KERNEL-BASED LEARNING

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Outline

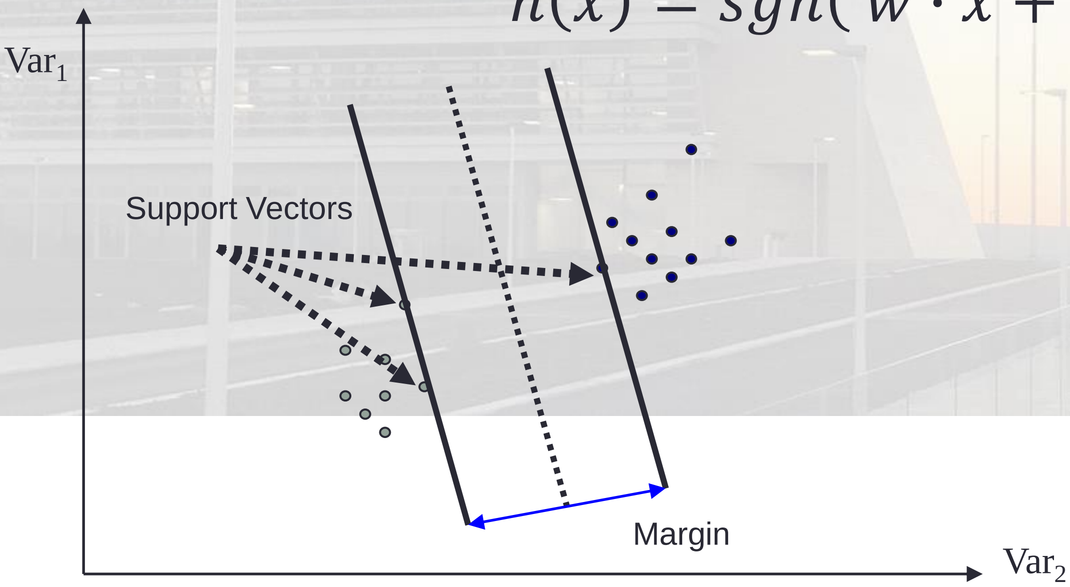
- Metodi Kernel
  - Motivazioni
  - Esempio
- Kernel standard
  - Polynomial kernel
  - String Kernel
- Introduzione a metodi Kernel *avanzati*
  - Tree kernels

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

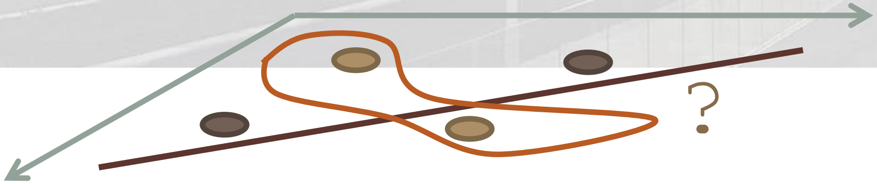
$$h(x) = sgn(\overrightarrow{w} \cdot \overrightarrow{x} + b) = sgn(\underbrace{\sum_{J=1}^{l} \alpha_j y_j \boxed{\overrightarrow{x_j} \cdot \vec{x}}}_{\text{Support Vectors}} + b)$$

