## KERNEL-BASED LEARNING

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## Outline

- Metodi Kernel
- Motivazioni
- Esempio
- Kernel standard
- Polynomial kernel
- String Kernel
- Introduzione a metodi Kernel avanzati
- Tree kernels


## Support Vector Machines

- Support Vector Machines (SVMs) are a machine learning paradigm based on the statistical learning theory [Vapnik, 1995]
- No need to remember everything, just the discriminating instances (i.e. the support vectors, SV)
- The classifier corresponds to the linear combination of SVs



## Support Vectors

Only the dot product is required

## Linear classifiers and separability

- In a R² space, 3 point can always be separable by a linear classifier
- but 4 points cannot always be shattered [Vapnik and Chervonenkis(1971)]
- One solution could be a more complex classifier
©Risk of over-fitting


## Linear classifiers and separability (2)

- ... but things change when projecting instances in a higher dimension feature space through a function $\phi$
- IDEA: It is better to have a more complex feature space instead a more complex function (i.e. learning algorithm)



## The kernel function

- In perceptrons and SVMs the learning algorithm only depends on the scalar product over pairs of example instance vectors
- Basically only the Gram-matrix is involved. In general, we call kernel the following function:

$$
K(\vec{x}, \vec{z})=\Phi(\vec{x}) \cdot \Phi(\vec{z})
$$

- The kernel corresponds to a scalar product over the transformed of initial objects $x$ and $z$
- If the mapping $\phi$ corresponds to the identity then the kernel is equal to the standard scalar product.
- Notice that the training in most learning machines (such as the perceptron) makes use of instances only through the kernel


## First Advantage: making instances linearly separable

$\rightarrow$


## An example: a mapping function

- Two masses $m_{l}$ and $m_{2}$, one is constrained
- A force $f_{a}$ is applied to the mass $m_{l}$
- Instead of applying an analyitical law we want to experiment
- The Features of individual experiments are masses $m_{1}, m_{2}$ and the appropriate orce $f_{a}$
- It is clear that the Newton law of gravity is involved:

$$
f\left(m_{1}, m_{2}, r\right)=C \frac{m_{1} m_{2}}{r^{2}}
$$

- The task corresponds to determine if $f\left(m_{1}, m_{2}, r\right)<f_{a}$


## An example: a mapping function (2)

$$
\vec{x}=\left(x_{1}, \ldots, x_{n}\right) \rightarrow \Phi(\vec{x})=\left(\Phi_{1}(\vec{x}), \ldots, \Phi_{k}(\vec{x})\right)
$$

- This law cannot be expressed linearly. A change of space:

$$
\left(f_{a}, m_{1}, m_{2}, r\right) \rightarrow(k, x, y, z)=\left(\ln f_{a}, \ln m_{1}, \ln m_{2}, \ln r\right)
$$

- holds as:

$$
\ln f\left(m_{1}, m_{2}, r\right)=\ln C+\ln m_{1}+\ln m_{2}-2 \ln r=c+x+y-2 z
$$

- The following hyperplane is the requested function $h()$ :

$$
\begin{aligned}
& \ln f_{a}-\ln m_{1}-\ln m_{2}+2 \ln r-\ln C=0 \\
& (I, I,-2,-I) \cdot\left(\ln m_{1}, \ln m_{2}, \ln r, \ln f_{a}\right)+\ln C=o,
\end{aligned}
$$

We can decide with no error if masses $m_{1}, m_{2}$ get closer or not

## Feature Spaces and Kernels

- Feature Space
- The input space is mapped into a new space $F$ with scalar product (called feature space) through a (non linear) trasformation $\phi$

$$
\phi=R^{N} \rightarrow F
$$

- The kernel function
- The evaluation require the computation of the scalar product over the trasformed
 vectors $\phi(x)$ but not the feature vectors themselves
- The scalr product is computed by a specialized function called kernel

$$
k(x, y)=(\phi(x) \cdot \phi(y))
$$

## Classification function: the dual form

$$
h(x)=\operatorname{sgn}(\vec{w} \cdot \vec{x}+b)=\operatorname{sgn}\left(\sum_{J=1}^{l} \alpha_{j} y_{j} \overrightarrow{x_{j}} \cdot \vec{x}+b\right)
$$

