Statistical learning on graphs

Jean-Philippe Vert
Jean-Philippe.Vert@ensmp.fr

ParisTech, Ecole des Mines de Paris
Institut Curie
INSERM U900

Seminar of probabilities, Institut Joseph Fourier, Grenoble, February 12, 2008.

Outline

Outline

Part 1

Statistical Learning with Positive Definite Kernels

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 $(a_1, a_2, \ldots, a_N) \in \mathbb{R}^N$:

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

Examples

Kernels for vectors

Classical kernels for vectors ($\mathcal{X} = \mathbb{R}^p$) include:

- The linear kernel

$$K_{lin}\left(\mathbf{x}, \mathbf{x}'\right) = \mathbf{x}^\top \mathbf{x}' \ .$$

- The polynomial kernel

$$K_{poly}\left(\mathbf{x}, \mathbf{x}'\right) = \left(\mathbf{x}^\top \mathbf{x}' + a\right)^d \ .$$

- The Gaussian RBF kernel:

$$K_{Gaussian}\left(\mathbf{x}, \mathbf{x}'\right) = \exp\left(-\frac{\| \mathbf{x} - \mathbf{x}' \|^2}{2\sigma^2}\right) \ .$$

Examples

Kernels for vectors

Classical kernels for vectors ($\mathcal{X} = \mathbb{R}^p$) include:

- The linear kernel

$$K_{lin}\left(\mathbf{x}, \mathbf{x}'\right) = \mathbf{x}^\top \mathbf{x}' \ .$$

- The polynomial kernel

$$K_{poly}\left(\mathbf{x}, \mathbf{x}'\right) = \left(\mathbf{x}^\top \mathbf{x}' + a\right)^d \ .$$

- The Gaussian RBF kernel:

$$K_{Gaussian}\left(\mathbf{x}, \mathbf{x}'\right) = \exp\left(-\frac{\| \mathbf{x} - \mathbf{x}' \|^2}{2\sigma^2}\right) \ .$$

Examples

Kernels for vectors

Classical kernels for vectors ($\mathcal{X} = \mathbb{R}^p$) include:

- The linear kernel

$$K_{lin}\left(\mathbf{x}, \mathbf{x}'\right) = \mathbf{x}^\top \mathbf{x}' \ .$$

- The polynomial kernel

$$K_{poly}\left(\mathbf{x}, \mathbf{x}'\right) = \left(\mathbf{x}^\top \mathbf{x}' + a\right)^d \ .$$

- The Gaussian RBF kernel:

$$K_{Gaussian}\left(\mathbf{x}, \mathbf{x}'\right) = \exp\left(-\frac{\| \mathbf{x} - \mathbf{x}' \|^2}{2\sigma^2}\right) \ .$$

P.d. kernels are inner products

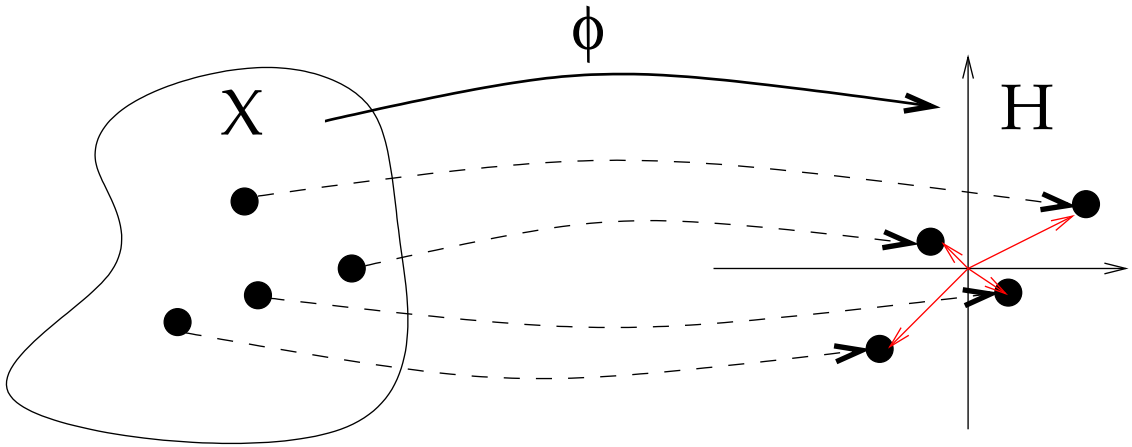
Theorem (Aronszajn, 1950)

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 $\mathcal{X}$:

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



Reproducing kernel Hilbert space

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).

Positive definite and reproducing kernels are the same

Theorem (Aronszajn, 1950)

K is a p.d. kernel if and only if there exists a RKHS having K as r.k.

Explicit construction of the RKHS

- If K is p.d., then the RKHS $\mathcal{H}$ is the vector subspace of $\mathbb{R}^{\mathcal{X}}$ spanned by the functions $\{K_{\mathbf{x}}\}_{\mathbf{x}\in\mathcal{X}}$ (and their pointwise limits).
- For any $f, g \in \mathcal{H}_0$, given by:

$$f = \sum_i a_i K_{\mathbf{x}_i} , \quad g = \sum_j b_j K_{\mathbf{y}_j} ,$$

the inner product is given by:

$$\langle f, g \rangle_{\mathcal{H}_0} := \sum_{i,j} a_i b_j K(\mathbf{x}_i, \mathbf{y}_j) , \quad \| f \|^2_{\mathcal{H}_0} = \sum_{i,j} a_i a_j K(\mathbf{x}_i, \mathbf{x}_j) .$$

Positive definite and reproducing kernels are the same

Theorem (Aronszajn, 1950)

K is a p.d. kernel if and only if there exists a RKHS having K as r.k.

Explicit construction of the RKHS

- If K is p.d., then the RKHS $\mathcal{H}$ is the vector subspace of $\mathbb{R}^{\mathcal{X}}$ spanned by the functions $\{K_{\mathbf{x}}\}_{\mathbf{x}\in\mathcal{X}}$ (and their pointwise limits).
- For any $f, g \in \mathcal{H}_0$, given by:

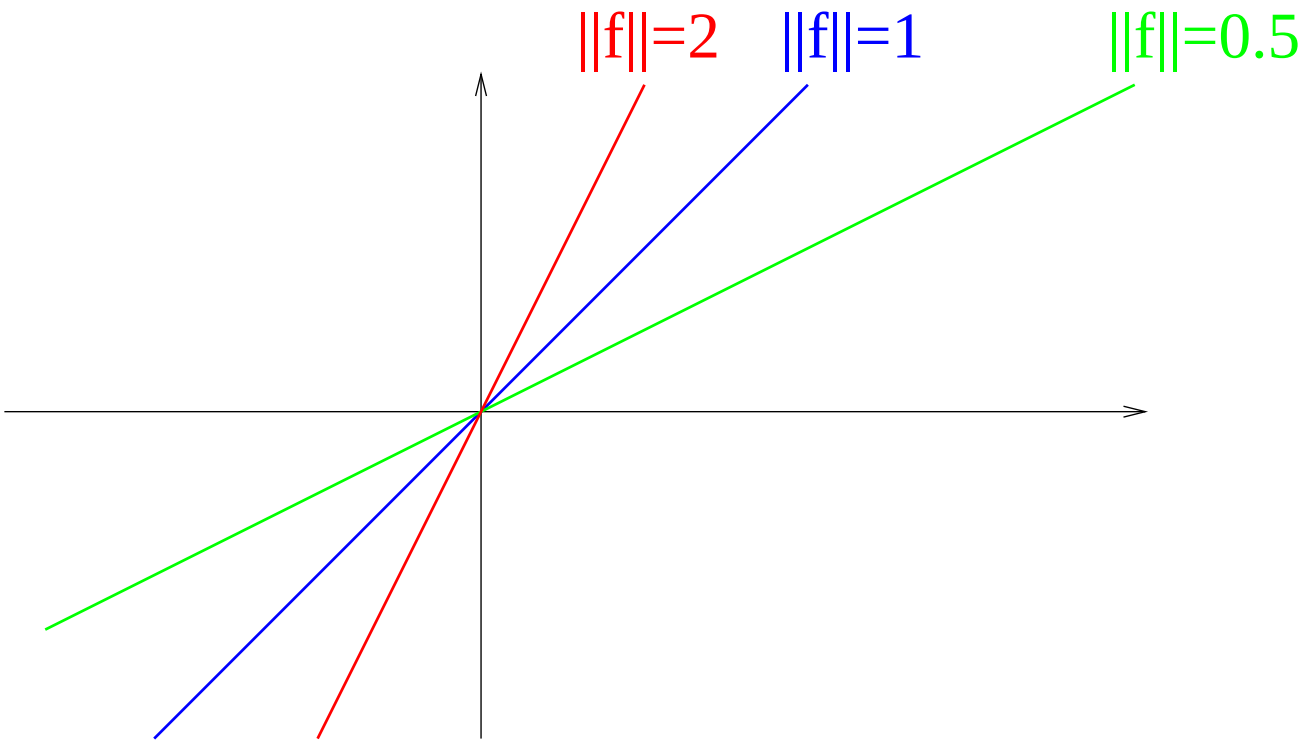
$$f = \sum_i a_i K_{\mathbf{x}_i} \,, \quad g = \sum_j b_j K_{\mathbf{y}_j} \,,$$

