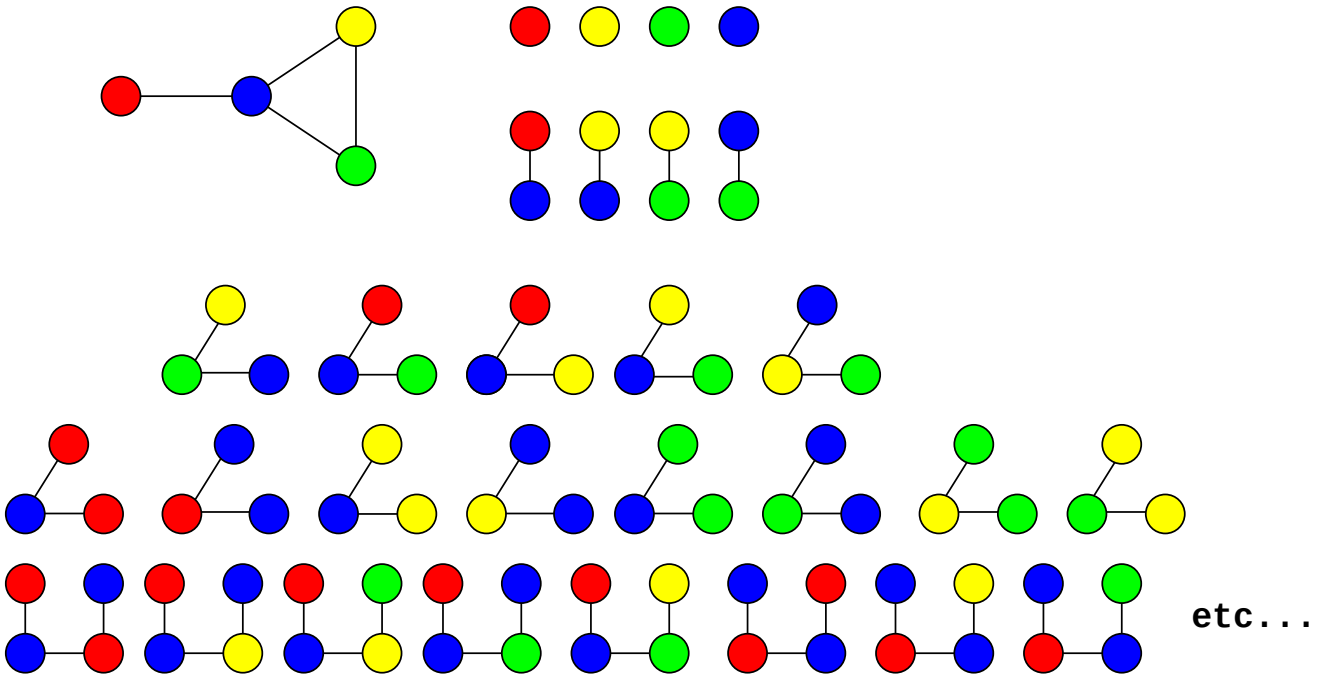
- It is intractable to compute complete graph kernels.
- It is intractable to compute the subgraph kernels.
- Restricting subgraphs to be linear does not help: it is also intractable to compute the path kernel.
- One approach to define polynomial time computable graph kernels is to have the feature space be made up of graphs homomorphic to subgraphs, e.g., to consider walks instead of paths.

Outline

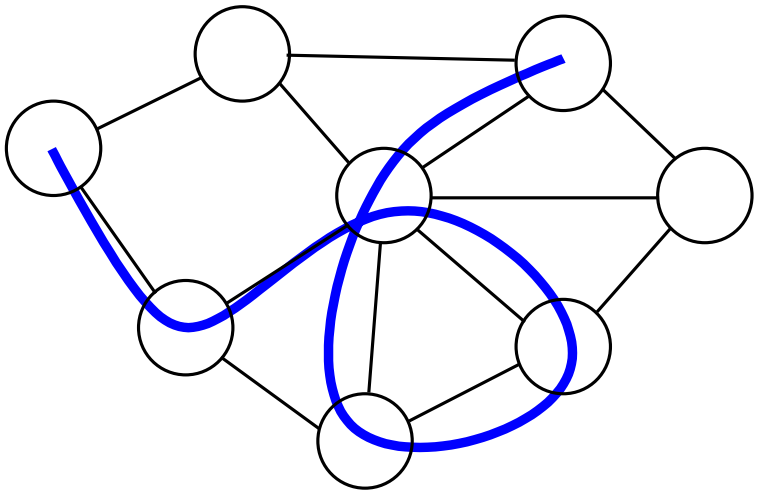
Walks

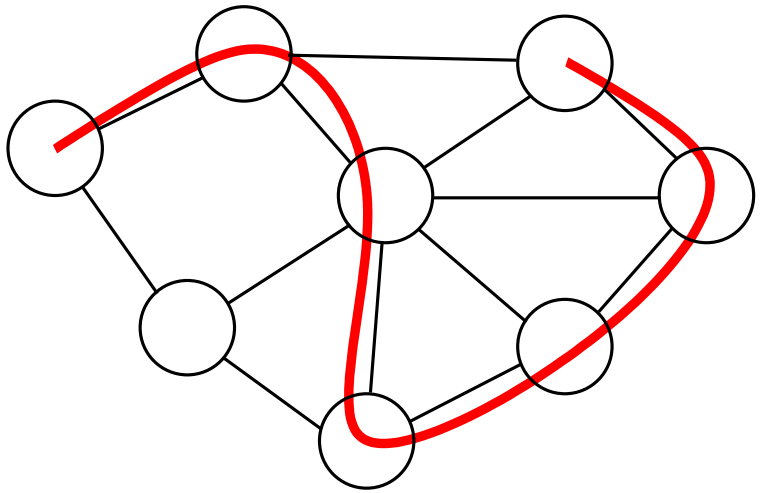
Definition

- 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:

$$K_{walk}(G_1, G_2) = \sum_{s \in \mathcal{S}} \Phi_s(G_1) \Phi_s(G_2) .$$

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Walk kernel examples

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).

- The geometric walk kernel is obtained (when it converges) with $\lambda_G(w) = \beta^{length(w)}$, for $\beta > 0$. In that case the feature space is of infinite dimension (Gärtner et al., 2003).

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Computation of walk kernels

Proposition

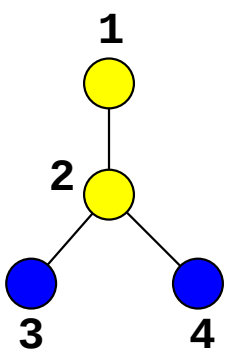
These three kernels (*n*th-order, random and geometric walk kernels) can be computed efficiently in polynomial time.

Product graph

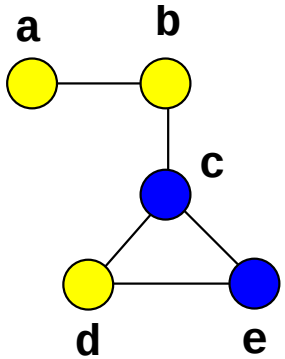
Definition

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:

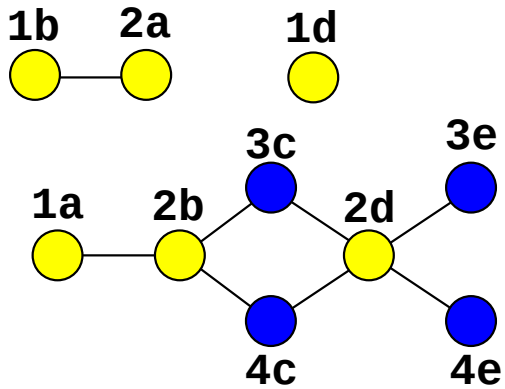
1. $V = \{(v_1, v_2) \in V_1 \times V_2 \ : \ v_1 \text{ and } v_2 \text{ have the same label}\}$,
2. $E = \left\{\left((v_1, v_2), (v_1', v_2')\right) \in V \times V \ : \ (v_1, v_1') \in E_1 \text{ and } (v_2, v_2') \in E_2\right\}$.



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

$$
\begin{aligned}
K_{walk}(G_1, G_2) &= \sum_{s \in \mathcal{S}} \Phi_s(G_1) \Phi_s(G_2) \\
&= \sum_{(w_1, w_2) \in \mathcal{W}(G_1) \times \mathcal{W}(G_1)} \lambda_{G_1}(w_1) \lambda_{G_2}(w_2) \mathbf{1}(l(w_1) = l(w_2)) \\
&= \sum_{w \in \mathcal{W}(G_1 \times G_2)} \lambda_{G_1 \times G_2}(w) \,.
\end{aligned}
$$

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&= \sum_{w \in \mathcal{W}(G_1 \times G_2)} \lambda_{G_1 \times G_2}(w)\,.
\end{aligned}
$$

Computation of the nth-order walk kernel

- For the nth-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:

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

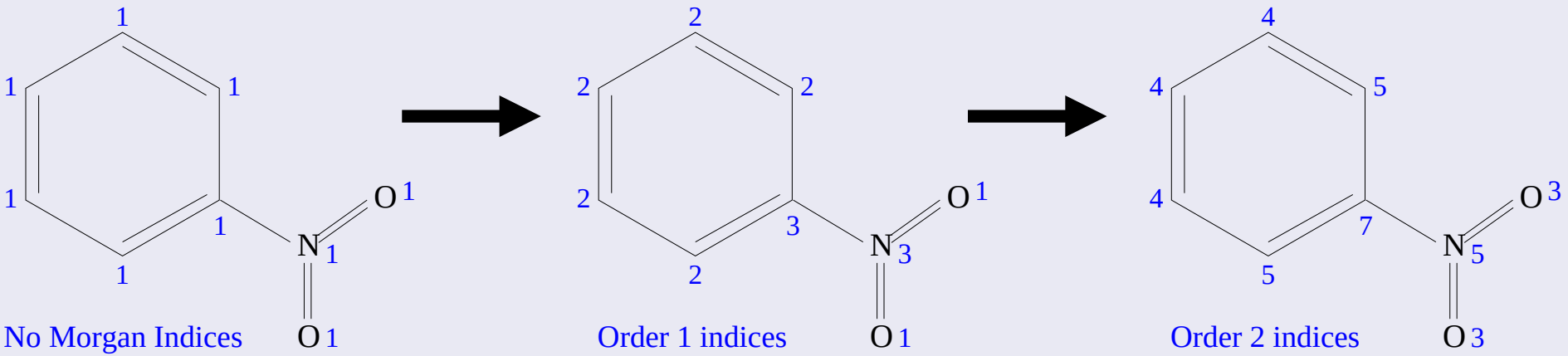
- Let Λ_i be the vector of $\lambda^i(v)$ and Λ_t be the matrix of $\lambda^t(v, v')$:

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

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

Extensions 1: label enrichment

Atom relabebling with the Morgan index (Mahé et al., 2004)

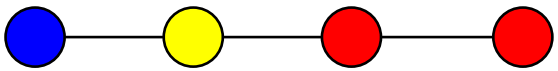


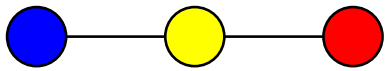
- Compromise between fingerprints and structural keys features.
- Other relabeling schemes are possible (graph coloring).
- Faster computation with more labels (less matches implies a smaller product graph).

Extension 2: Non-tottering walk kernel

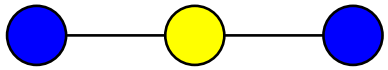
Tottering walks

A tottering walk is a walk $w = v_1 \dots v_n$ with $v_i = v_{i+2}$ for some i.





