


Kernels II

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Beginner's Workshop Machine Learning 2018

Agenda

Methods

- Kernel Ridge Regression
- Kernel PCA
- One-class SVM and SVDD

Kernels for specific Tasks

- Basic Kernels re-visited
- Kernels for Sequences
- Kernels for Graphs and Trees
- Kernels for Probabilistic Models

Learning Kernels

- Multiple Kernel Learning

Kernel Approximations

- Random Fourier Features

Why use kernels?

1. Efficient computation in high-dimensional feature spaces
2. Non-linear feature maps for complex decision surfaces
3. Abstraction from data representation and learning methods

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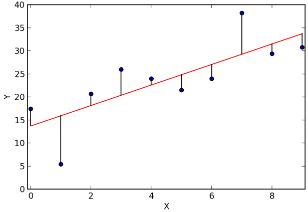
From OLS to Ridge Regression

The aim is to find a parameter vector $w_1 \in \mathbb{R}^d$ of a linear model $f_1(x) = b = \langle w_1, x \rangle$ that fits a given sample set $(x_i, b_i) \in \mathbb{R}^d \times \mathbb{R} \quad \forall i$ best. Hence, we are interested in solving the following least squares problem:

$$\min_{w \in \mathbb{R}^d} \sum_i (b_i - \langle w, x_i \rangle)^2$$

We introduce a regularization term $||w||^2$ into the optimization problem and a corresponding hyper-parameter $\lambda \geq 0$:

$$\min_{w \in \mathbb{R}^d} \mathcal{L}(w) = \min_{w \in \mathbb{R}^d} \lambda ||w||_2^2 + \sum_i (b_i - \langle w, x_i \rangle)^2$$



Solving the Ridge Regression Problem

For convenience we rephrase the latter into matrix notation.

$$\begin{aligned}\mathcal{L}(w) =& \lambda \|w\|^2 + \sum_i (b_i - \langle w, x_i \rangle)^2 \\ =& \lambda w^\mathsf{T} w + b^\mathsf{T} b - 2w^\mathsf{T} X b + w^\mathsf{T} X X^\mathsf{T} w\end{aligned}$$

$$\begin{aligned}\frac{\partial \mathcal{L}(w)}{\partial w} ! = 0 \Rightarrow 0 = 2\lambda w - 2Xb + 2XX^\mathsf{T} w \\ Xb = \lambda w + XX^\mathsf{T} w = (\lambda I + XX^\mathsf{T}) w \\ w = (\lambda I + XX^\mathsf{T})^{-1} Xb\end{aligned}$$

Kernel Ridge Regression Problem

We transform the data points into a (possibly very high dimensional) feature space using the feature mapping function $\phi : \mathbb{R}^d \to \mathcal{F}$. The resulting model, $f_2(x) = y = \langle w_2, \phi(x) \rangle$ with $w_2 \in \mathcal{F}$, retains the desired simplicity of linear functions while at the same time becoming much more expressive. The corresponding optimization problem arrives at:

$$\min_{w \in \mathcal{F}} \mathcal{L}(w) = \min_{w \in \mathcal{F}} \lambda \|w\|_2^2 + \sum_i \left(b_i - \langle w, \phi(x_i) \rangle\right)^2$$

which reads in matrix notation $\mathcal{L}(w) = \lambda w^\mathsf{T} w + b^\mathsf{T} b - 2 w^\mathsf{T} \Phi b + w^\mathsf{T} \Phi \Phi^\mathsf{T} w$. We can attempt to solve it the same way as ridge regression:

$$\frac{\partial \mathcal{L}(w)}{\partial w} ! = 0 \;\Rightarrow\; w = \left(\lambda I + \Phi \Phi^\mathsf{T}\right)^{-1} \Phi b \,,$$

which, unfortunately, does not help (i.e. $\Phi \Phi^\mathsf{T}$ is a covariance matrix in the possibly very high dimensional feature space!).