the inner product is given by:

$$\langle f, g \rangle_{\mathcal{H}_0} := \sum_{i,j} a_i b_j K\left(\mathbf{x}_i, \mathbf{y}_j\right) \,, \quad \| f \|^2_{\mathcal{H}_0} = \sum_{i,j} a_i a_j K\left(\mathbf{x}_i, \mathbf{x}_j\right) \,.$$

Example : RKHS of the linear kernel

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



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.

A useful property

Representer theorem (Kimeldorf and Wahba, 1971)

- 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:

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

admits a representation of the form:

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

Learning from data

General setting

- Observation: $\{z_1, \ldots, z_n\}$ where $z_i = (\mathbf{x}_i, y_i) \in \mathcal{X} \times \mathcal{Y}$
- Goal: learn a function $f : \mathcal{X} \to \mathbb{R}$
- Examples: density estimation, pattern recognition, regression, outlier detection, clustering, compression, low-dimensional embedding...

Learning from data

Empirical risk minimization (ERM)

1. Define a loss function $l(f, z)$ and a space of functions $\mathcal{F}$.
2. Minimize the empirical average loss over $\mathcal{F}$:

$$\hat{f} \in \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} l(f, z_i) \,.$$

General properties of ERM

- If $\mathcal{F}$ is not "too large" then the ERM is consistent ($\hat{f}$ is close to the best possible $f \in \mathcal{F}$ as the number of observations increases).
- If $\mathcal{F}$ is not "too small" then the best possible $f \in \mathcal{F}$ is a "good" solution.
- Challenge: choose a "small" $\mathcal{F}$ that contains "good" functions.

Learning from data

Empirical risk minimization (ERM)

1. Define a loss function $l(f, z)$ and a space of functions $\mathcal{F}$.
2. Minimize the empirical average loss over $\mathcal{F}$:

$$\hat{f} \in \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} l(f, z_i) \,.$$

General properties of ERM

- If $\mathcal{F}$ is not "too large" then the ERM is consistent ($\hat{f}$ is close to the best possible $f \in \mathcal{F}$ as the number of observations increases).
- If $\mathcal{F}$ is not "too small" then the best possible $f \in \mathcal{F}$ is a "good" solution.
- Challenge: choose a "small" $\mathcal{F}$ that contains "good" functions.

Learning with kernels

ERM in RKHS

- Take $\mathcal{F}$ to be a ball in the RKHS:

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

- Advantage: by controlling the "size" of $\mathcal{F}$ (related to B) the ERM principle works (consistency and theoretical rates of convergence).
- The kernel should be chosen s.t. some "good" functions have a small RKHS norm.

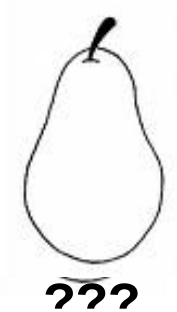
Example: pattern recognition


APPLE


APPLE


PEAR


PEAR


???


???


APPLE


PEAR


APPLE


APPLE


???

- Input variables $\mathbf{x} \in \mathcal{X}$
- Output $y \in \{-1, 1\}$.
- Training set $\mathcal{S} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$.

Large-margin classifiers

General setting

- For pattern recognition $\mathcal{Y} = \{-1, 1\}$.
- Goal: estimate a function $f : \mathcal{X} \to \mathbb{R}$ to predict $\mathbf{y}$ from the sign of $f(\mathbf{x})$
- The margin for a pair $(\mathbf{x}, \mathbf{y})$ is $\mathbf{y} f(\mathbf{x})$.
- Focusing on large margins ensures that $f(\mathbf{x})$ has the same sign as $\mathbf{y}$ and a large absolute value (confidence).
- Leads to 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.

ERM in for large-margin classifiers: Theory

Theoretical results

- The ERM estimator $\hat{f}_n$ solves:

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

- Let P an unknown distribution over $\mathcal{X} \times \mathcal{Y}$, assume $\mathcal{S} = (\mathbf{x}_i, y_i)_{i=1,\ldots,n}$ i.i.d. according to P.
- Assume K upper bounded by κ and ϕ Lipschitz with constant L_ϕ.
- For the ϕ-risk $R_\phi(f) = \mathbf{E}\phi\left(Yf\left(X\right)\right)$ we have:

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

ERM in for large-margin classifiers: 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:

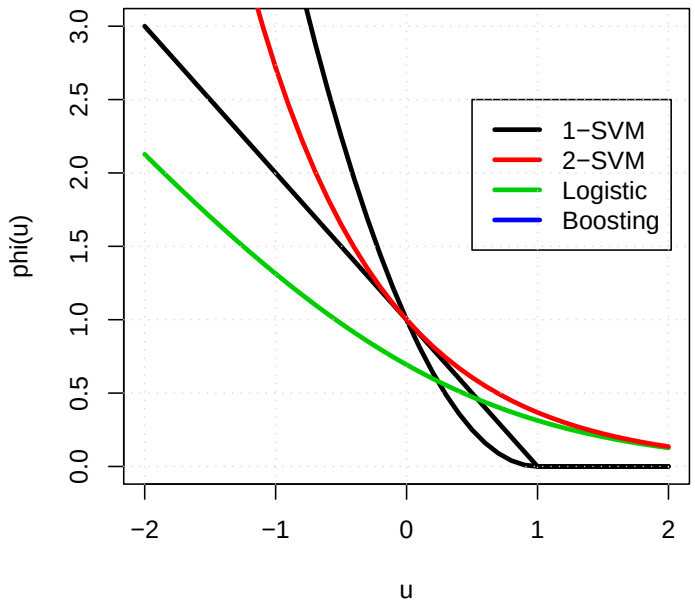
$$f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}) \ .$$

- 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}

Kernel methods: Summary

- 3 ways to map $\mathcal{X}$ to a Hilbert space:
  1. Explicitly define and compute $\Phi : \mathcal{X} \to \mathcal{H}$
  2. Define a p.d. kernel over $\mathcal{X}$
  3. Define a RKHS over $\mathcal{X}$
- The kernel trick allows to extend many linear algorithms to non-linear settings and to general data (even non-vectorial).
- 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 thanks to the representer theorem).
- We are now ready to learn with graphs by defining positive definite kernels for graphs!