Only the dot product is required



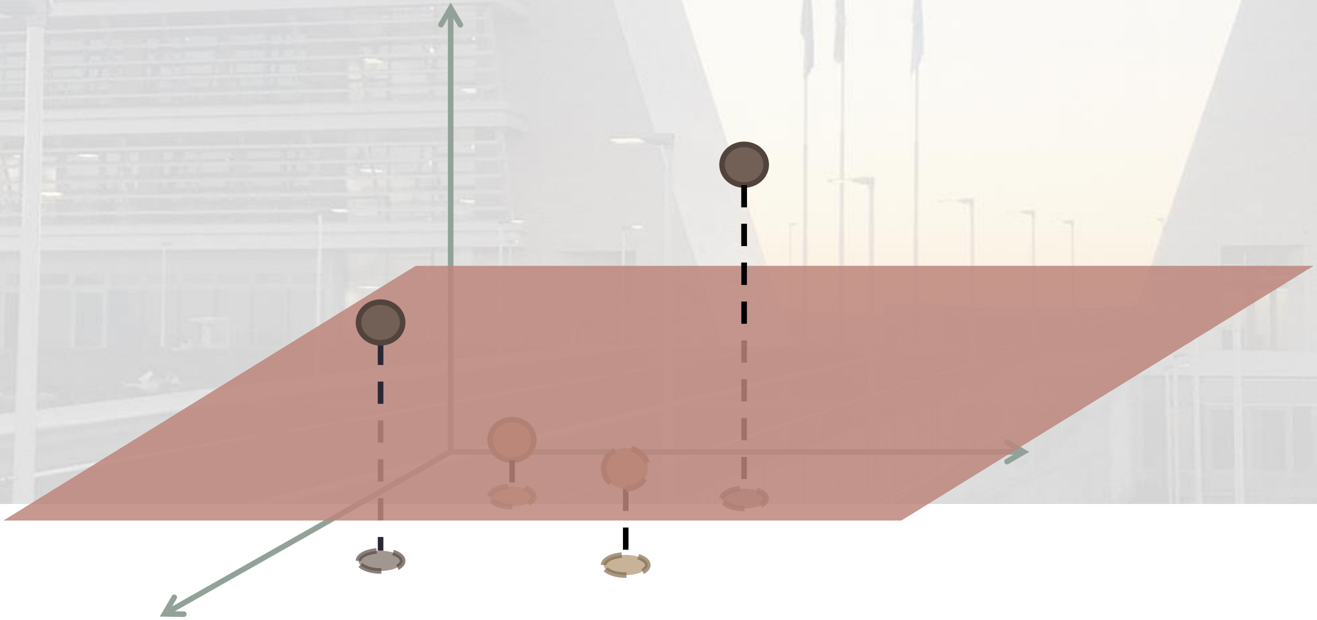
Linear classifiers and separability

- In a R^2 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

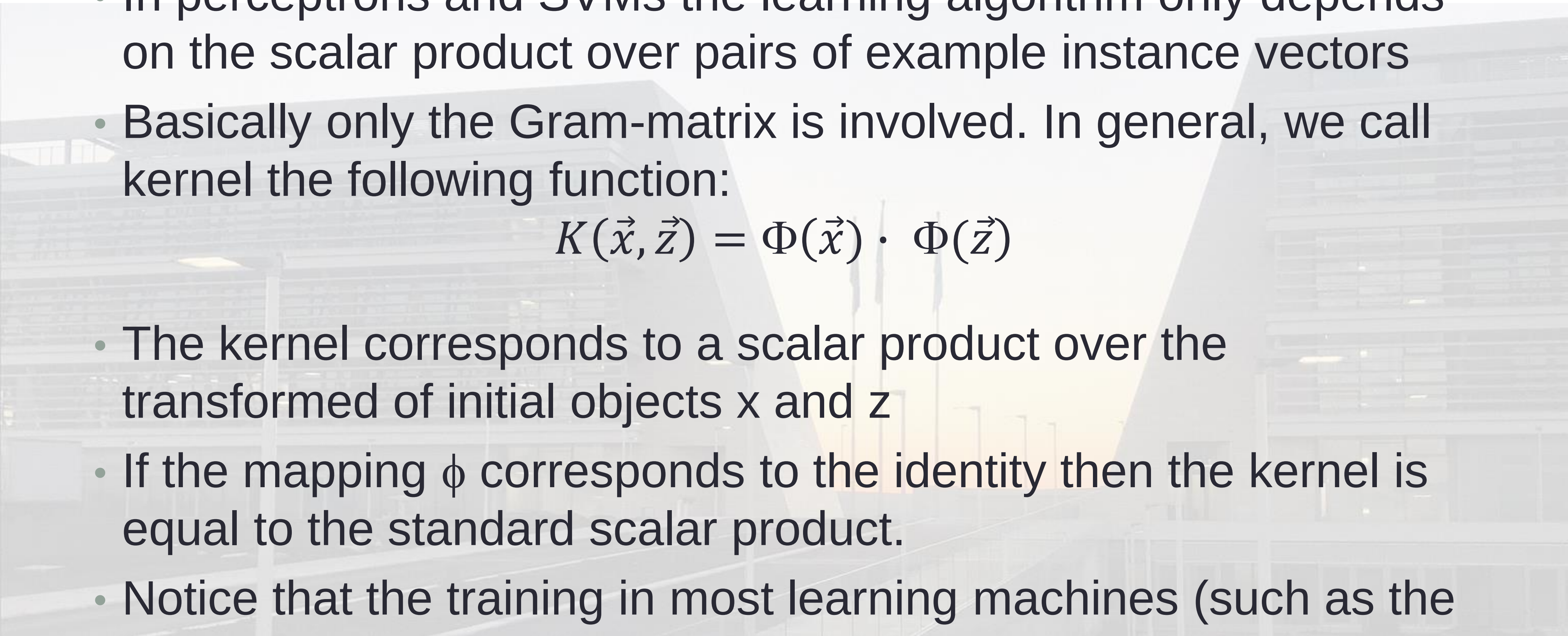


Linear classifiers and separability (2)

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



The kernel function

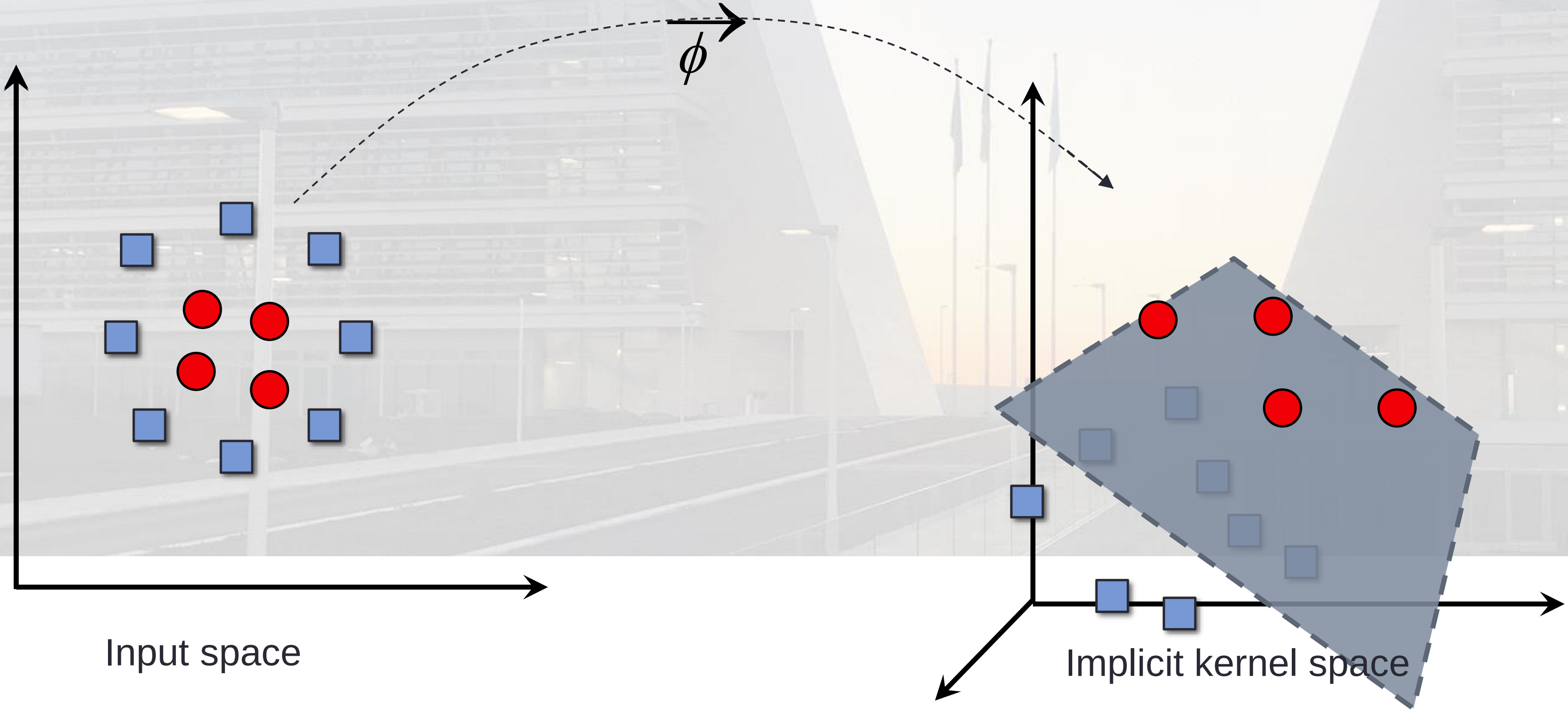


- In perceptrons and SVMs the learning algorithm only depends on the scalar product over pairs of example instance vectors
- Basically only the Gram-matrix is involved. In general, we call kernel the following function:

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

- The kernel corresponds to a scalar product over the transformed of initial objects x and z
- If the mapping ϕ 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

