Kernel-Based Learning & Multivariate Modeling

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Syllabus

Sep 10 Introduction to kernel-based learning

Sep 17 The SVM for classification, regression & novelty detection (I)

Oct 01 The SVM for classification, regression & novelty detection (II)

Oct 08 Kernel design (I): theoretical issues

Oct 15 Kernel design (II): practical issues

Oct 22 Kernelizing ML & stats algorithms

Oct 29 Advanced topics

Kernel design (II): practical issues

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

- Kernels on real vectors (whole families)
- Kernels on binary vectors (bitstrings = sets)
- General structured kernels:
  - All-subsets kernel
  - Convolution kernels
- Kernels on discrete structures:
  - Tree kernels
  - Graph kernels
- Kernels on distributions (generative kernels):
  - P-kernels
  - Marginalized kernels
- String kernels (text)

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

Kernel design (II): practical issues

All-subsets kernel

Consider a feature space with one feature for every subset $A \subseteq \{1, \ldots, d\}$ of the input variables:

For $\boldsymbol{x} \in \mathbb{R}^d$, feature A is given by $\phi_A(\boldsymbol{x}) = \prod_{i \in A} x_i$ (note $\phi_\emptyset(\boldsymbol{x}) = 1$)

The kernel is defined by the mapping $\phi : \boldsymbol{x} \to (\phi_A(\boldsymbol{x}))_{A \subseteq \{1,\ldots,d\}}$

$$\begin{aligned} k(\boldsymbol{x}, \boldsymbol{x'}) = \left\langle \phi(\boldsymbol{x}), \phi(\boldsymbol{x'}) \right\rangle &= \sum_{A \subseteq \{1,\ldots,d\}} \phi_A(\boldsymbol{x}) \phi_A(\boldsymbol{x'}) \\ &= \sum_{A \subseteq \{1,\ldots,d\}} \prod_{i \in A} x_i x'_i = \prod_{i=1}^{d} (1 + x_i x'_i) \end{aligned}$$

The last step is obtained by expanding $(1 + x_1 x'_1)(1 + x_2 x'_2) \ldots (1 + x_d x'_d)$

Kernel design (II): practical issues

All-subsets kernel

We have the freedom to downplay some features (and thus emphasize others) by introducing weighting factors $w_i \geq 0$ for each feature i:

$$\phi_A(\boldsymbol{x}) = \prod_{i \in A} \sqrt{w_i} x_i$$

therefore

$$k_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{x'}) = \prod_{i=1}^{d} (1 + w_i x_i x'_i)$$

Kernel design (II): practical issues

Bitstring/Binary variables/Sets

Let $\boldsymbol{x}, \boldsymbol{x'} \in \{0, 1\}^d$, representing absence/presence of a binary trait:

1. The Simple Matching Coefficient (SMC) is the fraction of $1 - 1$ matches, and it is a kernel on $\{0, 1\}^d$.

   Proof. For every $n \in \mathbb{N}$, and every choice $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \{0, 1\}^d$, we form the matrix $K = (k_{ij})$, where $k_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{1}{d}\boldsymbol{x}_i^\top \boldsymbol{x}_j$.

2. The Jaccard Coefficient is the fraction of $1 - 1$ matches among the traits present in either data vector, and it is a kernel on $\{0, 1\}^d$.

Kernel design (II): practical issues

Bitstring/Binary variables/Sets

- Given two sets $A, B \subset U$, where U is finite, consider

$$k(A,B) = \frac{1}{|U|} \sum_{a \in A} \sum_{b \in B} k_{\text{base}}(a,b)$$

- If k_{base} is the overlap kernel $k(a,b) = \begin{cases} 1 & \text{if } a = b; \\ 0 & \text{otherwise.} \end{cases}$

  we get $k(A,B) = \dfrac{|A \cap B|}{|U|}$, the equivalent of the SMC.

- The equivalent of the Jaccard kernel would be $k(A,B) = \dfrac{|A \cap B|}{|A \cup B|}$.