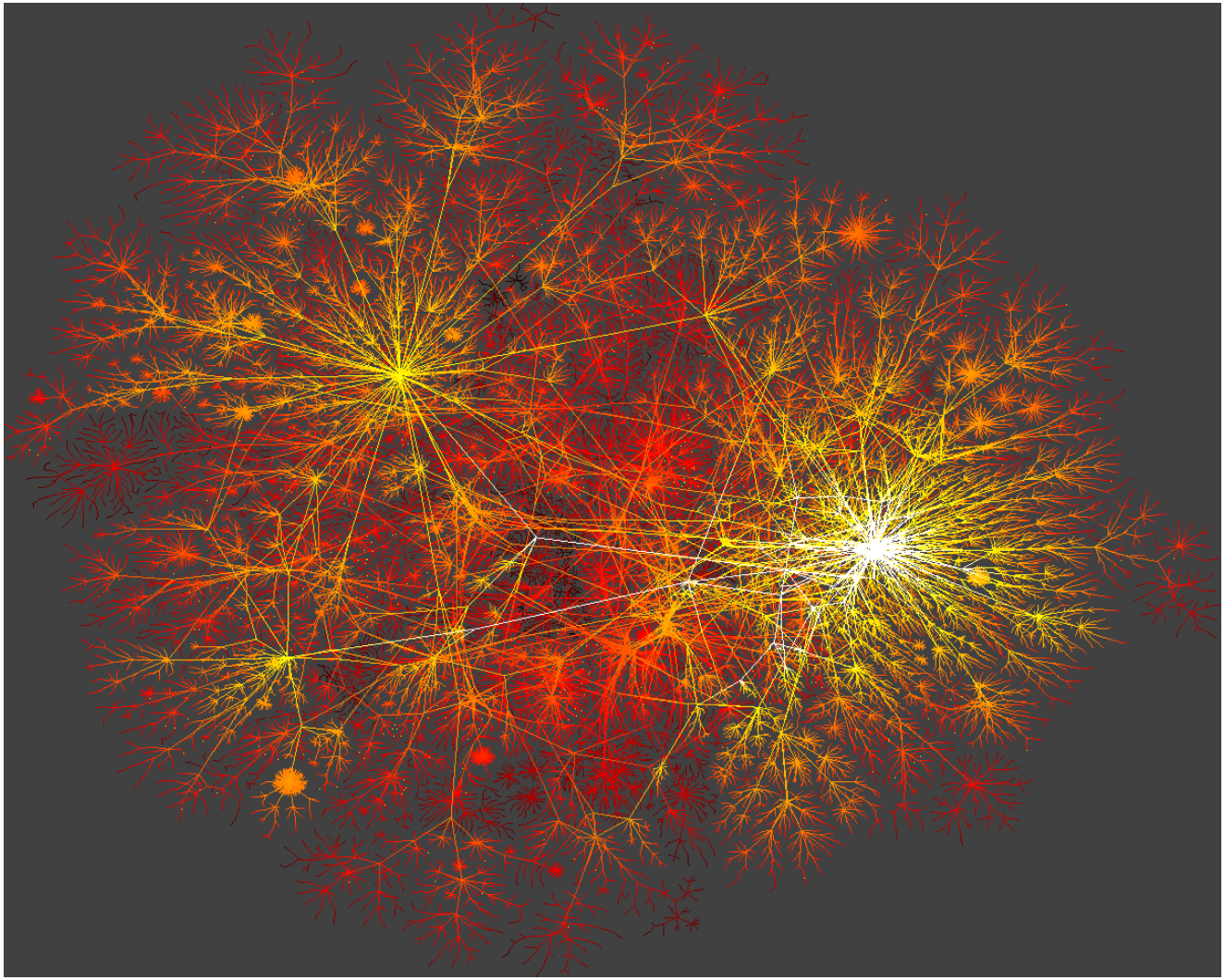
Part 2

Kernels on Graphs

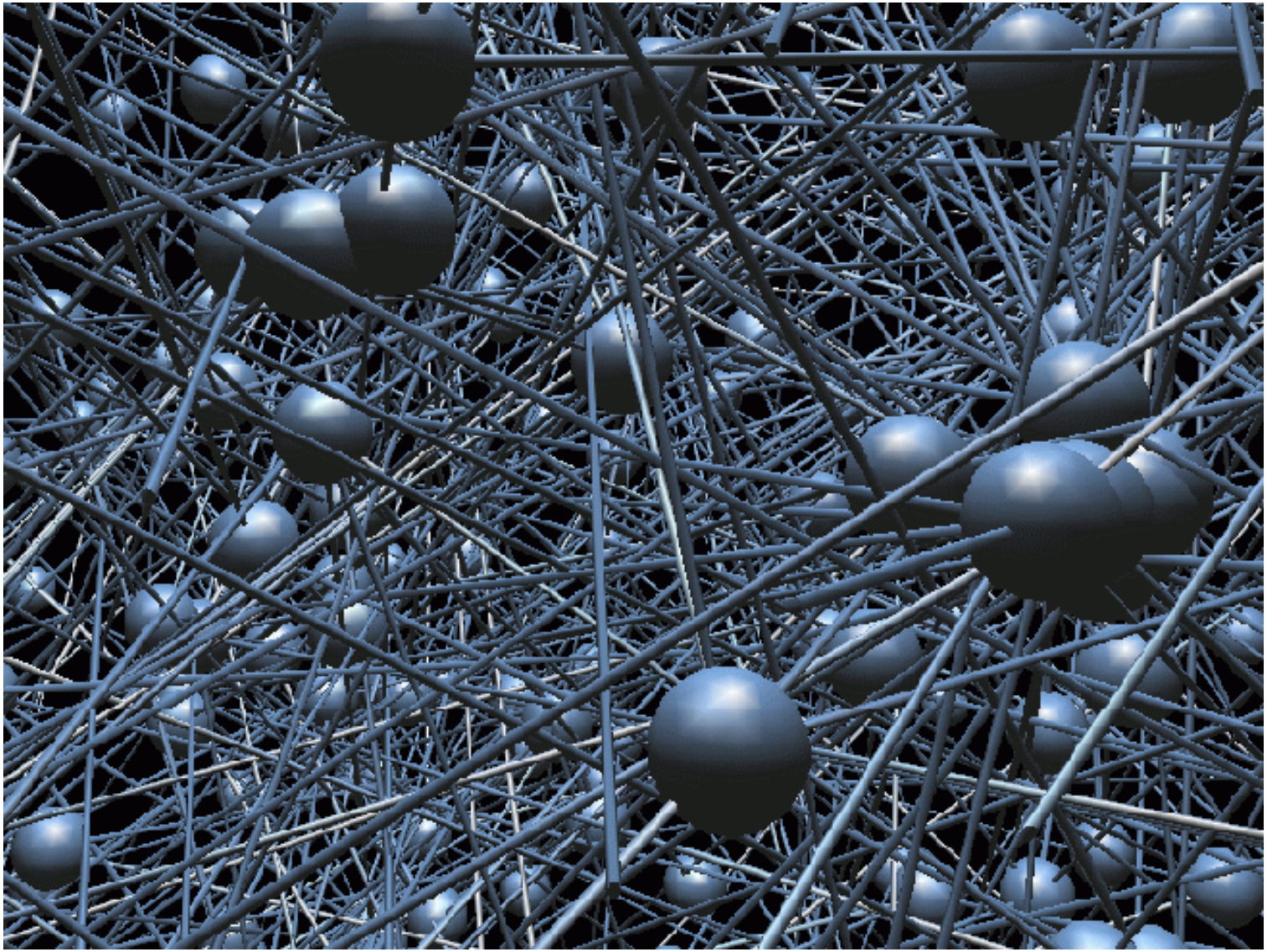
Outline

1. Statistical learning with positive definite kernels
2. Kernels on graphs
   - Motivation
   - Graph distance and p.d. kernels
   - Construction by regularization
   - The diffusion kernel
   - Harmonic analysis on graphs
   - Applications