Non-tottering

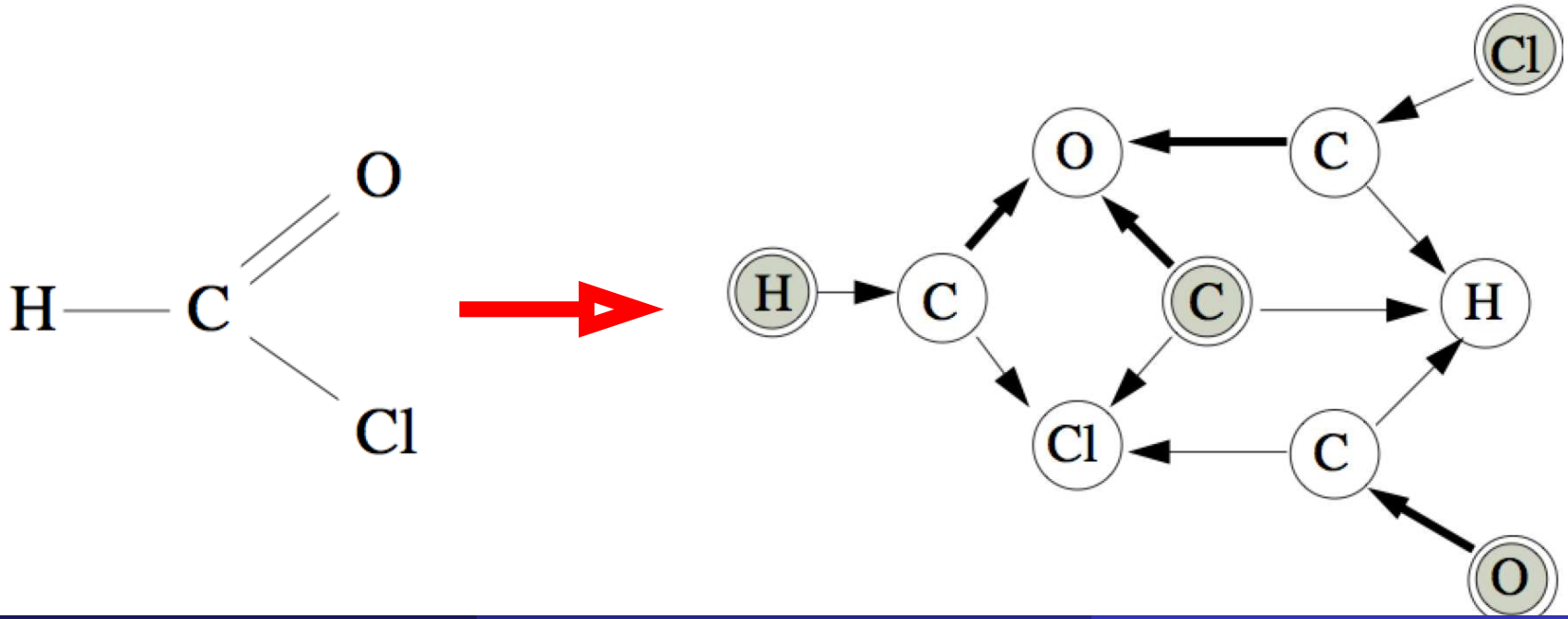


Tottering

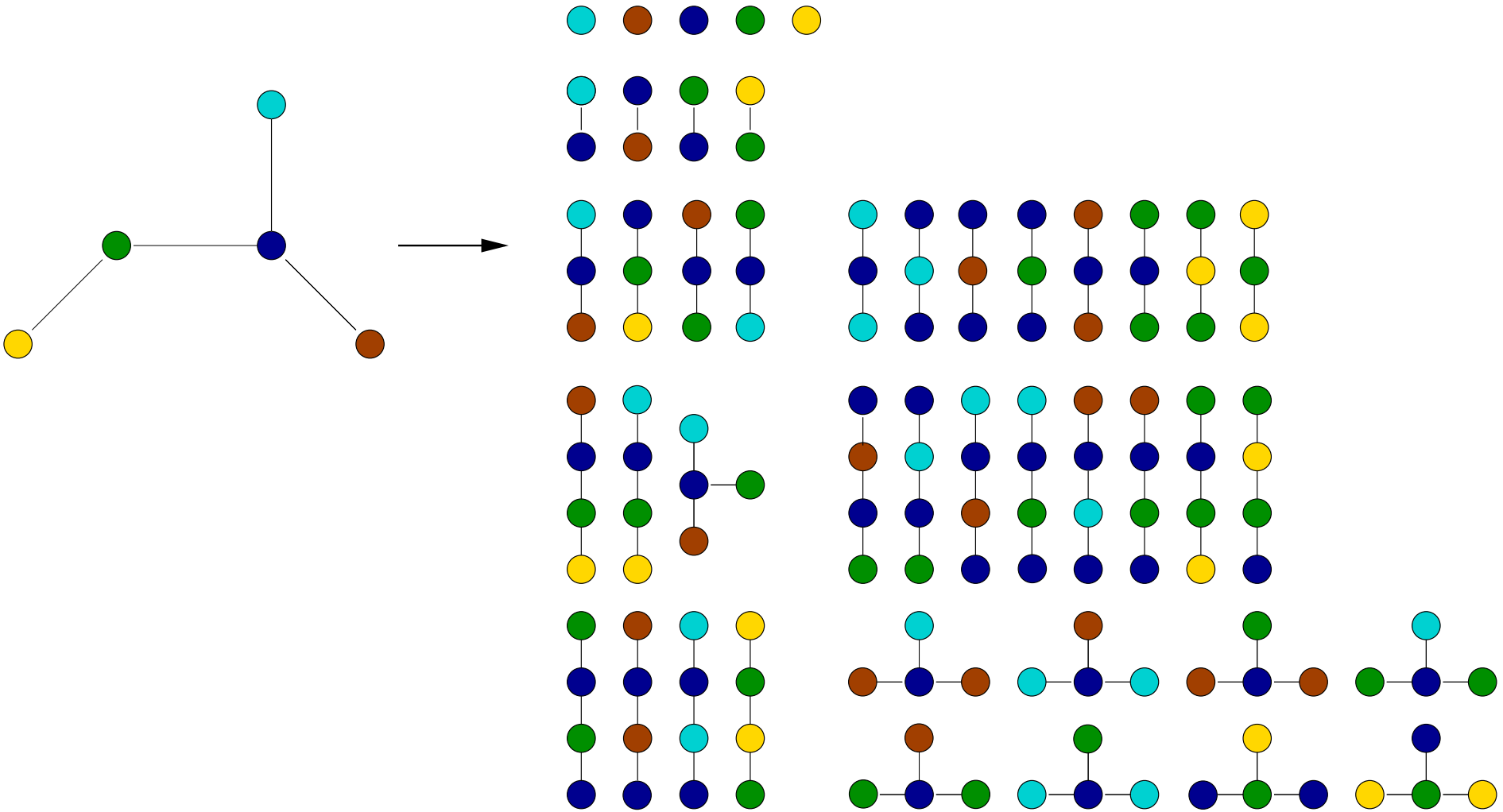
- Tottering walks seem irrelevant for many applications
- Focusing on non-tottering walks is a way to get closer to the path kernel (e.g., equivalent on trees).

Computation of the non-tottering walk kernel (Mahé et al., 2005)

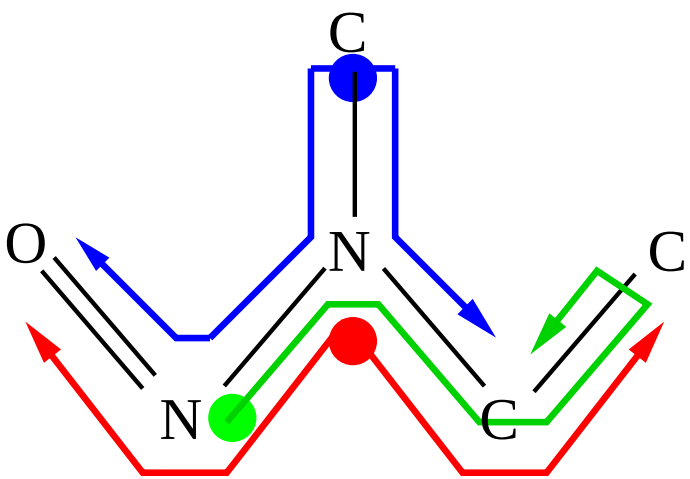
- Second-order Markov random walk to prevent tottering walks
- Written as a first-order Markov random walk on an augmented graph
- Normal walk kernel on the augmented graph (which is always a directed graph).

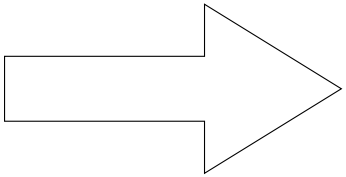


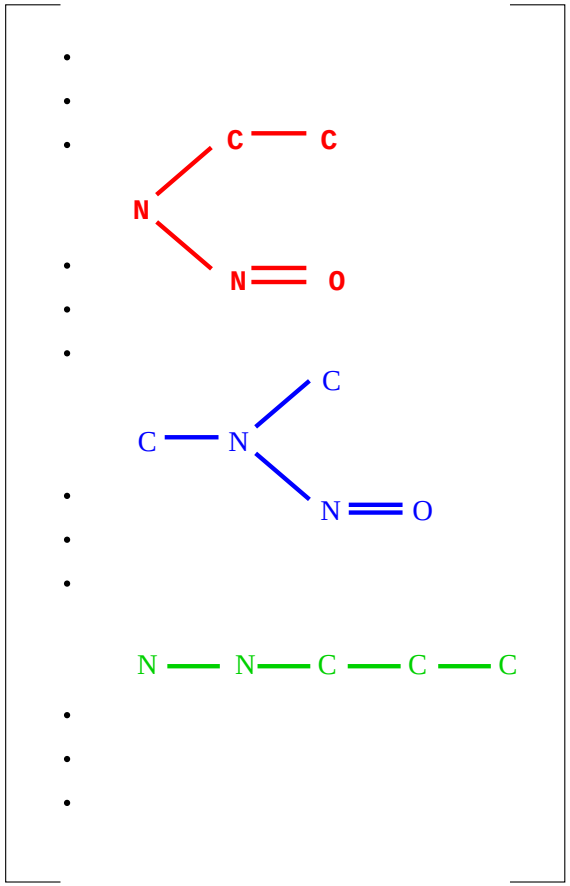
Extension 3: Subtree kernels



Example: Tree-like fragments of molecules







Computation of the subtree kernel (Ramon and Gärtner, 2003; Mahé and Vert, 2009)

- Like the walk kernel, amounts to compute the (weighted) number of subtrees in the product graph.
- Recursion: if $\mathcal{T}(v, n)$ denotes the weighted number of subtrees of depth n rooted at the vertex v, then:

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

  where $\mathcal{N}(v)$ is the set of neighbors of v.
- Can be combined with the non-tottering graph transformation as preprocessing to obtain the non-tottering subtree kernel.

Outline

Application in chemoinformatics (Mahé et al., 2005)

MUTAG dataset

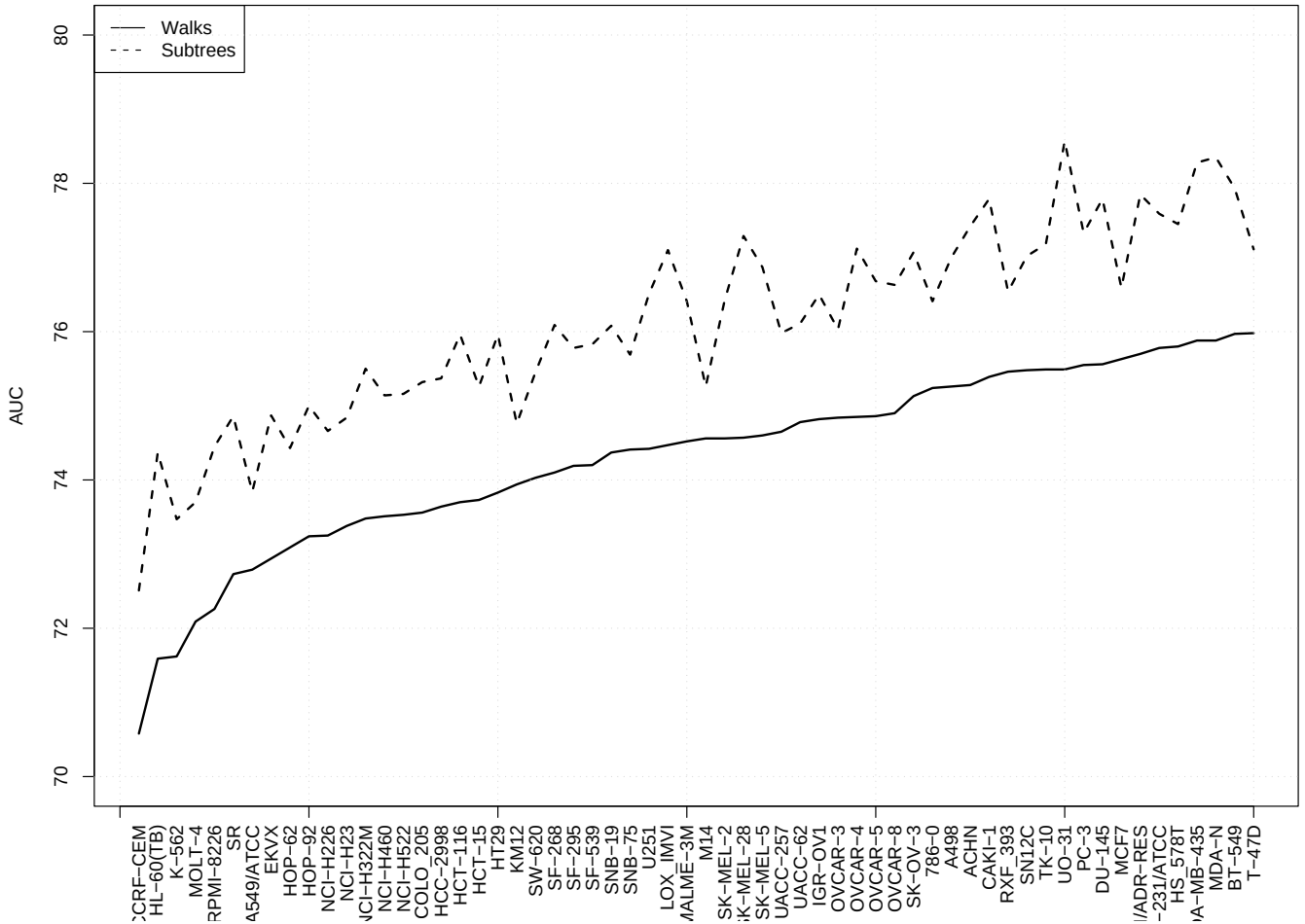
- aromatic/hetero-aromatic compounds
- high mutagenic activity /no mutagenic activity, assayed in *Salmonella typhimurium*.
- 188 compouunds: 125 + / 63 -