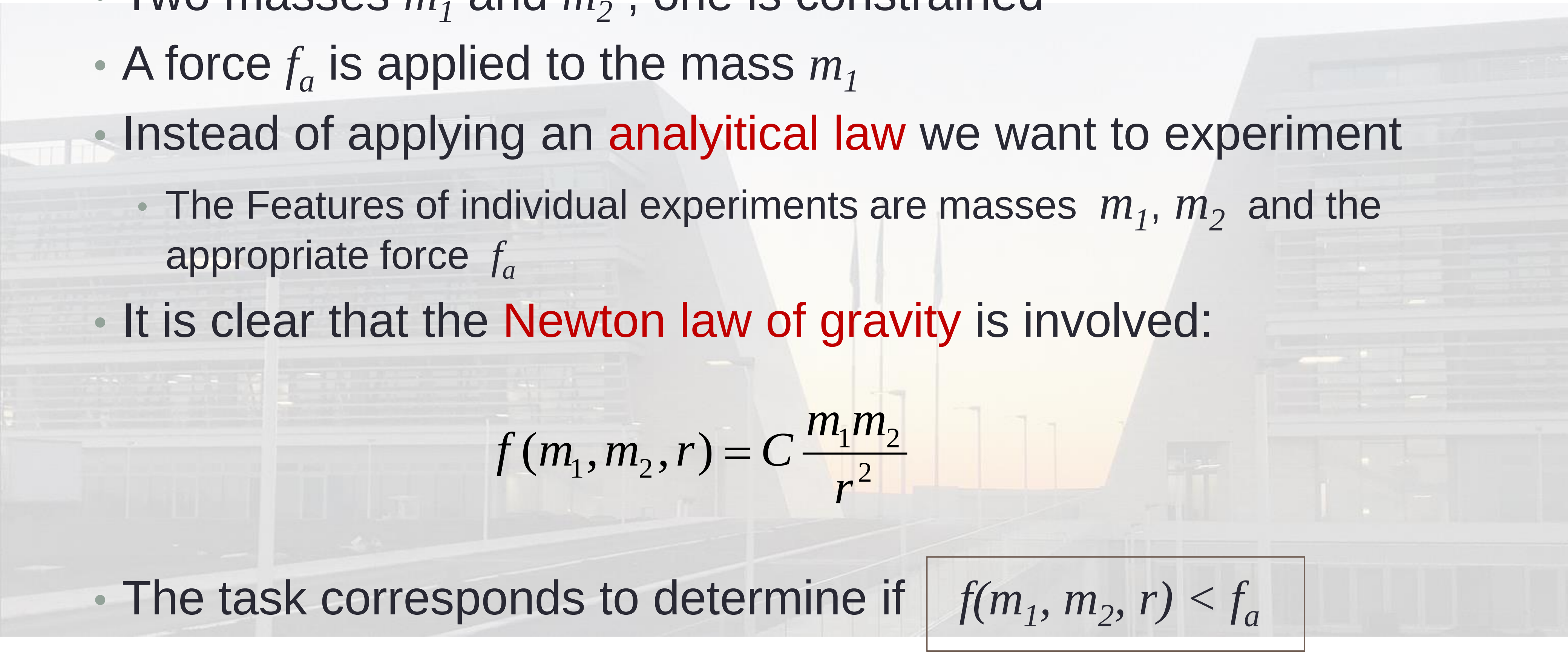
First Advantage:
making instances linearly separable



Input space

Implicit kernel space

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 force 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 $\boxed{f(m_1, m_2, r) < f_a}$

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:

$$(f_a, m_1, m_2, r) \to (k, x, y, z) = (\ln f_a, \ln m_1, \ln m_2, \ln r)$$

- holds as:

$$\ln f(m_1, m_2, r) = \ln C + \ln m_1 + \ln m_2 - 2\ln r = c + x + y - 2z$$

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

$$\ln f_a - \ln m_1 - \ln m_2 + 2\ln r - \ln C = 0$$

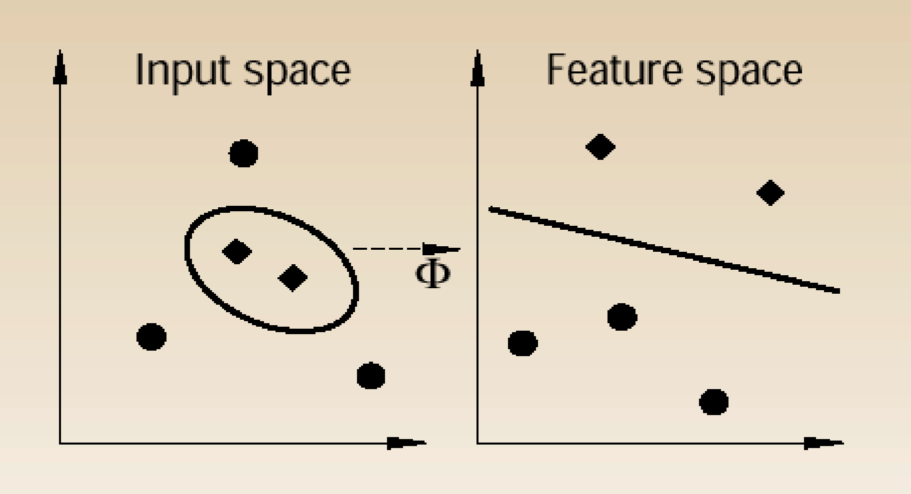
$$(1,1,-2,-1)\cdot(\ln m_1, \ln m_2, \ln r, \ln f_a) + \ln C = 0,$$

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

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

- 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 … x_l

A kernelized perceptron

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

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

$$= sgn(\textstyle\sum_{J=1}^{l} \alpha_j y_j k(\overrightarrow{x_j}, \vec{x}) + b)$$

- … 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

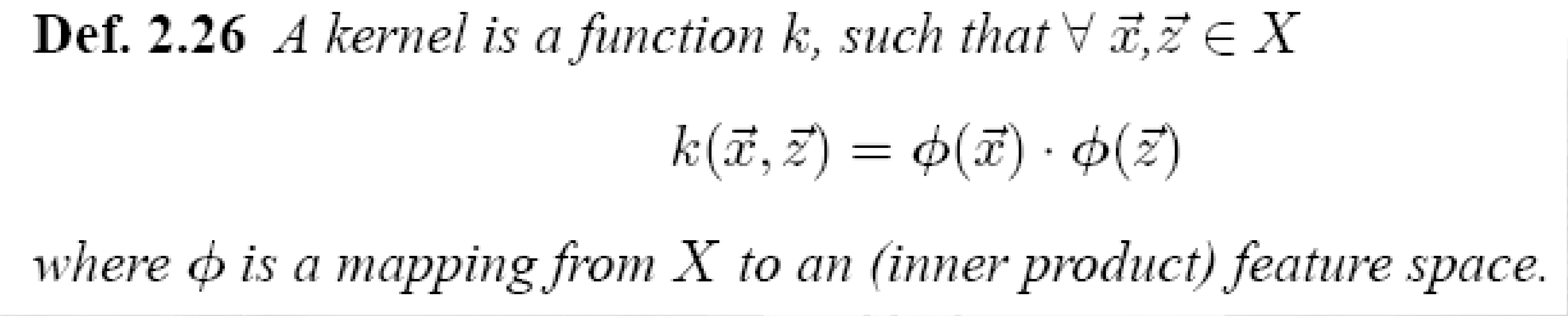
- In Soft Margin SVMs we need to maximize :

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

- By using kernel functions we rewrite the problem as:

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

What makes a function a kernel function?