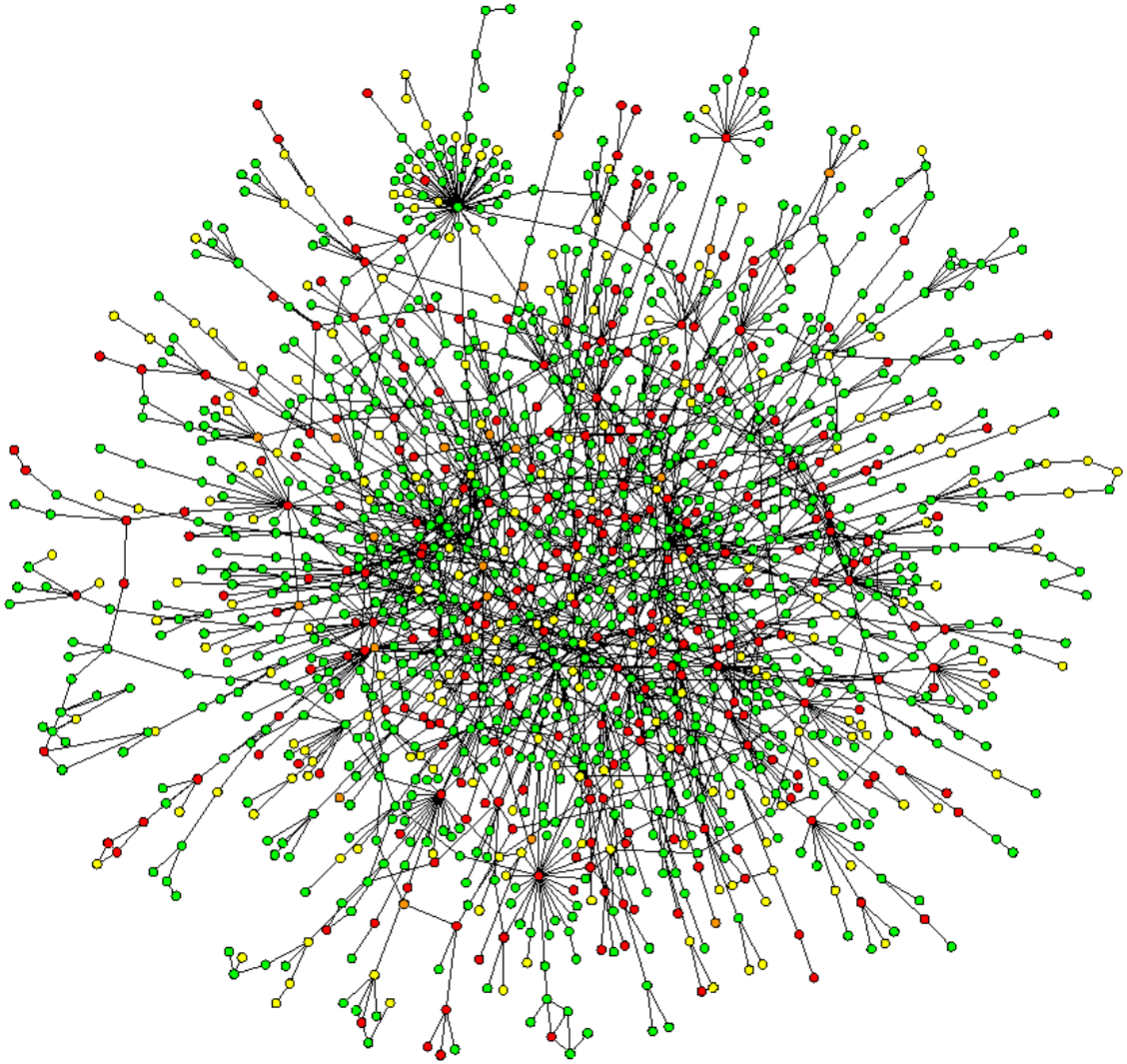
Example: web



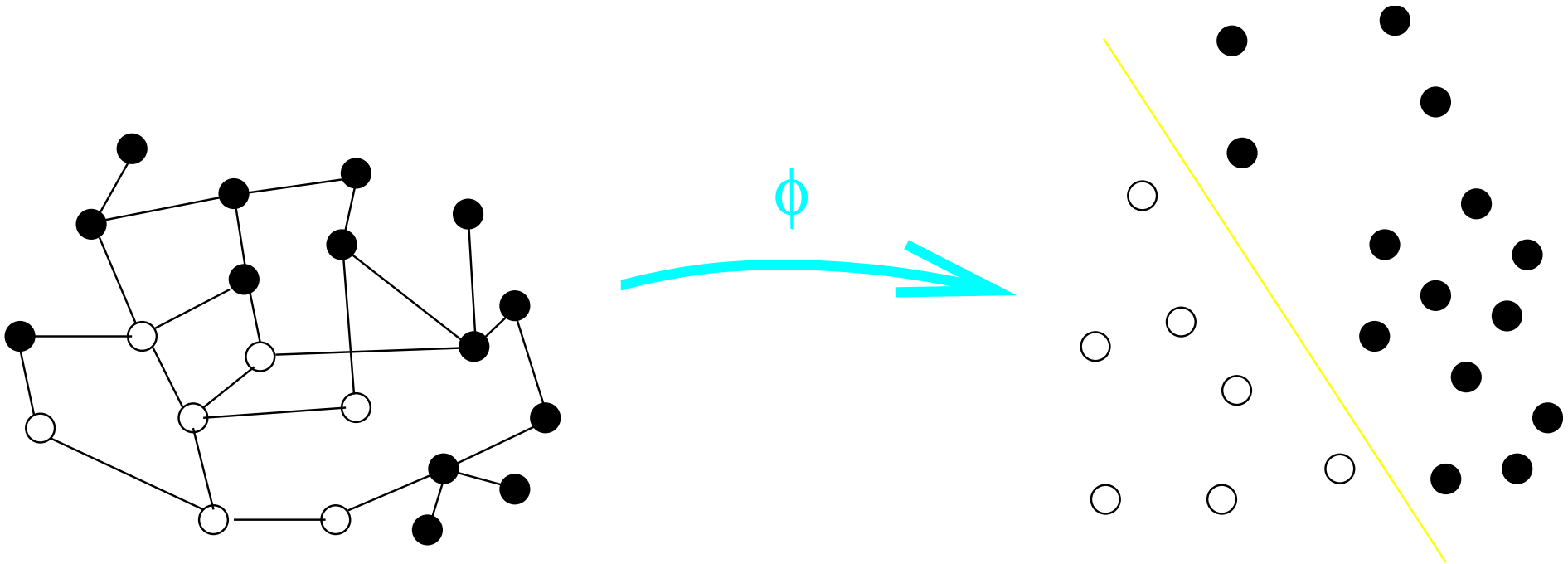
Example: social network



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)?

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)?

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, i.e.:

$$\forall t>0\,,\quad \exp\left(-td_K\left(\mathbf{x},\mathbf{x}'\right)^2\right)\text{ is p.d.}$$

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.*

Graph distance

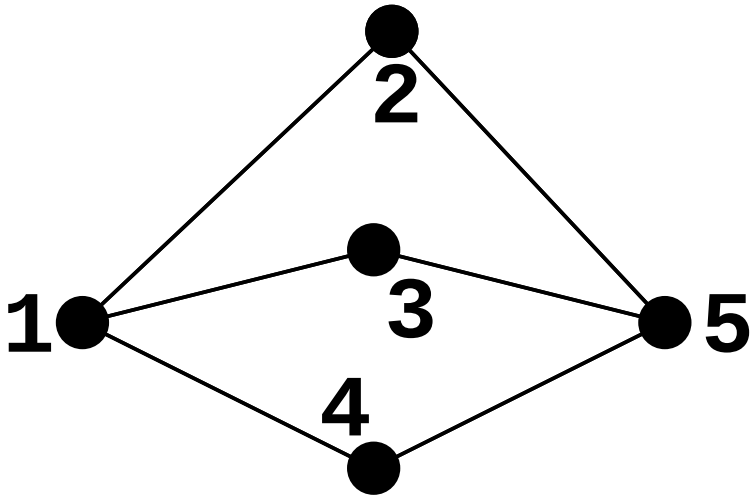
Graph embedding in a Hilbert space

- 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.*

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.