Kernel design (II): practical issues

Generative kernels

Given a probability distribution on $\mathcal{X} \times \mathcal{Z}$, we can compare data points by assigning a high value if both have high conditional probability:

$$k(\boldsymbol{x}, \boldsymbol{x'}) = \sum_{z \in \mathcal{Z}} p(\boldsymbol{x}|z) p(\boldsymbol{x'}|z) P(z) \qquad \text{discrete case}$$

$$k(\boldsymbol{x}, \boldsymbol{x'}) = \int_{\mathcal{Z}} p(\boldsymbol{x}|z) p(\boldsymbol{x'}|z) p(z) \, dz \qquad \text{continuous case}$$

The feature maps are $(\phi(\boldsymbol{x}))_z = p(\boldsymbol{x}|z)\sqrt{p(z)}$

Idea: $p(\boldsymbol{x}, \boldsymbol{x'}, z) = p(\boldsymbol{x}, \boldsymbol{x'}|z) p(z) = p(\boldsymbol{x}|z) p(\boldsymbol{x'}|z) p(z)$

Kernel design (II): practical issues

Generative kernels

Given a probability distribution on $\mathcal{X} \times \mathcal{Z}$, and a kernel on $\mathcal{X} \times \mathcal{Z}$ pairs, we can define:

$$k(\boldsymbol{x}, \boldsymbol{x'}) = \sum_{z} \sum_{z'} k\Big((\boldsymbol{x}, z), (\boldsymbol{x'}, z')\Big) p(z|\boldsymbol{x}) p(z'|\boldsymbol{x'})$$

Typical applications of generative kernels are found in **graphical models**:

- $\mathcal{X}$ are the **observed** variables and $\mathcal{Z}$ are the **hidden** (latent) variables
- A kernel for the observed ones is obtained by taking the expectation w.r.t. the hidden ones (*marginalizing* them away)
- Examples: HMMs for sequences or stochastic context-free grammars for RNA sequences –see "Kernel methods in genomics and computational biology" by J.P. Vert

Kernel design (II): practical issues

The Spectrum (aka n-Gram) kernel

- Let Σ be a finite alphabet: an n-Gram is a block of n adjacent characters in Σ

  Define $k(\boldsymbol{x}, \boldsymbol{x}') := \sum_{s \in \Sigma^n} |s \in \boldsymbol{x}| \cdot |s \in \boldsymbol{x}'|$

  Example: Word `aababc` in alphabet $\Sigma = \{\mathtt{a}, \mathtt{b}, \mathtt{c}\}$, $n = 2$:

aa	ab	ac	ba	bb	bc	...
1	2	0	1	0	1	...

- While the feature space is large, the feature vectors are sparse; this kernel can be computed in $O(|\boldsymbol{x}| + |\boldsymbol{x}'|)$ time and memory (the actual number of distinct n-Grams in a text is very small)

Kernel design (II): practical issues

Kernels from graphs

- 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 $S_{N\times N}$ whose entries are the weights of the edges and consider $S^2 = SS$ (S need not be symmetric)

- Typical use: **connectivity matrix** of G: the (i, j) element of S^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 S^2 is the number of common friends between data points i and j (it can be thought of as a measure of their similarity)

Kernel design (II): practical issues

Kernels from graphs

Notes:

- The entries of S may be real-valued numbers (e.g., symmetric bounded similarities)
- Higher powers of S measure higher-order similarities
- Only the even powers are guaranteed to be PSD

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

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

1. If S is symmetric, then $S = U\Lambda U^T$ (spectral decomposition), so $S^2 = (U\Lambda U^T)(U\Lambda U^T) = U\Lambda^2 U^T$.

2. In general, we have $S^k = U\Lambda^k U^T$ and therefore:

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

   is an example of a **diffusion** kernel.

Kernel design (II): practical issues

A worked example

Suppose we have designed a “kernel” on **mistery** objects $\boldsymbol{x}, \boldsymbol{x'}$ in $\mathcal{X} = [-1, +1]^d$ from a set of D descriptors $f_i : \mathcal{X} \rightarrow \mathbb{R}$ as the function:

$$k(\boldsymbol{x}, \boldsymbol{x'}) = \frac{\left(\sum_{i=1}^{D} f_i(\boldsymbol{x}) f_i(\boldsymbol{x'}) + \theta \right)^3}{\sqrt{\theta - \exp(-||\boldsymbol{x} - \boldsymbol{x'}||^2)}}$$

where $\theta \in \mathbb{R}$ is a free parameter.

