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



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



Linear classifiers and separability (2)

- ... but things change when projecting instances in a higher dimension feature space through a function ϕ
- **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
- Notice that the training in most learning machines (such as the perceptron) makes use of instances only through the kernel

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First Advantage: making instances linearly separable



An example: a mapping function

- Two masses m_1 and m_2 , one is constrained
- A force f_a is applied to the mass m_1
- 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:

$$f(m_1, m_2, r) = C \frac{m_1 m_2}{r^2}$$

• The task corresponds to determine if

$$f(m_1, m_2, r) < f_a$$

An example: a mapping function (2)

$$\vec{x} = (x_1, \dots, x_n) \to \Phi(\vec{x}) = (\Phi_1(\vec{x}), \dots, \Phi_k(\vec{x}))$$

- This law cannot be expressed linearly. A change of space:
 (f_a, m₁, m₂, r) → (k, x, y, z) = (ln f_a, ln m₁, ln m₂, ln r)
 holds as: ln f(m₁, m₂, r) = ln C + ln m₁ + ln m₂ - 2ln r = c + x + y - 2z
 The following homeomorphisms is the respected function h().
- The following hyperplane is the requested function h(): $\ln f_a - \ln m_1 - \ln m_2 + 2\ln r - \ln C = 0$

$$(1,1,-2,-1) \cdot (\ln m_1, \ln m_2, \ln r, \ln f_a) + \ln C = 0,$$

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 ϕ

$$\phi = R^N \to F$$

- 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

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

- 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 $x_1 \dots x_l$

A kernelized perceptron

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

$$h(x) = sgn(\vec{w} \cdot \Phi(\vec{x}) + b) = sgn(\sum_{J=1}^{l} \alpha_j y_j \Phi(\vec{x_j}) \cdot \Phi(\vec{x}) + b)$$
$$= sgn(\sum_{J=1}^{l} \alpha_j y_j k(\vec{x_j}, \vec{x}) + b)$$

and during training the on-line adjustment steps become:

$$y_i(\sum_{j=1}^l \alpha_j y_j \Phi(\overrightarrow{x_j}) \cdot) \Phi(\overrightarrow{x_i}) + b) = \sum_{j=1}^l \alpha_j y_i y_j k(\overrightarrow{x_j}, \overrightarrow{x_i}) + b)$$

Kernels in Support Vector Machines

• In Soft Margin SVMs we need to maximize :

$$\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} + \frac{1}{2C} \vec{\alpha} \cdot \vec{\alpha} - \frac{1}{C} \vec{\alpha} \cdot \vec{\alpha}$$

• By using kernel functions we rewrite the problem as:

$$\begin{cases} maximize \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \left(k(o_i, o_j) + \frac{1}{C} \delta_{ij} \right) \\ \alpha_i \ge 0, \quad \forall i = 1, ..., m \\ \sum_{i=1}^{m} y_i \alpha_i = 0 \end{cases}$$

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 ϕ is a mapping from X to an (inner product) feature space.

Only such type of functions support implicit mappings such as

$$\vec{x} = (x_1, \dots, x_n) \in \mathbb{R}^n \rightarrow \Phi(\vec{x}) = (\Phi_1(\vec{x}), \dots, \Phi_m(\vec{x})) \in \mathbb{R}^m$$

What makes a function a kernel function? (2)

Def. B.11 Eigen Values

Given a matrix $\mathbf{A} \in \mathbb{R}^m \times \mathbb{R}^n$, an egeinvalue λ and an egeinvector $\vec{x} \in \mathbb{R}^n - {\vec{0}}$ are such that

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

Def. B.12 Symmetric Matrix A square matrix $A \in \mathbb{R}^n \times \mathbb{R}^n$ is symmetric iff $A_{ij} = A_{ji}$ for $i \neq j$ i = 1, ..., mand j = 1, ..., n, i.e. iff A = A'.

