Machine Learning

MIRI Master

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LECTURE 14 : Learning with kernels

Learning with kernels (I): The SVM

Linear regression revisited

- **Problem**: We wish to find a function $y(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} + b$ which best models a data set $D = \{(\boldsymbol{x}_1, t_1), \ldots, (\boldsymbol{x}_N, t_N)\} \subset \mathbb{R}^d \times \mathbb{R}$

- Then we minimize the regularized (aka penalized) empirical error:

$$E^\lambda_{\text{emp}}(y) = \sum_{n=1}^{N} \Big(t_n - y(\boldsymbol{x}_n)\Big)^2 + \lambda \sum_{i=1}^{d} w_i^2 = \|\boldsymbol{t} - X\boldsymbol{w}\|^2 + \lambda \|\boldsymbol{w}\|^2$$

  The parameter $\lambda > 0$ defines a trade-off between the fit to the data and the complexity of the vector $\boldsymbol{w}$

Learning with kernels (I): The SVM

Linear regression revisited

Setting $\frac{\partial E^{\lambda}_{\text{emp}}(y)}{\partial \boldsymbol{w}} = 0$, we obtain the (regularized) normal equations:

$$-2X^{\mathsf{T}}(\boldsymbol{t} - X\boldsymbol{w}) + 2\lambda \boldsymbol{w} = 0$$

with solution

$$\widehat{\boldsymbol{w}} = (X^{\mathsf{T}}X + \lambda I_d)^{-1} X^{\mathsf{T}}\boldsymbol{t}$$

and therefore

$$y(\boldsymbol{x}) = \widehat{\boldsymbol{w}}^{\top}\boldsymbol{x}$$

Learning with kernels (I): The SVM

Linear regression revisited

It turns out that the regularized solution can be written as:

$$\widehat{\boldsymbol{w}} = \sum_{n=1}^{N} \alpha_n \boldsymbol{x}_n, \qquad \widehat{\boldsymbol{w}} = \begin{pmatrix} \widehat{w}_1 \\ \widehat{w}_2 \\ \vdots \\ \widehat{w}_d \end{pmatrix}$$

$$y(\boldsymbol{x}) = \sum_{n=1}^{N} \alpha_n (\boldsymbol{x}_n{}^\top \boldsymbol{x}), \qquad \boldsymbol{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{pmatrix}$$

The new vector of parameters is given by $\boldsymbol{\alpha} = (XX^\top + \lambda I_N)^{-1}\boldsymbol{t}$

Learning with kernels (I): The SVM

Linear regression revisited

So we have the **primal** and the **dual** forms for $y(\boldsymbol{x})$:

$$y(\boldsymbol{x}) = \widehat{\boldsymbol{w}}^\top \boldsymbol{x} \quad \text{and} \quad y(\boldsymbol{x}) = \sum_{n=1}^{N} \alpha_n (\boldsymbol{x}_n{}^\top \boldsymbol{x})$$

The dual form is usually more convenient when $d \gg N$:

- the primal requires the computation & inversion of $X^\mathsf{T} X + \lambda I_d$, requiring $O(Nd^2 + d^3)$ operations
- the dual requires the computation & inversion of $XX^\mathsf{T} + \lambda I_N$, requiring $O(dN^2 + N^3)$ operations

Learning with kernels (I): The SVM

Key aspects of kernel methods

How can we achieve non-linear regression?

A **feature map** is a function $\phi : \mathbb{R}^d \to \mathbb{R}^M$:

$$\phi(\boldsymbol{x}) = \Big(\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \cdots, \phi_M(\boldsymbol{x})\Big)^\mathsf{T}$$

- $\phi(\boldsymbol{x})$ is called the **feature vector**
- $\{\phi(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^d\}$ is the **feature space** (FS), and typically $M \gg d$.

Learning with kernels (I): The SVM

Key aspects of kernel methods

- Define $\Phi_{N\times M}$ the matrix of the $\phi(\boldsymbol{x}_n)$ as

$$\phi_{nm} = \phi_m(\boldsymbol{x}_n), n = 1, \ldots, N, m = 1, \ldots, M.$$

- Suppose we perform ridge regression on the Φ matrix

- The new regression function has the **primal** representation:

$$y(\boldsymbol{x}) = \widehat{\boldsymbol{w}}^\top \phi(\boldsymbol{x})$$

Note the primal now (explicitly) operates in feature space

Learning with kernels (I): The SVM

Key aspects of kernel methods

Given a feature map $\phi : \mathbb{R}^d \to \mathbb{R}^M$, we define its associated **kernel function** $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ as:

$$k(\boldsymbol{u}, \boldsymbol{v}) = \phi(\boldsymbol{u})^\top \phi(\boldsymbol{v}), \qquad \boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^d$$

- The feature space where k *implicitly* operates is $\mathbb{R}^M$
- For some feature maps, computing $k(\boldsymbol{u}, \boldsymbol{v})$ is independent of M

Learning with kernels (I): The SVM

Key aspects of kernel methods

Since $\widehat{\boldsymbol{w}} = \sum_{n=1}^{N} \alpha_n \phi(\boldsymbol{x}_n)$, the new regression function has the **dual** representation:

$$y(\boldsymbol{x}) = \sum_{n=1}^{N} \alpha_n (\phi(\boldsymbol{x}_n)^\top \phi(\boldsymbol{x})) = \sum_{n=1}^{N} \alpha_n k(\boldsymbol{x}_n, \boldsymbol{x})$$

The new vector of parameters is given by

$$\boldsymbol{\alpha} = (\mathbf{K} + \lambda I_N)^{-1} \boldsymbol{t}, \qquad \text{where } \mathbf{K} = \Big(k(\boldsymbol{x}_n, \boldsymbol{x}_m)\Big)$$