Kernel Ridge Regression

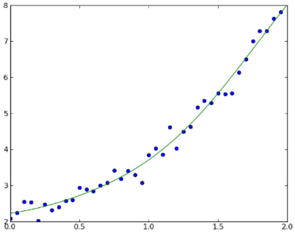
Now, we make use of a special case of the **Woodbury identity** for positive definite matrices P and R:

$$(P^{-1} + B^{\mathsf{T}} R^{-1} B)^{-1} B^{\mathsf{T}} R^{-1} = PB^{\mathsf{T}} (BPB^{\mathsf{T}} + R)^{-1}$$

In our problem, $R^{-1} = R = I$, $B^{\mathsf{T}} = \Phi$ and $P^{-1} = \lambda I$:

$$w = (\lambda I + \Phi\Phi^{\mathsf{T}})^{-1} \Phi b = \frac{1}{\lambda}\Phi(\frac{1}{\lambda}\Phi^{\mathsf{T}}\Phi + I)^{-1} b$$

$$w = \Phi(\Phi^{\mathsf{T}}\Phi + \lambda I)^{-1} b$$



which can be rephrased as $w = \sum_i \alpha_i \phi(x_i)$
with $\alpha = (\Phi^{\mathsf{T}}\Phi + \lambda I)^{-1} b = (K + \lambda I)^{-1} b$.

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Principle Components Analysis

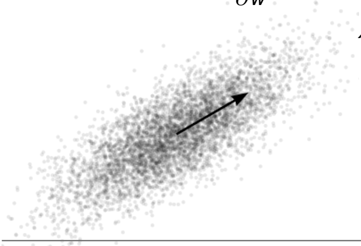
Find the direction of maximum variance w given (centered!) datapoints $x_1, \ldots, x_n \in \mathbb{R}^d$:

$$\max_w \quad \sum_i (w^\intercal x_i)^2 = w^\intercal X X^\intercal w \quad \text{subject to} \quad \|w\|^2 \leq 1\,.$$

Solve the corresponding Lagrangian $\mathcal{L}(w, \lambda) = w^\intercal X X^\intercal w - \lambda(w^\intercal w - 1)$ for w:

$$\frac{\partial \mathcal{L}(w, \lambda)}{\partial w} ! = 0 \;\Rightarrow\; 0 = 2XX^\intercal w - 2\lambda w$$

$$XX^\intercal w = \lambda w \quad \text{(=Eigenwert problem)}$$



Kernel Principle Components Analysis

From the unconstrained optimization problem (literally that's how we designed the OP), we know that the optimal solution of w will lie in the span of the data $w = \sum_i \alpha_i x_i = X\alpha$. Now lets do the feature map trick again:

$$\max_w \quad \sum_i (w^\mathsf{T}\phi(x_i))^2 = w^\mathsf{T}\Phi\Phi^\mathsf{T} w \quad \text{subject to} \quad \|w\|^2 \leq 1\,.$$

Solving is similar to standard PCA, i.e. the solution remains $\Phi\Phi^\mathsf{T} w = \lambda w$. Now, let's extend the solution:

$$\begin{aligned}
\Phi\Phi^\mathsf{T} w &= \lambda w \quad &&|\text{substitute } w = \Phi\alpha \\
\Phi\Phi^\mathsf{T}\Phi\alpha &= \lambda\Phi\alpha \quad &&|\cdot \Phi^\mathsf{T} \\
\Phi^\mathsf{T}\Phi\Phi^\mathsf{T}\Phi\alpha &= \lambda\Phi^\mathsf{T}\Phi\alpha \quad &&|\text{substitute } K = \Phi^\mathsf{T}\Phi \\
K^2\alpha &= \lambda K\alpha \quad &&\Rightarrow K\alpha = \lambda\alpha
\end{aligned}$$

Centering in feature space is important!

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What is One-class Classification?

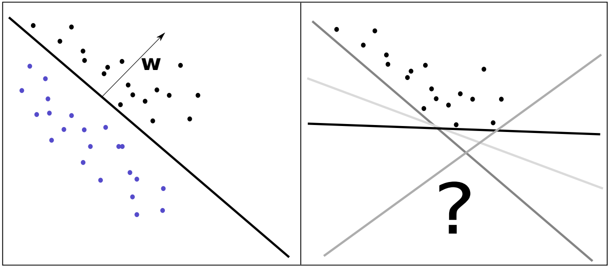
Learn common properties of given examples and be able to tell if a test point has the same properties or not:

- Assuming we know the data distribution $p(x)$ of our data. The task is, to reject all data points with $p(x) < \nu$ given a pre-defined threshold ν.
- Unfortunately, we usually don't know $p(\cdot)$ and estimation is really hard ...
- Therefore, we estimate a function $f(x) \in \{+1, -1\}$ that tells us whether $p(x) < \nu$ or not

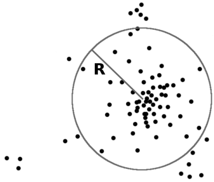
A Machine Learning Approach...