Results

10-fold cross-validation accuracy

Method	Accuracy
Progol1	81.4%
2D kernel	91.2%

2D Subtree vs walk kernels

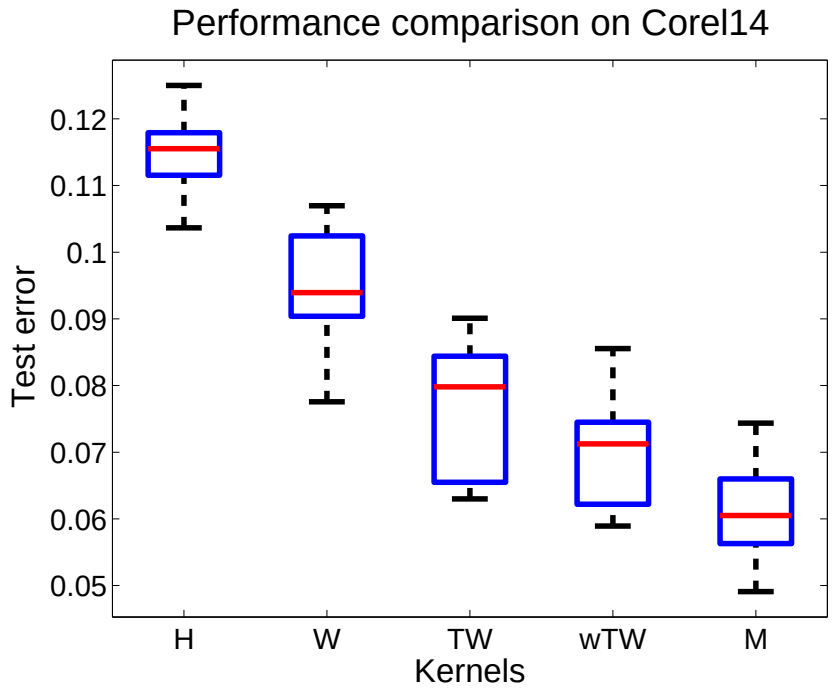


Screening of inhibitors for 60 cancer cell lines.

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).



Summary: graph kernels

What we saw

- Kernels do not allow to overcome the NP-hardness of subgraph patterns
- They allow to work with approximate subgraphs (walks, subtrees), in infinite dimension, thanks to the kernel trick
- However: using kernels makes it difficult to come back to patterns after the learning stage

Part 7

Kernels on graphs

Outline

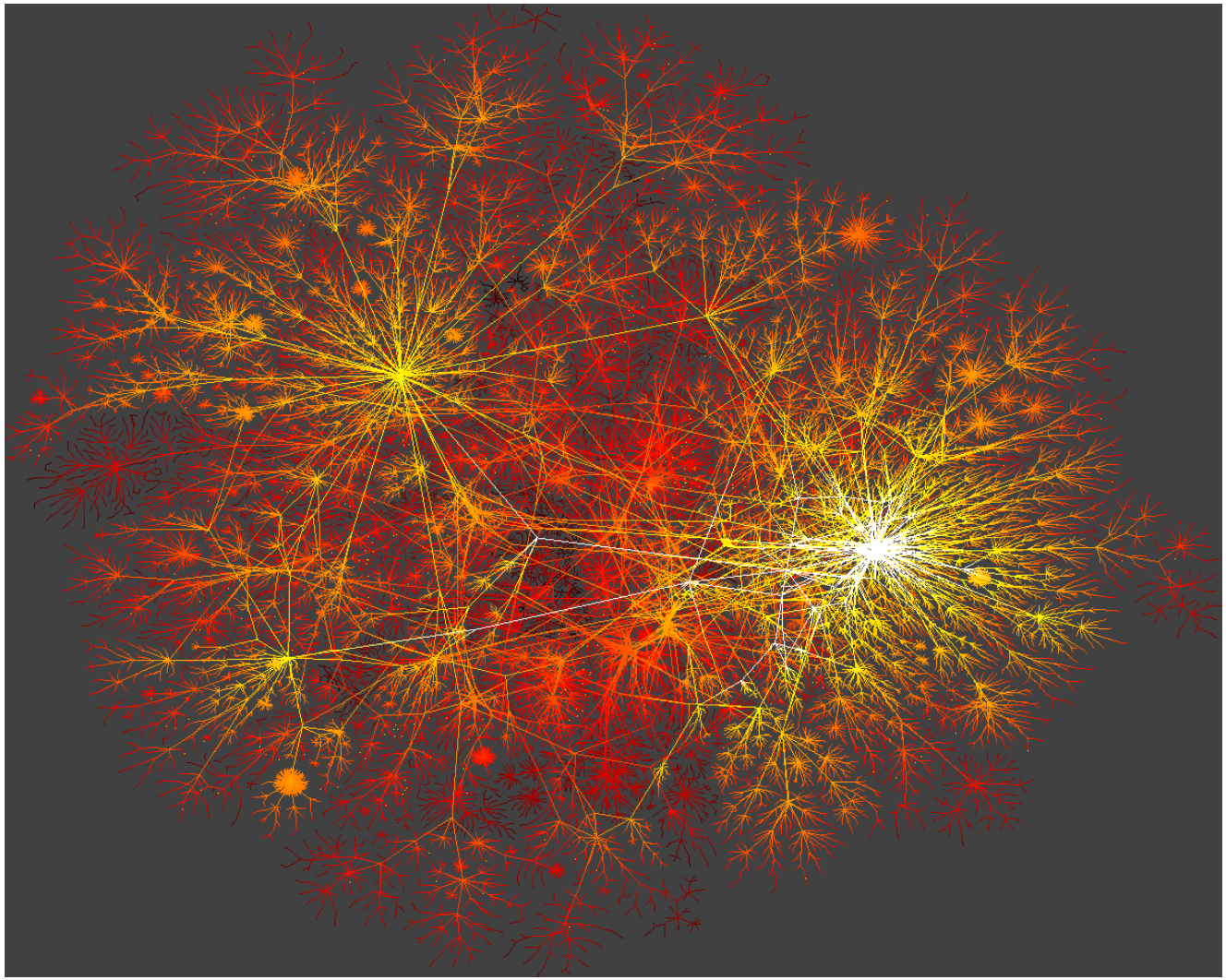
Graphs

Motivation

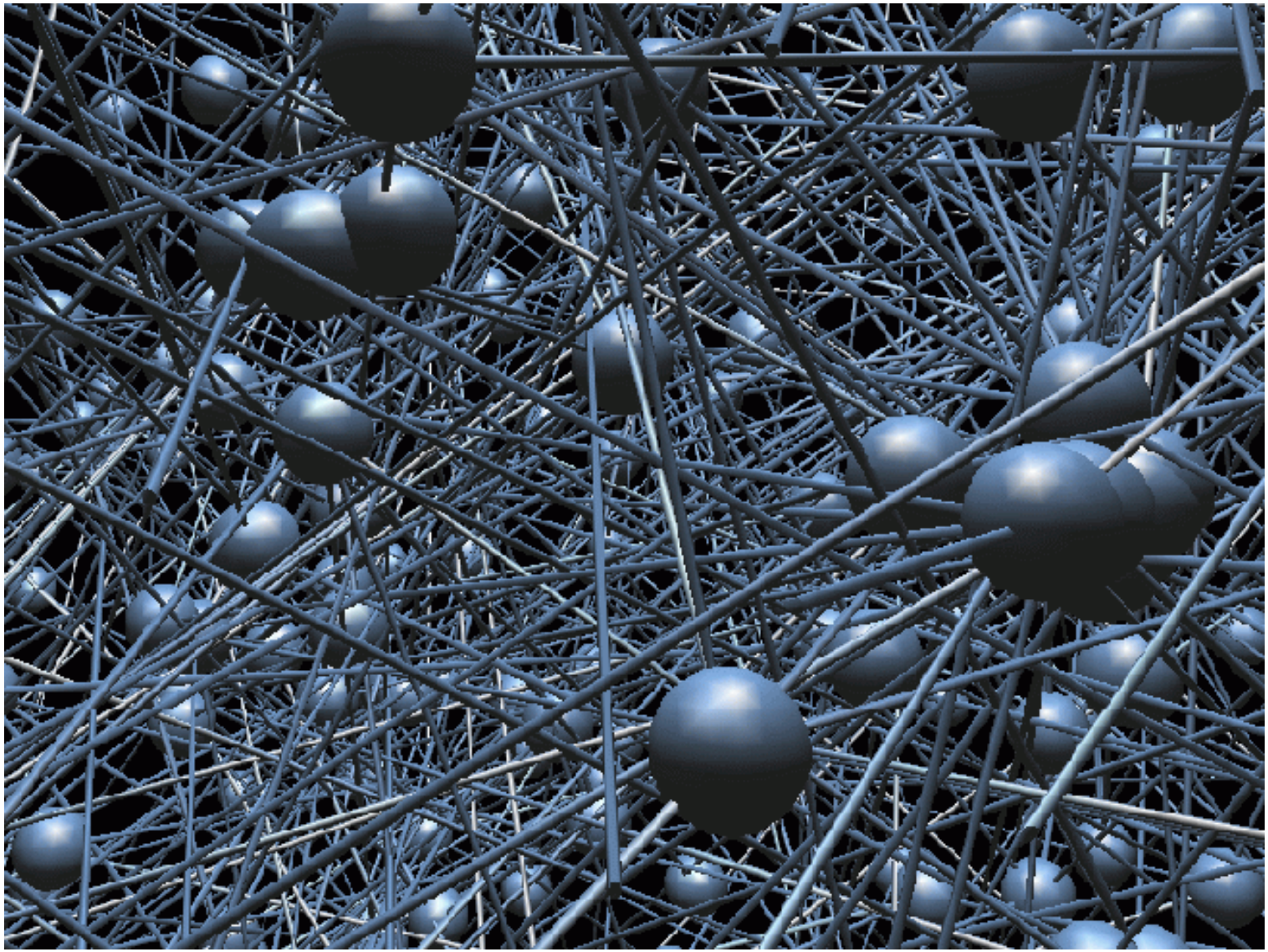
Many data come in the form of nodes in a graph for different reasons:

- by definition (interaction network, internet...)
- by discretization / sampling of a continuous domain
- by convenience (e.g., if only a similarity function if available)