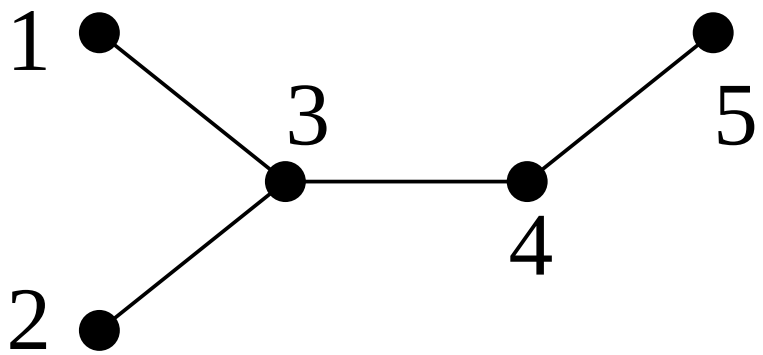
Proof

- 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

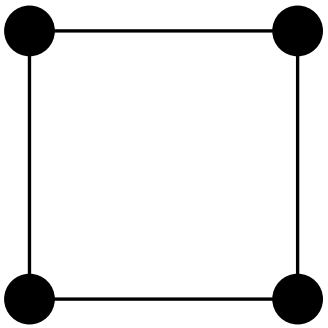


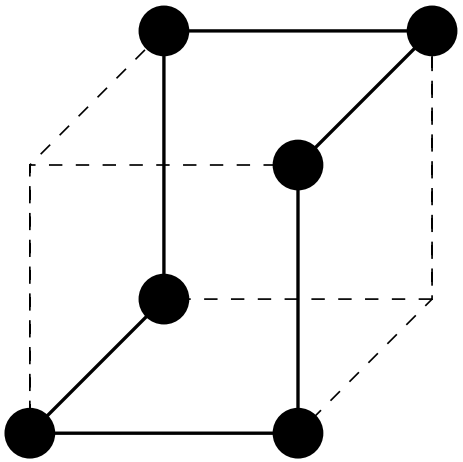
$$\left[e^{-d_G(i,j)}\right] = \begin{pmatrix} 1 & 0.14 & 0.37 & 0.14 & 0.05 \\ 0.14 & 1 & 0.37 & 0.14 & 0.05 \\ 0.37 & 0.37 & 1 & 0.37 & 0.14 \\ 0.14 & 0.14 & 0.37 & 1 & 0.37 \\ 0.05 & 0.05 & 0.14 & 0.37 & 1 \end{pmatrix}$$

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

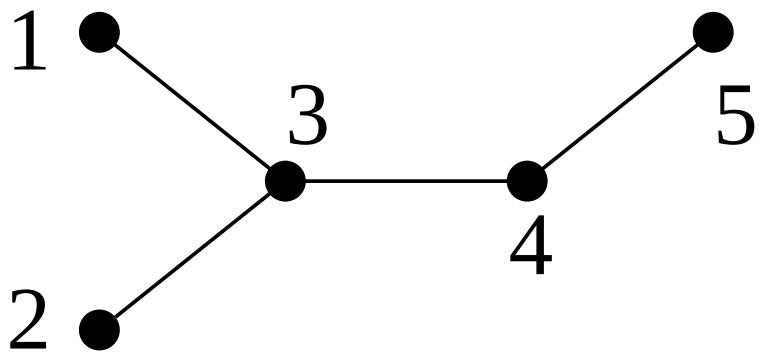
Motivation

- 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

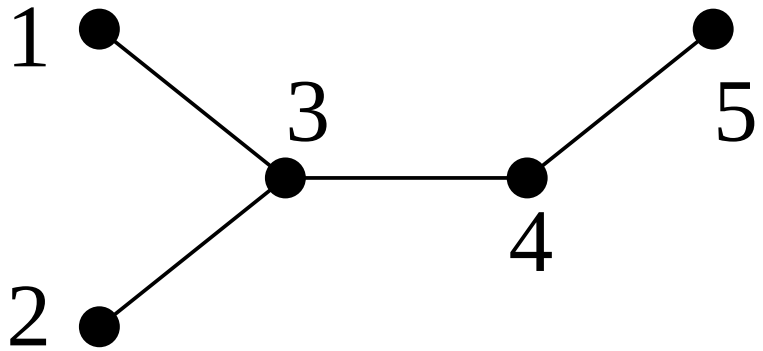


$$A = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \qquad D = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

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.*

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:

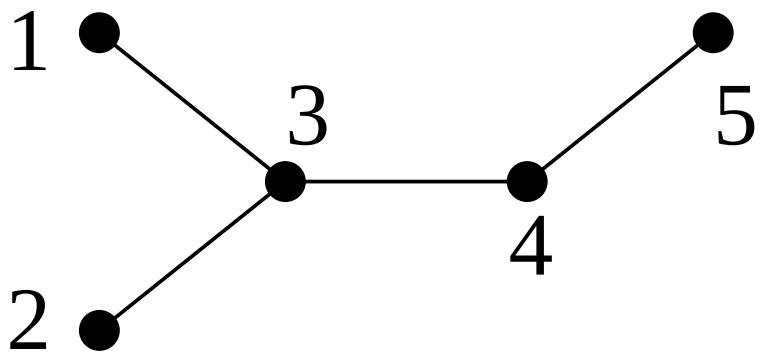
$$\begin{cases} \forall \mathbf{x} \in \mathcal{X}, & K_{\mathbf{x}} \in \mathcal{H} \ , \\ \forall \, (\mathbf{x}, f) \in \mathcal{X} \times \mathcal{H}, & \langle f, K_{\mathbf{x}} \rangle = f(\mathbf{x}) \ . \end{cases}$$

- $Ker(K) = Ker\,(L^*) = Ker\,(L)$, 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



$$L^* = \begin{pmatrix} 0.88 & -0.12 & 0.08 & -0.32 & -0.52 \\ -0.12 & 0.88 & 0.08 & -0.32 & -0.52 \\ 0.08 & 0.08 & 0.28 & -0.12 & -0.32 \\ -0.32 & -0.32 & -0.12 & 0.48 & 0.28 \\ -0.52 & -0.52 & -0.32 & 0.28 & 1.08 \end{pmatrix}$$

Outline

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 $K_{\mathbf{x}_0}(\mathbf{x}, 0) = \delta_{\mathbf{x}_0}(\mathbf{x})$.

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:

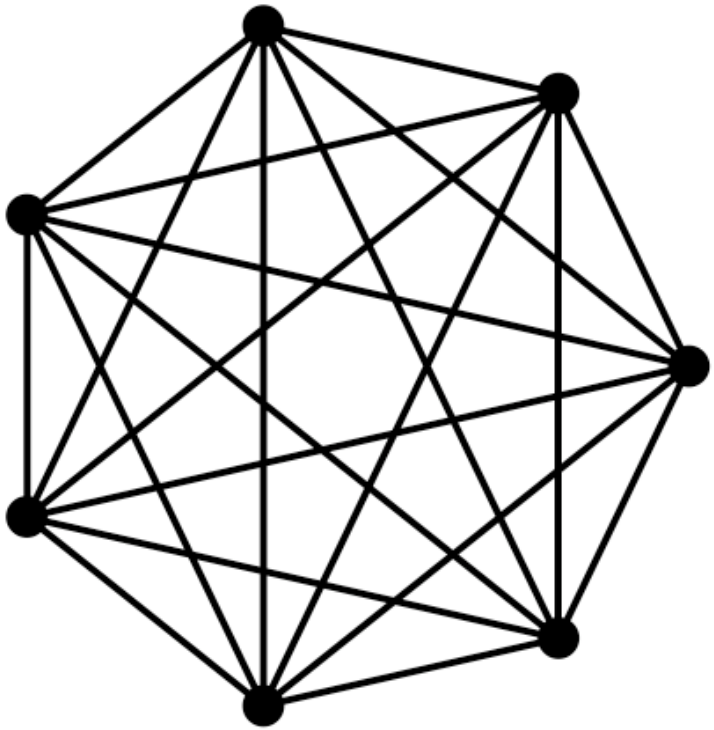
$$f_t = f_0 e^{-tL}$$

- This suggest to consider:

$$K = e^{-tL}$$

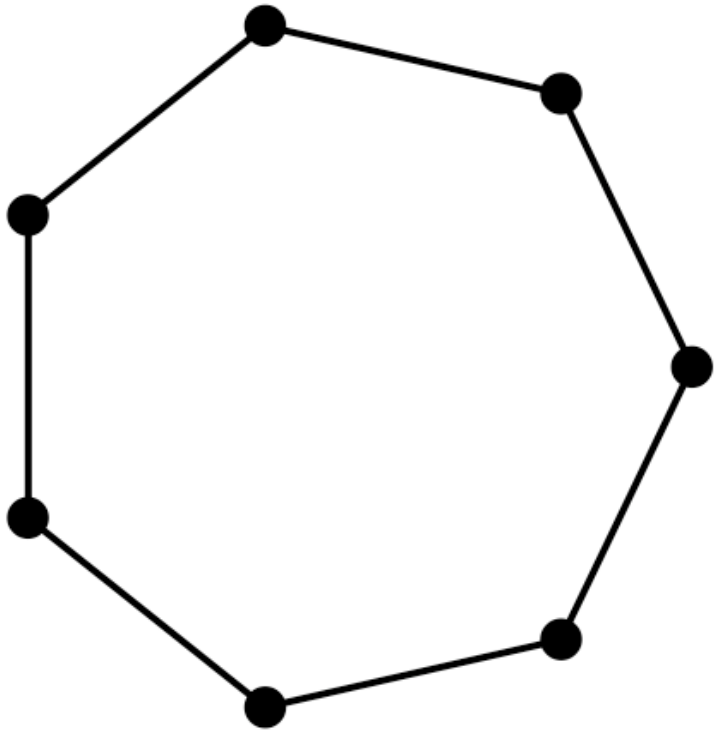
which is indeed symmetric positive semi-definite. We call it the diffusion kernel or heat kernel.