Def. B.13 Positive (Semi-) definite Matrix A square matrix $A \in \mathbb{R}^n \times \mathbb{R}^n$ 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 φ, 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

• If
$$d=2$$
 and $k(x, y) = (x \cdot y)^d$
 $x, y \in R^2$

$$(x \cdot y)^{2} = \left(\begin{bmatrix} x_{1} \\ x_{2} \end{bmatrix} \cdot \begin{bmatrix} y_{1} \\ y_{2} \end{bmatrix} \right)^{2} = \left(\begin{bmatrix} x_{1}^{2} \\ \sqrt{2} x_{1} x_{2} \\ x_{2}^{2} \end{bmatrix} \cdot \begin{bmatrix} y_{1}^{2} \\ \sqrt{2} y_{1} y_{2} \\ y_{2}^{2} \end{bmatrix} \right)$$
$$= (\phi(x) \cdot \phi(y)) = k(x, y)$$

Polynomial kernel



https://www.youtube.com/watch?v=3liCbRZPrZA

Polynomial Kernel (*n* dimensions)



General Polynomial Kernel (*n* dimensions)

$$(\vec{x} \cdot \vec{z} + c)^2 = \left(\sum_{i=1}^n x_i z_i + c\right)^2 = \left(\sum_{i=1}^n x_i z_i + c\right) \left(\sum_{j=1}^n x_i z_i + c\right) =$$
$$= \sum_{i=1}^n \sum_{j=1}^n x_i x_j z_i z_j + 2c \sum_{i=1}^n x_i z_i + c^2 =$$
$$= \sum_{i,j \in \{1,..,n\}} (x_i x_j) (z_i z_j) + \sum_{i=1}^n \left(\sqrt{2c} x_i\right) \left(\sqrt{2c} z_i\right) + c^2$$

Polynomial kernel and the conjunction of features

- The initial vectors can be mapped into a higher dimensional space (*c*=1) $\Phi(\langle x_1, x_2 \rangle) \rightarrow (x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1)$
- More expressive, as (x₁x₂) encodes original feature pairs, e.g. stock+market vs. downtown+market are contributing (when occurring) togheter
- We can smartly compute the scalar product as

$$\Phi(\vec{x}) \times \Phi(\vec{z}) = (x_1^2, x_2^2, \sqrt{2}x_1 x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1) \times (z_1^2, z_2^2, \sqrt{2}z_1 z_2, \sqrt{2}z_1, \sqrt{2}z_2, 1) =$$

$$= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 x_2 z_1 z_2 + 2x_1 z_1 + 2x_2 z_2 + 1 =$$

$$= (x_1 z_1 + x_2 z_2 + 1)^2 = (\vec{x} \times \vec{z} + 1)^2 = K_{p2} (\vec{x}, \vec{z})$$

The Architecture of an SVM

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

$$f(x) = \operatorname{sgn}(\sum_{i=1}^{l} v_i(\phi(x) \cdot \phi(x_i)) + b)$$
$$= \operatorname{sgn}(\sum_{i=1}^{l} v_i k(x, x_i) + b)$$

 $\phi(x_i)$ 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:
$$k(\vec{x}_i, \vec{x}_j) = \vec{x}_i \cdot \vec{x}_j$$

- Polinomiale potenza di p: $k(\vec{x}_i, \vec{x}_j) = (1 + \vec{x}_i \cdot \vec{x}_j)^p$
- Gaussiana (radial-basis function network):

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

• Percettrone a due stadi:

$$k(\vec{x}_i, \vec{x}_j) = \tanh(\beta_1 + \beta_0 \vec{x}_i \cdot \vec{x}_j)^p$$

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!!)

• $k(s,t) = \vec{s} \times \vec{t}$

- We will see how vectors \vec{s} and \vec{t} are defined in \mathbb{R}^{∞} , 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

B, a, n, k, Ba, Ban, Bank, an, ank, nk, Bn, Bnk, Bk and ak are the substrings of *Bank*.

R, a, n, k, Ra, Ran, Rank, an, ank, nk, Rn, Rnk, Rk and ak are the substrings of *Rank*.

 $\phi(\text{Bank}) = (\lambda, 0, \lambda, \lambda, \lambda, \lambda, \lambda^2, \lambda^2, \lambda^3, 0, \lambda^4, 0, \lambda^2, \lambda^3, \lambda^3, \dots$ $\phi(\text{Rank}) = (0, \lambda, \lambda, \lambda, \lambda, \lambda, 0, 0, 0, \lambda^3, 0, \lambda^4, \lambda^2, \lambda^3, \lambda^3, \dots$ $B, R, a, n, k, Ba, Ra, Ban, Ran, Bank, Rank, an, ank, ak \dots$

•Common substrings:

– a, n, k, an, ank, nk, ak

Notice how these are the same subsequences as between

Schrianak and Rank



Formally ...