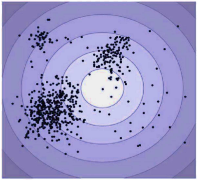
– Convert measurements to vector space and use famous SVM. Easy! Isn't it?

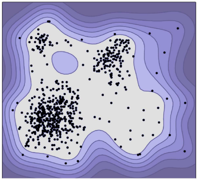
– No! (a) We have no ground truth, (b) most data points exhibit normal behavior, (c) new classes of object might occur during application



Support Vector Data Description (SVDD)





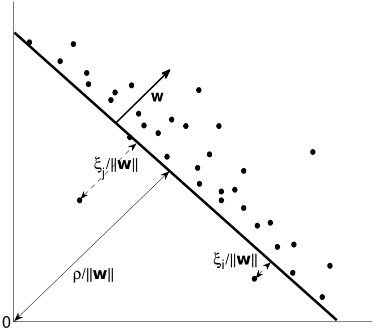


Support Vector Data Description (SVDD)

- Compute minimal enclosing sphere with center c and radius R
- Anomaly score as the distance to center c, that is $f(x) = \|\phi(x) - c\|$
- Accept data point x if $f(x) \leq R$ and ...

  ...reject x if $f(x) > R$

One-class Support Vector Machines (OC-SVM)



One-class SVM

- Separate data from origin with hyperplane with maximum distance to origin
- Model function: $f(x) = \langle w, \phi(x) \rangle - \rho$

OC-SVM: Optimization Problem

Primal optimization problem $0 < \nu \leq 1$

$$\min_{w,\rho,\xi} \quad \frac{1}{2}\|w\|^2 - \rho + \frac{1}{n\nu}\sum_{i=1}^{n}\xi_i$$

$$\text{s.t.} \quad \forall_{i=1}^{n} : \langle w, \phi(x_i)\rangle \geq \rho - \xi_i \quad \text{and} \quad \xi_i \geq 0$$

Lagrange: $\mathcal{L} = \frac{1}{2}\|w\|^2 - \rho + \frac{1}{n\nu}\sum_{i=1}^{n}\xi_i + \sum_i \alpha_i\left(\rho - \xi_i - \langle w, \phi(x_i)\rangle\right) - \sum_i \beta_i\xi_i$ with $\alpha_i, \beta_i \geq 0$.

$$\frac{\partial\mathcal{L}}{\partial w} = 0 \Rightarrow w = \sum_{i}^{n}\alpha_i\phi(x_i)$$

$$\frac{\partial\mathcal{L}}{\partial \xi_i} = 0 \Rightarrow \frac{1}{n\nu} - \alpha_i - \beta_i = 0 \Rightarrow 0 \leq \alpha_i \leq \frac{1}{n\nu}$$

$$\frac{\partial\mathcal{L}}{\partial \rho} = 0 \Rightarrow 1 = \sum_{i}^{n}\alpha_i$$

OC-SVM: Optimization Problem

Primal optimization problem $0 < \nu \leq 1$

$$\min_{w,\rho,\xi} \quad \frac{1}{2}\|w\|^2 - \rho + \frac{1}{n\nu}\sum_{i=1}^{n}\xi_i$$

$$\text{s.t.} \quad \forall_{i=1}^{n} : \langle w, \phi(x_i)\rangle \geq \rho - \xi_i \quad \text{and} \quad \xi_i \geq 0$$

Dual optimization problem

$$\max_{\alpha} \quad -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j K(x_i, x_j)$$

$$\text{s.t.} \quad \sum_{i=1}^{n}\alpha_i = 1 \quad \text{and} \quad 0 \leq \alpha_i \leq \frac{1}{n\nu} \quad \forall i$$

And expansion $w = \sum_i^n \alpha_i \phi(x_i)$

Question: What happens for $\nu = 1$?