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

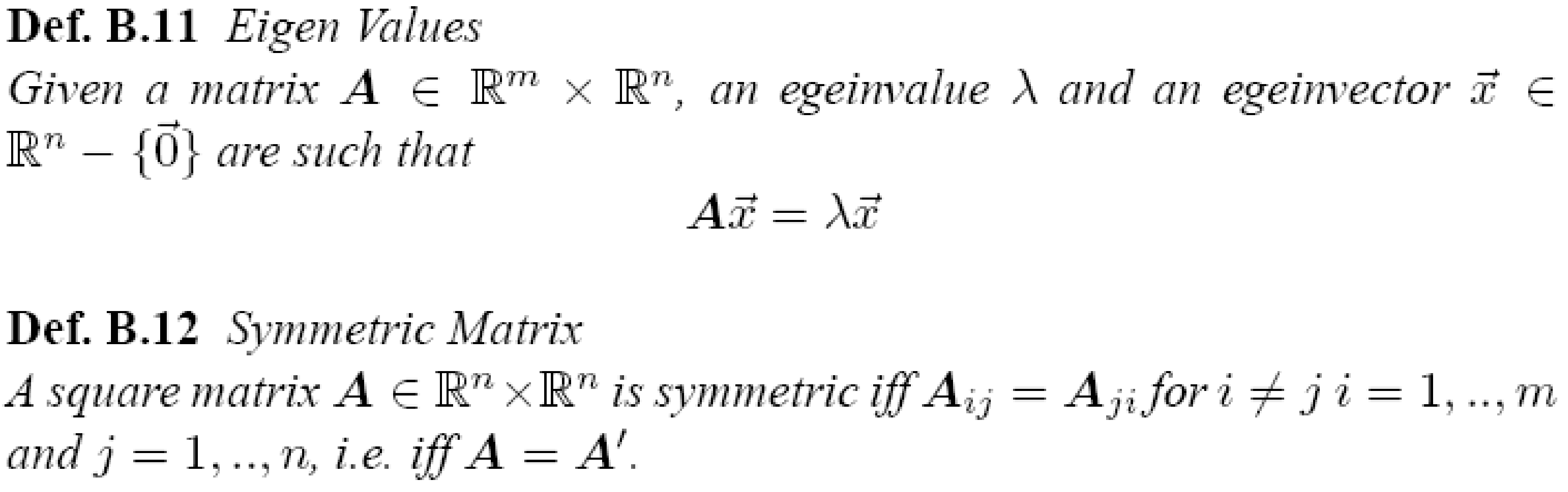
$$k(\vec{x}, \vec{z}) = \phi(\vec{x}) \cdot \phi(\vec{z})$$

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

Only such type of functions support implicit mappings such as

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

What makes a function a kernel function? (2)



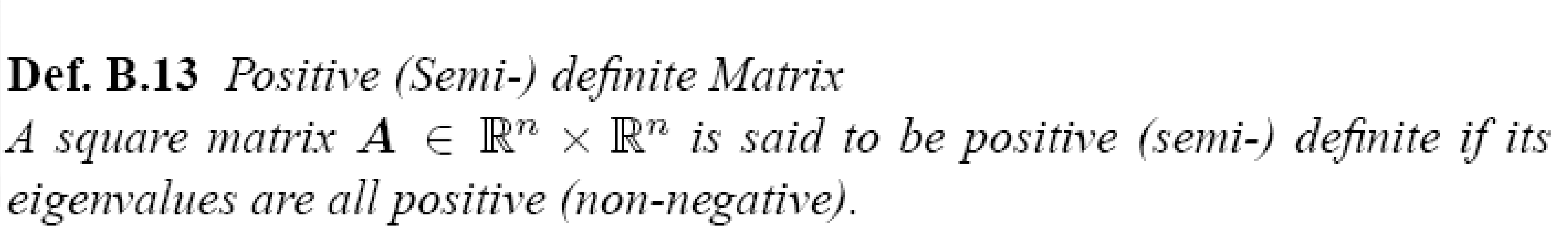
Def. B.11 *Eigen Values*

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

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

Def. B.12 *Symmetric Matrix*

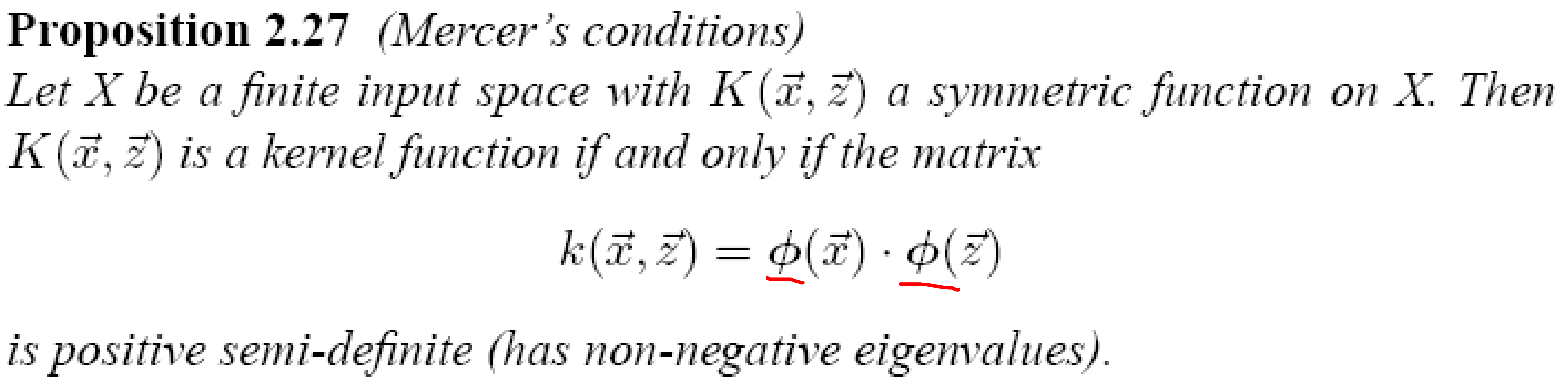
A square matrix $\boldsymbol{A} \in \mathbb{R}^n \times \mathbb{R}^n$ *is symmetric iff* $\boldsymbol{A}_{ij} = \boldsymbol{A}_{ji}$ *for* $i \neq j$ $i = 1, .., m$ *and* $j = 1, .., n$, *i.e. iff* $\boldsymbol{A} = \boldsymbol{A}'$.