Sottosequenza di indici ordinati e
non contigui di
$$(I, ... |s|)$$

 $\vec{I} = (i_1, ..., i_{|u|})$ $u = s[\vec{I}]$, substring of s defined by \vec{I}
 $\phi_u(s) = \sum_{\vec{I}:u=s[\vec{I}]} \lambda^{l(\vec{I})}$, con $l(\vec{I}) = i_{|u|} - i_1 + 1$
 $K(s,t) = \sum_{u \in \Sigma^*} \phi_u(s) \cdot \phi_u(t) = \sum_{u \in \Sigma^*} \sum_{\vec{I}:u=s[\vec{I}]} \lambda^{l(\vec{I})} \sum_{\vec{J}:u=t[\vec{J}]} \lambda^{l(\vec{J})} =$
 $= \sum_{u \in \Sigma^*} \sum_{\vec{I}:u=s[\vec{I}]} \sum_{\vec{J}:u=t[\vec{J}]} \lambda^{l(\vec{I})+l(\vec{J})}$, con $\Sigma^* = \bigcup_{n=0}^{\infty} \Sigma^n$

An example of string kernel computation

-
$$\phi_{a}(Bank) = \phi_{a}(Rank) = \lambda^{(i_{1}-i_{1}+1)} = \lambda^{(2-2+1)} = \lambda$$
,

-
$$\phi_n(\text{Bank}) = \phi_n(\text{Rank}) = \lambda^{(i_1-i_1+1)} = \lambda^{(3-3+1)} = \lambda$$
,

-
$$\phi_{\mathbf{k}}(\mathbf{Bank}) = \phi_{\mathbf{k}}(\mathbf{Rank}) = \lambda^{(i_1-i_1+1)} = \lambda^{(4-4+1)} = \lambda$$
,

-
$$\phi_{an}(Bank) = \phi_{an}(Rank) = \lambda^{(i_1-i_2+1)} = \lambda^{(3-2+1)} = \lambda^2$$
,

$$\begin{array}{l} - \ \phi_{\mathrm{ank}}(\mathrm{Bank}) = \phi_{\mathrm{ank}}(\mathrm{Rank}) = \lambda^{(i_1 - i_3 + 1)} = \lambda^{(4 - 2 + 1)} = \lambda^3, \\ \phi_{\mathrm{nk}}(\mathrm{Bank}) = \phi_{\mathrm{nk}}(\mathrm{Rank}) = \lambda^{(i_1 - i_2 + 1)} = \lambda^{(4 - 3 + 1)} = \lambda^2, \\ \phi_{\mathrm{ak}}(\mathrm{Bank}) = \phi_{\mathrm{ak}}(\mathrm{Rank}) = \lambda^{(i_1 - i_2 + 1)} = \lambda^{(4 - 2 + 1)} = \lambda^3. \end{array}$$

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

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?



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

$$\vec{x}_1 \cdot \vec{x}_2 = \phi(T_1) \cdot \phi(T_2) = K(T_1, T_2) = \\ = \sum_{n_1 \in T_1} \sum_{n_2 \in T_2} \Delta(n_1, n_2)$$

[Collins and Duffy, ACL 2002] evaluate Δ in O(n²):

$$\begin{split} &\Delta(n_1,n_2)=0, \text{ if the productions are different else} \\ &\Delta(n_1,n_2)=1, \text{ if pre-terminals else} \\ &\Delta(n_1,n_2)=\prod_{j=1}^{nc(n_1)}(1+\Delta(ch(n_1,j),ch(n_2,j))) \end{split}$$

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?



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

Decay factor $\Delta(n_1, n_2) = \lambda, \quad \text{if pre-terminals else}$ $\Delta(n_1, n_2) = \lambda \prod_{j=1}^{nc(n_1)} (1 + \Delta(ch(n_1, j), ch(n_2, j)))$ Normalization $K'(T_1, T_2) = \frac{K(T_1, T_2)}{\sqrt{K(T_1, T_1) \times K(T_2, T_2)}}$

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 $\Delta(n_1, n_2) = 0;$

- else

$$\Delta(n_1, n_2) = 1 + \sum_{\vec{J}_1, \vec{J}_2, l(\vec{J}_1) = l(\vec{J}_2)} \prod_{i=1}^{l(\vec{J}_1)} \Delta(c_{n_1}[\vec{J}_{1i}], c_{n_2}[\vec{J}_{2i}])$$

• By adding two decay factors we obtain:

$$\mu \left(\lambda^2 + \sum_{\vec{J}_1, \vec{J}_2, l(\vec{J}_1) = l(\vec{J}_2)} \lambda^{d(\vec{J}_1) + d(\vec{J}_2)} \prod_{i=1}^{l(\vec{J}_1)} \Delta(c_{n_1}[\vec{J}_{1i}], c_{n_2}[\vec{J}_{2i}]) \right)$$

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

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

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 function 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

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