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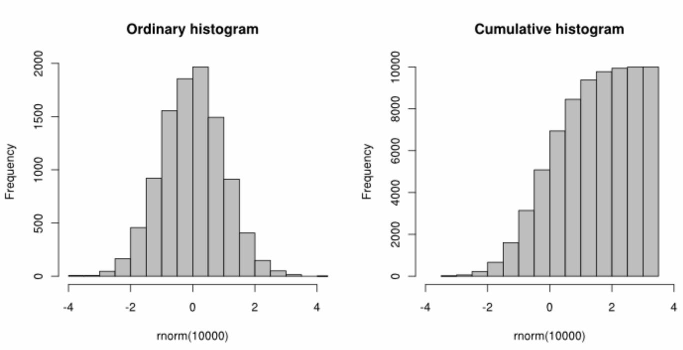
Examples

- Exponential and Laplacian Kernel
- Hyperbolic Tangent (Sigmoid) Kernel
- (Inverse) Multiquadric Kernel
- Circular and Spherical Kernel
- Power Kernel (Sahbi and Fleuret, 2004)
- Log Kernel
- Spline Kernel (Gunn, 1998)
- Bessel Kernel
- Cauchy Kernel (Basag, 2008)
- Chi-Square Kernel (Vedaldi and Zisserman, 2011)
- Wavelet kernel (Zhang et al, 2004)
- **Histogram Intersection Kernels** (Barla et al., ICIP 2003)

Histogram Intersection Kernel (Barla et al., ICIP 2003)

Definition (Histogram)

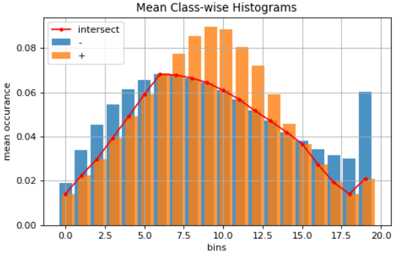
A histogram is an accurate representation of the distribution of numerical data. It is an estimate of the probability distribution of a continuous variable.

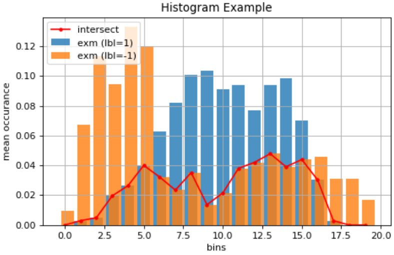


Histogram Intersection Kernel (Barla et al., ICIP 2003)

Assume data points are histograms consisting of B bins each. Then the histogram intersection kernel K is defined as:

$$K(x, y) = \sum_{b=1}^{B} \min(x_b, y_b) = \frac{1}{2} \sum_{b=1}^{B} (x_b + y_b - |x_b - y_b|)$$





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Examples

- Weighted Degree Kernel (Rätsch et al., Bioinformatics, 2005)
- Spectrum Kernel (Leslie et al., Pac. Symp. Biocomputing 2002)
- **Bag-of-words Kernel**

What are sequences?

Alphabet

An alphabet $\mathcal{A}$ is a finite set of discrete symbols.

- DNA, $\mathcal{A} = \{A, C, G, T\}$
- Natural language text, $\mathcal{A} = \{a, b, c, \ldots, A, B, C, \ldots\}$

Sequence

A sequence x is concatenation of symbols from $\mathcal{A}$, i.e. $x \in \mathcal{A}^*$.

- $\mathcal{A}^n$ is the set of all sequences of length n
- $\mathcal{A}^*$ is the set of all sequences of arbitrary length
- $|x|$ is the length of sequence x

Embedding Sequences

Characterize sequences using a language $L \subset \mathcal{A}^*$

Feature space spanned by frequencies of words $w \in L$

Feature Map

A function $\phi : \mathcal{A}^* \to \mathbb{R}^{|L|}$ mapping sequences to $\mathbb{R}^{|L|}$ given by

$$x \mapsto \left(\#_w(x)\sqrt{N_w}\right)_{w \in L}$$

where $\#_w(x)$ returns the frequency of w in sequence x.