- On the right form, instances only appear in the scalar product
- The ony thing that is needed is the Gram matrix,

$$
G=\left(\left\langle\mathbf{x}_{i} \cdot \mathbf{x}_{j}\right\rangle\right)_{i, j=1}^{l}
$$

i.e. the explicit computation of the scalar product over any pair of training instances $x_{1} \ldots x_{l}$

## A kernelized perceptron

- We can rewrite the decision function of a perceptron by taking into account a kernel:

$$
\begin{aligned}
h(x) & =\operatorname{sgn}(\vec{w} \cdot \Phi(\vec{x})+b)=\operatorname{sgn}\left(\sum_{J=1}^{l} \alpha_{j} y_{j} \Phi\left(\overrightarrow{x_{j}}\right) \cdot \Phi(\vec{x})+b\right) \\
& =\operatorname{sgn}\left(\sum_{J=1}^{l} \alpha_{j} y_{j} k\left(\overrightarrow{x_{j}}, \vec{x}\right)+b\right)
\end{aligned}
$$

- ... and during training the on-line adjustment steps become:

$$
\left.\left.y_{i}\left(\sum_{J=1}^{l} \alpha_{j} y_{j} \Phi\left(\overrightarrow{x_{j}}\right) \cdot\right) \Phi\left(\overrightarrow{x_{i}}\right)+b\right)=\sum_{J=1}^{l} \alpha_{j} y_{i} y_{j} k\left(\overrightarrow{x_{j}}, \overrightarrow{x_{i}}\right)+b\right)
$$

## Kernels in Support Vector Machines

- In Soft Margin SVMs we need to maximize :

$$
\sum_{i=1}^{m} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{m} y_{i} y_{j} \alpha_{i} \alpha_{j} \vec{x}_{i} \cdot \vec{x}_{j}+\frac{1}{2 C} \vec{\alpha} \cdot \vec{\alpha}-\frac{1}{C} \vec{\alpha} \cdot \vec{\alpha}
$$

- By using kernel functions we rewrite the problem as:

$$
\left\{\begin{array}{l}
\text { maximize } \sum_{i=1}^{m} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{m} y_{i} y_{j} \alpha_{i} \alpha_{j}\left(k\left(o_{i}, o_{j}\right)+\frac{1}{C} \delta_{i j}\right) \\
\alpha_{i} \geq 0, \quad \forall i=1, \ldots, m \\
\sum_{i=1}^{m} y_{i} \alpha_{i}=0
\end{array}\right.
$$

## What makes a function a kernel function?

Def. 2.26 $A$ kernel is a function $k$, such that $\forall \vec{x}, \vec{z} \in X$

$$
k(\vec{x}, \vec{z})=\phi(\vec{x}) \cdot \phi(\vec{z})
$$

where $\phi$ is a mapping from $X$ to an (inner product) feature space.

Only such type of functions support implicit mappings such as

$$
\vec{x}=\left(x_{1}, \ldots, x_{n}\right) \in R^{n} \rightarrow \Phi(\vec{x})=\left(\Phi_{1}(\vec{x}), \ldots, \Phi_{m}(\vec{x})\right) \in R^{m}
$$

## What makes a function a kernel function? (2)

Def. B. 11 Eigen Values
Given a matrix $\boldsymbol{A} \in \mathbb{R}^{m} \times \mathbb{R}^{n}$, an egeinvalue $\lambda$ and an egeinvector $\vec{x} \in$ $\mathbb{R}^{n}-\{\overrightarrow{0}\}$ are such that

$$
A \vec{x}=\lambda \vec{x}
$$

Def. B. 12 Symmetric Matrix
A square matrix $\boldsymbol{A} \in \mathbb{R}^{n} \times \mathbb{R}^{n}$ is symmetric iff $\boldsymbol{A}_{i j}=\boldsymbol{A}_{j i}$ for $i \neq j i=1, . ., m$ and $j=1, .$. , n, i.e. iff $\boldsymbol{A}=\boldsymbol{A}^{\prime}$.

Def. B. 13 Positive (Semi-) definite Matrix
A square matrix $\boldsymbol{A} \in \mathbb{R}^{n} \times \mathbb{R}^{n}$ is said to be positive (semi-) definite if its eigenvalues are all positive (non-negative).

