Graph kernels

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Graph based Representation in Pattern Recognition 2011

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.

Outline

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:

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

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

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

Examples

If $\chi = \mathbb{R}^n$, classical kernels include:

- Linear kernel:

$$K(x,y) = x^t y$$

- Polynomial kernel

$$K(x,y) = (x^t y)^d + c,\ c \in \mathbb{R}, d \in \mathbb{N}$$

- Cosinus kernel:

$$K(x,y) = \frac{x^t y}{\|x\| \|y\|}$$

- Rational kernel:

$$K(x,y) = 1 - \frac{\|x-y\|^2}{\|x-y\|^2 + b}, b \in \mathbb{R} - \{0\}$$

- Gaussian Kernel

$$K(x,y) = exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right), \sigma \in \mathbb{R} - \{0\}$$

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:

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

A basic example

- Let $\chi = \mathbb{R}^2$ and $k(x,y) = (x^t y)^2 + 1$
- For any $x = (x_1, x_2)$ and $y = (y_1, y_2)$ we have:

$$\begin{array}{rcl} k(x,y) & = & (x_1 y_1 + x_2 y_2)^2 + 1 \\ & = & 1 + x_1^2 y_1^2 + x_2^2 y_2^2 + 2 x_1 x_2 y_1 y_2 \end{array}$$

- The function φ from $\mathbb{R}^2$ to $\mathbb{R}^4$ defined by:

$$\varphi(x) = \begin{pmatrix} 1 \\ x_1^2 \\ x_2^2 \\ \sqrt{2} x_1 x_2 \end{pmatrix}$$

- Satisfies

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

- Remark: An hyperplane in $\mathcal{H} = \mathbb{R}^4$ corresponds to a quadric of $\mathbb{R}^2$.

$$< \varphi(x), n > = K \Rightarrow n_1 + n_2 x_1^2 + n_3 x_2^2 + n_4 \sqrt{2} x_1 x_2 = K$$

The Kernel Trick

- Linear classifier become non-linear using kernels

- Problem: φ is usually unknown.
- Many methods only need scalar product between data (not explicit coordinates) $\Rightarrow$ replace scalar product by kernel.
- E.g. k-NN:

$$
\begin{aligned}
d_K^2(x_1,x_2) &= \|\varphi(x_1)-\varphi(x_2)\|^2 \\
&= <\varphi(x_1)-\varphi(x_2),\varphi(x_1)-\varphi(x_2)> \\
&= <\varphi(x_1),\varphi(x_1)> + <\varphi(x_2),\varphi(x_2)> -2<\varphi(x_1),\varphi(x_2)> \\
d_K(x_1,x_2) &= k(x_1,x_1)+k(x_2,x_2)-2k(x_1,x_2)
\end{aligned}
$$

- Kernel trick
  - Algorithm defined in $\mathcal{H} \Rightarrow$ (linear methods,non linear separation),
  - Data stored in χ.

Interesting but so what...

Outline

Kernel and strutured data

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

- Edit Path $h = e_1 \ldots, e_n \in P(G, G')$

$$G \underset{e_1}{\rightarrow} \ldots \underset{e_n}{\rightarrow} G'$$

e_i: removal/insertion/relabelling operation.

- Cost of an edit path:

$$C(h) = \sum_{i=1}^{n} c(e_i)$$

- Graph Edit distance

$$d(G, G') = min_{h=e_1, \ldots, e_n \in P(G,G')} C(h)$$

A work intensively explored by Neuhauss & Bunke (see citations on last slide)

Graph prototypes Let $\{G_1, \ldots, G_n\}$

$$G \rightarrow vect(G) = (d(G, G_i))_{i=\{1,\ldots,n\}} \Rightarrow K(G, G') =< Vect(G), Vect($$

Diffusion Kernels

- Let B^S be a similarity matrix over S=$\{G_1, \ldots, G_n\}$. E.g.:

$$B^S(G_i, G_j) = exp(-\frac{d(G_i, G_j)^2}{2\sigma})$$

- "Force" definite positiveness:

$$K^S = exp(\lambda B^S) = \sum_{k=1}^{+\infty} \frac{\lambda^k}{k!}(B^S)^k$$

  with an appropriate choice of λ is definite positive.

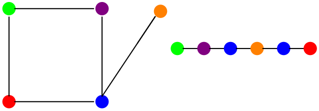
$$k^S(G_i, G_j) = K^S_{i,j}$$

  is thus a valid kernel defined on $\{G_1, \ldots, G_n\}$.

- Drawback: Any incoming data G defines a new problem on $S \cup \{G\}$.

Walk kernels

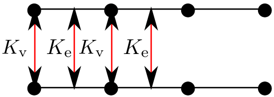
- Walks: Let $G = (V, E)$. $W = (v_1, \ldots, v_n)$ is a walk iff $(v_i, v_{i+1}) \in E, \forall i \in \{1, \ldots, n-1\}$.



is a walk

- Kernel between walks

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



Walks kernels

- Walk kernels :

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

- Covers different Graph kernels[Vert 2007,Vishwanathan et al. 2010]:

$$If\ \lambda_G(h) = \begin{cases} 1\ iff\ |h| = n & K \text{is a nth order walk kernel} \\ P_G(h)(Markov\ RW) & K \text{is a random walk/marginalized kern} \\ \beta^{|h|} & K \text{is a geometric kernel} \end{cases}$$

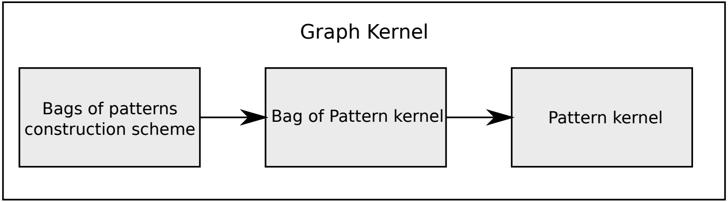
$$P_G(h) = p_s(h_1)\Pi_{i=1}^{n} p_t(h_i | h_{i-1}) p_q(h_n) \text{ with } |h| = n$$

- Connection with diffusion algorithms on product graphs. May be computed “efficiently” using matrix inversion.
- Walks may induce totering problems: Walks with arbitrary length on the same set of edges and vertices.
- Framework extended to tree-pattern [Vert 2006, Bach 2007]

Finite Bag kernels

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

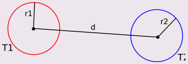
Three independent step to design a graph kernel.

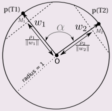


Haussler99

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

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

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

Conclusion

Kernel

Direct comparison

- Vector Description
- Edit Distance
- Regularization of similarity criterion

Bags of Patterns

Infinite

- Type of Pattern (Walks,Trees)
- Walk attenuation
  - Markov,
  - geometric,
  - n^{th} order.

Finite

- Type of Pattern (Paths, Trails, Trees)
- Bag selection,
- Bag comparison
- Pattern kernel

- Graph kernels provide an implicit embedding of graphs,
- Many statistical tools may be used using the kernel trick,
- The interpretation of operations performed in the implicit Hilbert space is controled by the similarity criterion defined by the kernel (e.g. mean).

Thank you for your attention !

Questions ?

References

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Kernels and infinite Bags

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Kernels and finite Bags

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- Next talk.