Example: complete graph



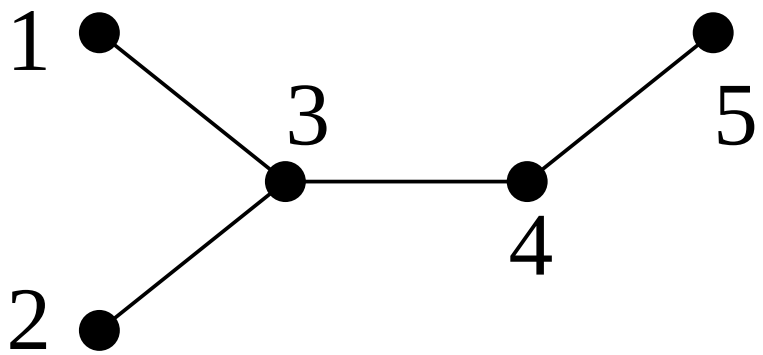
$$K_{i,j} = \begin{cases} \frac{1+(m-1)e^{-tm}}{m} & \text{for } i = j, \\ \frac{1-e^{-tm}}{m} & \text{for } i \neq j. \end{cases}$$

Example: closed chain



$$K_{i,j} = \frac{1}{m} \sum_{\nu=0}^{m-1} \exp\left[-2t\left(1 - \cos\frac{2\pi\nu}{m}\right)\right] \cos\frac{2\pi\nu(i-j)}{m}.$$

Example



$$e^{-L} = \begin{pmatrix} 0.50 & 0.13 & 0.24 & 0.10 & 0.04 \\ 0.13 & 0.50 & 0.24 & 0.10 & 0.04 \\ 0.24 & 0.24 & 0.24 & 0.18 & 0.10 \\ 0.10 & 0.10 & 0.18 & 0.32 & 0.30 \\ 0.04 & 0.04 & 0.10 & 0.30 & 0.52 \end{pmatrix}$$

Outline

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

- For any function $f \in \mathbb{R}^m$, let:

$$\hat{f}_i = u_i^\top f$$

be the Fourier coefficients of f (projection of f onto the eigenbasis of K).

- The RKHS norm of f is then:

$$\| f \|_{K_t}^2 = f^\top K^{-1} f = \sum_{i=1}^m e^{t\lambda_i} \hat{f}_i^2.$$

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.

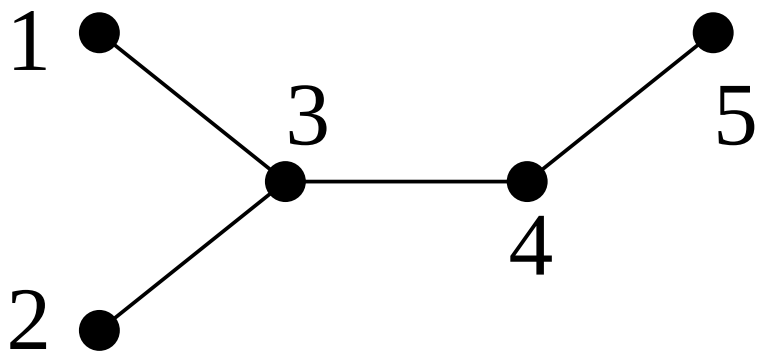
Example : regularized Laplacian

$$r(\lambda) = \frac{1}{\lambda + \epsilon}, \qquad \epsilon > 0$$

$$K = \sum_{i=1}^{m} \frac{1}{\lambda_i + \epsilon} u_i u_i^\top = (L + \epsilon I)^{-1}$$

$$\| f \|_K^2 = f^\top K^{-1} f = \sum_{i \sim j} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j) \right)^2 + \epsilon \sum_{i=1}^{m} f(\mathbf{x}_i)^2 .$$

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

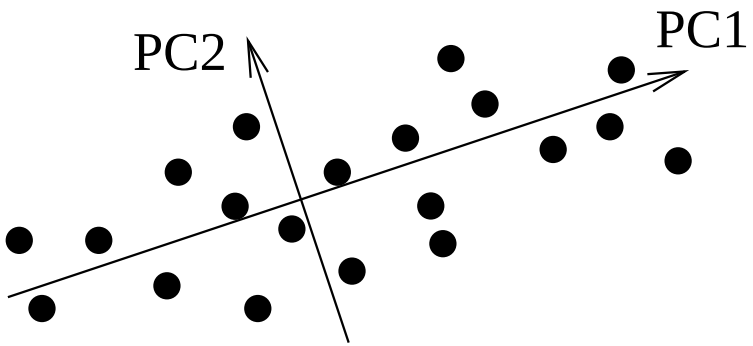
- A classical relaxation of graph partitioning is:

$$\min_{f \in \mathbb{R}^{\mathcal{X}}} \sum_{i \sim j} (f_i - f_j)^2 \quad \text{s.t.} \sum_i f_i^2 = 1$$

- This can be rewritten

$$\max_f \sum_i f_i^2 \text{ s.t.} \quad \| f \|_{\mathcal{H}} \leq 1$$

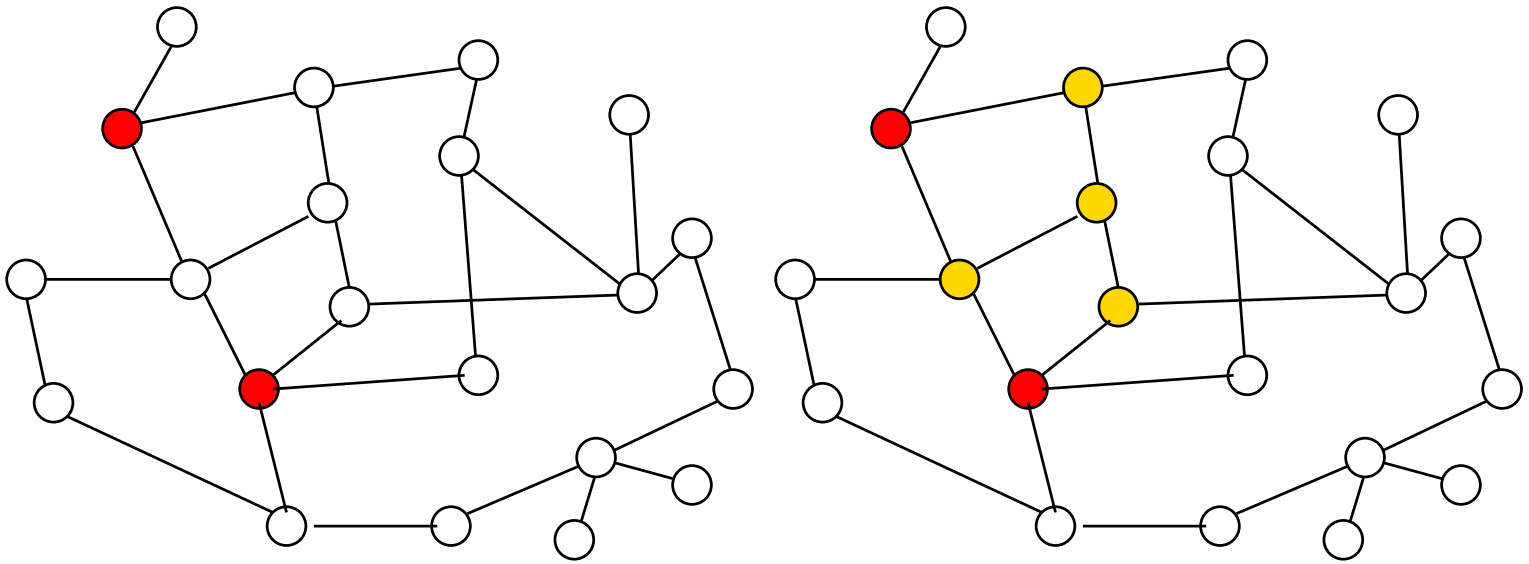
- This is principal component analysis in the RKHS ("kernel PCA")