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*

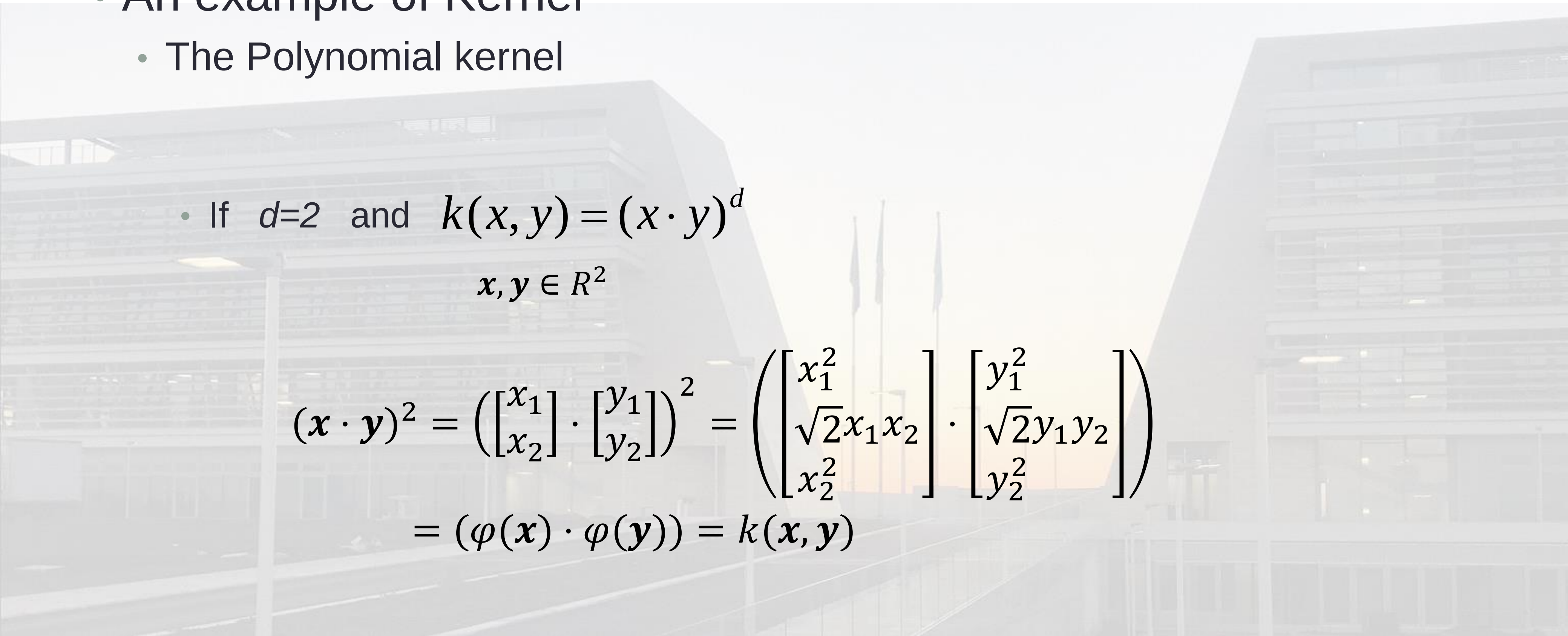
$$k(\vec{x},\vec{z}) = \underline{\phi}(\vec{x}) \cdot \underline{\phi}(\vec{z})$$

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



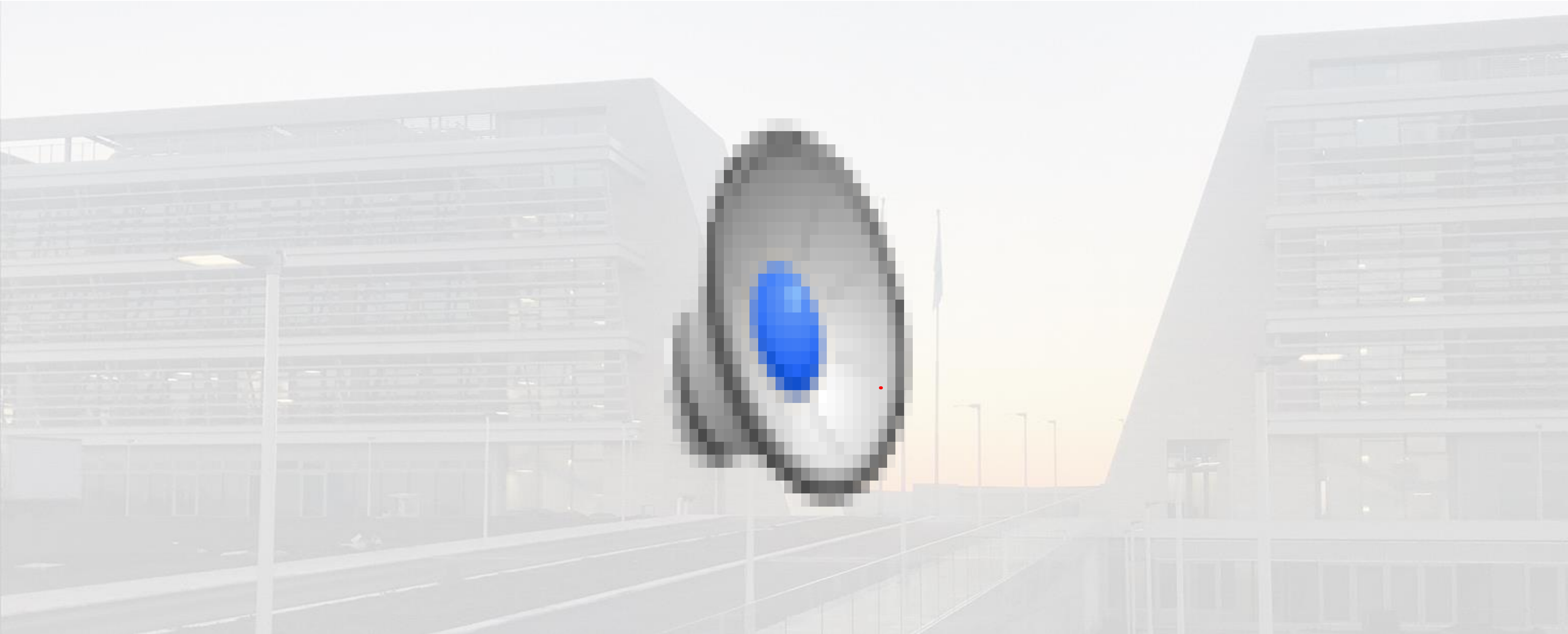
- If *d=2* and $k(x, y) = (x \cdot y)^d$

