# Introduction to machine learning 

Masters M2MO \& MIDS

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## Today

- Kernels
- Kernel SVM
- Kernel regression


## Supervised learning setting

- We observe a training dataset $D$ of pairs $\left(x_{i}, y_{i}\right)$ for $i=1, \ldots, n$
- Features $x_{i} \in \mathbb{R}^{d}$ and labels $y_{i} \in \mathbb{R}$ (regression) or $y_{i} \in\{-1,1\}$ (binary classification)
- Given a features vector $x \in \mathbb{R}^{d}$, we want to predict the label $y$


## Features engineering

- Given raw features $x_{1}, \ldots, x_{n} \in \mathbb{R}^{d}$, we can construct new features
- For instance, we can add second order polynomials of the features

$$
x_{i, j}^{2}, \quad x_{i, j} \times x_{i, k} \quad \text { for any } \quad 1 \leq j, k \leq d
$$

- It increases the number of features, hence the dimension of the model weights $w$ learned from it


## A feature map

- Consider a feature map $\varphi: \mathbb{R}^{d} \rightarrow \mathbb{H}$ that "adds" all these new features
- $\mathbb{H}$ is an Hilbert space (eventually infinite dimensional), endowed with an inner product $\langle\cdot, \cdot\rangle_{\mathbb{H}}$
- The decision boundary $x \rightarrow\langle w, \varphi(x)\rangle+b=0$ is not an hyperplane anymore (but $\varphi(x) \rightarrow\langle w, \varphi(x)\rangle+b=0$ is)

A common belief: increasing dimension of features space makes data almost linearly separable


The polynomial mapping $\varphi: \mathbb{R}^{2} \rightarrow \mathbb{R}^{6}$ for $x=\left(x_{1}, x_{2}\right) \in \mathbb{R}^{2}$

$$
\varphi(x)=\left(x_{1}^{2}, x_{2}^{2}, \sqrt{2} x_{1} x_{2}, \sqrt{2} x_{1}, \sqrt{2} x_{2}, 1\right)
$$

solves the XOR (Exclusive OR) classification problem


XOR : label $y_{i}$ is blue iff one of the coordinates of $x_{i}$ equals 1.

- Blue and red points cannot be linearly separated in $\mathbb{R}^{2}$
- But they can using the mapping $\varphi$, using the hyperplane $x_{1} x_{2}=0$

This mapping $\varphi$ is call polynomial mapping of order 2 .
Note that for $x, x^{\prime} \in \mathbb{R}^{2}$ we have

$$
\begin{aligned}
\left\langle\varphi(x), \varphi\left(x^{\prime}\right)\right\rangle & =\left\langle\left[\begin{array}{c}
x_{1}^{2} \\
x_{1}^{2} \\
x_{2}^{2} \\
\sqrt{2} x_{1} x_{2} \\
\sqrt{2} x_{1} \\
\sqrt{2} x_{2} \\
1
\end{array}\right],\left[\begin{array}{c}
x_{1}^{2} \\
x_{1}^{\prime 2} \\
x_{2}^{\prime 2} \\
\sqrt{2} x_{1}^{\prime} x_{2}^{\prime} \\
\sqrt{2} x_{1}^{\prime} \\
\sqrt{2} x_{2}^{\prime} \\
1
\end{array}\right]\right\rangle \\
& =\left(x 1 x_{1}^{\prime}+x_{2} x_{2}^{\prime}+1\right)^{2} \\
& =\left(\left\langle x, x^{\prime}\right\rangle+1\right)^{2}
\end{aligned}
$$

This motivates the definition of

$$
K\left(x, x^{\prime}\right)=\left\langle\varphi(x), \varphi\left(x^{\prime}\right)\right\rangle=\left(\left\langle x, x^{\prime}\right\rangle+c\right)^{q}
$$

where $q \in \mathbb{N}-\{0\}$ and $c>0$. In this case $K$ is called the polynomial kernel of degree $q$.