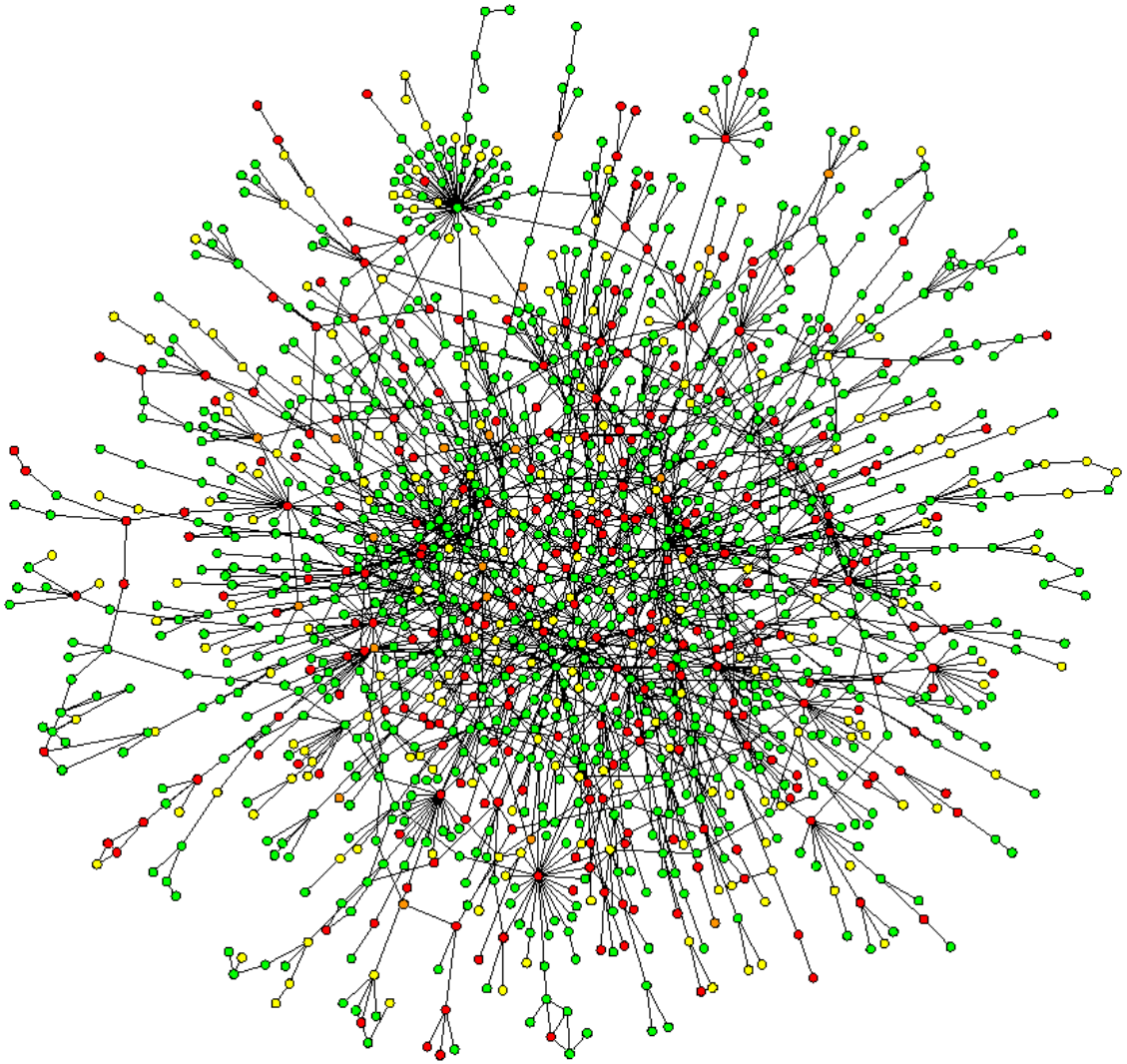
Example: web



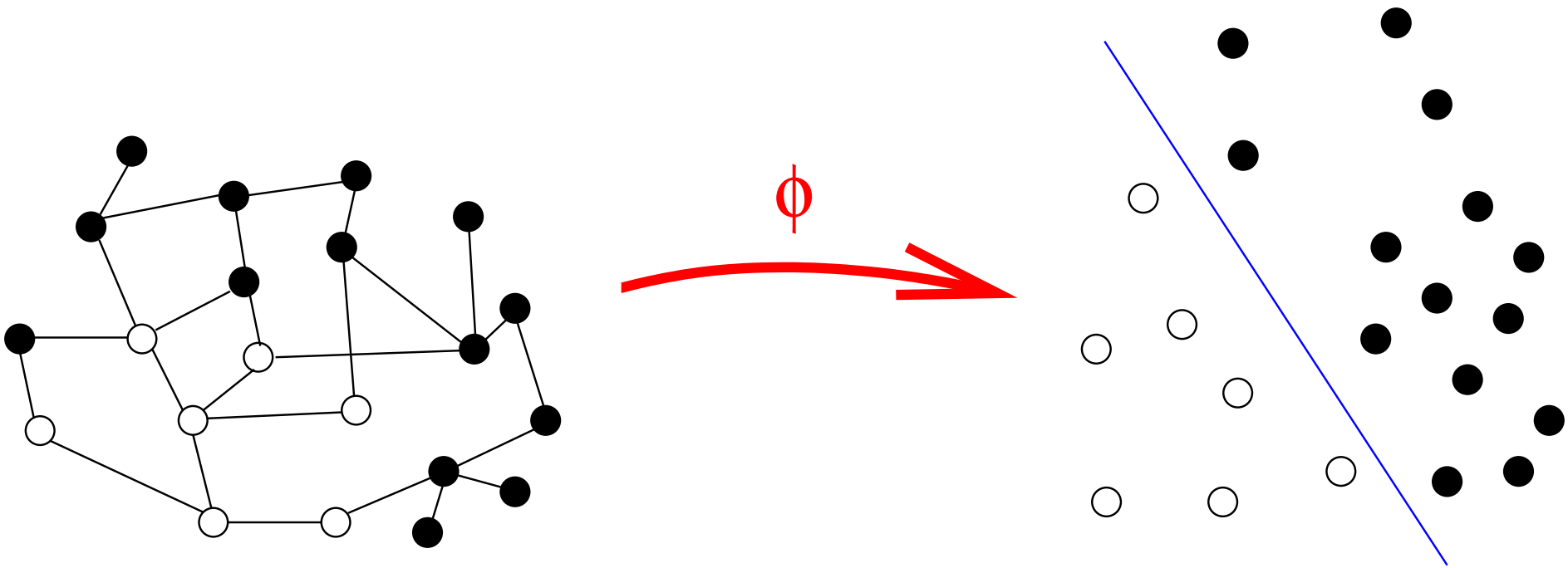
Example: social network



Example: protein-protein interaction



Kernel on a graph



- We need a kernel $K(\mathbf{x}, \mathbf{x}')$ between nodes of the graph.
- Example: predict gene protein functions from high-throughput protein-protein interaction data.

General remarks

Strategies to make a kernel on a graph

- $\mathcal{X}$ being finite, any symmetric semi-definite matrix K defines a valid p.d. kernel on $\mathcal{X}$.
- How to "translate" the graph topology into the kernel?
  - Direct geometric approach: $K_{i,j}$ should be "large" when $\mathbf{x}_i$ and $\mathbf{x}_j$ are "close" to each other on the graph?
  - Functional approach: $\| f \|_K$ should be "small" when f is "smooth" on the graph?
  - Link discrete/continuous: is there an equivalent to the continuous Gaussien kernel on the graph (e.g., limit by fine discretization)?

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Outline

Conditionally p.d. kernels

Hilbert distance

- Any p.d. kernels is an inner product in a Hilbert space

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

- It defines a Hilbert distance:

$$d_K\left(\mathbf{x},\mathbf{x}'\right)^2=K\left(\mathbf{x},\mathbf{x}\right)+K\left(\mathbf{x}',\mathbf{x}'\right)-2K\left(\mathbf{x},\mathbf{x}'\right)$$

- $-d_K^2$ is conditionally positive definite (c.p.d.), i.e.:

$$\forall t>0\,,\quad \exp\left(-td_K\left(\mathbf{x},\mathbf{x}'\right)^2\right)\ \text{is p.d.}$$

Example

A direct approach

- For $\mathcal{X} = \mathbb{R}^n$, the inner product is p.d.:

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}' \,.$$

- The corresponding Hilbert distance is the Euclidean distance:

$$d_K\left(\mathbf{x}, \mathbf{x}'\right)^2 = \mathbf{x}^\top \mathbf{x} + \mathbf{x}'^\top \mathbf{x} - 2\mathbf{x}\top\mathbf{x}' = ||\mathbf{x} - \mathbf{x}'||^2 \,.$$

- $-d_K^2$ is conditionally positive definite (c.p.d.), i.e.:

$$\forall t > 0\,, \quad \exp\left(-t||\mathbf{x} - \mathbf{x}'||^2\right) \text{ is p.d.}$$

Graph distance

Graph embedding in a Hilbert space

- Given a graph $G = (V, E)$, the graph distance $d_G(x, x')$ between any two vertices is the length of the shortest path between x and x'.
- We say that the graph $G = (V, E)$ can be embedded (exactly) in a Hilbert space if $-d_G$ is c.p.d., which implies in particular that $\exp(-t d_G(x, x'))$ is p.d. for all $t > 0$.

Lemma

- *In general graphs can not be embedded exactly in Hilbert spaces.*
- *In some cases exact embeddings exists, e.g.:*
  - *trees can be embedded exactly,*
  - *closed chains can be embedded exactly.*

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Lemma

- *In general graphs can not be embedded exactly in Hilbert spaces.*
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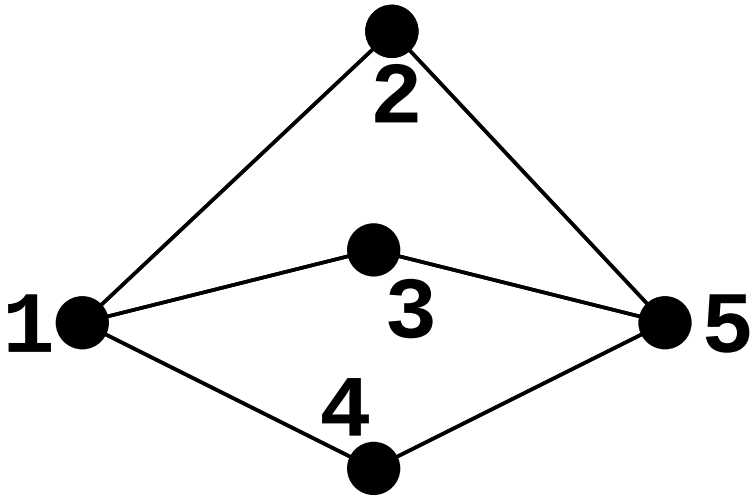
Example: non-c.p.d. graph distance



$$d_G = \begin{pmatrix} 0 & 1 & 1 & 1 & 2 \\ 1 & 0 & 2 & 2 & 1 \\ 1 & 2 & 0 & 2 & 1 \\ 1 & 2 & 2 & 0 & 1 \\ 2 & 1 & 1 & 1 & 0 \end{pmatrix}$$

$$\lambda_{\min}\left(\left[e^{(-0.2 d_G(i,j))}\right]\right) = -0.028 < 0\,.$$

Graph distance on trees are c.p.d.

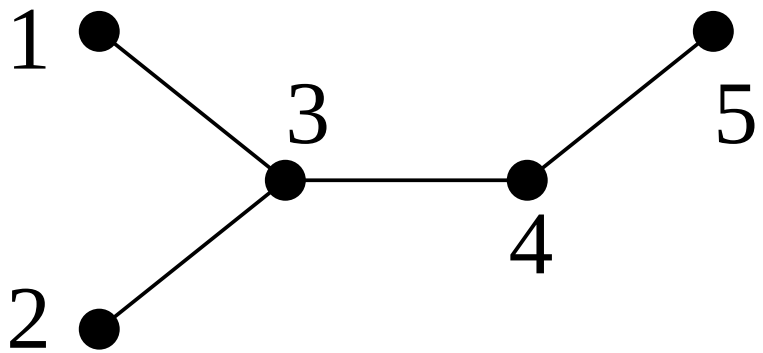
Proof

- Let $G = (V, E)$ a tree
- Fix a root $x_0 \in V$
- Represent any vertex $x \in V$ by a vector $\Phi(x) \in \mathbb{R}^{|E|}$, where $\Phi(x)_i = 1$ is the i-th edge is in the (unique) path between x and x_0, 0 otherwise.
- Then:

$$d_G(x, x') = \| \Phi(x) - \Phi(x') \|^2 ,$$

and therefore $-d_G$ is c.p.d., in particular $\exp(-t d_G(x, x'))$ is p.d. for all $t > 0$.