Refinement of embedding using weighting constants N_w

Normalization, often $\|\phi(x)\|_1 = 1$ or $\|\phi(x)\|_2 = 1$

Generic Sequence Kernel

Generic Sequence Kernel

A sequence kernel $K : \mathcal{A}^* \times \mathcal{A}^* \to \mathbb{R}$ over ϕ is defined by

$$K(x, y) = \langle \phi(x), \phi(y) \rangle = \sum_{w \in L} \#_w(x) \#_w(y) N_w \ .$$

By definition K is an inner product in $\mathbb{R}^{|L|}$ and thus symmetric and positive semi-definite.

Feature space induced by ϕ explicit but sparse.

Bag-of-Words Kernel

Characterization of sequences by non-overlapping words.

$$x = \text{"Hasta la vista, baby."} \longrightarrow \{\text{"Hasta", "la", "vista", "baby"}\}$$

Bag-of-Words Kernel

Sequence kernel using embedding language containing words

$$L = \text{Dictionary (explicit) or } L = (A \setminus D)^* \text{ (implicit)}$$

with $D \subset A$ delimiter symbols, e.g. punctation and space.

Extension using stemming techniques, "helping" $\Rightarrow$ "help"

Weighting to control contribution of words

Bag-of-Words: Example

Bag of Words Example

Document 1

The quick brown fox jumped over the lazy dog's back.

Document 2

Now is the time for all good men to come to the aid of their party.

Term	Document 1	Document 2
aid	0	1
all	0	1
back	1	0
brown	1	0
come	0	1
dog	1	0
fox	1	0
good	0	1
jump	1	0
lazy	1	0
men	0	1
now	0	1
over	1	0
party	0	1
quick	1	0
their	0	1
time	0	1

Stopword List

for
is
of
the
to

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Examples

- Diffusion Kernel (Kondor and Lafferty, 2002)
- Approximate tree kernels (Rieck et al., JMLR 2010)
- Graphlet Kernel (Borgwardt, Petri, et al., MLG 2007)
- Cyclic Pattern Kernel (Horvath et al., KDD 2004)
- Subtree Kernel (Ramon and Gaertner, 2004)
- Edit-Distance Kernel (Neuhaus and Bunke, 2006)
- Weighted Decomposition Kernel (Menchetti et al., ICML 2005)
- Optimal Assignment Kernel (Froehlich et al., ICML 2005)
- Shortest-Path Kernel (Borgwardt and Kriegel, ICDM 2005)
- **Random Walks Kernel** (Kashima et al., ICML 2003, Gaertner et al., COLT 2003)

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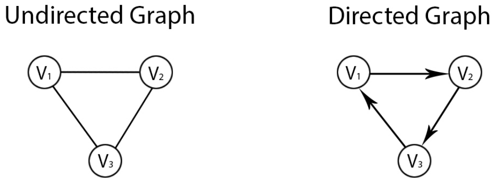
What is a graph?

Definition (Graph)

A graph G is an ordered pair $G = (V, E)$ comprising a set $V = (v_i)_{i=1,\dots,n}$ of n vertices together with a set $E \subset V \times V$ of edges (which are 2-element subsets of V.



e.g. $G_{undirected} = (V, E)$ with $E = \{(v_1, v_2), (v_1, v_3), (v_2, v_3)\}$ and $V = \{v_1, v_2, v_3\}$. Such graphs can be represented by their respective adjacency matrix $A \in \{0, 1\}^{|V| \times |V|}$ with $a_i j = 1$ if $(v_i, v_j) \in E$.

Graph Comparison Problem

Definition (Graph Comparison Problem)

Given two graphs G and G' from the space of graphs $\mathcal{G}$. The problem of graph comparison is to find a mapping

$$s : \mathcal{G} \times \mathcal{G} \rightarrow \mathbb{R}$$

such that $s(G, G')$ quantifies the (dis)similiarity between G and G'.

Important for, e.g.

- Function prediction of chemical compounds
- Structural comparison and function prediction of protein structures
- Comparison of social networks
- Analysis of semantic structures in Natural Language Processing
- Comparison of UML diagrams

Solutions I: Subgraph Isomorphism

Principle

Graph Isomorphism

Find a mapping f of the vertices of G_1 to the vertices of G_2 such that G_1 and G_2 are identical; i.e. (x, y) is an edge of G_1 iff $(f(x), f(y))$ is an edge of G_2. Then f is an isomorphism, and G_1 and G_2 are called isomorphic.