Given a "raw feature" space $\mathcal{X}$ (often $\mathcal{X}=\mathbb{R}^{d}$ ), a function

$$
K: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}
$$

is called a kernel over $\mathcal{X}$.
Definition. We say that a kernel $K$ is symmetric iff

$$
K\left(x, x^{\prime}\right)=K\left(x^{\prime}, x\right)
$$

for any $x, x^{\prime} \in \mathcal{X}$

Definition. We say that a kernel is PDS (positive definite symetric) iff

- it is symmetric
- for any $N \in \mathbb{N}$ and any $\left\{x_{1}, \ldots x_{N}\right\} \subset \mathcal{X}$ we have

$$
\boldsymbol{K}=\left[K\left(x_{i}, x_{j}\right)\right]_{1 \leq i, j \leq N} \succeq 0
$$

meaning that $K$ is positive semi-definite (symmetric), or equivalently that

$$
u^{\top} \boldsymbol{K} u=\sum_{1 \leq i, j \leq N} u_{i} u_{j} K\left(x_{i}, x_{j}\right) \geq 0
$$

for any $u \in \mathbb{R}^{N}$, or equivalently that all eigenvalues of $K$ are non-negative.
For a sample $x_{1}, \ldots, x_{n}$ we call $\boldsymbol{K}=\left[K\left(x_{i}, x_{j}\right)\right]_{1 \leq i, j \leq n}$ the Gram matrix of this sample.

Definition. Hadamard product $\boldsymbol{A} \odot \boldsymbol{B}$ between two matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ (or vectors) with the same dimensions is given by

$$
(\boldsymbol{A} \odot \boldsymbol{B})_{i, j}=\boldsymbol{A}_{i, j} \odot \boldsymbol{B}_{i, j}
$$

Theorem. The sum, product, pointwise limit and composition with a power series $\sum_{n \geq 0} a_{n} x^{n}$ with $a_{n} \geq 0$ for all $n \geq 0$ preserves the PDS property.

Proof. Consider two $N \times N$ Gram matrices $\boldsymbol{K}, \boldsymbol{K}^{\prime}$ of PDS kernels $K, K^{\prime}$ and take $u \in \mathbb{R}^{N}$. Observe that

$$
u^{\top}\left(\boldsymbol{K}+\boldsymbol{K}^{\prime}\right) u=u^{\top} \boldsymbol{K} u+u^{\top} \boldsymbol{K}^{\prime} u \geq 0
$$

So PDS is preserved by the sum and finite sums by reccurence.

Now, to prove that the product $\boldsymbol{K} \odot \boldsymbol{K}^{\prime}$ is PDS, write $\boldsymbol{K}=\boldsymbol{M} \boldsymbol{M}^{\top}$, where $\boldsymbol{M}$ is the square-root of $\boldsymbol{K}$ (which is SDP) and note that

$$
\begin{aligned}
u^{\top}\left(\boldsymbol{K} \odot \boldsymbol{K}^{\prime}\right) u & =\sum_{1 \leq i, j \leq N} u_{i} u_{j} \boldsymbol{K}_{i, j} \boldsymbol{K}_{i, j}^{\prime}=\sum_{1 \leq i, j \leq N} \sum_{k=1}^{N} u_{i} u_{j} \boldsymbol{M}_{i, k} \boldsymbol{M}_{k, j} \boldsymbol{K}_{i, j}^{\prime} \\
& =\sum_{k=1}^{N} z_{k}^{\top} \boldsymbol{K}^{\prime} z_{k} \geq 0
\end{aligned}
$$

with $z_{k}=u \odot M_{\bullet, k}$.
This proves that finite products of PDS kernels is PDS.

Assume that $K_{n} \rightarrow K$ as $n \rightarrow+\infty$ pointwise, where $K_{n}$ is a sequence of PDS kernels.
It means that any associated sequence of Gram matrices $\boldsymbol{K}_{n}$ and the its limit $\boldsymbol{K}$ satisfies $\boldsymbol{K}_{n} \rightarrow \boldsymbol{K}$ entrywise, so that for any $u \in \mathbb{R}^{N}$ we have

$$
u^{\top} \boldsymbol{K}_{n} u \rightarrow u^{\top} \boldsymbol{K} u
$$

so $u^{\top} \boldsymbol{K} u \geq 0$ since $u^{\top} \boldsymbol{K}_{n} u \rightarrow u$ for all $n$.
This proves stability of PDS property under pointwise limit.

Now, let $K$ be a kernel such that $\left|K\left(x, x^{\prime}\right)\right|<r$ for all $x, x^{\prime} \in \mathcal{X}$ and $\sum_{n \geq 0} a_{n} x^{n}$ a power series with radius of convergence $r$.