## What makes a function a kernel function? (3)

Proposition 2.27 (Mercer's conditions)
Let $X$ be a finite input space with $K(\vec{x}, \vec{z})$ a symmetric function on $X$. Then $K(\vec{x}, \vec{z})$ is a kernel function if and only if the matrix

$$
k(\vec{x}, \vec{z})=\phi(\vec{x}) \cdot \phi(\vec{z})
$$

is positive semi-definite (has non-negative eigenvalues).

- IDEA: If the Gram matrix is positive semi-definite then the mapping $\phi$, such that $F$ is an inner-product space whose scalar product corresponds to the kernel $k(. .$.$) , exists$
- In $F$ the separability should be easier


## Feature Spaces and Kernels

- An example of Kernel
- The Polynomial kernel

$$
\text { - If } \begin{aligned}
& d=2 \text { and } k(x, y)=(x \cdot y)^{d} \\
& x, y \in R^{2} \\
& \qquad \begin{aligned}
(x \cdot y)^{2}= & \left(\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right] \cdot\left[\begin{array}{l}
y_{1} \\
y_{2}
\end{array}\right]\right)^{2}=\left(\left[\begin{array}{l}
x_{1}^{2} \\
\sqrt{2} x_{1} x_{2} \\
x_{2}^{2}
\end{array}\right] \cdot\left[\begin{array}{l}
y_{1}^{2} \\
\sqrt{2} y_{1} y_{2} \\
y_{2}^{2}
\end{array}\right]\right) \\
= & (\phi(x) \cdot \phi(y))=k(x, y)
\end{aligned}
\end{aligned}
$$

## Polynomial kernel

## Polynomial Kernel ( $n$ dimensions)

$$
\begin{aligned}
(\vec{x} \cdot \vec{z})^{2} & =\left(\sum_{i=1}^{n} x_{i} z_{i}\right)^{2}
\end{aligned}=\left(\sum_{i=1}^{n} x_{i} z_{i}\right)\left(\sum_{j=1}^{n} x_{i} z_{i}\right), ~\left(\sum_{i=1}^{n} \sum_{j=1}^{n} x_{i} x_{j} z_{i} z_{j}=\sum_{i, j \in\{1, \ldots, n\}}\left(x_{i} x_{j}\right)\left(z_{i} z_{j}\right) .\right.
$$

## General Polynomial Kernel (n dimensions)

$$
\begin{aligned}
& (\vec{x} \cdot \vec{z}+c)^{2}=\left(\sum_{i=1}^{n} x_{i} z_{i}+c\right)^{2}=\left(\sum_{i=1}^{n} x_{i} z_{i}+c\right)\left(\sum_{j=1}^{n} x_{i} z_{i}+c\right)= \\
& =\sum_{i=1}^{n} \sum_{j=1}^{n} x_{i} x_{j} z_{i} z_{j}+2 c \sum_{i=1}^{n} x_{i} z_{i}+c^{2}= \\
& =\sum_{i, j \in\{1, ., n\}}\left(x_{i} x_{j}\right)\left(z_{i} z_{j}\right)+\sum_{i=1}^{n}\left(\sqrt{2 c} x_{i}\right)\left(\sqrt{2 c} z_{i}\right)+c^{2}
\end{aligned}
$$

## Polynomial kernel and the conjunction of features

- The initial vectors can be mapped into a higher dimensional space ( $c=1$ )

$$
\Phi\left(<x_{1}, x_{2}>\right) \rightarrow\left(x_{1}^{2}, x_{2}^{2}, \sqrt{2} x_{1} x_{2}, \sqrt{2} x_{1}, \sqrt{2} x_{2}, 1\right)
$$