Example

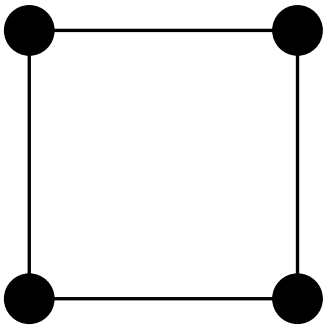


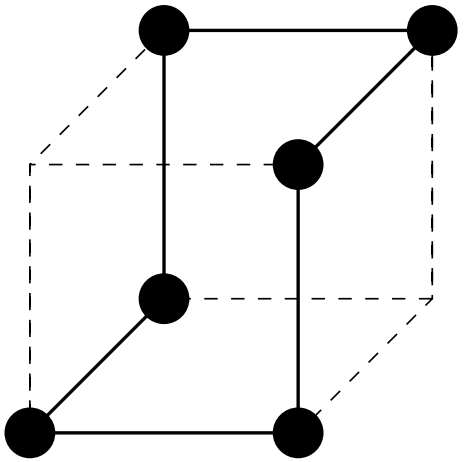
$$\left[e^{-d_G(i,j)}\right] = \begin{pmatrix} 1 & 0.14 & 0.37 & 0.14 & 0.05 \\ 0.14 & 1 & 0.37 & 0.14 & 0.05 \\ 0.37 & 0.37 & 1 & 0.37 & 0.14 \\ 0.14 & 0.14 & 0.37 & 1 & 0.37 \\ 0.05 & 0.05 & 0.14 & 0.37 & 1 \end{pmatrix}$$

Graph distance on closed chains are c.p.d.

Proof: case $|V| = 2p$

- Let $G = (V, E)$ a cycle with an even number of vertices $|V| = 2p$
- Fix a root $x_0 \in V$, number the $2p$ edges from x_0 to x_0.
- Map the $2p$ edges in $\mathbb{R}^p$ to $(e_1, \ldots, e_p, -e_1, \ldots, -e_p)$
- Map a vertex v to the sum of the edges in the shortest path between x_0 and v.





Outline

Functional approach

Motivation

- How to make p.d. kernel on general graphs?
- Making a kernel is equivalent to defining a RKHS.
- There are intuitive notions of smoothness on a graph

Idea

- Define a priori a smoothness functional on the functions $f : \mathcal{X} \to \mathbb{R}$.
- Show that it defines a RKHS and identify the corresponding kernel

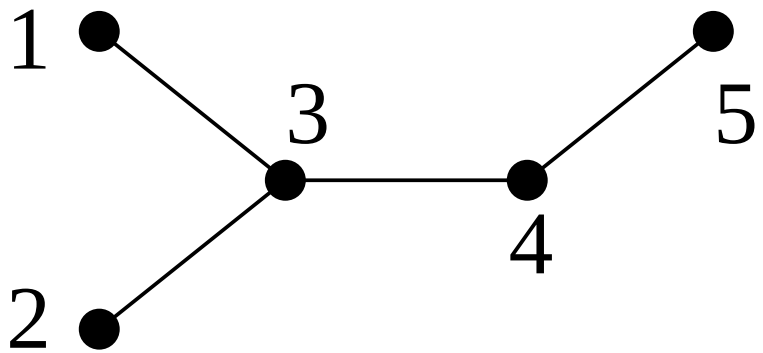
Notations

- $\mathcal{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$ is finite.
- For $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$, we note $\mathbf{x} \sim \mathbf{x}'$ to indicate the existence of an edge between $\mathbf{x}$ and $\mathbf{x}'$
- We assume that there is no self-loop $\mathbf{x} \sim \mathbf{x}$, and that there is a single connected component.
- The adjacency matrix is $A \in \mathbb{R}^{m \times m}$:

$$A_{i,j} = \begin{cases} 1 & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

- D is the diagonal matrix where $D_{i,i}$ is the number of neighbors of $\mathbf{x}_i$ ($D_{i,i} = \sum_{i=1}^{m} A_{i,j}$).

Example

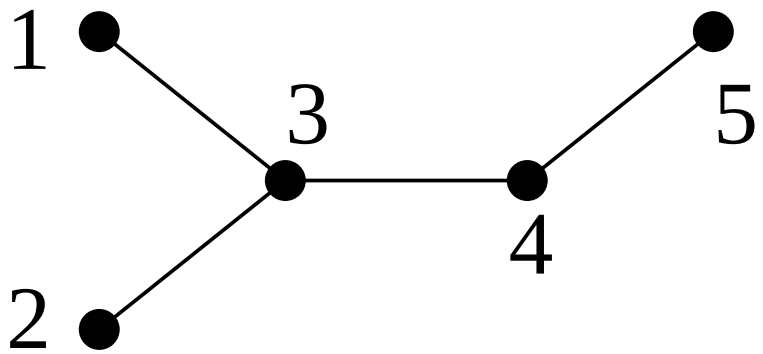


$$A = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \qquad D = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Graph Laplacian

Definition

The Laplacian of the graph is the matrix $L = D - A$.



$$L = D - A = \begin{pmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

Properties of the Laplacian

Lemma

Let $L = D - A$ be the Laplacian of a connected graph:

- *For any $f : \mathcal{X} \to \mathbb{R}$,*

$$\Omega(f) := \sum_{i \sim j} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j)\right)^2 = f^\top L f$$

- *L is a symmetric positive semi-definite matrix*
- *0 is an eigenvalue with multiplicity 1 associated to the constant eigenvector $\mathbf{1} = (1, \ldots, 1)$*
- *The image of L is*

$$Im(L) = \left\{ f \in \mathbb{R}^m : \sum_{i=1}^m f_i = 0 \right\}$$

Proof: link between $\Omega(f)$ and L

$$
\begin{aligned}
\Omega(f) &= \sum_{i \sim j} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j)\right)^2 \\
&= \sum_{i \sim j} \left(f(\mathbf{x}_i)^2 + f(\mathbf{x}_j)^2 - 2 f(\mathbf{x}_i) f(\mathbf{x}_j)\right) \\
&= \sum_{i=1}^{m} D_{i,i} f(\mathbf{x}_i)^2 - 2 \sum_{i \sim j} f(\mathbf{x}_i) f(\mathbf{x}_j) \\
&= f^\top D f - f^\top A f \\
&= f^\top L f
\end{aligned}
$$

Proof: eigenstructure of L

- L is symmetric because A and D are symmetric.
- For any $f \in \mathbb{R}^m$, $f^\top L f = \Omega(f) \geq 0$, therefore the (real-valued) eigenvalues of L are ≥ 0 : L is therefore positive semi-definite.
- f is an eigenvector associated to eigenvalue 0
  iff $f^\top L f = 0$
  iff $\sum_{i \sim j} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j)\right)^2 = 0$,
  iff $f(\mathbf{x}_i) = f(\mathbf{x}_j)$ when $i \sim j$,
  iff f is constant (because the graph is connected).
- L being symmetric, $Im(L)$ is the orthogonal supplement of $Ker(L)$, that is, the set of functions orthogonal to $\mathbf{1}$. $\square$

Our first graph kernel

Theorem

The set $\mathcal{H} = \left\{ f \in \mathbb{R}^m : \sum_{i=1}^m f_i = 0 \right\}$ *endowed with the norm:*

$$\Omega(f) = \sum_{i \sim j} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j) \right)^2$$

is a RKHS whose reproducing kernel is L^**, the pseudo-inverse of the graph Laplacian.*

In case of...

Pseudo-inverse of L

Remember the pseudo-inverse L^* of L is the linear application that is equal to:

- 0 on $Ker(L)$
- L^{-1} on $Im(L)$, that is, if we write:

$$L = \sum_{i=1}^{m} \lambda_i u_i u_i^\top$$

the eigendecomposition of L:

$$L^* = \sum_{\lambda_i \neq 0} (\lambda_i)^{-1} u_i u_i^\top \ .$$

- In particular it holds that $L^*L = LL^* = \Pi_{\mathcal{H}}$, the projection onto $Im(L) = \mathcal{H}$.

Proof (1/2)

- Resticted to $\mathcal{H}$, the symmetric bilinear form:

$$\langle f, g \rangle = f^\top L g$$

  is positive definite (because L is positive semi-definite, and $\mathcal{H} = Im(L)$). It is therefore a scalar product, making of $\mathcal{H}$ a Hilbert space (in fact Euclidean).
- The norm in this Hilbert space $\mathcal{H}$ is:

$$\| f \|^2 = \langle f, f \rangle = f^\top L f = \Omega(f) \ .$$

Proof (2/2)

To check that $\mathcal{H}$ is a RKHS with reproducing kernel $K = L^*$, it suffices to show that:

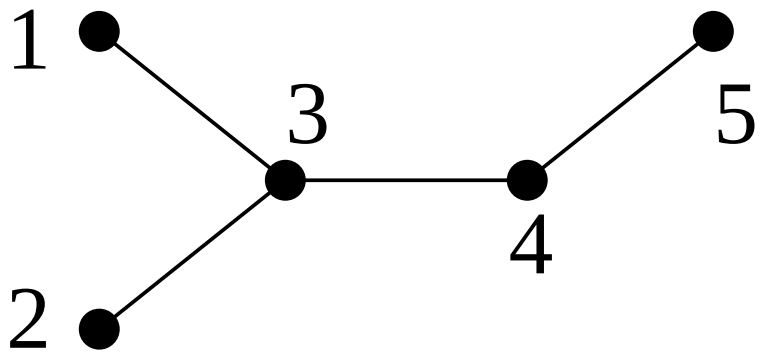
$$\begin{cases} \forall \mathbf{x} \in \mathcal{X}, & K_{\mathbf{x}} \in \mathcal{H} \ , \\ \forall \, (\mathbf{x}, f) \in \mathcal{X} \times \mathcal{H}, & \langle f, K_{\mathbf{x}} \rangle = f(\mathbf{x}) \ . \end{cases}$$

- $Ker(K) = Ker\,(L^*) = Ker\,(L)$, implying $K\mathbf{1} = 0$. Therefore, each row/column of K is in $\mathcal{H}$.
- For any $f \in \mathcal{H}$, if we note $g_i = \langle K(i, \cdot), f \rangle$ we get:

$$g = KLf = L^*Lf = \Pi_{\mathcal{H}}(f) = f \ .$$

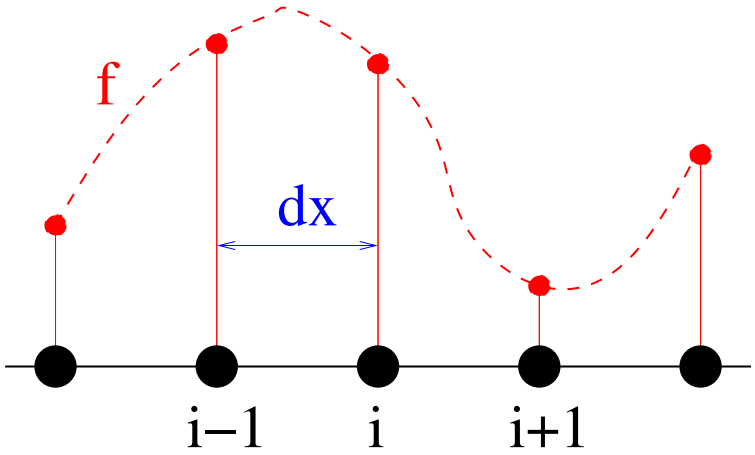
As a conclusion $K = L^*$ is the reproducing kernel of $\mathcal{H}$. $\square$

Example



$$L^* = \begin{pmatrix} 0.88 & -0.12 & 0.08 & -0.32 & -0.52 \\ -0.12 & 0.88 & 0.08 & -0.32 & -0.52 \\ 0.08 & 0.08 & 0.28 & -0.12 & -0.32 \\ -0.32 & -0.32 & -0.12 & 0.48 & 0.28 \\ -0.52 & -0.52 & -0.32 & 0.28 & 1.08 \end{pmatrix}$$

Interpretation of the Laplacian



$$
\begin{aligned}
\Delta f(x) &= f''(x) \\
&\sim \frac{f'(x + dx/2) - f'(x - dx/2)}{dx} \\
&\sim \frac{f(x + dx) - f(x) - f(x) + f(x - dx)}{dx^2} \\
&= \frac{f_{i-1} + f_{i+1} - 2f(x)}{dx^2} \\
&= -\frac{Lf(i)}{dx^2}.
\end{aligned}
$$

Interpretation of regularization

For $f = [0,1] \to \mathbb{R}$ and $x_i = i/m$, we have:

$$\begin{aligned}
\Omega(f) &= \sum_{i=1}^{m} \left(f\left(\frac{i+1}{m}\right) - f\left(\frac{i}{m}\right) \right)^2 \\
&\sim \sum_{i=1}^{m} \left(\frac{1}{m} \times f'\left(\frac{i}{m}\right) \right)^2 \\
&= \frac{1}{m} \times \frac{1}{m} \sum_{i=1}^{m} f'\left(\frac{i}{m}\right)^2 \\
&\sim \frac{1}{m} \int_0^1 f'(t)^2 dt.
\end{aligned}$$

Outline

Motivation

- Consider the normalized Gaussian kernel on $\mathbb{R}^d$:

$$K_t(\mathbf{x}, \mathbf{x}') = \frac{1}{(4\pi t)^{\frac{d}{2}}} \exp\left(-\frac{\| \mathbf{x} - \mathbf{x}' \|^2}{4t}\right).$$

- In order to transpose it to the graph, replacing the Euclidean distant by the shortest-path distance does not work.
- In this section we provide a characterization of the Gaussian kernel as the solution of a partial differential equation involving the Laplacian, which we can transpose to the graph: the diffusion equation.
- The solution of the discrete diffusion equation will be called the diffusion kernel or heat kernel.