By stability under sum and product, we have that

$$
\sum_{k=0}^{N} a_{n} K^{n}
$$

is PDS , and

$$
\lim _{N \rightarrow+\infty} \sum_{n=0}^{N} a_{n} K^{n}=\sum_{n \geq 0} a_{n} K^{n}
$$

remains PDS since PDS is kept under pointwise limit.
This concludes the proof of the theorem.

Theorem. The following inequality holds for $K, K^{\prime}$ two PDS kernels

$$
K\left(x, x^{\prime}\right)^{2} \leq K(x, x) K\left(x^{\prime}, x^{\prime}\right)
$$

for any $x, x^{\prime} \in \mathcal{X}$. It is called the Cauchy-Schwartz inequality for PSD kernels.

Proof. Take $x, x^{\prime} \in \mathcal{X}$ and consider the Gram matrix

$$
\boldsymbol{K}=\left[\begin{array}{cc}
K(x, x) & K\left(x, x^{\prime}\right) \\
K\left(x^{\prime}, x\right) & K\left(x^{\prime}, x^{\prime}\right)
\end{array}\right] .
$$

Since $K$ is PDS, then $K \succeq 0$, which entails that

$$
0 \leq \operatorname{det} \boldsymbol{K}=K(x, x) K\left(x^{\prime}, x^{\prime}\right)-K\left(x, x^{\prime}\right)^{2}
$$

Theorem [Reproducing kernel Hilbert space]. Let $K: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a PDS kernel. Then, there is a Hilbert space $\mathbb{H}$ endowed with an inner product $\langle\cdot, \cdot\rangle$ and a mapping $\varphi: \mathcal{X} \rightarrow \mathbb{H}$ such that

$$
K\left(x, x^{\prime}\right)=\left\langle\varphi(x), \varphi\left(x^{\prime}\right)\right\rangle
$$

and such that the reproducing property holds:

$$
h(x)=\langle h, K(x, \cdot)\rangle
$$

for any $h \in \mathbb{H}$ and $x \in \mathcal{X}$.
Proof. Available on the moodle. Think of $\mathbb{H}$ as containing limits of functions

$$
\sum_{i=1}^{N} a_{i} K\left(x_{i}, \cdot\right)
$$

for any $a_{1}, \ldots, a_{N} \in \mathbb{R}$ and $x_{1}, \ldots, x_{N} \in \mathcal{X}$.
Remark. Stresses the fact that a PDS kernel is some kind of similarity measure, since it is actually an inner product

- We say that $\mathbb{H}$ is a reproducting kernel Hilbert space associated to the kernel $K$.
- The Hilbert space $\mathbb{H}$ is called the features space associated to $K$
- The corresponding mapping $\varphi: \mathcal{X} \rightarrow \mathbb{H}$ is called the features mapping
- $\mathbb{H}$ is endowed with an inner product $\left\langle h, h^{\prime}\right\rangle$ for $h, h^{\prime} \in \mathbb{H}$ and a norm $\|h\|=\sqrt{\langle h, h\rangle}$
- The feature space might is not unique in general

In summary

- Choose a kernel $K$ you think relevant, if it's PDS, then there is a mapping $\varphi$ and a RKHS $\mathbb{H}$ for it
- Feature engineernig becomes kernel engineering with kernel methods

Definition. The normalized kernel $K^{\prime}$ associated to a kernel $K$ is given by

$$
K^{\prime}\left(x, x^{\prime}\right)=\frac{K\left(x, x^{\prime}\right)}{\sqrt{K(x, x) K\left(x^{\prime}, x^{\prime}\right)}}
$$

if $K(x, x) K\left(x^{\prime}, x^{\prime}\right)>0$ and $K\left(x, x^{\prime}\right)=0$ otherwise.
Theorem. If $K$ is a PDS kernel, its normalized kernel $K^{\prime}$ is PDS.
Remark. We have that $K\left(x, x^{\prime}\right)$ is the cosine of the angle between $\varphi(x)$ and $\varphi\left(x^{\prime}\right)$ if $K$ is a normalized kernel (if none is zero). Once again, $K\left(x, x^{\prime}\right)$ is a similarity measure between $x$ and $x^{\prime}$

Proof. Let $x_{1}, \ldots, x_{N} \in \mathcal{X}$ and $c \in \mathbb{R}^{N}$. If $K\left(x_{i}, x_{i}\right)=0$ or $K\left(x_{j}, x_{j}\right)=0$ then $K\left(x_{i}, x_{j}\right)=0$ using Cauchy-Schwartz, so $K^{\prime}\left(x_{i}, x_{j}\right)=0$.