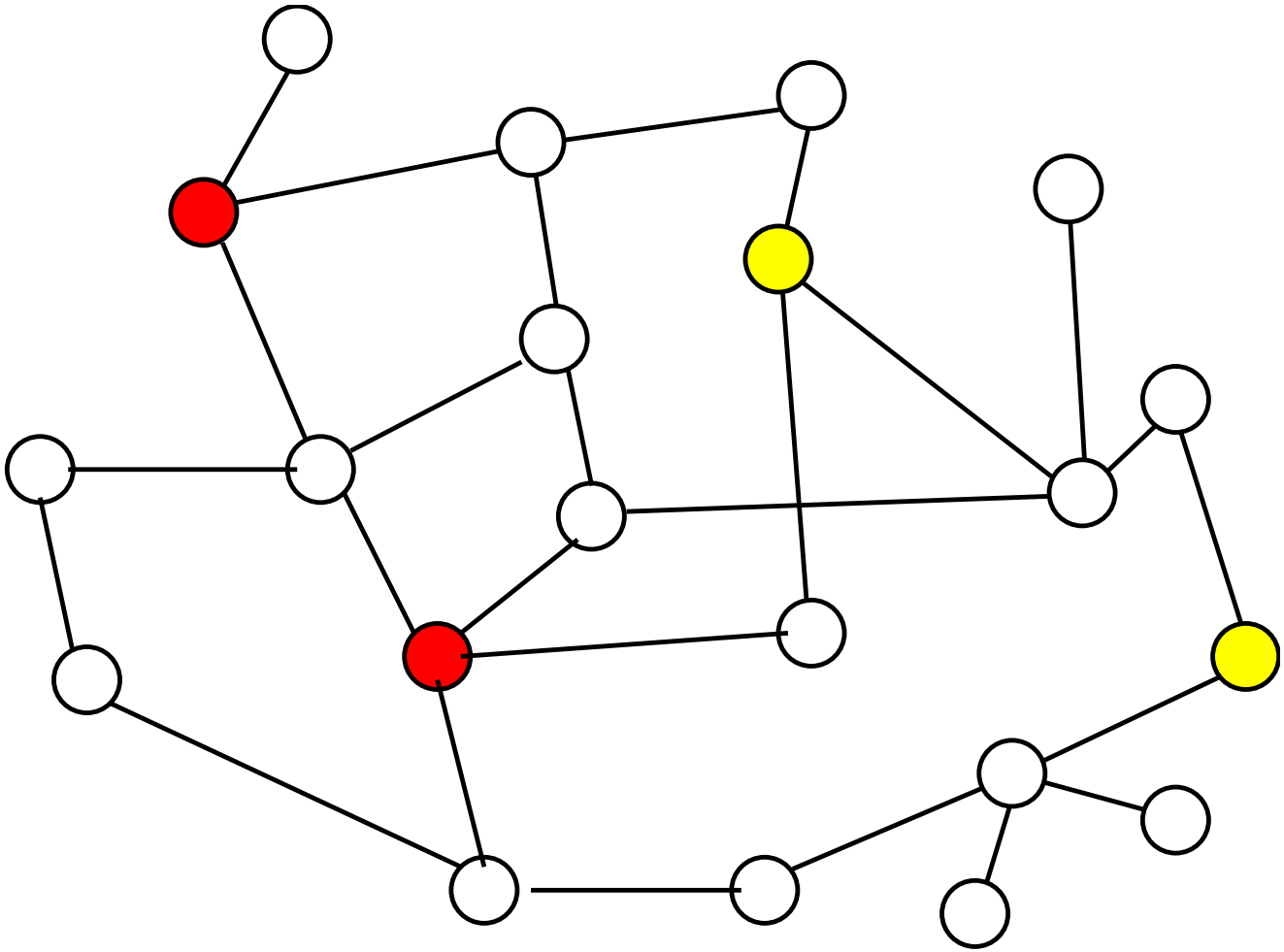
Applications 2: search on a graph

- Let $x_1, \ldots, x_q$ a set of q nodes (the query). How to find "similar" nodes (and rank them)?
- One solution:

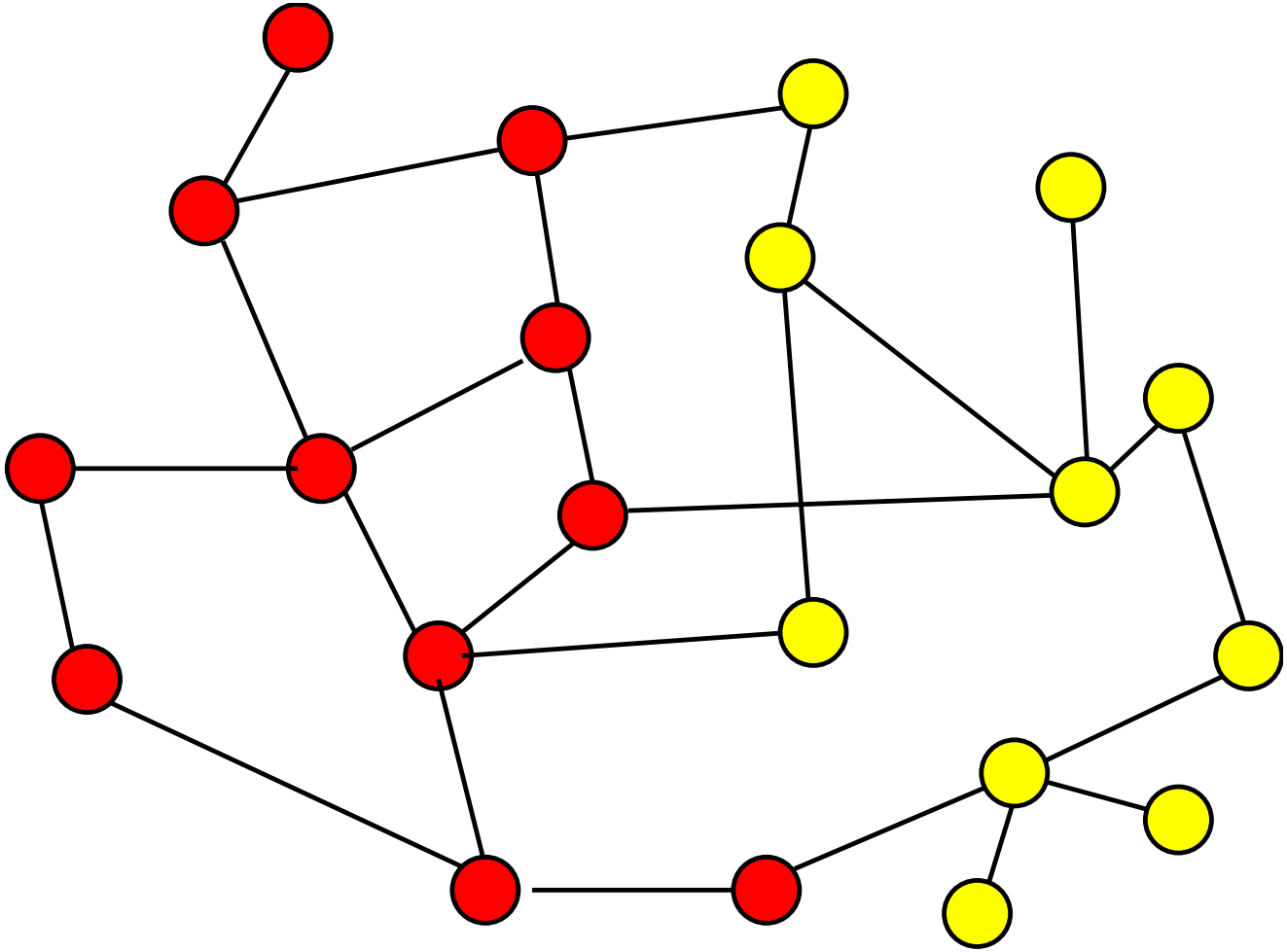
$$\min_f \| f \|_{\mathcal{H}} \quad \text{s.t.} \quad f(x_i) \geq 1 \text{ for } i = 1, \ldots, q.$$