$$\boldsymbol{x}, \boldsymbol{y} \in R^2$$

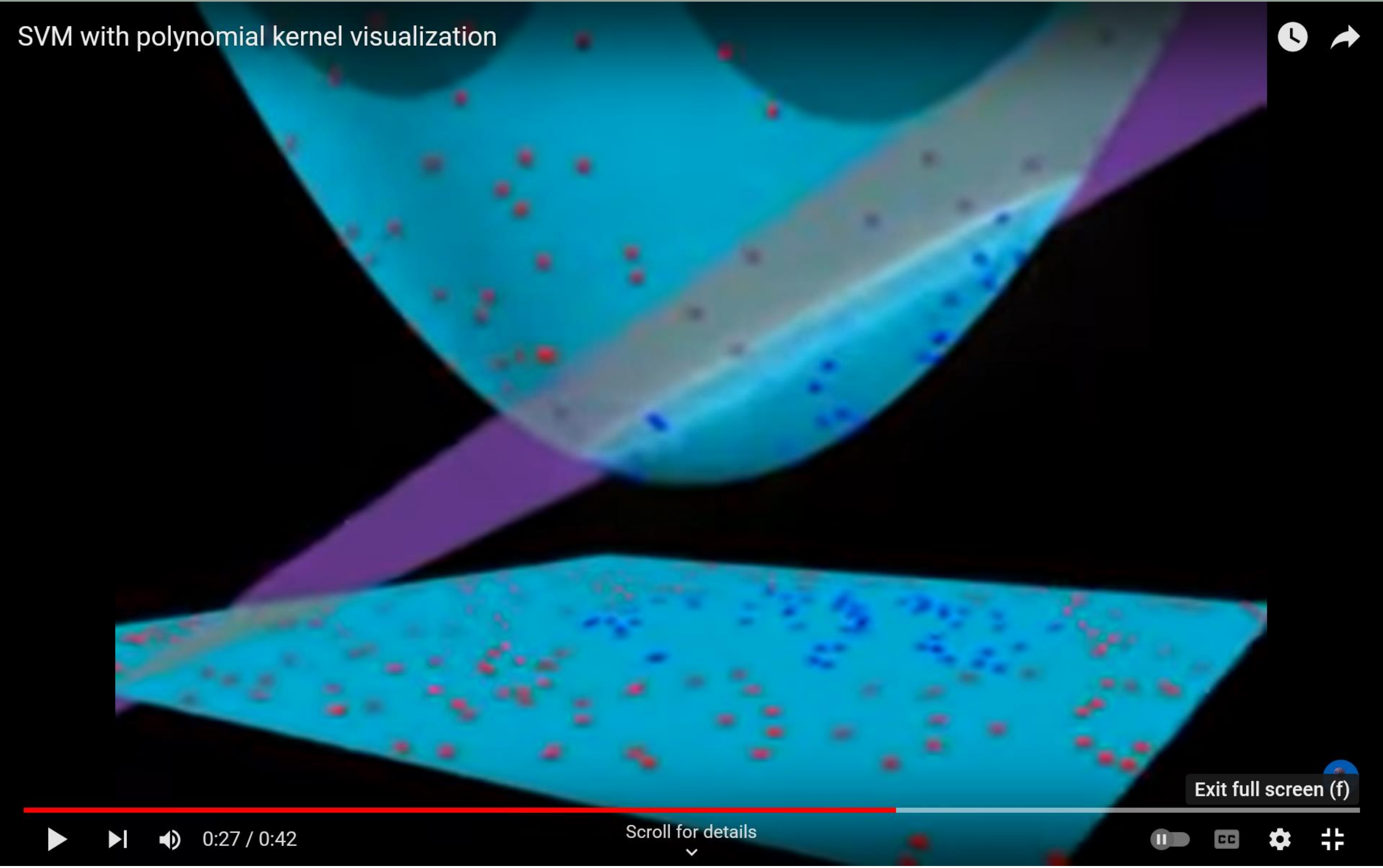
$$(\boldsymbol{x} \cdot \boldsymbol{y})^2 = \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}\right)^2 = \left(\begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \cdot \begin{bmatrix} y_1^2 \\ \sqrt{2}y_1y_2 \\ y_2^2 \end{bmatrix}\right)$$

$$= (\varphi(\boldsymbol{x}) \cdot \varphi(\boldsymbol{y})) = k(\boldsymbol{x}, \boldsymbol{y})$$

Polynomial kernel



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



SVM with polynomial kernel visualization

Polynomial Kernel (*n* dimensions)

$$\begin{aligned}
(\vec{x}\cdot\vec{z})^2 &= \Big(\sum_{i=1}^{n} x_i z_i\Big)^2 &&= \Big(\sum_{i=1}^{n} x_i z_i\Big)\Big(\sum_{j=1}^{n} x_i z_i\Big) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j z_i z_j &&= \sum_{i,j\in\{1,..,n\}} (x_i x_j)(z_i z_j) \\
&= \sum_{k=1}^{m} X_k Z_k &&= \vec{X}\cdot\vec{Z}
\end{aligned}$$

General Polynomial Kernel (*n* dimensions)

$$(\vec{x}\cdot\vec{z}+c)^2 = \Big(\sum_{i=1}^{n} x_i z_i + c\Big)^2 = \Big(\sum_{i=1}^{n} x_i z_i + c\Big)\Big(\sum_{j=1}^{n} x_i z_i + c\Big) =$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j z_i z_j + 2c\sum_{i=1}^{n} x_i z_i + c^2 =$$

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

Polynomial kernel and the conjunction of features

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

$$\Phi(< x_1, x_2 >) \rightarrow (x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1)$$

- More expressive, as (x_1x_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

$$\Phi(\vec{x})\times\Phi(\vec{z}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1)\times(z_1^2, z_2^2, \sqrt{2}z_1z_2, \sqrt{2}z_1, \sqrt{2}z_2, 1) =$$

$$= x_1^2z_1^2 + x_2^2z_2^2 + 2x_1x_2z_1z_2 + 2x_1z_1 + 2x_2z_2 + 1 =$$

$$= (x_1z_1 + x_2z_2 + 1)^2 = \boxed{(\vec{x}\times\vec{z} + 1)^2 = K_{p2}\ (\vec{x}, \vec{z})}$$