Kernel-Based Learning

Key aspects of kernel methods

- A feature map is of the general form $\phi : \mathcal{X} \to \mathcal{H}$. The associated kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is $k(\boldsymbol{u}, \boldsymbol{v}) = \langle \phi(\boldsymbol{u}), \phi(\boldsymbol{v}) \rangle_{\mathcal{H}}, \ \boldsymbol{u}, \boldsymbol{v} \in \mathcal{X}$

- $\mathcal{X}$ can be any space, $\mathcal{H}$ is any **Hilbert space**:

  - An abstract complete vector space possessing the structure of an inner product

  - Examples would be $\mathbb{R}^M$ or the l_2 space of square-summable sequences

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In our previous discussion, $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{H} = \mathbb{R}^M$

Learning with kernels (I): The SVM

Key aspects of kernel methods

Kernel-based methods consist of two ingredients:

1. The kernel function (this is non-trivial)

2. The algorithm taking kernels as input

   - Data items are embedded into a vector space (feature space FS)
   - Linear relations are sought among the elements of the FS
   - The coordinates of these images are not needed: only their pairwise inner products
   - These inner products can sometimes be computed efficiently and implicitly in the input space (kernel function)
   - The solution vector is expressed as a linear combination of the kernel centered at the data

Learning with kernels (I): The SVM

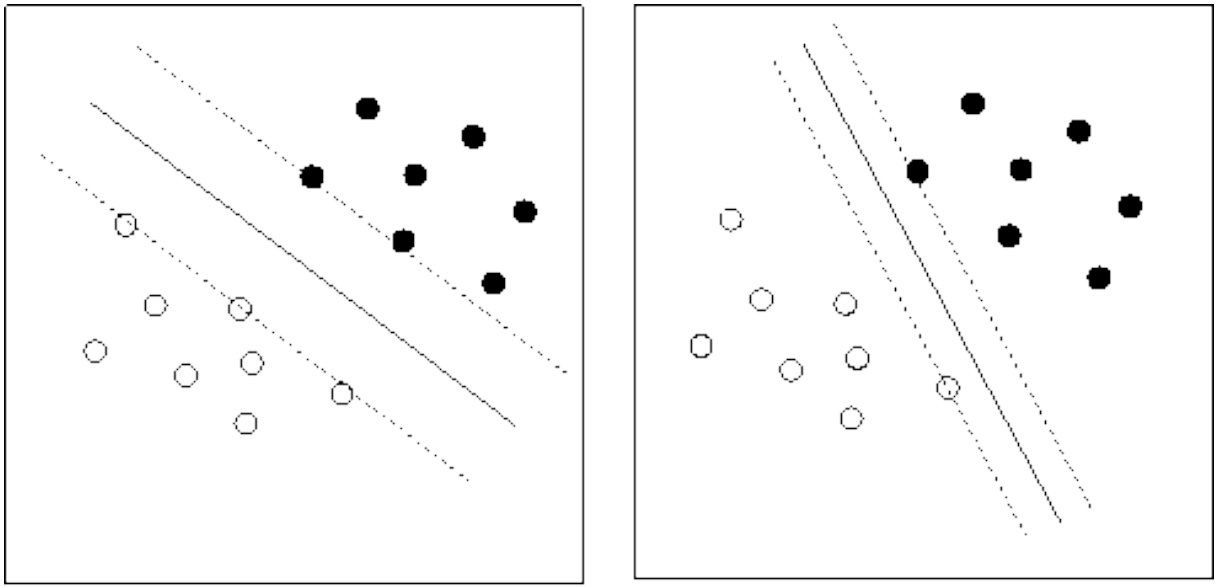
Key aspects of kernel methods

Many (classical and new) learning algorithms can be "kernelized":

- The Support Vector Machine (SVM) and the Relevance Vector Machine (RVM)
- Fisher Discriminant Analysis (KFDA), Principal Components Analysis (KPCA), Canonical Correlation Analysis (KCCA), ...
- Kernel (regularized) linear regression
- Kernel k-means, kernel kNN
- (less known or very recent): PLS, Parzen Windows, logistic regression, statistical tests, ...

Support Vector Machines

Preliminaries



(a) Larger margin (b) Smaller margin

Which solution is more likely to lead to better generalization?

Support Vector Machines

Preliminaries

Working Hypothesis (intuition):

The larger the margin, the better the generalization

- Criterion for building a two-class classifier:

  Maximize the **width of the margin** between the classes

- **margin** = empty area around the decision boundary, defined by the distance to the nearest training examples

  These examples will be called the **support vectors**

Goal: find the hyperplane (linear boundary) with the **largest margin**

Support Vector Machines

Formalisation

We have a data set $D = \{(\boldsymbol{x}_1, t_1), \ldots, (\boldsymbol{x}_N, t_N)\}$, with $\boldsymbol{x}_n \in \mathbb{R}^d$ and $t_n \in \{-1, +1\}$, describing a two class problem

We wish to find a function $y(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b$ which best models D

- We would like to find $\boldsymbol{w}, b$ such that:

  $\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b > 0$, when $t_n = +1$
  $\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b < 0$, when $t_n = -1$

- In short, $t_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) > 0$, or $t_n\, y(\boldsymbol{x}_n) > 0, \qquad 1 \leq n \leq N$

Support Vector Machines

Formalisation

- The quantity $t_n\, y(\boldsymbol{x}_n)$ is the **functional** margin of $\boldsymbol{x}_n$ (there will be an "error" whenever $t_n\, y(\boldsymbol{x}_n) < 0$)

- Given the plane $\pi : y(\boldsymbol{x}) = 0$ or $\pi : \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b = 0$, the distance $d(\boldsymbol{x}, \pi) = \frac{|y(\boldsymbol{x})|}{\|\boldsymbol{w}\|}$ is called the **geometrical margin** of $\boldsymbol{x}$