The diffusion equation

Lemma

For any $\mathbf{x}_0 \in \mathbb{R}^d$*, the function:*

$$K_{\mathbf{x}_0}(\mathbf{x}, t) = K_t(\mathbf{x}_0, \mathbf{x}) = \frac{1}{(4\pi t)^{\frac{d}{2}}} \exp\left(-\frac{\| \mathbf{x} - \mathbf{x}_0 \|^2}{4t}\right).$$

is solution of the diffusion equation:

$$\frac{\partial}{\partial t} K_{\mathbf{x}_0}(\mathbf{x}, t) = \Delta K_{\mathbf{x}_0}(\mathbf{x}, t).$$

with initial condition $K_{\mathbf{x}_0}(\mathbf{x}, 0) = \delta_{\mathbf{x}_0}(\mathbf{x})$

(proof = direct computation).

Discrete diffusion equation

For finite-dimensional $f_t \in \mathbb{R}^m$, the diffusion equation becomes:

$$\frac{\partial}{\partial t} f_t = -L f_t$$

which admits the following solution:

$$f_t = f_0 e^{-tL}$$

with

$$e^{tL} = I - tL + \frac{t^2}{2!} L^2 - \frac{t^3}{3!} L^3 + \dots$$

Diffusion kernel (Kondor and Lafferty, 2002)

This suggest to consider:

$$K = e^{-tL}$$

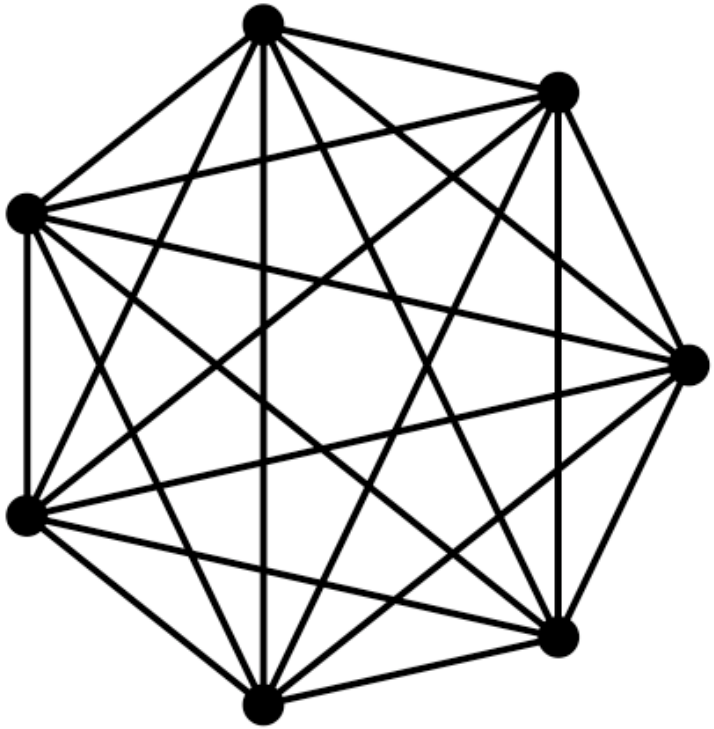
which is indeed symmetric positive semi-definite because if we write:

$$L = \sum_{i=1}^{m} \lambda_i u_i u_i^\top \quad (\lambda_i \geq 0)$$

we obtain:

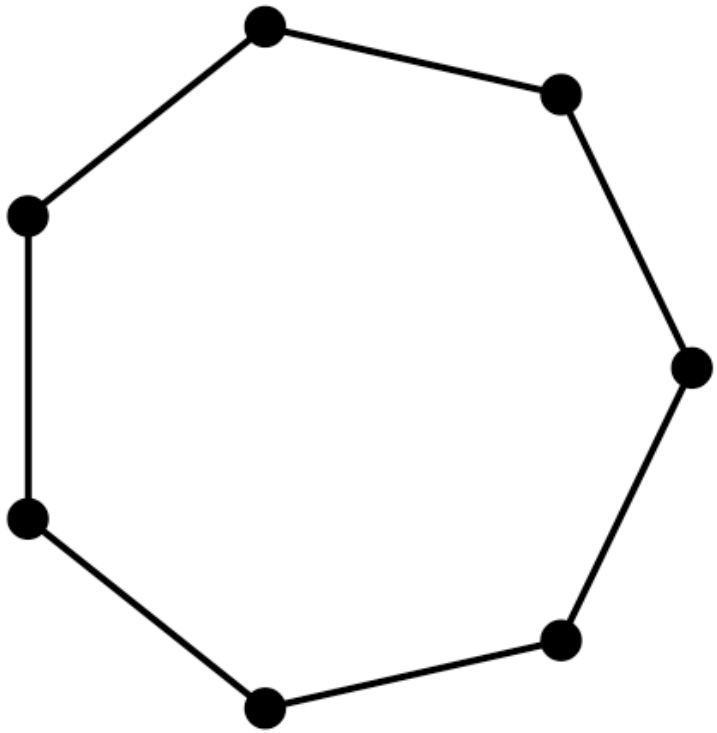
$$K = e^{-tL} = \sum_{i=1}^{m} e^{-t\lambda_i} u_i u_i^\top$$

Example: complete graph



$$K_{i,j} = \begin{cases} \frac{1+(m-1)e^{-tm}}{m} & \text{for } i = j, \\ \frac{1-e^{-tm}}{m} & \text{for } i \neq j. \end{cases}$$

Example: closed chain



$$K_{i,j} = \frac{1}{m} \sum_{\nu=0}^{m-1} \exp\left[-2t\left(1 - \cos\frac{2\pi\nu}{m}\right)\right] \cos\frac{2\pi\nu(i-j)}{m}.$$

Outline

Motivation

- In this section we show that the diffusion and Laplace kernels can be interpreted in the frequency domain of functions
- This shows that our strategy to design kernels on graphs was based on (discrete) harmonic analysis on the graph
- This follows the approach we developed for semigroup kernels!

Spectrum of the diffusion kernel

- Let $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_m$ be the eigenvalues of the Laplacian:

$$L = \sum_{i=1}^{m} \lambda_i u_i u_i^\top \quad (\lambda_i \geq 0)$$

- The diffusion kernel K_t is an invertible matrix because its eigenvalues are strictly positive:

$$K_t = \sum_{i=1}^{m} e^{-t\lambda_i} u_i u_i^\top$$

Norm in the diffusion RKHS

- Any function $f \in \mathbb{R}^m$ can be written as $f = K\left(K^{-1}f\right)$, therefore its norm in the diffusion RKHS is:

$$\| f \|_{K_t}^2 = \left(f^\top K^{-1}\right) K \left(K^{-1} f\right) = f^\top K^{-1} f \,.$$

- For $i = 1, \ldots, m$, let:

$$\hat{f}_i = u_i^\top f$$

be the projection of f onto the eigenbasis of K.

- We then have:

$$\| f \|_{K_t}^2 = f^\top K^{-1} f = \sum_{i=1}^m e^{t\lambda_i} \hat{f}_i^2 .$$

- This looks similar to $\int \left| \hat{f}(\omega) \right|^2 e^{\sigma^2 \omega^2} d\omega$ ...

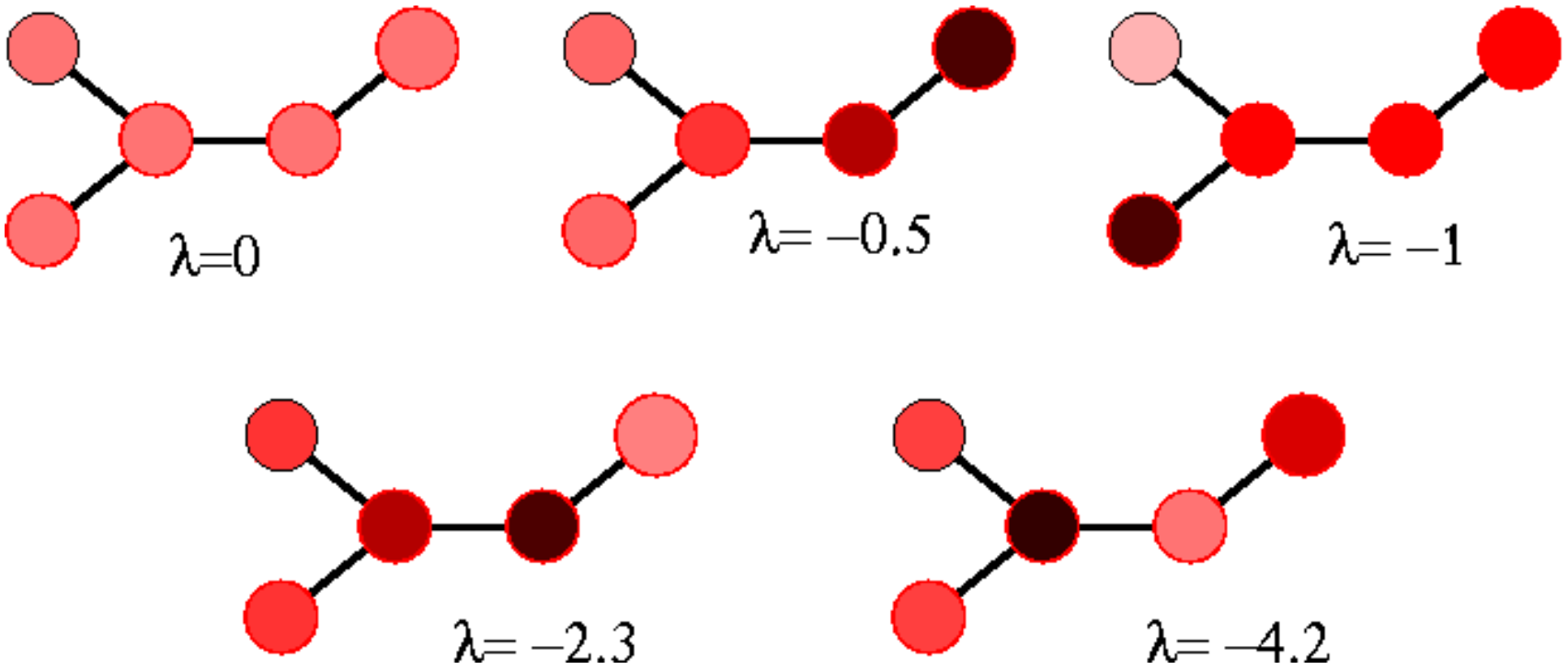
Discrete Fourier transform

Definition

The vector $\hat{f} = \left(\hat{f}_1, \ldots, \hat{f}_m\right)^\top$ is called the discrete Fourier transform of $f \in \mathbb{R}^n$

- The eigenvectors of the Laplacian are the discrete equivalent to the sine/cosine Fourier basis on $\mathbb{R}^n$.
- The eigenvalues λ_i are the equivalent to the frequencies ω^2
- Successive eigenvectors "oscillate" increasingly as eigenvalues get more and more negative.