Under what conditions does this expression define a kernel?

Kernel design (II): practical issues

A worked example

1. The numerator is simply the polynomial kernel of degree 3 applied to the descriptors and hence a kernel in itself for all $\theta \geq 0$

2. Since the denominator must be well-defined, we conclude that $\theta > 1$

3. Now define $f(z) = \dfrac{1}{\sqrt{\theta - z}}$, for $\theta > 1$

4. We find its Taylor series expansion as $f(z) = \sum_{n=0}^{\infty} a_n z^n$, with $a_n = \left(2^n \theta^{(2n+1)/2}\right)^{-1} \prod_{i=1}^{n} (2i-1)$, which is positive for all $\theta > 0$

5. Therefore both the denominator and numerator are kernels and so is their product, for $\theta > 1$ (note the kernel is *not* normalized)

Example in a real application domain

Handling missing values in microbiology

- Modern modelling problems are difficult for a number of reasons, including the challenge of dealing with a significant amount of missing information

- **Missing values** almost always represent a serious problem because they force to preprocess the dataset and a good deal of effort is normally put in this part of the modelling

- In order to process such datasets with kernel methods, an imputation procedure is then deemed a necessary but demanding step

Example in a real application domain

Handling missing values in microbiology

- The study of fecal source pollution in waterbodies is a major problem in ensuring the welfare of human populations

- **Microbial source tracking** (MST) methods attempt to identify the source of contamination, allowing for improved risk analysis and better water management

- The available dataset includes 148 observations about 10 chemical, microbial, and eukaryotic markers of fecal pollution in water

- All variables (except the class variable) are binary, i.e., they signal the presence or absence of a particular marker

Example in a real application domain

Handling missing values in microbiology

Origin	HF183	HF134	CF128	Humito	Pomito	Bomito	ADO	DEN
Human :50	0 :68	0 :81	0 :104	0 :35	0 :83	0 :78	0 :56	0 :80
Cow :26	1 :40	1 :26	1 : 5	1 :79	1 :32	1 :32	1 :59	1 :34
Poultry:31	**?**:31	**?**:32	**?**:30	**?**:25	**?**:24	**?**:29	**?**:24	**?**:25
Pig :32								

Summary (counts) table for the full dataset. The first column is the target class. The symbol **?** denotes a missing value.

The percentage of missing values is around 19.8 %, and all the predictive variables have percentages between 17 % and 23 %

Example in a real application domain

Handling missing values in microbiology

Let the symbol **?** denote a missing element, for which only equality is defined. Let $k : X \times X \to \mathbb{R}$ be a symmetric kernel in X and P a probability mass function (PMF) in X. Then the function $k^{\textbf{?}}(x, y)$ given by

$$k^{\textbf{?}}(x,y) = \begin{cases} k(x,y), & \text{if } x, y \neq \textbf{?} \text{ ;} \\ g(x) = \sum\limits_{y' \in X} P(y')k(x,y'), & \text{if } x \neq \textbf{?} \text{ and } y = \textbf{?}\text{;} \\ g(y) = \sum\limits_{x' \in X} P(x')k(x',y), & \text{if } x = \textbf{?} \text{ and } y \neq \textbf{?}\text{;} \\ G = \sum\limits_{x' \in X} P(x') \sum\limits_{y' \in X} P(y')k(x',y'), & \text{if } x = y = \textbf{?} \end{cases}$$

is a kernel in $X \cup \{\textbf{?}\}$.