So, we can assume $K\left(x_{i}, x_{i}\right)>0$ for all $i=1, \ldots, N$ and write the following:

$$
\begin{aligned}
\sum_{1 \leq i, j \leq N} \frac{c_{i} c_{j} K\left(x_{i}, x_{j}\right)}{\sqrt{K\left(x_{i}, x_{i}\right) K\left(x_{j}, x_{j}\right)}} & =\sum_{1 \leq i, j \leq N} \frac{c_{i} c_{j}\left\langle\varphi\left(x_{i}\right), \varphi\left(x_{j}\right)\right\rangle}{\left\|\varphi\left(x_{i}\right)\right\|\left\|\varphi\left(x_{j}\right)\right\|} \\
& =\left\|\sum_{i=1}^{N} \frac{c_{i} \varphi\left(x_{i}\right)}{\left\|\varphi\left(x_{i}\right)\right\|}\right\|^{2} \geq 0
\end{aligned}
$$

which proves the theorem.
Remark. If $K$ is a normalized kernel, then

$$
\|\varphi(x)\|=\langle\varphi(x), \varphi(x)\rangle=K(x, x)=1
$$

for any $x \in \mathcal{X}$

The polynomial kernel. For $c>0$ and $q \in \mathbb{N}-\{0\}$ we define the polynomial kernel

$$
K\left(x, x^{\prime}\right)=\left(\left\langle x, x^{\prime}\right\rangle+c\right)^{q} .
$$

It is a PDS kernel
Proof. It is the power of the PDS kernel $\left(x, x^{\prime}\right) \mapsto\left\langle x, x^{\prime}\right\rangle+b$.
We already computed its mapping $\varphi(x)$ : it contains all the monomials of degree less than $q$ of the coordinates of $x$

The RBF kernel (Radial Basis Function). For $\gamma>0$ it is given by

$$
K\left(x, x^{\prime}\right)=\exp \left(-\gamma\left\|x-x^{\prime}\right\|_{2}^{2}\right)
$$

Theorem. The RBF kernel is a PDS and normalized kernel.
Proof. First remark that

$$
\begin{aligned}
\exp \left(-\gamma\left\|x-x^{\prime}\right\|_{2}^{2}\right) & =\frac{\exp \left(2 \gamma\left\langle x, x^{\prime}\right\rangle\right)}{\exp \left(\gamma\|x\|^{2}\right) \exp \left(\gamma\left\|x^{\prime}\right\|^{2}\right)} \\
& =\frac{K^{\prime}\left(x, x^{\prime}\right)}{\sqrt{K^{\prime}(x, x) K^{\prime}\left(x^{\prime}, x^{\prime}\right)}}
\end{aligned}
$$

with $K^{\prime}\left(x, x^{\prime}\right)=\exp \left(2 \gamma\left\langle x, x^{\prime}\right\rangle\right)$ and that $K^{\prime}$ is PDS since

$$
K^{\prime}\left(x, x^{\prime}\right)=\sum_{n \geq 0} \frac{\left(2 \gamma\left\langle x, x^{\prime}\right\rangle\right)^{n}}{n!}
$$

namely a series of the PDS kernel $\left(x, x^{\prime}\right) \mapsto 2 \gamma\left\langle x, x^{\prime}\right\rangle$.

The tanh kernel. Also called the sigmoid kernel

$$
K^{\prime}\left(x, x^{\prime}\right)=\tanh \left(a\left\langle x, x^{\prime}\right\rangle+c\right)=\frac{e^{a\left\langle x, x^{\prime}\right\rangle+c}-e^{a\left\langle x, x^{\prime}\right\rangle+c}}{e^{a\left\langle x, x^{\prime}\right\rangle+c}+e^{a\left\langle x, x^{\prime}\right\rangle+c}}
$$

for $a, c>0$. It is again a PDS kernel (same argument as for the RBF kernel).

Remark. By far, the RBF kernel is the most widely used: uses as a similarity measure the Euclidean norm More mathematical details are covered in the exercices.

Kernel based algorithms how to use kernels for classification and regression?