Subgraph Isomorphism

Subgraph isomorphism asks if there is a subset of edges and vertices of G_1 that is isomorphic to a smaller graph G_2.

Advantages

– Captures topological similarities between graphs accurately

Disadvantages

– Runtime may grow exponentially with the number of nodes

Solutions II: Graph Edit Distances

Principle

- Count operations that are necessary to transform G_1 into G_2
- Assign costs to different types of operations (edge/node insertion/deletion, modification of labels)

Advantages

- Captures partial similarities between graphs
- Allows for noise in the nodes, edges and their labels
- Flexible way of assigning costs to different operations

Disadvantages

- Contains subgraph isomorphism check as one intermediate step
- Choosing cost function for different operations is difficult

Solutions III: Topological Descriptors

Principle

- Map each graph to a feature vector
- Use distances and metrics on vectors for learning on graphs

Advantages

- Reuses known and efficient tools for feature vectors

Disadvantages

- Efficiency comes at a price: feature vector transformation leads to loss of topological information

Example: Random Walks Kernel

Principle

- Count common walks in two input graphs G and G'
- Walks are sequences of nodes that allow repetitions of nodes

Elegant computation

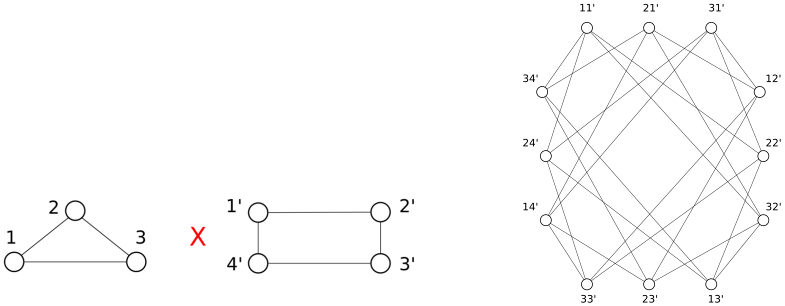
- Walks of length k can be computed using the k-th power of the adjacency matrix $A \in \mathbb{R}^{n \times n}$
- Construct direct product graph of G and G'
- Count walks in this product graph $G_x = (V_x, E_x)$
- Each walk in the product graph corresponds to one walk in G and G'

$$K(G, G') = \sum_{i,j=1}^{|V_x|} [\sum_k \lambda^k A_x^k]_{ij}$$

Example: Direct product of two graphs

Definition (Direct Product Graph)

Given two graphs $G = (V, E)$ and $G' = (V', E')$, their direct product G_x is a new graph with $V_x = \{(v_i, v_r') : v_i \in V, v_r' \in V'\}$ and $E_x = \{((v_i, v_r'), (v_j, v_s')) : (v_i, v_j) \in E \wedge (v_r', v_s') \in E'\}$.



[Vishwanathan et al., JMLR, 2010]

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Examples

- Probability Product Kernels (Jebara et al., JMLR, 2004)
- Bhattacharyya kernel (Jebara et al., JMLR, 2004)
- Expected likelihood kernel (Jebara et al., JMLR, 2004)
- Bayesian Kernel (Alashwal et al., WOSET, 2009)
- TOP kernel (Tsuda et al., NIPS, 2002)
- **Fisher Kernel** (Jaakkola and Haussler, 1999)

The Fisher Kernel (Jaakkola and Haussler, 1999)

Suppose that we are given a probabilistic model of our data $p(x, \theta)$ which is parameterized by θ. Then the Fisher kernel for two datapoints x and x' is defined as the inner product (with special normalization) of the derivatives (with respect to the parameters θ) of the log-likelihoods $p(x|\theta)$ and $p(x'|\theta)$:

$$K(x, x') = s(x, \theta)^\intercal Z_\theta^{-1} s(x', \theta)$$

$$s(x, \theta) = \frac{\partial}{\partial \theta} \log p(x|\theta)$$

Z denotes the Fisher information matrix: $Z_\theta = \mathbb{E}_x[s(x, \theta)s(x, \theta)^\intercal |\theta]$

Practically, the Z_θ is replace by the identity matrix.