- More expressive, as ( $x_{1} x_{2}$ ) encodes original feature pairs, e.g. stock+market vs. downtown+market are contributing (when occurring) togheter
- We can smartly compute the scalar product as

$$
\begin{aligned}
\Phi(\vec{x}) \times \Phi(\vec{z}) & =\left(x_{1}^{2}, x_{2}^{2}, \sqrt{2} x_{1} x_{2}, \sqrt{2} x_{1}, \sqrt{2} x_{2}, 1\right) \times\left(z_{1}^{2}, z_{2}^{2}, \sqrt{2} z_{1} z_{2}, \sqrt{2} z_{1}, \sqrt{2} z_{2}, 1\right)= \\
& =x_{1}^{2} z_{1}^{2}+x_{2}^{2} z_{2}^{2}+2 x_{1} x_{2} z_{1} z_{2}+2 x_{1} z_{1}+2 x_{2} z_{2}+1= \\
& =\left(x_{1} z_{1}+x_{2} z_{2}+1\right)^{2}=(\vec{x} \times \vec{z}+1)^{2}=K_{p 2}(\vec{x}, \vec{z})
\end{aligned}
$$

## The Architecture of an SVM

- It is a non linear classifier (based on a kernel)
- Decision function:

$$
\begin{aligned}
f(x) & =\operatorname{sgn}\left(\sum_{i=1}^{l} v_{i}\left(\phi(x) \cdot \phi\left(x_{i}\right)\right)+b\right) \\
& =\operatorname{sgn}\left(\sum_{i=1}^{l} v_{i} k\left(x, x_{i}\right)+b\right)
\end{aligned}
$$

$\phi\left(x_{i}\right)$ substitutes every training instamce $x_{i}$
$v_{i}=\alpha_{i} y_{i}$
$v_{i}$ are the solutions of the optimization problem

The mapping function is never computed, but is implict in the kernel estimation

## Esempi di Funzioni Kernel

- Lineare: $k\left(\vec{x}_{i}, \vec{x}_{j}\right)=\vec{x}_{i} \cdot \vec{x}_{j}$
- Polinomiale potenza di p: $k\left(\vec{x}_{i}, \vec{x}_{j}\right)=\left(1+\vec{x}_{i} \cdot \vec{x}_{j}\right)^{p}$
- Gaussiana (radial-basis function network):

$$
k\left(\vec{x}_{i}, \vec{x}_{j}\right)=e^{-\frac{\left\|\vec{x}_{i}-\vec{x}_{j}\right\|^{2}}{2 \sigma^{2}}}
$$

- Percettrone a due stadi:

$$
k\left(\vec{x}_{i}, \vec{x}_{j}\right)=\tanh \left(\beta_{1}+\beta_{0} \vec{x}_{i} \cdot \vec{x}_{j}\right)^{p}
$$

## String Kernel

- Given two strings, the number of matches between their substrings is computed
- E.g. Bank and Rank
- B, a, n, k, Ba, Ban, Bank, an, ank, nk
- R, a , n, k, Ra, Ran, Rank, an, ank, nk
- String kernel over sentences and texts
- Huge space but there are efficient algorithms
- Lodhi, Huma; Saunders, Craig; Shawe-Taylor, John; Cristianini, Nello; Watkins, Chris (2002). "Text classification using string kernels". Journal of Machine Learning Research: 419-444.


## String kernel

- A function that give two strings $s$ and $t$ is able to compute a real number $k(s, t)$ such that
- two vectors exist $\vec{s}$ and $\vec{t}$
- $\vec{s}$ and $\vec{t}$ are unique for $s$ and $t$
- (the vectors represents strings by embedding their crucial properties!!)
- $\mathrm{k}(\mathrm{s}, \mathrm{t})=\vec{s} \times \vec{t}$
- We will see how vectors $\vec{s}$ and $\vec{t}$ are defined in $\mathbb{R}^{\infty}$, as the numer of strings of arbitrary length over an alphabet is infinite
- IDEA: Define a space whereas each substring is a dimension


## Kernel tra Bank e Rank

$\mathrm{B}, \mathrm{a}, \mathrm{n}, \mathrm{k}, \mathrm{Ba}, \mathrm{Ban}, \mathrm{Bank}, \mathrm{an}, \mathrm{ank}, \mathrm{nk}, \mathrm{Bn}, \mathrm{Bnk}, \mathrm{Bk}$ and ak are the substrings of Bank.
$\mathrm{R}, \mathrm{a}, \mathrm{n}, \mathrm{k}, \mathrm{Ra}$, Ran, Rank, an, ank, $\mathrm{nk}, \mathrm{Rn}, \mathrm{Rnk}, \mathrm{Rk}$ and ak are the substrings of Rank.