- Let's recall the primal and dual formulation of the SVM

Linear SVM. Primal problem is
$\min _{w \in \mathbb{R}^{d}, b \in \mathbb{R}, s \in \mathbb{R}^{n}} \frac{1}{2}\|w\|_{2}^{2}+C \sum_{i=1}^{n} s_{i}$
subject to $y_{i}\left(\left\langle x_{i}, w\right\rangle+b\right) \geq 1-s_{i}$ and $s_{i} \geq 0$ for all $i=1, \ldots, n$
or equivalently

$$
\underset{w \in \mathbb{R}^{d}, b \in \mathbb{R}}{\operatorname{argmin}} \frac{1}{2}\|w\|_{2}^{2}+C \sum_{i=1}^{n} \ell\left(y_{i},\left\langle x_{i}, w\right\rangle+b\right)
$$

where $\ell\left(y, y^{\prime}\right)=\max \left(0,1-y y^{\prime}\right)=\left(1-y y^{\prime}\right)_{+}$is the hinge loss
Label prediction given by

$$
y=\operatorname{sgn}(\langle x, w\rangle+b)
$$


$\mathbf{w} \cdot \mathbf{x}+b=-\grave{i}$

Kernel SVM: replace $x_{i}$ by $\varphi\left(x_{i}\right)$. In the primal this leads to

$$
\underset{w \in \mathbb{R}^{d}, b \in \mathbb{R}^{2}}{\operatorname{argmin}} \frac{1}{2}\|w\|_{2}^{2}+C \sum_{i=1}^{n} \ell\left(y_{i},\left\langle\varphi\left(x_{i}\right), w\right\rangle+b\right)
$$

Label prediction is given by

$$
y=\operatorname{sgn}(\langle\varphi(x), w\rangle+b)
$$

In the primal, you need to compute $\varphi(x)$ !

Dual problem is
$\max _{\alpha \in \mathbb{R}^{n}} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j}\left\langle x_{i}, x_{j}\right\rangle$
subject to $0 \leq \alpha_{i} \leq C$ and $\sum_{i=1}^{n} \alpha_{i} y_{i}=0$ for all $i=1, \ldots, n$
and the label prediction using dual variables

$$
x \mapsto \operatorname{sgn}(\langle w, x\rangle+b)=\operatorname{sgn}\left(\sum_{i=1}^{n} \alpha_{i} y_{i}\left\langle x, x_{i}\right\rangle+b\right)
$$

depends only on the features $x_{i}$ via their inner products $\left\langle x_{i}, x_{j}\right\rangle$

Fundamental remark. The dual problem depends only on the features via their inner products

Given some kernel $K$, let's replace the "raw" inner products $\left\langle x_{i}, x_{j}\right\rangle$ by the "new" inner products $K\left(x_{i}, x_{j}\right)=\left\langle\varphi\left(x_{i}\right), \varphi\left(x_{j}\right)\right\rangle$

The kernel trick. Once again, to train the SVM with a kernel, you don't need to know or compute the $\varphi\left(x_{i}\right)$

## The kernel SVM

$\max _{\alpha \in \mathbb{R}^{n}} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} K\left(x_{i}, x_{j}\right)$
subject to $0 \leq \alpha_{i} \leq C$ and $\sum_{i=1}^{n} \alpha_{i} y_{i}=0$ for all $i=1, \ldots, n$ and the label prediction using dual variables

$$
x \mapsto \operatorname{sgn}\left(\sum_{i=1}^{n} \alpha_{i} y_{i} K\left(x, x_{i}\right)+b\right)
$$

with the intercept given by

$$
b=y_{i}-\sum_{j=1}^{n} \alpha_{j} y_{j} K\left(x_{j}, x_{i}\right)
$$

for any $i$ such that $0<\alpha_{i}<C$ (cf previous lecture)

This proves that the hypothesis solution writes

$$
h(x)=\operatorname{sgn}\left(\sum_{i=1}^{n} \alpha_{i} y_{i} K\left(x, x_{i}\right)+b\right),
$$

namely a combination of functions $K\left(x_{i}, \cdot\right)$ where $x_{i}$ are the support vectors.