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Recap: Support Vector Machine

Primal SVM:

$$\min_{\tilde{w},b,\xi} \quad \frac{1}{2}\|\tilde{w}\|^2 + C\sum_i \xi_i$$

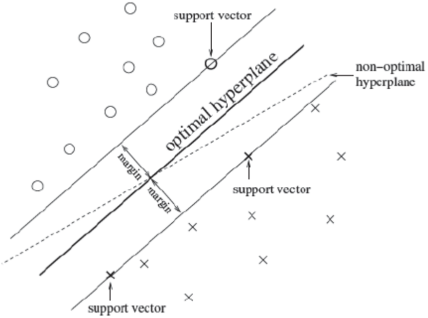
subject to $\quad y_i(\langle \tilde{w}, \phi(x_i)\rangle + b) \geq 1 - \xi_i$

$$\xi_i \geq 0, \quad i = 1, \ldots, n$$

Dual SVM:

$$\max_{\alpha} \quad \sum_i \alpha_i - \frac{1}{2}\sum_{ij} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$

subject to $\quad \sum_i \alpha_i y_i = 0, \quad 0 \leq \alpha_i \leq C, \quad i = 1$



Agenda

Methods

- Kernel Ridge Regression
- Kernel PCA
- One-class SVM and SVDD

Kernels for specific Tasks

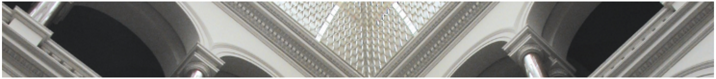
- Basic Kernels re-visited
- Kernels for Sequences
- Kernels for Graphs and Trees
- Kernels for Probabilistic Models

Learning Kernels

- Multiple Kernel Learning

Kernel Approximations

- Random Fourier Features



Technische Universität Berlin

Idea of MKL

Instead of selecting a single, best kernel, why not learn combinations of all suitable kernels?
Hence, in multiple kernel learning, we want to find a weighted combination of kernels $K = \sum_t d_t K_t$ (for $d_t \geq 0$ and $\|d\|_p^2 = 1$) that solves the problem best.

Problem: How to adjust weighting parameters d_t?

Solution:

1. A weighted kernel can be expressed as inner product of weighted feature maps:

$$K(x, y) = \sum_t d_t K_t(x, y) = \sum_t d_t \langle \phi_t(x), \phi_t(y) \rangle = \sum_t \langle \sqrt{d_t}\phi_t(x), \sqrt{d_t}\phi_t(y) \rangle$$

2. Weighting the parameters instead of the features:

$$\langle \tilde{w}_t, \sqrt{d_t}\phi_t(x) \rangle = \langle \sqrt{d_t}\tilde{w}_t, \phi_t(x) \rangle = \langle \sqrt{d_t}\tilde{w}_t, \phi_t(x) \rangle$$

3. Substituting $\sqrt{d_t}\tilde{w}_t = w_t$ and hence, $\tilde{w} = \frac{1}{\sqrt{d_t}} w_t$

Multiple Kernel Learning (SVM)

Primal MKL-SVM:

$$\min_{w,b,d,\xi} \quad \frac{1}{2}\sum_t d_t^{-1}\|w_t\|^2 + C\sum_i \xi_i$$

$$\text{subject to} \quad y_i\big(\sum_t \langle w_t, \phi_t(x_i)\rangle + b\big) \geq 1 - \xi_i$$

$$\xi_i \geq 0, \quad d_t \geq 0, \quad \|d\|_p^2 \leq 1, \quad i = 1, \ldots, n, \; t = 1, \ldots, T$$

Dual MKL-SVM:

$$\max_{\alpha} \quad \min_{d_t \geq 0, \|d\|_p^2 \leq 1} \quad \overbrace{\sum_i \alpha_i - \frac{1}{2}\sum_{ij}\alpha_i\alpha_j y_i y_j \sum_t d_t K_t(x_i, x_j)}^{J(\alpha,d)}$$

$$\text{subject to} \quad \sum_i \alpha_i y_i = 0 \quad 0 \leq \alpha_i \leq C \; i = 1, \ldots, n$$

Multiple Kernel Learning (SVM)

Algorithm 1 Algorithm (Multiple Kernel Learning for SVM)

Require: x, y, C, p-norm and a list of kernels K_t

Initialize kernel mixture coefficients such that $\|d^{z=0}\|_p = 1$

while Until Convergence **do**

(Step 1) solve standard SVM problem: $\alpha^{z+1} = \arg\max_{\alpha:0\leq\alpha_i\leq C} J(\alpha, d^z)$ s.t. $\sum_{i=1}^n \alpha_i y_i = 0$