The Architecture of an SVM

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

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

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

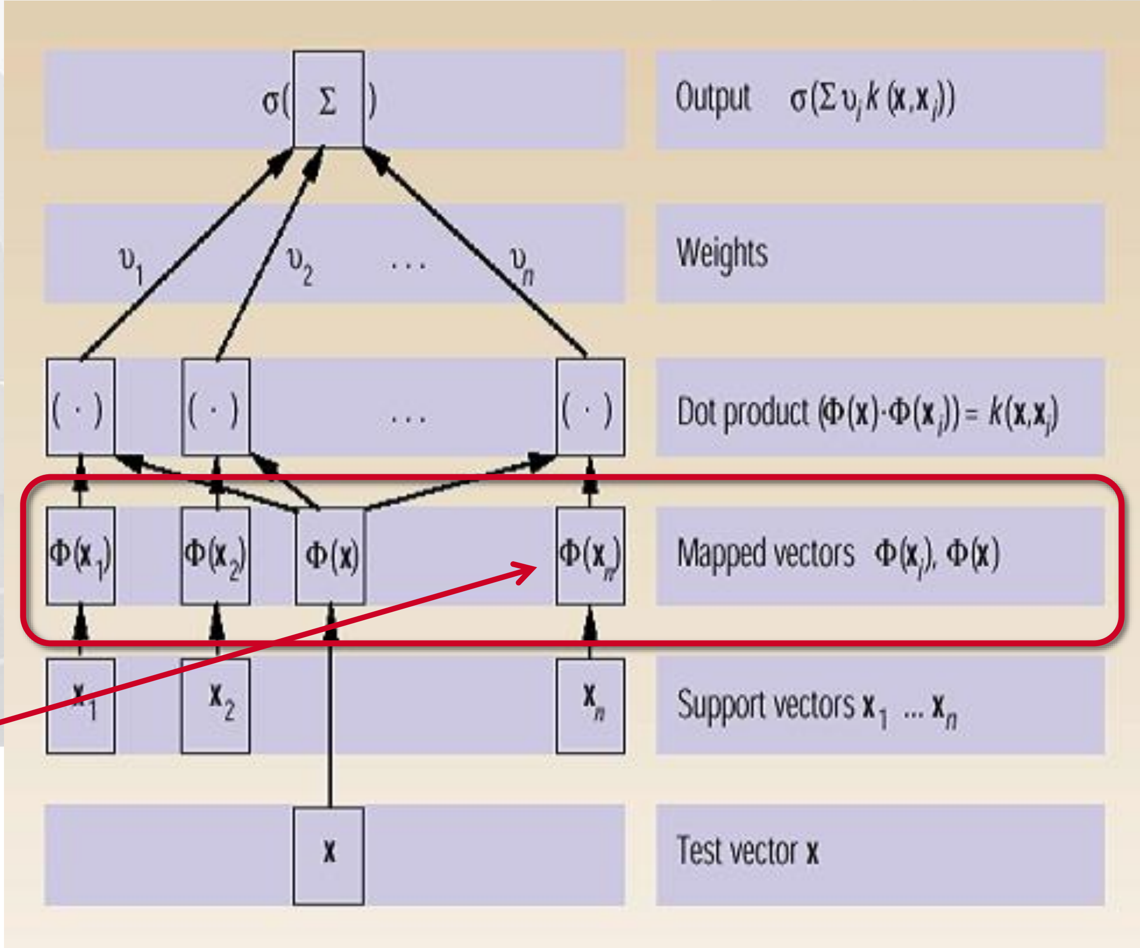
$\phi(x_i)$ *substitutes every*

training instamce x_i

$v_i = \alpha_i y_i$

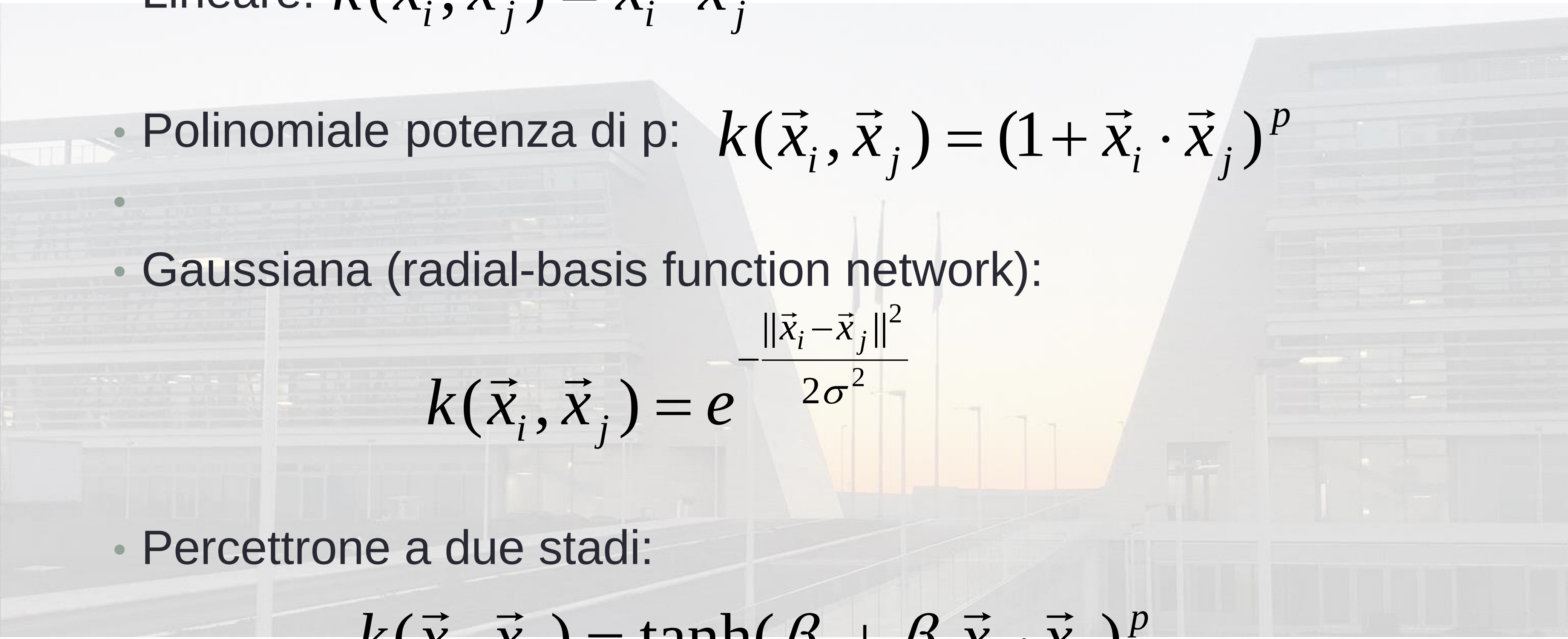
v_i *are the solutions*

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:

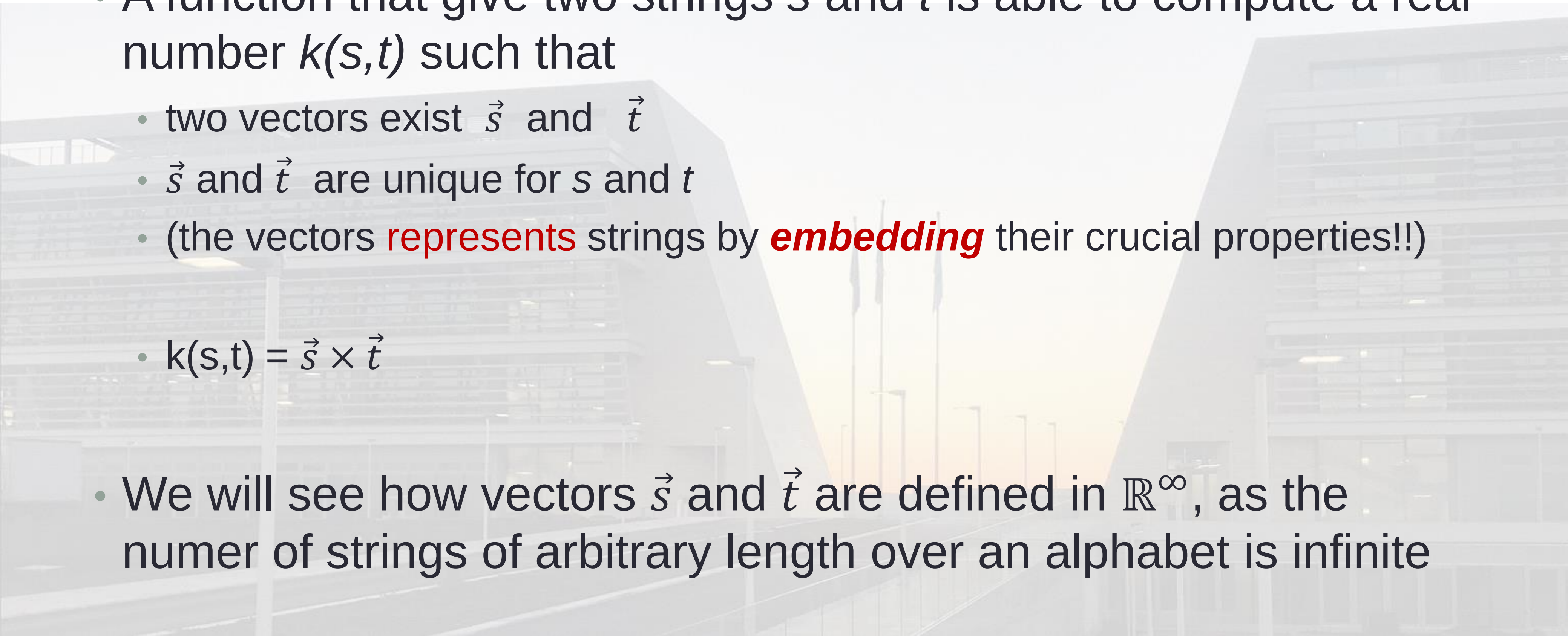
$$k(\vec{x}_i, \vec{x}_j) = \tanh(\beta_1 + \beta_0 \vec{x}_i \cdot \vec{x}_j)^p$$

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 $\mathbb{R}^\infty$, 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*

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*.