Example in a real application domain

Handling missing values in microbiology

For the particular case of binary variables $x, y \in \{v_1, v_2\}$, a convenient approach is to define the kernel:

$$k_{0/1}(x, y) = \mathbb{I}_{\{x=y\}}$$

where

$$\mathbb{I}_{\{z\}} = \begin{cases} 1 & \text{if } z \text{ is true} \\ 0 & \text{if } z \text{ is false} \end{cases}$$

Example in a real application domain

Handling missing values in microbiology

Consider now $\boldsymbol{x}, \boldsymbol{y} \in \{0, 1\}^d$. When we apply the Theorem to this kernel, we obtain an extended multivariate kernel:

$$\mathcal{K}_1(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{d} \sum_{i=1}^{d} \begin{cases} 1 & \text{if } x_i = y_i = 1 \ ; \\ P_i(x_i), & \text{if } x_i \neq \textbf{?} \text{ and } y_i = \textbf{?}; \\ P_i(y_i), & \text{if } x_i = \textbf{?} \text{ and } y_i \neq \textbf{?}; \\ (P_i(0))^2 + (P_i(1))^2, & \text{if } x_i = y_i = \textbf{?}; \\ 0, & \text{otherwise} \end{cases}$$

This kernel is a generalization of the classical *Simple Matching Coefficient*, proposed by Sokal and Michener for numerical taxonomy

Example in a real application domain

Handling missing values in microbiology

Let the symbol **?** denote a missing element, for which only equality is defined. Let $k : X \times X \to \mathbb{R}$ be a symmetric kernel in $X = \{0, 1\}^d$. Let $c(\boldsymbol{x})$ be the set of completions of $\boldsymbol{x}$. Given two vectors $\boldsymbol{x}, \boldsymbol{y} \in X$, the function

$$\mathcal{K}_2(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{|c(\boldsymbol{x})||c(\boldsymbol{y})|} \sum_{\boldsymbol{x}' \in c(\boldsymbol{x})} \sum_{\boldsymbol{y}' \in c(\boldsymbol{y})} k(\boldsymbol{x}', \boldsymbol{y}') \tag{1}$$

is a kernel in $X \cup \{\textbf{?}\}$.

Example in a real application domain

Handling missing values in microbiology

			10x10cv for each class			
Approach	C	10x10cv	Human	Cow	Poultry	Swine
$\mathcal{K}_1$	2.0	79.3	95.4	64.5	75.2	69.4
$\mathcal{K}_2$	1.6	78.2	92.6	62.8	71.8	74.2
MI-1	1.0	79.9	92.7	66.4	69.4	80.2
MI-2	1.0	79.0	94.5	57.5	70.8	78.8

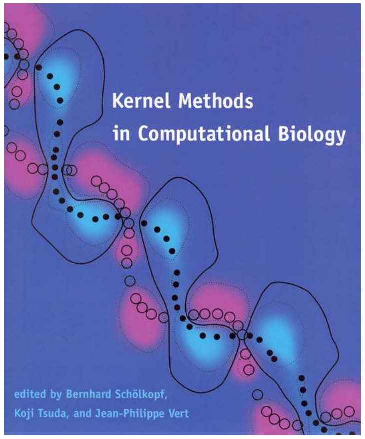
Mean 10x10cv accuracies for the four approaches to handle missing values. Also shown are best cost parameter C and detailed class performance.

(*joint work with G. Nebot, T. Aluja and V. Kobayashi*)

Kernel design (II): practical issues

More Kernels!

Kernels abound in computational biology and computational chemistry (e.g., phylogenetic profiles, protein 3D structures)


Kernel Methods
in Computational Biology
edited by Bernhard Schölkopf,
Koji Tsuda, and Jean-Philippe Vert

Example: the prediction of **interacting proteins** to reconstruct an interaction network can be posed as a binary classification problem: given a pair of proteins, do they interact or not?

⟶ we need kernel between *pairs* of proteins!

Kernel design (II): practical issues

More Kernels!

The available data is about each single protein; it is then natural to derive kernels for **pairs** of proteins k_{pair} from any kernel k for **single** proteins:

$$k_{\text{pair}}\Big((A,B),(C,D)\Big) := k(A,C)k(B,D) + k(A,D)k(B,C)$$

(there is usually no order in a protein pair, so we try both matches)

· Using Product Kernels to Predict Protein Interactions. *Advances in Biochemical Engineering/Biotechnology* (110), pp 215-245 (2007)

· Kernel methods for predicting protein-protein interactions. *Bioinformatics*. 2005

Kernel design (II): practical issues

Conclusions

- The power of kernel methods partly relies in the ability to process virtually any sort of data as soon as a valid kernel is defined

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

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

- Theoretical analyses are needed on the implications of the kernel choice for the success of specific kernel-based methods