## $\phi$

$$
\begin{aligned}
\phi(\operatorname{Bank})= & \left(\lambda, 0, \lambda, \lambda, \lambda, \lambda^{2}, \lambda^{2}, \lambda^{3}, 0, \lambda^{4}, 0, \lambda^{2}, \lambda^{3}, \lambda^{3},\right. \\
\phi(\text { Rank })= & \left(0, \lambda, \lambda, \lambda, \lambda, 0,0,0, \lambda^{3}, 0, \lambda^{4}, \lambda^{2}, \lambda^{3}, \lambda^{3},\right. \\
& B, R, a, n, k, \text { Ba, Ra, Ban, Ran, Bank, Rank, an, ank, ak } \ldots
\end{aligned}
$$

-Common substrings:

$$
-a, n, k, a n, a n k, n k, a k
$$

- Notice how these are the same subsequences as between
-Schrianak and Rank


## Formally ...

Sottosequenza di indici ordinati e

$$
\begin{aligned}
& s=s_{1}, \ldots, s_{|s|} \text { non contigui di }(I, \ldots|s|) \\
& \vec{I}=\left(i_{1}, \ldots, i_{|u|}\right) \quad u=s[\vec{I}], \text { substring of } s \text { defined by } \vec{I} \\
& \phi_{u}(s)=\sum_{\vec{I}: u=s[\vec{I}]} \lambda^{l(\vec{I})} \text {, con } l(\vec{I})=i_{|u|}-i_{1}+1 \\
& K(s, t)=\sum_{u \in \Sigma^{*}} \phi_{u}(s) \cdot \phi_{u}(t)=\sum_{u \in \Sigma^{*}} \sum_{\vec{I}: u=s[\vec{I}]} \lambda^{l(\vec{I})} \sum_{\vec{J}: u=t[\vec{J}]} \lambda^{l(\vec{J})}= \\
& =\sum_{u \in \Sigma^{*}} \sum_{\vec{I}: u=s[\vec{I}]} \sum_{\vec{J}: u=t[\vec{J}]} \lambda^{l(\vec{I})+l(\vec{J})} \quad, \text { con } \Sigma^{*}=\bigcup_{n=0}^{\infty} \Sigma^{n}
\end{aligned}
$$

## An example of string kernel computation

- $\phi_{\mathrm{a}}($ Bank $)=\phi_{\mathrm{a}}(\mathrm{Rank})=\lambda^{\left(i_{1}-i_{1}+1\right)}=\lambda^{(2-2+1)}=\lambda$,
- $\phi_{\mathrm{n}}(\operatorname{Bank})=\phi_{\mathrm{n}}(\mathrm{Rank})=\lambda^{\left(i_{1}-i_{1}+1\right)}=\lambda^{(3-3+1)}=\lambda$,
- $\phi_{\mathrm{k}}(\operatorname{Bank})=\phi_{\mathrm{k}}(\operatorname{Rank})=\lambda^{\left(i_{1}-i_{1}+1\right)}=\lambda^{(4-4+1)}=\lambda$,
- $\phi_{\mathrm{an}}(\mathrm{Bank})=\phi_{\mathrm{an}}(\mathrm{Rank})=\lambda^{\left(i_{1}-i_{2}+1\right)}=\lambda^{(3-2+1)}=\lambda^{2}$,
- $\phi_{\text {ank }}($ Bank $)=\phi_{\text {ank }}(\operatorname{Rank})=\lambda^{\left(i_{1}-i_{3}+1\right)}=\lambda^{(4-2+1)}=\lambda^{3}$,

$$
\begin{aligned}
& \phi_{\mathrm{nk}}(\mathrm{Bank})=\phi_{\mathrm{nk}}(\mathrm{Rank})=\lambda^{\left(i_{1}-i_{2}+1\right)}=\lambda^{(4-3+1)}=\lambda^{2} \\
& \phi_{\mathrm{ak}}(\mathrm{Bank})=\phi_{\mathrm{ak}}(\mathrm{Rank})=\lambda^{\left(i_{1}-i_{2}+1\right)}=\lambda^{(4-2+1)}=\lambda^{3}
\end{aligned}
$$

It follows that $K(\operatorname{Bank}, \operatorname{Rank})=\left(\lambda, \lambda, \lambda, \lambda^{2}, \lambda^{3}, \lambda^{2}, \lambda^{3}\right) \cdot\left(\lambda, \lambda, \lambda, \lambda^{2}, \lambda^{3}, \lambda^{2}, \lambda^{3}\right)$ $=3 \lambda^{2}+2 \lambda^{4}+2 \lambda^{6}$.