ϕ

	B	R	a	n	k	Ba	Ra	Ban	Ran	Bank	Rank	an	ank	ak	…
ϕ(Bank)= (	λ	0	λ	λ	λ	λ^2	λ^2	λ^3	0	λ^4	0	λ^2	λ^3	λ^3	…
ϕ(Rank)= (	0	λ	λ	λ	λ	0	0	0	λ^3	0	λ^4	λ^2	λ^3	λ^3	…

- 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 (1, … |s|)

$s = s_1, \ldots, s_{|s|}$

$\vec{I} = (i_1, \ldots, i_{|u|})$ $\quad u = s[\vec{I}]$, substring of *s* defined by $\vec{I}$

$$\phi_u(s) = \sum_{\vec{I}:u=s[\vec{I}]} \lambda^{l(\vec{I})}, \text{ con } l(\vec{I}) = i_{|u|} - i_1 + 1$$

$$K(s,t) = \sum_{u \in \Sigma^*} \phi_u(s) \cdot \phi_u(t) = \sum_{u \in \Sigma^*} \sum_{\vec{I}:u=s[\vec{I}]} \lambda^{l(\vec{I})} \sum_{\vec{J}:u=t[\vec{J}]} \lambda^{l(\vec{J})} =$$

$$= \sum_{u \in \Sigma^*} \sum_{\vec{I}:u=s[\vec{I}]} \sum_{\vec{J}:u=t[\vec{J}]} \lambda^{l(\vec{I})+l(\vec{J})}, \text{ con } \Sigma^* = \bigcup_{n=0}^{\infty} \Sigma^n$$

An example of string kernel computation

- $\phi_{\mathrm{a}}(\mathrm{Bank}) = \phi_{\mathrm{a}}(\mathrm{Rank}) = \lambda^{(i_1-i_1+1)} = \lambda^{(2-2+1)} = \lambda,$
- $\phi_{\mathrm{n}}(\mathrm{Bank}) = \phi_{\mathrm{n}}(\mathrm{Rank}) = \lambda^{(i_1-i_1+1)} = \lambda^{(3-3+1)} = \lambda,$
- $\phi_{\mathrm{k}}(\mathrm{Bank}) = \phi_{\mathrm{k}}(\mathrm{Rank}) = \lambda^{(i_1-i_1+1)} = \lambda^{(4-4+1)} = \lambda,$
- $\phi_{\mathrm{an}}(\mathrm{Bank}) = \phi_{\mathrm{an}}(\mathrm{Rank}) = \lambda^{(i_1-i_2+1)} = \lambda^{(3-2+1)} = \lambda^2,$
- $\phi_{\mathrm{ank}}(\mathrm{Bank}) = \phi_{\mathrm{ank}}(\mathrm{Rank}) = \lambda^{(i_1-i_3+1)} = \lambda^{(4-2+1)} = \lambda^3,$

$\phi_{\mathrm{nk}}(\mathrm{Bank}) = \phi_{\mathrm{nk}}(\mathrm{Rank}) = \lambda^{(i_1-i_2+1)} = \lambda^{(4-3+1)} = \lambda^2,$

$\phi_{\mathrm{ak}}(\mathrm{Bank}) = \phi_{\mathrm{ak}}(\mathrm{Rank}) = \lambda^{(i_1-i_2+1)} = \lambda^{(4-2+1)} = \lambda^3.$

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

Kernel Combination and normalization

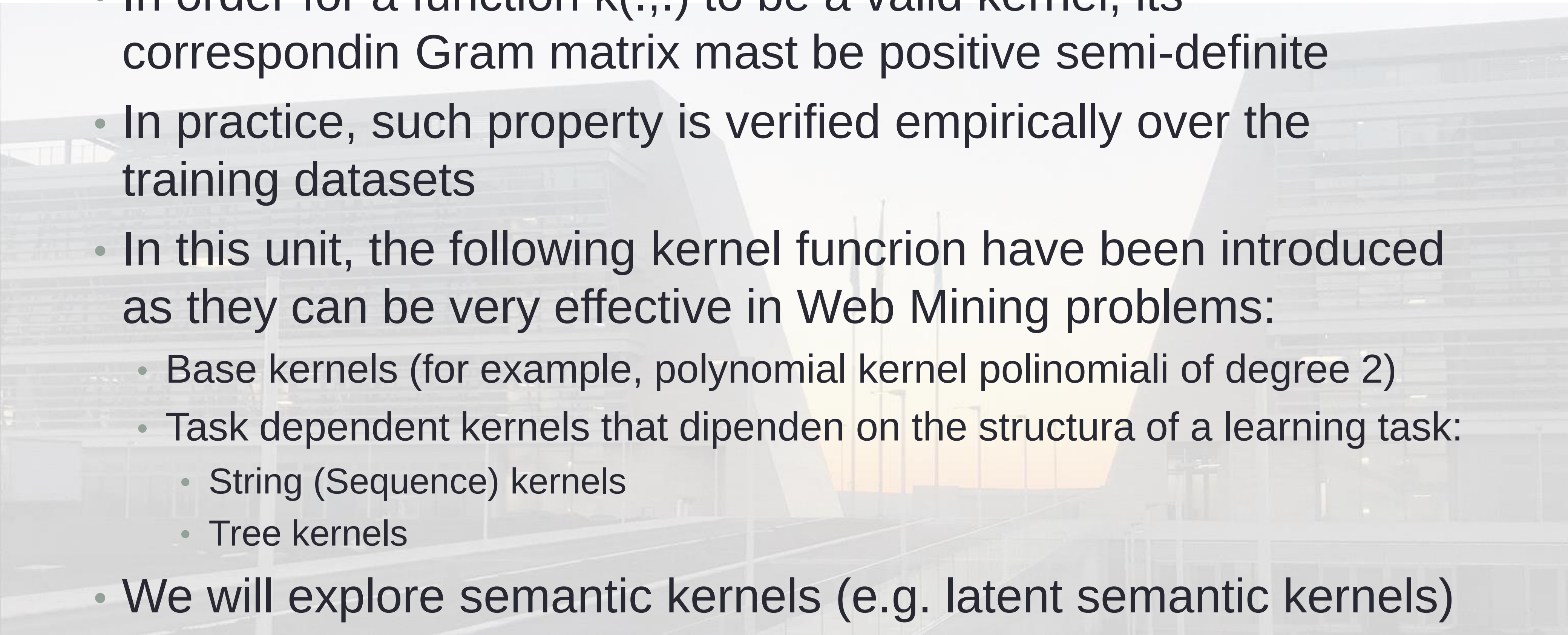
- Kernels can be easily combined so that the evidences captured by several kernel functions can contribute to the learning algorithm
  - The sum of kernels is a valid kernel
  - The product of kernels is a valid kernel
- We can also Normalize the implicit space operating directly only the kernel function

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

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

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