For the RBF kernel, the decision function is

$$
x \mapsto \sum_{i: \alpha_{i} \neq 0} \alpha_{i} y_{i} \exp \left(-\gamma\left\|x-x_{i}\right\|_{2}^{2}\right)+b
$$

It is a mixture of Gaussian "densities". Let's recall that the $x_{i}$ with $\alpha_{i} \neq 0$ are the support vectors

$$
x \mapsto \sum_{i: \alpha_{i} \neq 0} \alpha_{i} y_{i} \exp \left(-\gamma\left\|x-x_{i}\right\|_{2}^{2}\right)+b
$$



The kernel trick is not only for the SVM
Representer theorem. If $K$ is a PDS kernel and $\mathbb{H}$ its corresponding RKHS, we have that for any increasing function $g$ and any function $L: \mathbb{R}^{n} \rightarrow \mathbb{R}$ that the optimization problem

$$
\underset{h \in \mathbb{H}}{\operatorname{argmin}} g(\|h\|)+L\left(h\left(x_{1}\right), \ldots, h\left(x_{n}\right)\right)
$$

admits only solutions of the form

$$
h=\sum_{i=1}^{n} \alpha_{i} K\left(x_{i}, \cdot\right)
$$

## Kernel ridge regression.

- Consider this time a continuous label $y_{i} \in \mathbb{R}$, features $x_{i} \in \mathcal{X}$ for $i=1, \ldots, n$ and a features mapping $\varphi: \mathcal{X} \rightarrow \mathbb{H}$ with PDS kernel $K$
- Kernel ridge regression considers the problem

$$
\underset{w}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \ell\left(y_{i},\left\langle w, \varphi\left(x_{i}\right)\right\rangle\right)+\frac{\lambda}{2}\|w\|_{2}^{2}\right\}
$$

where $\lambda$ is a penalization parameter, and $\ell\left(y, y^{\prime}\right)=\frac{1}{2}\left(y-y^{\prime}\right)^{2}$ is the least-squares loss

- Can be written as

$$
\underset{w}{\operatorname{argmin}} F(x) \text { with } \quad F(w)=\|y-\boldsymbol{X} w\|_{2}^{2}+\lambda\|w\|_{2}^{2}
$$

with $\boldsymbol{X}$ the matrix with rows containing the $\varphi\left(x_{i}\right)$ and $y=\left[y_{1} \cdots y_{n}\right] \in \mathbb{R}^{n}$

- This problem is strongly convex, and admits a global minimum iff

$$
\nabla F(w)=0 \quad \text { namely } \quad\left(\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \boldsymbol{I}\right) w=\boldsymbol{X}^{\top} y
$$

- Note that $\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \boldsymbol{I}$ is always invertible. Thus kernel ridge allows admits a closed-form solution
- Requires to solve a $D \times D$ linear system, where $D$ is the dimension of $\mathbb{H}$
- What if $D$ is large ?
- Let's us the kernel trick, as we did for SVM
- Representer theorem says that we can find $\alpha$ such that

$$
h(x)=\langle w, \varphi(x)\rangle=\sum_{i=1}^{n} \alpha_{i} K\left(x_{i}, x\right)=\sum_{i=1}^{n} \alpha_{i}\left\langle\varphi\left(x_{i}\right), \varphi(x)\right\rangle
$$

for any $x \in \mathcal{X}$

- This means that

$$
w=\boldsymbol{X}^{\top} \alpha
$$

Now, use the following trick: for any matrix $\boldsymbol{X}$, we have

$$
\left(\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^{\top}=\boldsymbol{X}^{\top}\left(\boldsymbol{X} \boldsymbol{X}^{\top}+\lambda \boldsymbol{I}\right)^{-1}
$$

This entails

$$
w=\left(\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^{\top} y=\boldsymbol{X}^{\top}\left(\boldsymbol{X} \boldsymbol{X}^{\top}+\lambda \boldsymbol{I}\right)^{-1} y
$$

which gives (note that $\left.\left(\boldsymbol{X} \boldsymbol{X}^{\top}\right)_{i, j}=\left\langle\varphi\left(x_{i}\right), \varphi\left(x_{j}\right)\right\rangle=K\left(x_{i}, x_{j}\right)\right)$

$$
\alpha=(\boldsymbol{K}+\lambda \boldsymbol{I})^{-1} y
$$

Proof of the trick. Note that

$$
\left(\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \boldsymbol{I}\right) \boldsymbol{X}^{\top}=\boldsymbol{X}^{\top}\left(\boldsymbol{X} \boldsymbol{X}^{\top}+\lambda \boldsymbol{I}\right)
$$

Multiplying on the left by $\left(\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \boldsymbol{I}\right)^{-1}$ leads to

$$
\boldsymbol{X}^{\top}=\left(\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^{\top}\left(\boldsymbol{X} \boldsymbol{X}^{\top}+\lambda \boldsymbol{I}\right)
$$

and then on the right by $\left(\boldsymbol{X} \boldsymbol{X}^{\top}+\lambda \boldsymbol{I}\right)^{-1}$ concludes with

$$
\left(\boldsymbol{X} \boldsymbol{X}^{\top}+\lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^{\top}=\left(\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^{\top}
$$

A cute trick. But let's do it like we did for the SVMs (just to be sure...)