- The optimal separating hyperplane (OSH) is the one that maximizes the geometrical margin for linearly separable data:

$$\max_{\boldsymbol{w},b} \left\{ \min_{1 \leq n \leq N} d(\boldsymbol{x}_n, \pi) \right\} \qquad \text{subject to } t_n \left(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b \right) > 0 \ (1 \leq n \leq N)$$

Support Vector Machines

Formalisation

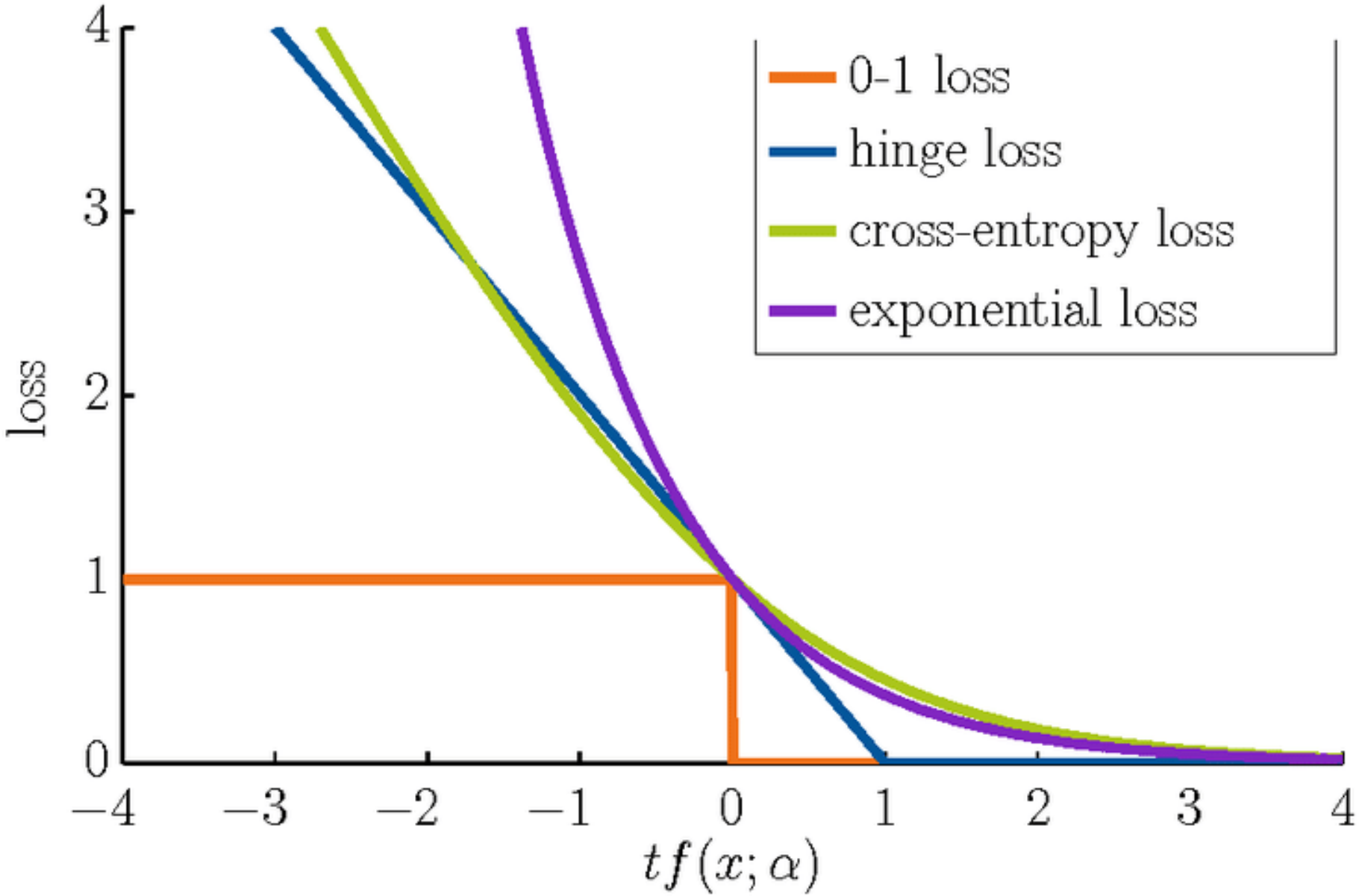
- Rescaling $\boldsymbol{w}, b$ such that $|\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b| = 1$ for the points closest to the hyperplane, we obtain $|\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b| \geq 1$

- The **support vectors** (SV) are the $\boldsymbol{x}_n$ such that $|\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b| = 1$

- The loss is $\max(1 - t_n\, y(\boldsymbol{x}_n), 0) = (1 - t_n\, y(\boldsymbol{x}_n))_+$ (**hinge loss**)