(Step 2) optimize the kernel weights: $d^{z+1} = \arg\min_{d_t\geq 0} J(\alpha^{z+1}, d)$ s.t. $\|d\|_p^2 \leq 1$

z=z+1

end while

return Trained parameter vector $\alpha^\star$, weights d^*

Step 2 can be solved analytically: $d_t = \frac{\|w_t\|_2^{\frac{2}{p+1}}}{\left(\sum_{t'} \|w_{t'}\|_2^{\frac{2p}{p+1}}\right)^{\frac{1}{p}}}$ with expansions $w_t = d_t \sum_i \alpha_i y_i \phi(x_i)$.

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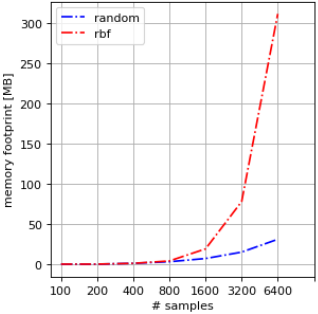
Why Approximations?

Although kernels are very versatile and often easier to construct than explicit feature maps, they quickly show their limits in large-scale and big data setting due to their quadratic scaling:



We would like to build a feature function given a specific choice of kernel such that $K(x, y) \approx \langle \phi(x), \phi(y) \rangle$.

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Approximating Kernels: Theory

Theorem (Bochner)

Assume that K is a normalized, positive definite, translation-invariant (real) kernel (i.e. $K(x, y) = K(x - y)$ and $K(0) = 1$) then it can be represented as the Fourier transform of a probability distribution:

$$
\begin{aligned}
K(\Delta) &= \int \exp(iw^T\Delta)p(w)dw \\
&= \mathbb{E}_{w\sim p}[\exp(iw^T\Delta)] = \mathbb{E}_{w\sim p}[\cos(w^T\Delta)] = \mathbb{E}_{w\sim p}[\cos(w^T(x-y))] \\
&= \mathbb{E}_{w\sim p}[\cos(w^Tx)\cos(w^Ty) + \sin(w^Tx)\sin(w^Ty)] \\
&= \mathbb{E}_{w\sim p}[[\cos(w^Tx), \sin(w^Tx)] \cdot [\cos(w^Ty), \sin(w^Ty)]^T]
\end{aligned}
$$

Hence, we can approximate K using D $\sin(w^Tx)$ and $\cos(w^Tx)$ features with randomly sampled $w \sim p$ and the empirical expectation:

$$K(x, y) \approx \frac{1}{D}\sum_d [\cos(w_d^Tx), \sin(w_d^Tx)] \cdot [\cos(w_d^Ty), \sin(w_d^Ty)]^T$$

Approximating Gaussian Kernels: Application

- If the kernel is Gaussian with unit variance $K(\Delta) = \exp(-\|\Delta\|^2/2)$ then the corresponding sampling distribution is $p(w) = (2\pi)^{-\frac{|\mathcal{X}|}{2}} \exp(-\|w\|^2/2)$
- Variant: The kernel is approximated by sampling only cos-features (instead of cos and sin) but with an additional shift $b \sim unif(0, 2\pi)$.

Algorithm 2 Algorithm (Random Fourier Features)

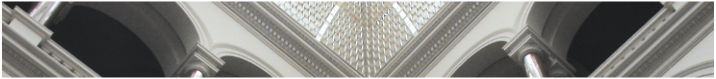
Require: Input data $x_i \in \mathcal{X}$, $i = 1, \ldots, n$, number of random features D

Sample $j = 1, \ldots, D$ offsets $b_j \sim unif(0, 2\pi)$

Sample $j = 1, \ldots, D$ $|\mathcal{X}|$-dimensional parameters $w_j \sim \mathcal{N}(0, 1)$

Construct the approximate feature map $\phi(x) = \sqrt{(\frac{2}{D})}[\cos(w_1^T x + b_1), \ldots, \cos(w_D^T x + b_D)]^T$

return transformed data $\phi(x_i) \in \mathbb{R}^D$, $i = 1, \ldots, n$



Thank you!