Graph kernels

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Séminaire LORIA 2012

Motivation

Structural Pattern Recognition

- 🙂 Rich description of objects
- 🙁 Poor properties of graph's space does not allow to readily generalize/combine sets of graphs

Statistical Pattern Recognition

- 🙁 Global description of objects
- 🙂 Numerical spaces with many mathematical properties (metric, vector space, ...).

Motivation

Analyse large famillies of structural and numerical objects using a **unified** framework based on pairwise similarity.

Kernels : Definition

- A kernel k is a **symmetric** similarity measure on a set χ

$$\forall (x,y) \in \chi^2,\ k(x,y) = k(y,x)$$

- k is said to be **definite positive** (d.p.) iff k is symmetric and iff:

$$\left.\begin{array}{lcl} \forall (x_1,\dots,x_n) & \in & \chi^n \\ \forall (c_1,\dots,c_n) & \in & \mathbb{R}^n \end{array}\right\} \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j k(x_i,x_j) \geq 0$$

- $K = (k(x_i,x_j))_{(i,j)\in\{1,\dots,n\}}$ is the Gramm matrix of k. k is d.p. iff:

$$\forall c \in \mathbb{R}^n - \{0\},\ c^t K c \geq 0$$

Kernels and scalar products

Aronszajn 1950 :

A kernel k is d.p. on a space χ
if and only if
it exists

- one Hilbert space $\mathcal{H}$ and
- a function $\varphi : \chi \rightarrow \mathcal{H}$

such that:

$$k(x, y) = < \varphi(x), \varphi(y) >$$

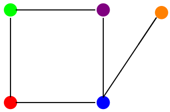
Outline

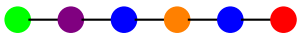
Kernel and strutured data

The kernel trick provides an implicit embedding whose metric is defined from our similarity criterion (the kernel).

Walk kernels

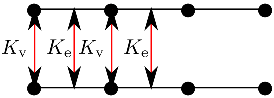
- Walks: Let $G = (V, E)$. $W = (v_1, \dots, v_n)$ is a walk iff $(v_i, v_{i+1}) \in E, \forall i \in \{1, \dots, n-1\}$.



 is a walk

- Kernel between walks

$$K(h,h') = \begin{cases} 0 & \text{if } |h| \neq [h'| \text{ and} \\ K_v(v_1, v'_1).\Pi_{i=1}^{|h|} K_e(e_i, e'_i) K_v(v_{i+1}, v'_{i+1}) & \text{otherwize} \end{cases}$$



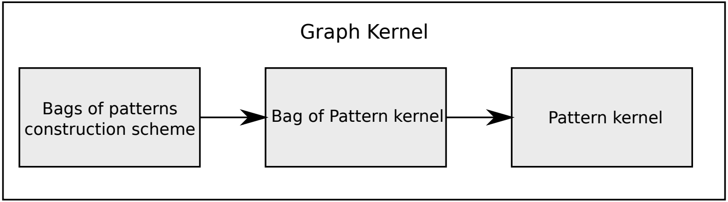
- Walk kernels :

$$K(G_1, G_2) = \sum_{h \in \mathcal{W}(G_1)} \sum_{h' \in \mathcal{W}(G_2)} K(h,h') \lambda_{G_1}(h) \lambda_{G_2}(h')$$

Finite Bag kernels

$$\left.\begin{array}{ccc} G & \rightarrow & B(G) \\ G' & \rightarrow & B(G') \end{array}\right\} K(G,G') = K(B(G),B(G'))$$

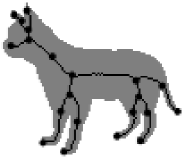
Three independent step to design a graph kernel.



Questions :

Which type of graph best capture object's properties ?
Shape recognition:

- Shape described by skeletons encoded by graphs $G = (V, E, \omega)$.
  - V:
    - extremities/intersection of branches or
    - abrupt changes of the radius along a branch.
  - E:
    - branches of the skeleton.
    - Each edge is weighted by a function ω encoding the length of the boundary which contributed to the branch [Torsello04].



Chemoinformatic: $G = (V, E, \mu, \nu)$

- V set of atoms, μ atom's type,
- E set of bounds, ν bound's type.

Questions :

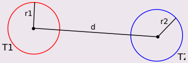
- Which type of graph best capture object's properties ?
- Which pattern should we choose ?
  - Paths,
  - Sub trees,
  - Sub graphs.
  - Sub combinatorial maps,...
- How to build a bag which minimizes the loss of information ?
  - All patterns up to a given size ?
  - More relevant patterns ?
    - Shape recognition: A priori information $\rightarrow$ covering problem
    - Chemoinformatics: Multiple kernel learning with one kernel per pattern.
- How to define a kernel between bags

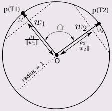
Bag of paths kernels
shape recognition

Haussler99

$$K_{\text{mean}}(T_1, T_2) = \frac{1}{|T_1|}\frac{1}{|T_2|}\sum_{t\in T_1}\sum_{t\in T_2} K_{\text{pattern}}(t, t'),$$

More complex kernels





(Desobry 2005)

$$K'(x, y) = \frac{K(x,y)}{\sqrt{K(x,x)K(y,y)}}$$
$$K'(x, x) = \|\varphi'(x)\|^2 = 1$$

Normalized kernel

Weighted mean kernel

$$\begin{array}{lcl} K_{\text{weighted}}(T_1, T_2) & = & \frac{1}{|T_1|}\frac{1}{|T_2|}\sum_{t\in T_1}\sum_{t'\in T_2}\lambda_{T_1}(t)\lambda_{T_2}(t')K_{\text{pattern}}(t, t'), \\ \lambda_{T_i}(t) & = & <\varphi(t), \mu_{T_i}>^d \end{array}$$

Bag of paths kernels
chemoinformatic

Basic

$$K_{\text{mean}}(G_1, G_2) = \sum_{t \in T(G_1) \cap T(G_2)} K(f_t(G_1), f_t(G_2)),$$

Basic MKL

$$K_{\text{BMKL}}(G_1, G_2) = \sum_{t \in T(G_1) \cap T(G_2)} d_t K(f_t(G_1), f_t(G_2)),$$

Infinite MKL

$$K_{\text{IMKL}}(G_1, G_2) = \sum_{t \in \mathcal{T}} \sum_{t' \in \mathcal{T}, t' \leq t} d_{t,t'} K(f_t(G_1), f_{t'}(G_2)),$$

where $\mathcal{T} = T(G_1) \cup T(G_2)$

Pattern kernels
How to compare patterns

- Classical approach:

$$K_{\text{classic}}(t,t') = \begin{cases} 0 \quad \text{if } t \not\sim t', \\ \sum_{\varphi \in Isom(t,t')} \left(\prod_{i=1}^{|V|} K_v(\mu(v_i), \varphi(\mu(v_i' i))) \right) \\ \left(\prod_{i=1}^{|E|} K_e(\nu(e_i), \nu(e_i')) \right) \end{cases}$$

- Pb: Similar but not identical patterns are not comparable.
- Solutions :
  - Shape recognition : Use rewrittings
  - Chemoinformatics : Use edit distance.

Conclusion

- Our aim : Studdy properties of structure space and combine structural pattern recognition and machine learning/optimisation methods.

Thank you for your attention !

Questions ?

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Kernels and infinite Bags

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- Next talk.