## Tree Kernels

- String kernels adopt a structured approach to kernel estimation and are very useful in NLP and Web Mining tasks
- However, what has been defined over sequences can be profitably exploited also in the treatment of more complex structures
- Trees whose parent relationship determine subsequences in terms of
- Multiple paths from the root to the leaves
- Ordered sets of children (i.e. sequences of immediately dominated nodes) of every node in the tree
- Graphs, whose structure can be captured by several trees (subgraphs) and thus characterized by multiple subsequences


## Tree kernels

- Applications are related to text processing tasks such as
- Syntactic parsing, when SVM classification is useful to select the best parse tree among multiple legal grammatical interpretations
- Question Classification, where SVM classification is applied to the recognition of the target of a question (e.g. a person such as in "Who is the inventor of the light?" vs. a place as in "Where is Taji Mahal?"
or to pattern recognition (e.g. in bioinformatics the classification of protein structures)


## Tree Kernels

Modeling syntax in Natural Language learning task is complex, e.g.

- Question Classification
- Semantic role relations within predicate argument structures and


Tree kernels are natural way to exploit syntactic information from sentence parse trees

- useful to engineer novel and complex features.


## Tree structures and natural language

- PARSING: Breaking down a text into its component parts of speech (according to a formal grammar) with an explanation of the form, function, and syntactic relationship of each part
- INPUT: gives a talk
- Output : a costituency tree


Chomsky, N. 1957. Syntactic Structures. The Hague/Paris: Mouton.

## The Collins and Duffy's Tree Kernel



Given a costituency tree

## The overall fragment set

We can explode the syntactic tree in all syntactically motivated fragments

- For each node the production rules must be respected, i.e. we can remove " 0 or all children at a time"
- It is also known as Syntactic Tree Kernel



## Explicit feature space

Can we build a feature vector accounting on all this information?

$\vec{x}_{1} \cdot \vec{x}_{2}$ counts the number of common substructures

## Implicit Representation

Can we estimate the tree kernel in an implicit space?

- We can implicitly count the number of common subtrees
- We prevent to define feature vectors that consider ALL POSSIBLE SUBTREES, i.e. thousand of features
- The final model will not contain feature vectors, but TREES

$$
\begin{array}{r}
\vec{x}_{1} \cdot \vec{x}_{2}=\phi\left(T_{1}\right) \cdot \phi\left(T_{2}\right)=K\left(T_{1}, T_{2}\right)= \\
=\sum_{n_{1} \in l_{1}} \sum_{n_{2} \in r_{2}} \Delta\left(n_{1}, n_{2}\right)
\end{array}
$$

[Collins and Duffy, ACL 2002] evaluate $\Delta$ in $O\left(n^{2}\right)$ :
$\Delta\left(n_{1}, n_{2}\right)=0$, if the productions are different else $\Delta\left(n_{1}, n_{2}\right)=1$, if pre-terminals else
$\Delta\left(n_{1}, n_{2}\right)=\prod_{j=1}^{n c\left(n_{1}\right)}\left(1+\Delta\left(\operatorname{ch}\left(n_{1}, j\right), \operatorname{ch}\left(n_{2}, j\right)\right)\right)$

## Tree kernels are ... embedding tools

- Semantic Tree Kernels allows generating vectors that reflect syntactic/semantic information of sentences
- Who is the tallest man in the world?

- Which most similar sentences/trees/vectors?
- Who is the richest woman in the world?
- Who is the richest person in the world?
- Who is the fastest swimmer in the world?
- Who was murdered yesterday by the terrorist group?