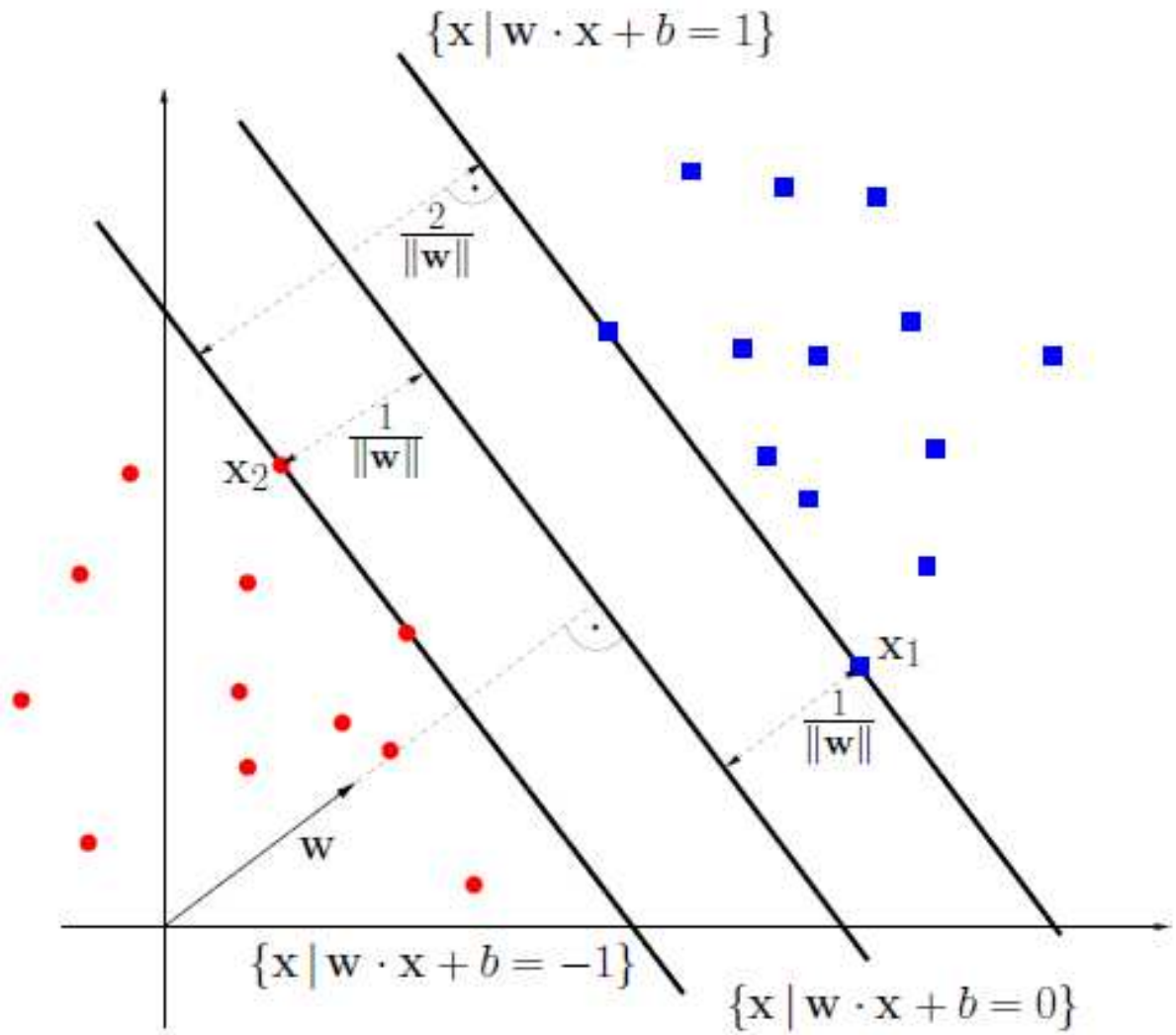
- The **margin** of the OSH is twice the distance to any SV:

  $\text{margin}(\text{OSH}) = 2\, d(\boldsymbol{x}_{\text{SV}}, \text{OSH}) = \dfrac{2}{\|\boldsymbol{w}\|}$, since $|y(\boldsymbol{x}_{\text{SV}})| = 1$


0-1 loss
hinge loss
cross-entropy loss
exponential loss
loss
4
3
2
1
0
−4
−3
−2
−1
0
1
2
3
4
$tf(x;\alpha)$

Support Vector Machines

Geometrical view



Support Vector Machines

A look on what's to come

1. We find the **canonical OSH** by solving

$$\underset{\boldsymbol{w},b}{\text{máx}} \left\{ \frac{2}{\|\boldsymbol{w}\|} \quad / \quad t_n \left(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b \right) \geq 1, \qquad 1 \leq n \leq N \right\}$$

2. The solution will be $\boldsymbol{w} = \sum_{n=1}^{N} t_n \alpha_n \boldsymbol{x}_n$, with $\alpha_n \geq 0$ (the **dual** form)

3. A fraction of the training $\boldsymbol{x}_n$ will have $\alpha_n = 0$ (**sparsity**); the $\boldsymbol{x}_n$ for which $\alpha_n > 0$ will coincide with the **support vectors**

4. The **discriminant function** will be written

$$y_{\text{SVM}}(\boldsymbol{x}) = \text{sgn}(\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b) = \text{sgn} \left(\sum_{n=1}^{N} t_n \alpha_n \langle \boldsymbol{x}, \boldsymbol{x}_n \rangle + b \right)$$

Support Vector Machines

Resolution

$$\textbf{minimize} \qquad \frac{1}{2}\|\boldsymbol{w}\|^2$$

$$\textbf{subject to} \quad t_n\left(\langle \boldsymbol{w}, \boldsymbol{x}_n\rangle + b\right) \geq 1, \qquad 1 \leq n \leq N$$

This is solved (numerically) by QP techniques:

- Quadratic (therefore convex) function subject to linear constraints
- Unique solution (or set of equivalent ones); therefore, NO LOCAL MINIMA

Support Vector Machines

Margin violations

- In practice, we allow small margin violations ε_n, for each $\boldsymbol{x}_n$:

$$\textbf{minimize} \qquad \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\varepsilon_n$$

$$\textbf{subject to} \quad t_n\left(\langle \boldsymbol{w}, \boldsymbol{x}_n\rangle + b\right) \geq 1 - \varepsilon_n, \qquad \varepsilon_n \geq 0, 1 \leq n \leq N$$

- The ε_n are **slack** variables, leading to a **soft margin** ($\varepsilon_n > 0$ implying the functional margin $t_n y(\boldsymbol{x}_n) < 1$)