An alternative formulation of

$$
\min _{w} \sum_{i=1}^{n}\left(y_{i}-\left\langle w, \varphi\left(x_{i}\right)\right\rangle\right)^{2}+\lambda\|w\|_{2}^{2}
$$

is given by

$$
\min _{w} \sum_{i=1}^{n}\left(y_{i}-\left\langle w, \varphi\left(x_{i}\right)\right\rangle\right)^{2} \text { subject to }\|w\|_{2}^{2} \leq r^{2}
$$

and also

$$
\min _{w} \sum_{i=1}^{n} s_{i}^{2} \text { subject to }\|w\|_{2}^{2} \leq r^{2} \text { and } s_{i}=y_{i}-\left\langle w, \varphi\left(x_{i}\right)\right\rangle
$$

Which leads to the following Lagrangian

$$
\begin{aligned}
L(w, s, \alpha, \lambda)= & \min _{w} \sum_{i=1}^{n} s_{i}^{2}+\min _{w} \sum_{i=1}^{n} \alpha_{i}\left(y_{i}-s_{i}-\left\langle w, \varphi\left(x_{i}\right)\right\rangle\right) \\
& +\lambda\left(\|w\|_{2}^{2}-r^{2}\right)
\end{aligned}
$$

so that the KKT conditions leads to the following properties:

$$
\begin{aligned}
& \nabla_{w} L=-\sum_{i=1}^{n} \alpha_{i} \varphi\left(x_{i}\right)+2 \lambda w \Rightarrow w=\frac{1}{2 \lambda} \sum_{i=1}^{n} \alpha_{i} \varphi\left(x_{i}\right) \\
& \nabla_{s_{i}} L=2 s_{i}-\alpha_{i} \Rightarrow s_{i}=\alpha_{i} / 2
\end{aligned}
$$

and the slackness complementary conditions:

$$
\alpha_{i}\left(y_{i}-s_{i}-\left\langle w, \varphi\left(x_{i}\right)\right\rangle\right)=0 \text { and } \lambda\left(\|w\|_{2}^{2}-r^{2}\right)=0
$$

Plugging the expressions of $w$ and $s_{i}$ in functions of $\alpha$ in $L$ gives after some algebra the dual objective

$$
\begin{aligned}
D(\alpha)=- & \lambda \sum_{i=1}^{n} \alpha_{i}^{2}+2 \sum_{i=1}^{n} \alpha_{i} y_{i} \\
& -\sum_{1 \leq i, j \leq n} \alpha_{i} \alpha_{j}\left\langle\varphi\left(x_{i}\right), \varphi\left(x_{j}\right)\right\rangle-\lambda r^{2}
\end{aligned}
$$

(where we replaced $2 \lambda \alpha_{i}$ by $\alpha_{i}$ ) which can be written matricially as

$$
\begin{aligned}
D(\alpha) & =-\lambda\|\alpha\|_{2}^{2}+2\langle\alpha, y\rangle-\alpha^{\top} \boldsymbol{X} \boldsymbol{X}^{\top} \alpha \\
& =2\langle\alpha, y\rangle-\alpha^{\top}(\boldsymbol{K}+\lambda \boldsymbol{I}) \alpha
\end{aligned}
$$

with optimum achieved for

$$
\alpha=(\boldsymbol{K}+\lambda \boldsymbol{I})^{-1} y
$$

(same as before, of course...)

## In summary

- Solving a problem in the dual benefits from the kernel trick
- Allows to construct complex non-linear decision functions
- OK if $n$ is not too large... (if the $n \times n$ Gram matrix $K$ fits in memory)
- Otherwise, stick to the primal! (and forget about kernels...)
- But don't forget about feature engineering (yes, again!)


## Thank you!