Application 3: Semi-supervised learning



Application 3: Semi-supervised learning



Application 4: Tumor classification from microarray data

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

Application 4: Tumor classification from microarray data

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

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:

$$f(x) = \sum_{i=1}^{p} \beta_i x_i + \beta_0 \ ,$$

- Interpretation: the weight β_i quantifies the influence of gene i for the classification

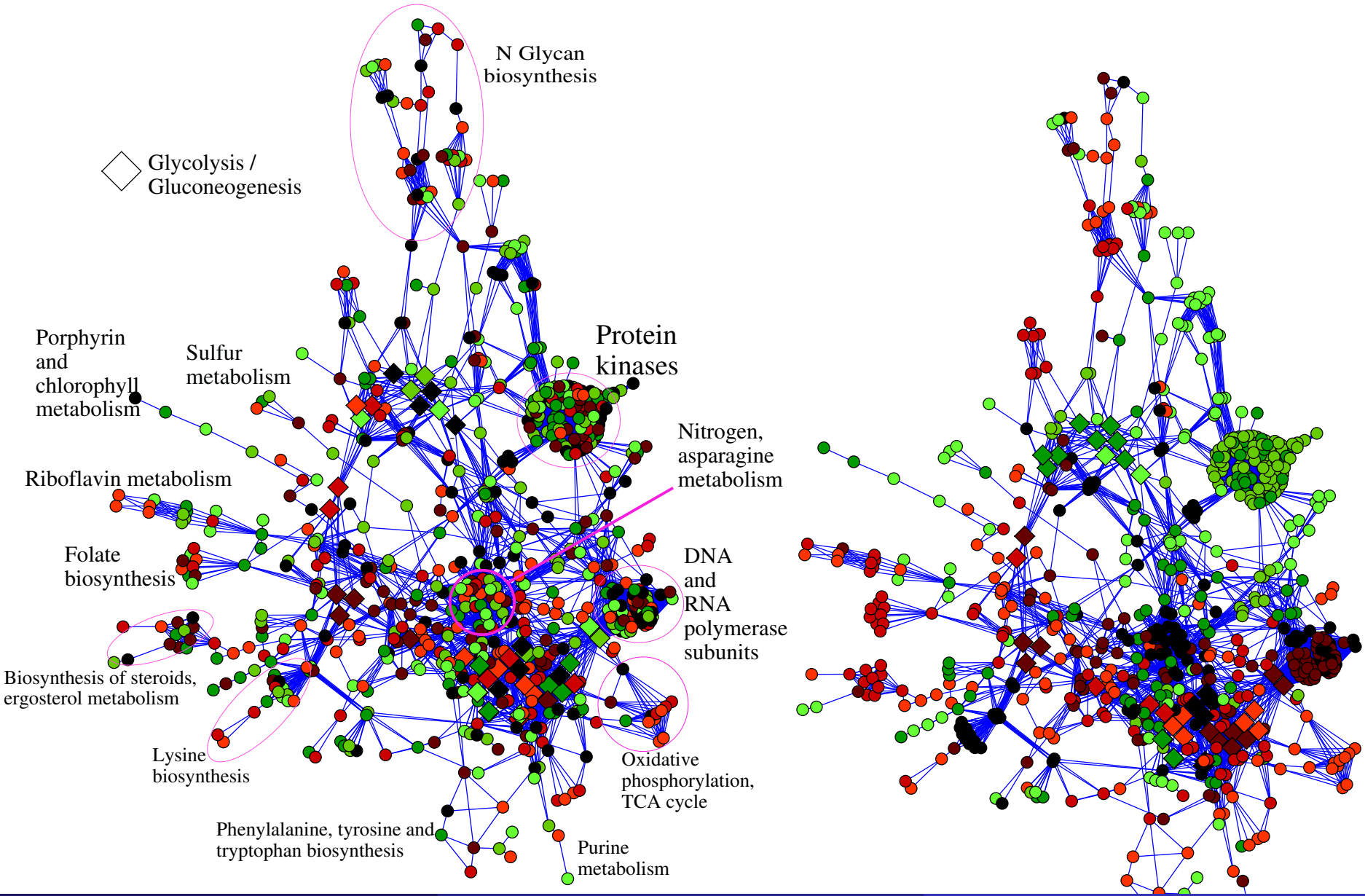
Pitfalls

- No robust estimation procedure exist for 100 samples in 10^5 dimensions!

Prior knowledge

- We know the functions of many genes, and how they interact together.
- This can be represented as a graph of genes, where connected genes perform some action together
- Prior knowledge: constraint the weights of genes that work together to be similar
- Mathematically: constrain the norm of the weight vector in the RKHS of the diffusion kernel.

Comparison


N Glycan biosynthesis
Glycolysis / Gluconeogenesis
Porphyrin and chlorophyll metabolism
Sulfur metabolism
Protein kinases
Nitrogen, asparagine metabolism
Riboflavin metabolism
Folate biosynthesis
DNA and RNA polymerase subunits
Biosynthesis of steroids, ergosterol metabolism
Lysine biosynthesis
Oxidative phosphorylation, TCA cycle
Phenylalanine, tyrosine and tryptophan biosynthesis
Purine metabolism

Conclusion

Conclusion

What we saw

- Extension of machine learning algorithms to graph data through the definition of positive definite kernels for and on graphs
- A variety of solutions have been proposed, borrowing ideas from graph algorithms and spectral graph theory.
- Increasingly used in real-world applications.

Unanswered question

- Theoretical foundations to guide the choice of kernel?
- How to design / choose / learn a kernel for a given application in practice?
- How to improve scalability of kernel methods + graph kernels to large datasets?

Further reading

Kernels and RKHS: general


N. Aronszajn.
Theory of reproducing kernels.
Trans. Am. Math. Soc., 68:337 – 404, 1950.


C. Berg, J. P. R. Christensen, and P. Ressel.
Harmonic analysis on semigroups.
Springer-Verlag, New-York, 1984.


G. Wahba.
Spline Models for Observational Data, volume 59 of *CBMS-NSF Regional Conference Series in Applied Mathematics*.
SIAM, Philadelphia, 1990.

Further reading

Learning with kernels


V. N. Vapnik.
Statistical Learning Theory.
Wiley, New-York, 1998.


B. Schölkopf and A. J. Smola.
Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond.
MIT Press, Cambridge, MA, 2002.


J. Shawe-Taylor and N. Cristianini.
Kernel Methods for Pattern Analysis.
Cambridge University Press, 2004.


B. Schölkopf, K. Tsuda, and J.-P. Vert.
Kernel Methods in Computational Biology.
MIT Press, 2004.

Further reading

Kernels on graphs


R. I. Kondor and J. Lafferty.
Diffusion Kernels on Graphs and Other Discrete Input.
In *ICML 2002*, 2002.


J.-P. Vert and M. Kanehisa.
Graph-driven features extraction from microarray data using diffusion kernels and kernel CCA.
In Suzanna Becker, Sebastian Thrun, and Klaus Obermayer, editors, *Adv. Neural Inform. Process. Syst.*, pages 1449–1456. MIT Press, 2003.


F. Rapaport, A. Zynoviev, M. Dutreix, E. Barillot, and J.-P. Vert.
Classification of microarray data using gene networks.
BMC Bioinformatics, 8:35, 2007.