Example: eigenvectors of the Laplacian



Generalization

This observation suggests to define a whole family of kernels:

$$K_r = \sum_{i=1}^{m} r(\lambda_i) u_i u_i^\top$$

associated with the following RKHS norms:

$$\| f \|_{K_r}^2 = \sum_{i=1}^{m} \frac{\hat{f}_i^2}{r(\lambda_i)}$$

where $r : \mathbb{R}^+ \to \mathbb{R}_*^+$ is a non-increasing function.

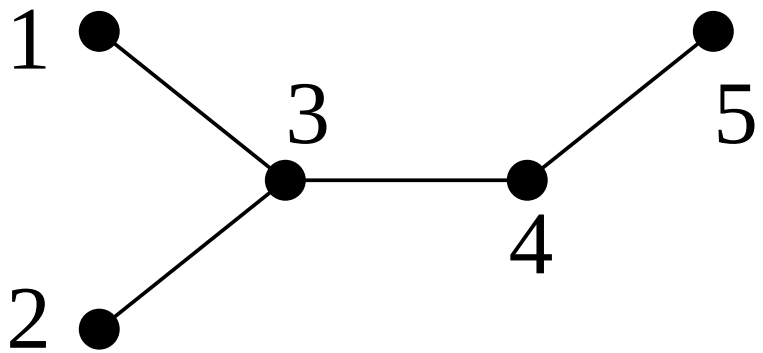
Example : regularized Laplacian

$$r(\lambda) = \frac{1}{\lambda + \epsilon}, \qquad \epsilon > 0$$

$$K = \sum_{i=1}^{m} \frac{1}{\lambda_i + \epsilon} u_i u_i^\top = (L + \epsilon I)^{-1}$$

$$\| f \|_K^2 = f^\top K^{-1} f = \sum_{i \sim j} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j) \right)^2 + \epsilon \sum_{i=1}^{m} f(\mathbf{x}_i)^2 .$$

Example



$$(L+I)^{-1} = \begin{pmatrix} 0.60 & 0.10 & 0.19 & 0.08 & 0.04 \\ 0.10 & 0.60 & 0.19 & 0.08 & 0.04 \\ 0.19 & 0.19 & 0.38 & 0.15 & 0.08 \\ 0.08 & 0.08 & 0.15 & 0.46 & 0.23 \\ 0.04 & 0.04 & 0.08 & 0.23 & 0.62 \end{pmatrix}$$

Outline

Applications 1: graph partitioning

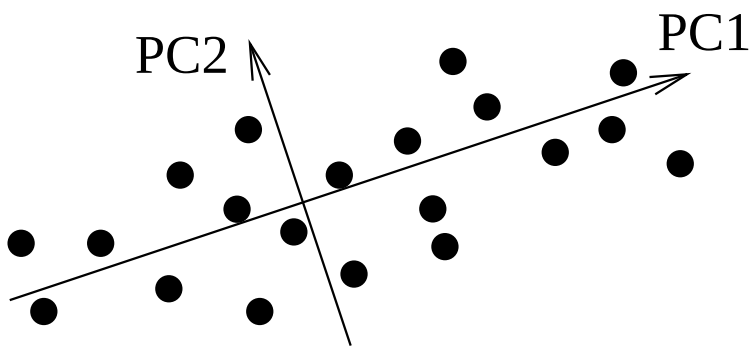
- A classical relaxation of graph partitioning is:

$$\min_{f \in \mathbb{R}^{\mathcal{X}}} \sum_{i \sim j} (f_i - f_j)^2 \quad \text{s.t.} \sum_i f_i^2 = 1$$

- This can be rewritten

$$\max_f \sum_i f_i^2 \text{ s.t.} \quad \| f \|_{\mathcal{H}} \leq 1$$

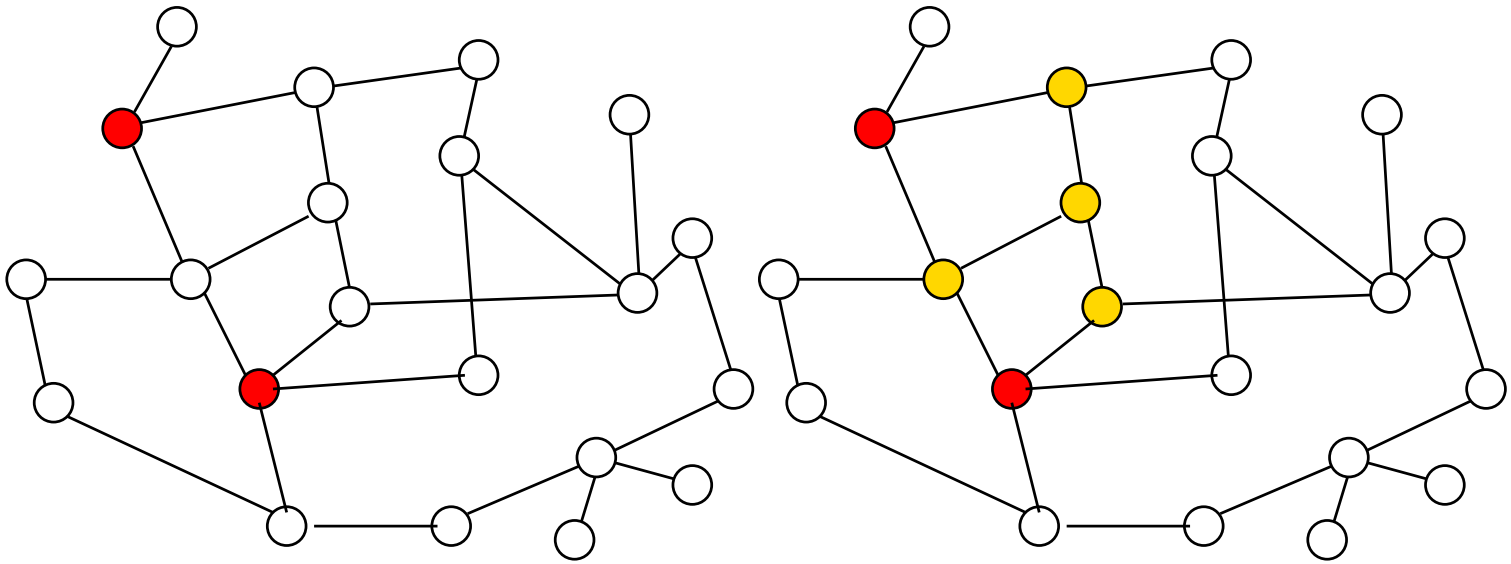
- This is principal component analysis in the RKHS ("kernel PCA")



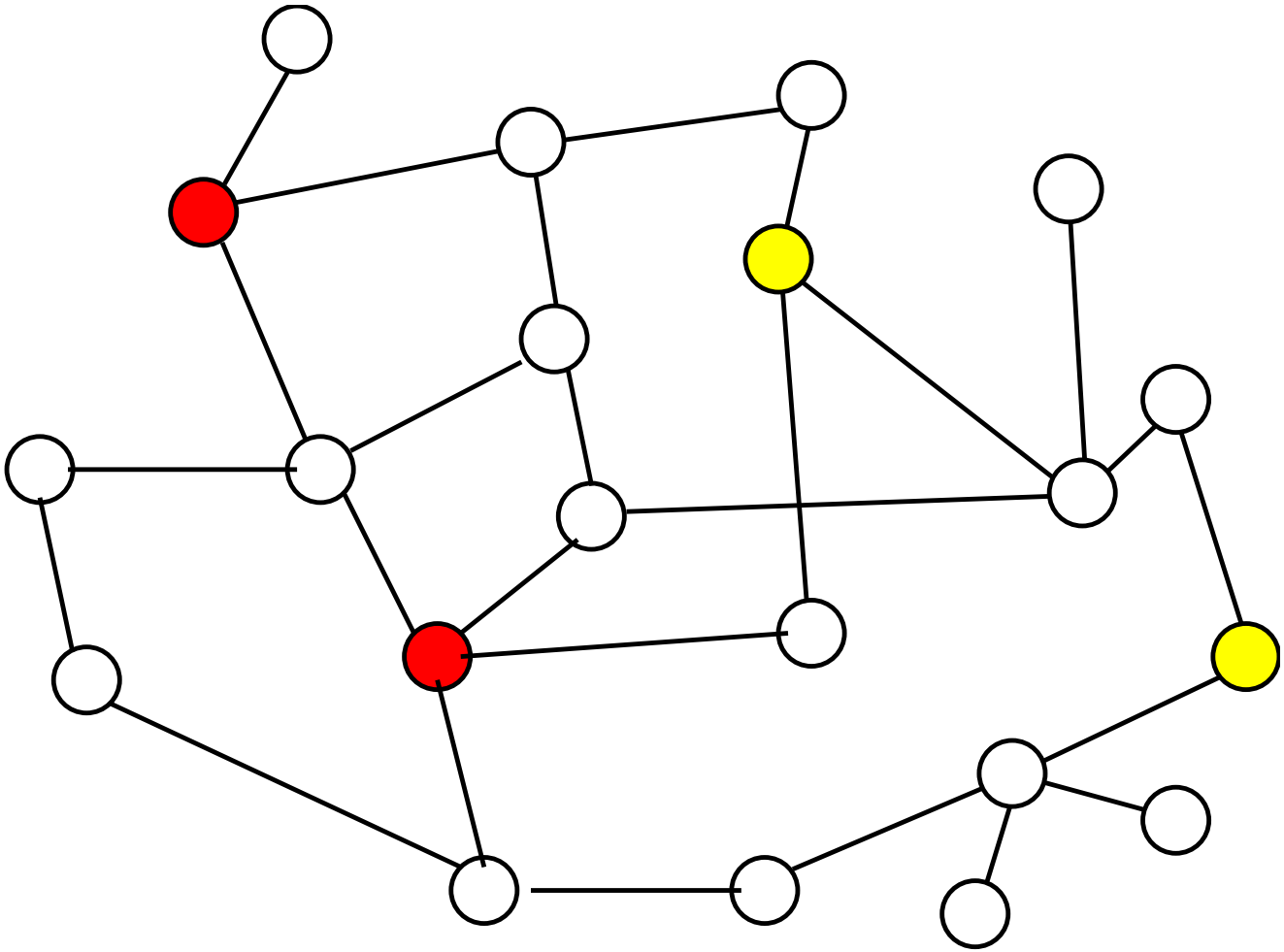
Applications 2: search on a graph

- Let $x_1, \ldots, x_q$ a set of q nodes (the query). How to find "similar" nodes (and rank them)?
- One solution:

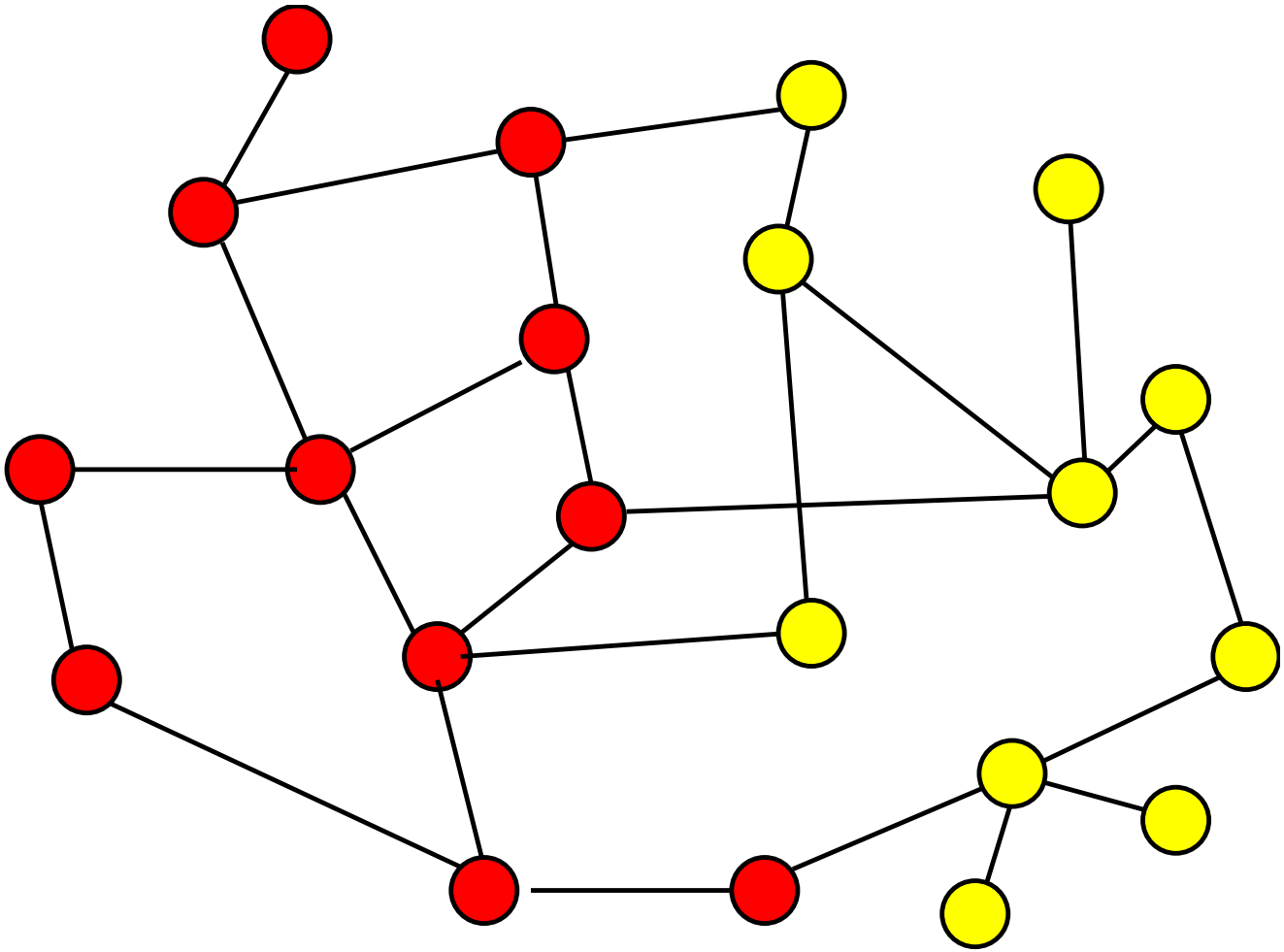
$$\min_f \| f \|_{\mathcal{H}} \quad \text{s.t.} \quad f(x_i) \geq 1 \text{ for } i = 1, \ldots, q.$$