Support Vector Machines

Lagrangian form (primal)

- We first construct the Lagrangian:

$$\mathcal{L} = \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_{n=1}^{N} \alpha_n \Big\{ t_n \left(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b \right) - 1 + \varepsilon_n \Big\} + C \sum_{n=1}^{N} \varepsilon_n - \sum_{n=1}^{N} \mu_n \varepsilon_n$$

- The $\alpha_n, \mu_n \geq 0$ are the *Lagrange multipliers* (auxiliary variables to cope with the constraints)

- The solution is the saddle point of $\mathcal{L}$:

  1. the minimum of $\mathcal{L}$ is taken with respect to $\boldsymbol{w}, b$

  2. the maximum of $\mathcal{L}$ is taken with respect to the α_n

Support Vector Machines

Lagrangian form

The gradient of $\mathcal{L}$ with respect to $\boldsymbol{w}, b$ must vanish:

$$\frac{\partial \mathcal{L}}{\partial b} = \sum_{n=1}^{N} \alpha_n t_n = 0, \quad \frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_{n=1}^{N} \alpha_n t_n \boldsymbol{x}_n = 0, \quad \frac{\partial \mathcal{L}}{\partial \varepsilon_n} = C - \alpha_n - \mu_n = 0$$

In addition, the so-called **KKT complementarity conditions** hold:

$$\alpha_n \Big(t_n \left(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b \right) - 1 + \varepsilon_n \Big) = 0, \ 1 \leq n \leq N$$

Support Vector Machines

Dual formulation

The Lagrangian $\mathcal{L}$ is convex; its optimization is equivalent to the maximization of its **dual problem** $\mathcal{L}_D$:

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maximize $$\mathcal{L}_D = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m t_n t_m \langle \boldsymbol{x}_n, \boldsymbol{x}_m \rangle$$

subject to $0 \leq \alpha_n \leq C, \quad 1 \leq n \leq N,$ **and** $\sum_{n=1}^{N} \alpha_n t_n = 0$

- Note how neither $\mu_n, \varepsilon_n, \boldsymbol{w}, b$ appear in the dual form
- Maximization is only with respect to the α_n

Support Vector Machines

Result

- The discriminant function is:

$$y_{\mathsf{SVM}}(\boldsymbol{x}) = \mathsf{sgn}\left(\sum_{n=1}^{N} \alpha_n t_n \, \langle \boldsymbol{x}_n, \boldsymbol{x} \rangle + b\right)$$

  with $\alpha_n > 0$ *only* for the support vectors (for the rest, $\alpha_n = 0$).

- By setting $C = \infty$ we are in the *hard* margin case

  $\Rightarrow C$ represents a tradeoff between **margin width** and **training error**

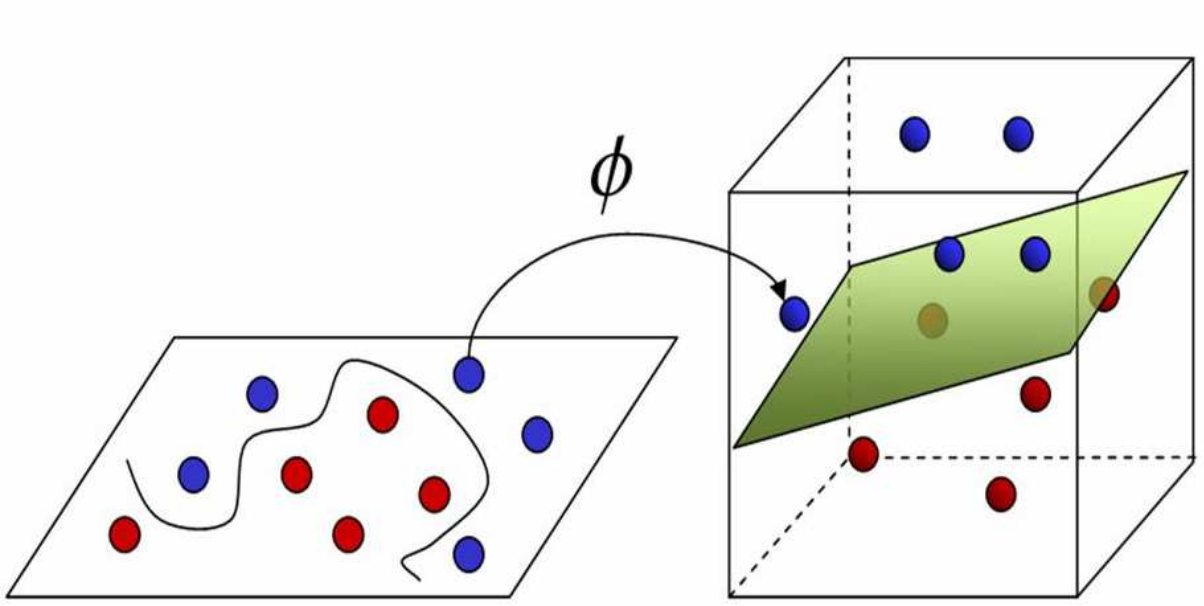
- $b = -\left(\sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n t_n \, \alpha_m t_m \, \langle \boldsymbol{x}_n, \boldsymbol{x}_m \rangle\right) / \left(\sum_{n=1}^{N} \alpha_n\right)$

Support Vector Machines

General feature maps

Recall the idea of mapping input data into some Hilbert space (called the *feature space*) via a non-linear mapping $\phi : \mathcal{X} \to \mathcal{H}$

The associated kernel function is $k(\boldsymbol{u}, \boldsymbol{v}) = \langle \phi(\boldsymbol{u}), \phi(\boldsymbol{v}) \rangle, \ \boldsymbol{u}, \boldsymbol{v} \in \mathcal{X}$