## Weighting in grammatical tree kernels

In the kernel estimation different subtrees are taken in account different times

- Es: in the following trees, one fragment will contribute twice to the overall kernel



## Weighting

- A decay factor can be used, so the contribution of the embedded trees is reduced.
- The normalization of Tree Kernel estimation corresponds to the normalization of the explicit feature vector

$$
\begin{aligned}
& \text { Decay factor } \\
& \Delta\left(n_{1}, n_{2}\right)=\lambda, \text { if pre-terminals else } \\
& \Delta\left(n_{1}, n_{2}\right)=\lambda \prod_{j=1}^{n c\left(n_{1}\right)}\left(1+\Delta\left(\operatorname{ch}\left(n_{1}, j\right), \operatorname{ch}\left(n_{2}, j\right)\right)\right) \\
& \text { Normalization }^{\prime} K^{\prime}\left(T_{1}, T_{2}\right)=\frac{K\left(T_{1}, T_{2}\right)}{\sqrt{K\left(T_{1}, T_{1}\right) \times K\left(T_{2}, T_{2}\right)}}
\end{aligned}
$$

## Partial Tree [Moschitti,2006]

- A Syntactic Tree satisfies completely a grammar rule, i.e. the constraint is "remove 0 or all children at a time".
- Partial Tree Kernel (PTK) relaxes such constraint we get more general substructures
- It allows gaps in the production rules in the same fashion of the sequence kernel



## Partial Tree Kernel

- if the node labels of $n_{1}$ and $n_{2}$ are different then $\Delta\left(n_{1}, n_{2}\right)=0$;
- else

$$
\Delta\left(n_{1}, n_{2}\right)=1+
$$

$$
\sum_{\vec{J}_{1}, \vec{J}_{2}, l\left(\vec{J}_{1}\right)=l\left(\vec{J}_{2}\right)} \prod_{i=1}^{l\left(\vec{J}_{1}\right)}
$$

- By adding two decay factors we obtain:

$$
\mu\left(\lambda^{2}+\sum_{\vec{J}_{1}, \vec{J}_{2}, l\left(\vec{J}_{1}\right)=l\left(\vec{J}_{2}\right)} \lambda^{d\left(\vec{J}_{1}\right)+d\left(\vec{J}_{2}\right)} \prod_{i=1}^{l\left(\vec{J}_{1}\right)} \Delta\left(c_{n_{1}}\left[\vec{J}_{1 i}\right], c_{n_{2}}\left[\vec{J}_{2 i}\right]\right)\right)
$$

## Kernel Combination and normalization

- Kernels can be easily combined so that the evidences captured by several kernel functions can contribute to the learning algorithm
- The sum of kernels is a valid kernel
- The product of kernels is a valid kernel
- We can also Normalize the implicit space operating directly only the kernel function

$$
\begin{aligned}
\hat{K}(s, t) & =\langle\hat{\phi}(s) \cdot \hat{\phi}(t)\rangle=\left\langle\frac{\phi(s)}{\|\phi(s)\|} \cdot \frac{\phi(t)}{\|\phi(t)\|}\right\rangle \\
& =\frac{1}{\|\phi(s)\|\|\phi(t)\|}\langle\phi(s) \cdot \phi(t)\rangle=\frac{K(s, t)}{\sqrt{K(s, s) K(t, t)}}
\end{aligned}
$$

## Summary

- The dual form of the SVM optimization problem ONLY depends on the scalar product between training examples and NOT from their explicit vector representation (likewise the perceptron)
- This suggests to exploit this property in order to:
- Define efficient functions able to compute the scalar product out from the original representation (i.e. from the input space)
- Exploit more complex representations (i.e. more expressive feature spaces) in implicit way
- This corresponds to search the model in feature spaces able to:
- Preserve the mathematical properties sufficient to guarantee convergence (i.e. the minimization of the expected error)
- Support training and classification by a limited complexity (e.g. no need to build large dimensional representations of input instances)


## Summary (2)

- In order for a function k(.,.) to be a valid kernel, its correspondin Gram matrix mast be positive semi-definite
- In practice, such property is verified empirically over the training datasets
- In this unit, the following kernel funcrion have been introduced as they can be very effective in Web Mining problems:
- Base kernels (for example, polynomial kernel polinomiali of degree 2)
- Task dependent kernels that dipenden on the structura of a learning task:
- String (Sequence) kernels
- Tree kernels
- We will explore semantic kernels (e.g. latent semantic kernels) later in the course


## References

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