Application 3: Semi-supervised learning



Application 3: Semi-supervised learning



Application 4: Tumor classification from microarray data (Rapaport et al., 2006)

Data available

- Gene expression measures for more than $10k$ genes
- Measured on less than 100 samples of two (or more) different classes (e.g., different tumors)

Goal

- Design a classifier to automatically assign a class to future samples from their expression profile
- Interpret biologically the differences between the classes

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Linear classifiers

The approach

- Each sample is represented by a vector $x = (x_1, \ldots, x_p)$ where $p > 10^5$ is the number of probes
- Classification: given the set of labeled sample, learn a linear decision function:

$$f(x) = \sum_{i=1}^{p} \beta_i x_i + \beta_0 \ ,$$

  that is positive for one class, negative for the other
- Interpretation: the weight β_i quantifies the influence of gene i for the classification

Linear classifiers

Pitfalls

- No robust estimation procedure exist for 100 samples in 10^5 dimensions!
- It is necessary to reduce the complexity of the problem with prior knowledge.

Example : Norm Constraints

The approach

A common method in statistics to learn with few samples in high dimension is to constrain the norm of β, e.g.:

- Euclidean norm (support vector machines, ridge regression): $\| \beta \|_2 = \sum_{i=1}^{p} \beta_i^2$
- L_1-norm (lasso regression) : $\| \beta \|_1 = \sum_{i=1}^{p} | \beta_i |$

Pros

- Good performance in classification

Cons

- Limited interpretation (small weights)
- No prior biological knowledge

Example 2: Feature Selection

The approach

Constrain most weights to be 0, i.e., select a few genes (< 20) whose expression are enough for classification. Interpretation is then about the selected genes.

Pros

- Good performance in classification
- Useful for biomarker selection
- Apparently easy interpretation

Cons

- The gene selection process is usually not robust
- Wrong interpretation is the rule (too much correlation between genes)

Pathway interpretation

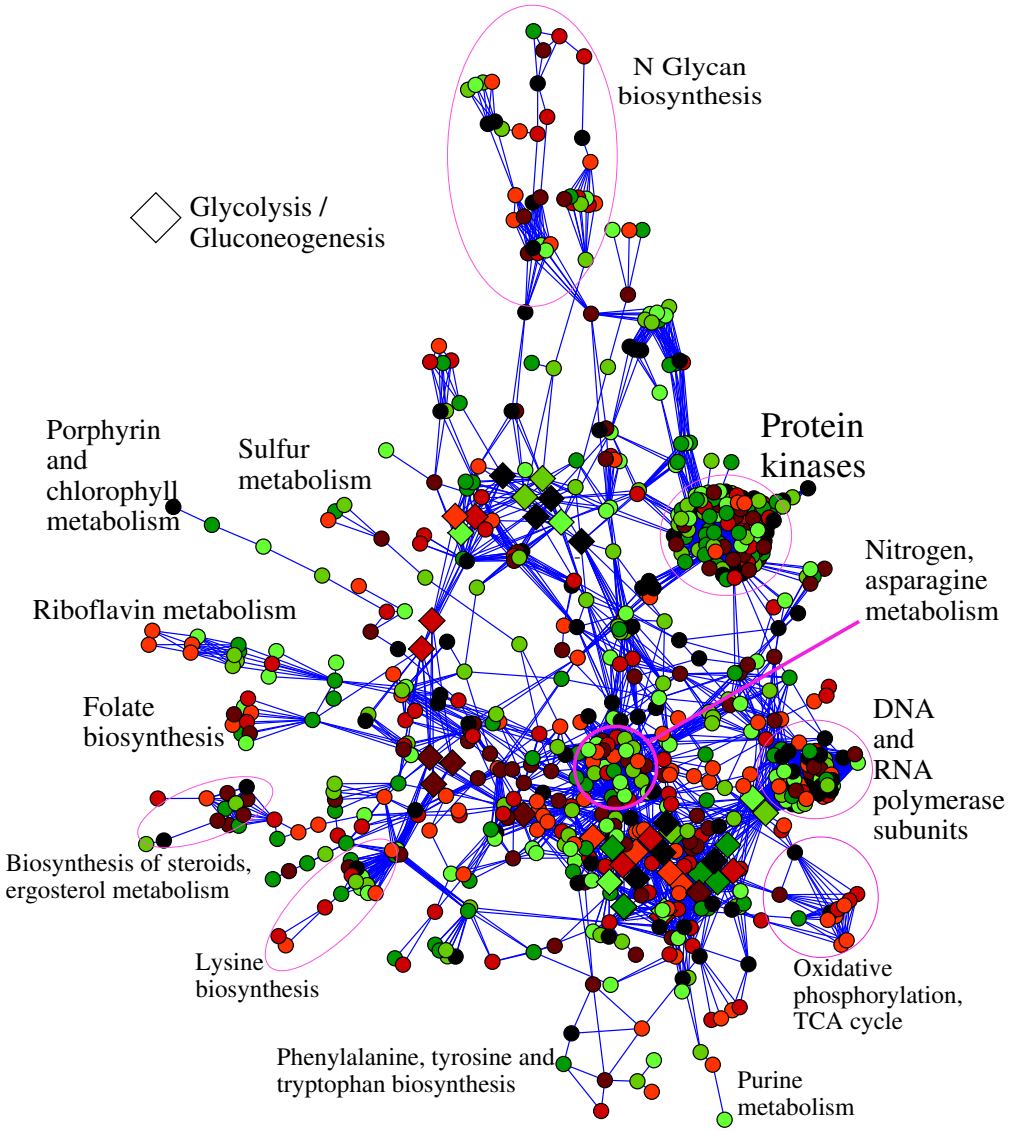
Motivation

- Basic biological functions are usually expressed in terms of pathways and not of single genes (metabolic, signaling, regulatory)
- Many pathways are already known
- How to use this prior knowledge to constrain the weights to have an interpretation at the level of pathways?

Solution (Rapaport et al., 2006)

- Constrain the diffusion RKHS norm of β
- Relevant if the true decision function is indeed smooth w.r.t. the biological network

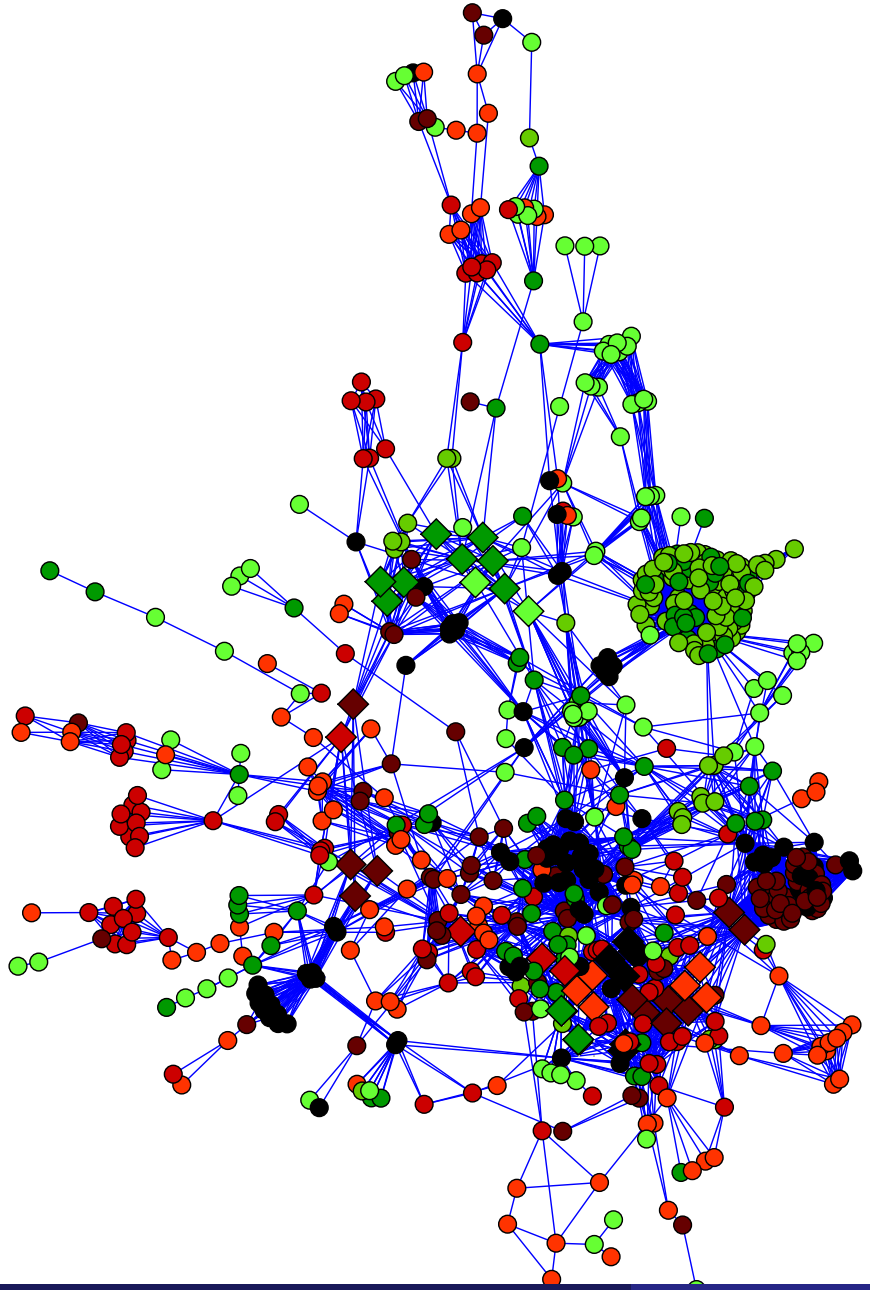
Pathway interpretation



Bad example

- The graph is the complete known metabolic network of the budding yeast (from KEGG database)
- We project the classifier weight learned by a SVM
- Good classification accuracy, but no possible interpretation!

Pathway interpretation



Good example

- The graph is the complete known metabolic network of the budding yeast (from KEGG database)
- We project the classifier weight learned by a spectral SVM
- Good classification accuracy, and good interpretation!

Conclusion

What we saw

- Basic definitions of p.d. kernels and RKHS
- How to use RKHS in machine learning
- The importance of the choice of kernels, and how to include “prior knowledge” there.
- Several approaches for kernel design (there are many!)
- Review of kernels for strings and on graphs

What we did not see

- How to automatize the process of kernel design (kernel selection? kernel optimization?)
- How to deal with non p.d. kernels (tends to become the rule in applications)
- Applications beyond bioinformatics (there are many!).

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