Support Vector Machines

SVM training ... back to the OSH

- We now substitute $\boldsymbol{x}_n$ by $\phi(\boldsymbol{x}_n)$, then build the OSH in $\mathcal{H}$

- The discriminant function becomes:

$$y_{\text{SVM}}(\boldsymbol{x}) = \text{sgn}\left(\sum_{n=1}^{N} \alpha_n t_n k(\boldsymbol{x}, \boldsymbol{x}_n) + b\right)$$

- The dual of the new QP problem is formulated exactly as before, replacing $\langle \boldsymbol{x}_n, \boldsymbol{x}_m \rangle$ with $k(\boldsymbol{x}_n, \boldsymbol{x}_m)$

Support Vector Machines

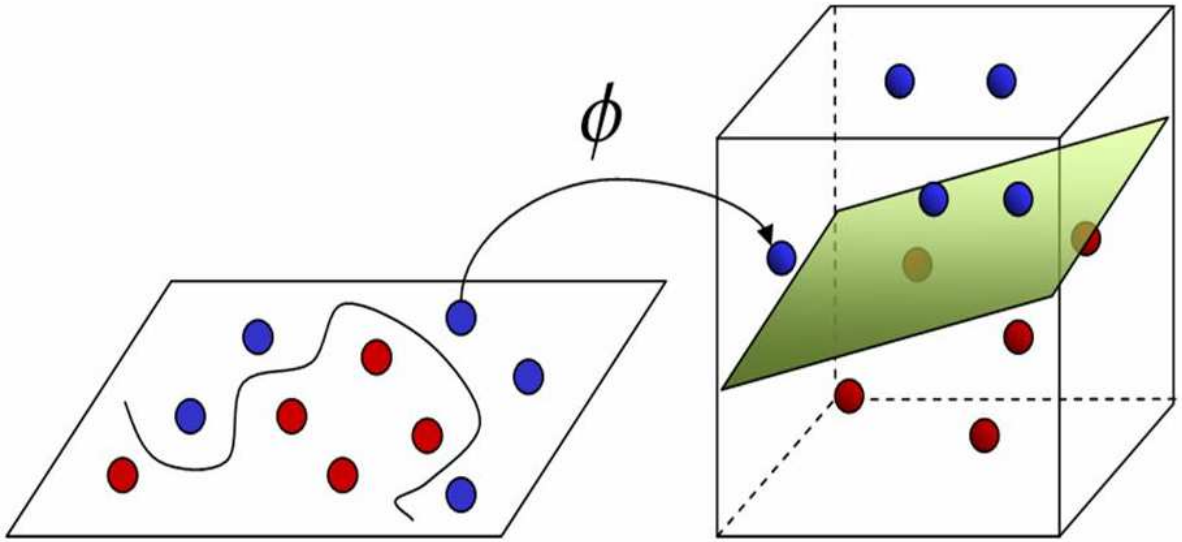
In conclusion ...

- (⇑) No local minima, no initial conditions, few parameters to set
- (⇑) Provide with a compact description of original data
- (⇑) Decision surfaces can be RBFs, polynomials, multilayer perceptrons, ...
- (⇑) Accept any data type as input
- (⇑) Explicit complexity control via C, ϵ and the kernel parameters
- (⇑) Less affected by large input dimensions than other methods
- (⇑) Excellent practical performance: OCR, text categorization, face detection, ...

- (⇓) Training requires solving a QP problem
- (⇓) Choice of best kernel is an open issue; **kernel design** is an active area of research
- (⇓) Sometimes fraction of SVs very high (indicating a poor model)
- (⇓) Performance usually depends on a careful choice of the parameters

Learning with kernels (II): Kernel functions

A kernel function implicitly defines a map $\phi : \mathcal{X} \to \mathcal{H}$ from an input space of objects $\mathcal{X}$ into some Hilbert space $\mathcal{H}$ (called the *feature space*). The "kernel trick" consists in performing the mapping and the inner product simultaneously by defining its associated kernel function:



$$k(\boldsymbol{u}, \boldsymbol{v}) = \langle \phi(\boldsymbol{u}), \phi(\boldsymbol{v}) \rangle_{\mathcal{H}}, \ \boldsymbol{u}, \boldsymbol{v} \in \mathcal{X},$$

Learning with kernels (II): Kernel functions

The Kernel Trick

- Suppose we take $k(\boldsymbol{u}, \boldsymbol{v}) = \langle \boldsymbol{u}, \boldsymbol{v} \rangle^d$ (a simple choice).
- What is the underlying mapping ϕ here?

  $\Longrightarrow$ Answer: this choice of kernel corresponds to a map ϕ leading into the space spanned by all products of exactly d dimensions of $\mathbb{R}^n$.
- Let us take, for instance, $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^2$, and take $d = 2$:

$$k(\boldsymbol{u}, \boldsymbol{v}) = \langle \boldsymbol{u}, \boldsymbol{v} \rangle^2 = \left[\left\langle \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \right\rangle \right]^2$$

$$= (u_1 v_1 + u_2 v_2)^2 = (u_1 v_1)^2 + 2 u_1 v_1 u_2 v_2 + (u_2 v_2)^2$$

$$= u_1^2 v_1^2 + (\sqrt{2} u_1 u_2)(\sqrt{2} v_1 v_2) + u_2^2 v_2^2$$

$$= \left\langle \begin{pmatrix} u_1^2 \\ \sqrt{2} u_1 u_2 \\ u_2^2 \end{pmatrix}, \begin{pmatrix} v_1^2 \\ \sqrt{2} v_1 v_2 \\ v_2^2 \end{pmatrix} \right\rangle = \langle \phi(\boldsymbol{u}), \phi(\boldsymbol{v}) \rangle$$

- Therefore, $\phi : \mathbb{R}^2 \longrightarrow \mathbb{R}^3$ with $\phi(\boldsymbol{x}) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)^T$

Learning with kernels (II): Kernel functions

Characterization of Kernels

Definition: A symmetric function k is called **positive semi-definite** in $\mathcal{X}$ if:

for every $N \in \mathbb{N}$, and every choice $\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N \in \mathcal{X}$,

the matrix $\mathbf{K} = (k_{ij})$, where $k_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$ is **positive semi-definite**.

Theorem: k admits the existence of a map $\phi : \mathcal{X} \to \mathcal{H}$ s.t.

$\mathcal{H}$ is a Hilbert space and $k(\boldsymbol{u}, \boldsymbol{v}) = \langle \phi(\boldsymbol{u}), \phi(\boldsymbol{v}) \rangle_{\mathcal{H}}$

if and only if k is a positive semi-definite symmetric function in $\mathcal{X}$.

Learning with kernels (II): Kernel functions

On positive semi-definiteness

There are many equivalent characterizations of the psd (*positive semi-definite*) property for real symmetric matrices. Here are some:

1. $A_{d\times d}$ is psd if and only if all of its eigenvalues are non-negative.

2. $A_{d\times d}$ is psd if and only if the determinants of all of its leading principal minors are non-negative.

3. $A_{d\times d}$ is psd if and only if there is a psd matrix B such that $BB^T = A$ (this matrix B is unique and called the square root of A).

4. $A_{d\times d}$ is psd if and only if, $\forall \boldsymbol{c} \in \mathbb{R}^d,\ \boldsymbol{c}^T A \boldsymbol{c} \geq 0$.

Learning with kernels (II): Kernel functions

General linear kernel

If $A_{d\times d}$ is a psd matrix, then the function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ given by $k(\boldsymbol{u}, \boldsymbol{v}) = \boldsymbol{u}^T A \boldsymbol{v}$ is a kernel.

Proof. Since A is psd we can write it in the form $A = BB^T$. For every $N \in \mathbb{N}$, and every choice $\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N \in \mathbb{R}^d$, we form the matrix $K = (k_{ij})$, where $k_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \boldsymbol{x}_i^T A \boldsymbol{x}_j$. Then for every $\boldsymbol{c} \in \mathbb{R}^N$:

$$\sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j k_{ij} = \sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j \boldsymbol{x}_i^T A \boldsymbol{x}_j = \sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j (B^T \boldsymbol{x}_i)^T (B^T \boldsymbol{x}_j)$$

$$= \left\| \sum_{i=1}^{N} c_i (B^T \boldsymbol{x}_i) \right\|^2 \geq 0. \qquad \text{Note that } \phi(\boldsymbol{x}) = B^T \boldsymbol{x}$$

Learning with kernels (II): Kernel functions

Summary of kernel properties

If k, k' are kernels on $\mathbb{R}^d$, k'' is a kernel on $\mathbb{R}^N$, $a, b \geq 0$, and $\phi : \mathbb{R}^d \to \mathbb{R}^N$, then the following functions are kernels on $\mathbb{R}^d$:

1. $k(\boldsymbol{u}, \boldsymbol{v}) + k'(\boldsymbol{u}, \boldsymbol{v})$

2. $ak(\boldsymbol{u}, \boldsymbol{v}) + b$

3. $k(\boldsymbol{u}, \boldsymbol{v})k'(\boldsymbol{u}, \boldsymbol{v})$

4. $k''(\phi(\boldsymbol{u}), \phi(\boldsymbol{v}))$

Learning with kernels (II): Kernel functions

Normalization

If k is a kernel, then so is:

$$k_n(\boldsymbol{u}, \boldsymbol{v}) := \frac{k(\boldsymbol{u}, \boldsymbol{v})}{\sqrt{k(\boldsymbol{u}, \boldsymbol{u})}\sqrt{k(\boldsymbol{v}, \boldsymbol{v})}}$$

Moreover,

$$\begin{aligned} |k_n(\boldsymbol{u}, \boldsymbol{v})| &\leq 1 \\ k_n(\boldsymbol{u}, \boldsymbol{u}) &= 1 \end{aligned}$$

Learning with kernels (II): Kernel functions

Polynomial combinations

1. If k is a kernel and p is a polynomial of degree m with positive coefficients, then the function

$$k_p(\boldsymbol{u}, \boldsymbol{v}) = p(k(\boldsymbol{u}, \boldsymbol{v}))$$

   is also a kernel.

2. The special case where k is linear and $p(z) = (az + 1)^m$ leads to the so-called **polynomial kernel**

Learning with kernels (II): Kernel functions

Polynomial combinations

Consider the kernel family:

$$\Big\{k_i(\boldsymbol{u},\boldsymbol{v}) = \alpha_i\Big(\langle \boldsymbol{u},\boldsymbol{v}\rangle + a_i\Big)^{\beta_i} \;/\; \beta_i \in \mathbb{N}, \alpha_i > 0, a_i \geq 0\Big\}$$

For any $q > 0 \in \mathbb{N}$,

$$\sum_{i=0}^{q} k_i(\boldsymbol{u},\boldsymbol{v})$$

is a kernel.

Learning with kernels (II): Kernel functions

Polynomial combinations

Consider the particular case $a_i = 0, \beta_i = i$ and $\alpha_i = \frac{\alpha^i}{i!}$, for some real $\alpha > 0$, and take the limit $q \to \infty$.

The obtained series is convergent for all α and the resulting kernel is:

$$\sum_{i=0}^{\infty} \frac{\alpha^i}{i!}(\langle \boldsymbol{u}, \boldsymbol{v} \rangle)^i = e^{\alpha \langle \boldsymbol{u}, \boldsymbol{v} \rangle}$$

Assume that $u, v \in \mathbb{R}$; then $\exp(\alpha u v) = \langle \phi(u), \phi(v) \rangle$ with $\phi(z) = \left(\sqrt{\frac{\alpha^i}{i!}} z^i \right)_{i=0}^{\infty}$, and therefore we have designed a feature space of infinite dimension!

Learning with kernels (II): Kernel functions

Translation invariant and radial kernels

We say that a kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is:

Translation invariant if it has the form $k(\boldsymbol{u}, \boldsymbol{v}) = T(\boldsymbol{u} - \boldsymbol{v})$, where $T : \mathbb{R}^d \to \mathbb{R}$ is a differentiable function.

Radial if it has the form $k(\boldsymbol{u}, \boldsymbol{v}) = t(\|\boldsymbol{u} - \boldsymbol{v}\|)$, where $t : [0, \infty) \to [0, \infty)$ is a differentiable function.

Radial kernels fulfill $k(\boldsymbol{u}, \boldsymbol{u}) = t(0)$.

Learning with kernels (II): Kernel functions

The Gaussian kernel

Consider the function $t(z) = \exp(-\gamma z^2), \gamma > 0$. The resulting radial kernel is known as the **Gaussian RBF kernel**:

$$k(\boldsymbol{u}, \boldsymbol{v}) = \exp(-\gamma \|\boldsymbol{u} - \boldsymbol{v}\|^2)$$

Note that some people call it the RBF kernel *par excellence*!

You can also find it as:

$$k(\boldsymbol{u}, \boldsymbol{v}) = \exp\left(-\frac{\|\boldsymbol{u} - \boldsymbol{v}\|^2}{2\sigma^2}\right)$$

Learning with kernels (II): Kernel functions

Euclidean space $\mathbb{R}^d$, but not only

- Kernels on sets/bitstrings
- Graph kernels
- Generative kernels (on probability distributions)
- Convolution kernels (on combinatorial structures)
- Tree kernels
- String kernels (text)

... and many others (functional data, categorical data, ...)

Learning with kernels (II): Kernel functions

A kernel for set comparison

Given two sets A, B, consider

$$k(A, B) = \sum_{a \in A} \sum_{b \in B} k_{\text{base}}(a, b)$$

If k_{base} is the overlap kernel:

$$k(a, b) = \begin{cases} 1 & \text{if } a = b; \\ 0 & \text{otherwise.} \end{cases}$$

we get $k(A, B) = |A \cap B|$. Remarkably, $k(A, B) = \dfrac{|A \cap B|}{|A \cup B|}$ is also a kernel.

Learning with kernels (II): Kernel functions

Kernels for/from graphs (I)

- Consider a graph $G = (V, E)$, where the set of vertices (nodes) V are the data points and E is the set of edges. Call $N = |V|$, the number of nodes
- The idea is to compute a (base) matrix $B_{N \times N}$ whose entries are the weights of the edges and consider $B^2 = BB$ (B need not be symmetric)
- Typical use: **connectivity matrix** of G: the (i, j) element of B^2 is the number of paths of length exactly 2 between i and j

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Examples:

1. protein-protein interactions
2. people-to-people interactions

In 2, the (i, j) element of B^2 is the number of common friends between data points i and j (it can be thought of as a measure of their similarity)

Learning with kernels (II): Kernel functions

Kernels for/from graphs (II)

Notes:

1. The entries of B may be real-valued numbers (e.g., symmetric bounded similarities)

2. Higher powers of B measure higher-order similarities

3. Only the even powers are guaranteed to be PSD

Consider, for a given $\lambda \in (0, 1)$:

$$\sum_{k=0}^{\infty} \frac{1}{k!} \lambda^k B^k = \exp(\lambda B)$$

If B is symmetric, then $B = U \Lambda U^T$ is its spectral decomposition, so $B^2 = (U \Lambda U^T)(U \Lambda U^T) = U \Lambda^2 U^T$. In general, we have $B^k = U \Lambda^k U^T$ and therefore:

$$K = \exp(\lambda B) = U \exp(\lambda \Lambda) U^T$$

is an example of a **diffusion** kernel (the name comes from the *heat equation* in physics)

Learning with kernels (II): Kernel functions

Popular choices for the Kernel

Polynomial kernels (relation to GLDs)

$$k(\boldsymbol{u}, \boldsymbol{v}) = (\langle \boldsymbol{u}, \boldsymbol{v} \rangle + 1)^d, \ d \in \mathbb{N}$$

Gaussian RBF kernels (relation to RBFNNs)

$$k(\boldsymbol{u}, \boldsymbol{v}) = \exp\left(-\gamma \|\boldsymbol{u} - \boldsymbol{v}\|^2\right) \ \gamma > 0 \in \mathbb{R}$$

Laplacian RBF kernels (relation to ???)

$$k(\boldsymbol{u}, \boldsymbol{v}) = \exp\left(-\gamma \|\boldsymbol{u} - \boldsymbol{v}\|\right) \ \gamma > 0 \in \mathbb{R}$$

Sigmoidal kernels (relation to MLPs)

$$k(\boldsymbol{u}, \boldsymbol{v}) = g(\alpha \langle \boldsymbol{u}, \boldsymbol{v} \rangle + \beta)$$

with g a sigmoidal (e.g., logistic, tanh, ...) and particular choices for α, β.

Learning with kernels (II): Kernel functions

Afterthoughts

1. Importance of designing kernels that do not constitute explicit inner products between objects, and therefore fully exploit the kernel trick.

2. Possibility of learning the kernel function (or the kernel matrix) from the training data.

3. Need more research for handling special situations –like missing, imprecise or not-applicable (NA) values.

4. Theoretical analyses on the implications of the kernel choice for the success of kernel-based methods.