Nonlinear supervised learning with kernels

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Kernel methods

- Widely used in machine learning.
- Extend algorithms such as SVMs to define non-linear decision boundaries.

Idea

- Implicitly defining an inner product in a high-dimensional space.
- Replacing the original inner product in the input space with positive definite kernels immediately extends algorithms such as SVMs to a non-linear separation in the input space.

Kernel methods

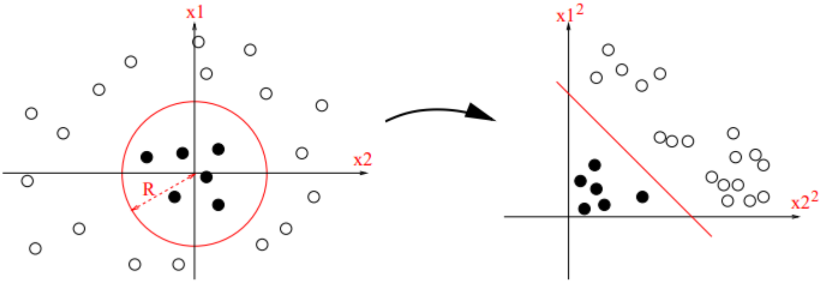
SVM

In practice, linear separation is often not possible.

Implicit lifting to a higher dimensional space

- Use more complex functions to separate the two sets
- Use a non-linear mapping φ from the input space $\mathcal{X}$ to a higher-dimensional space $\mathcal{H}$, where linear separation is possible.

Polynomial mapping

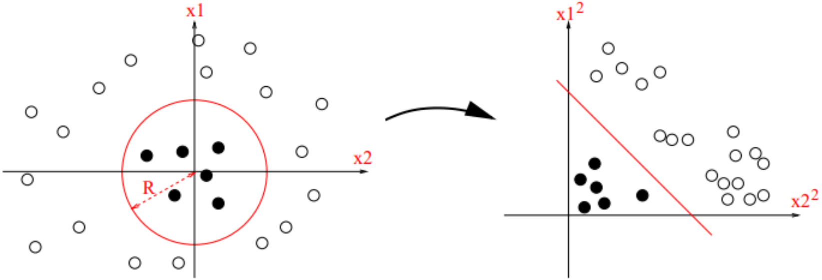


Polynomial mapping

The **polynomial** mapping $\varphi : \mathbb{R}^2 \to \mathbb{R}^3$ for $x = (x_1, x_2) \in \mathbb{R}^2$

$$\varphi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

solves the classification problem: label $Y_i = 1$ if the data point is in the circle of radius R.



Note that for $x, \tilde{x} \in \mathbb{R}^2$ we have

$$\begin{aligned}\langle \varphi(x), \varphi(x') \rangle &= x_1^2 \tilde{x}_1^2 + x_2^2 \tilde{x}_2^2 + 2 x_1 x_2 \tilde{x}_1 \tilde{x}_2 \\ &= \langle x, \tilde{x} \rangle^2 .\end{aligned}$$

Some definitions

Definition (Kernel)

A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a kernel over $\mathcal{X}$.

The idea is to define a kernel k such that

$$\forall (x, x') \in \mathcal{X} \times \mathcal{X}, \qquad k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}.$$

- for some mapping $\varphi = \mathcal{X} \to \mathcal{H}$ to a Hilbert space $\mathcal{H}$
- $\mathcal{H}$ is called a feature space

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- for some mapping $\varphi = \mathcal{X} \to \mathcal{H}$ to a Hilbert space $\mathcal{H}$
- $\mathcal{H}$ is called a feature space

Interpretation: k can be interpreted as a similarity measure between elements of the input space $\mathcal{X}$ (or the "raw feature" space).

Kernel trick in ML

- Many machine learning algorithms (in particular, linear SVMs) can be expressed only in terms of inner products between vectors
- Computing the explicit mappings $\varphi(x_1), \varphi(x_2)$ and their inner product $\langle \varphi(x_1), \varphi(x_2) \rangle_{\mathcal{H}}$ can be computationally expensive!
- Kernel trick: avoid the explicit mapping $\varphi(x)$ by directly computing the inner product $\langle \varphi(x_1), \varphi(x_2) \rangle_{\mathcal{H}}$ via the kernel function $k(x_1, x_2)$

Good properties of kernels

Efficiency:

- k is often significantly more efficient to compute than φ and an inner product in $\mathcal{H}$.
- in several common examples, the computation of $k(x, x')$ can be achieved in $O(\dim \mathcal{X})$ while that of $\langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$ typically requires $O(\dim(\mathcal{H}))$ work, with $\dim(\mathcal{H}) \gg N$.
- in some cases, $\dim(\mathcal{H}) = \infty$.

Flexibility:

- No need to explicitly define or compute a mapping φ
- The kernel k can be arbitrarily chosen so long as the existence of φ is guaranteed, i.e. k satisfies Mercer's condition

More definitions on kernels

Definition (Symmetry)

We say that a kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is symmetric if for all $(x, x') \in \mathcal{X} \times \mathcal{X}$

$$k(x, x') = k(x', x).$$

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Definition (Positive Definite Symmetric (PDS) kernel)

We say that a kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is Positive Definite Symmetric (PDS) if for any $\{x_1, \ldots, x_n\} \subset \mathcal{X}$ the matrix $K := (k(x_i, x_j))_{1 \leqslant i,j \leqslant n}$ is symmetric positive semidefinite (SPSD), i.e.

$$K := (k(x_i, x_j))_{1 \leqslant i,j \leqslant n} \succeq 0.$$

More definitions on kernels

Recall that K is SPSD if

- the eigenvalues of K are all non-negative,
- or, for any vector $u \in \mathbb{R}^n$

$$u^T K u = \sum_{ij} u_i u_j k(x_i, x_j) \geqslant 0$$

(with K symmetric).

For a sample $x_1, \dots, x_n$ we call $K = [K(x_i, x_j)]_{1 \leqslant i,j \leqslant n}$ the Gram matrix of this sample.

Some properties of "stability"

Definition (Hadamard product)

$A \odot B$ between two matrices A and B (or vectors) with the same dimensions is given by

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

Theorem

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

Proof I

(Sum) Consider two $n \times n$ Gram matrices K, K' of PDS kernels K, K' and take $u \in \mathbb{R}^n$. Observe that

$$u^\top (K + K')u = u^\top Ku + u^\top K'u \geqslant 0$$

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

Proof II

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

$$\begin{aligned} u^\top (K \odot K') u &= \sum_{1 \leqslant i,j \leqslant n} u_i u_j K_{i,j} K'_{i,j} \\ &= \sum_{1 \leqslant i,j \leqslant n} \sum_{k=1}^{n} u_i u_j M_{i,k} M_{k,j} K'_{i,j} \\ &= \sum_{k=1}^{n} z_k^\top K' z_k \geqslant 0 \end{aligned}$$

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

Proof III

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

$$u^\top K_\ell u \to u^\top K u$$

so $u^\top K u \geqslant 0$ since $u^\top K_\ell u \to u$ for all ℓ. This proves stability of PDS property under pointwise limit.

(Composition w/ a power series) Now, let K be a kernel such that $|K(x, x')| < r$ for all $x, x' \in \mathcal{X}$ and $\sum_{\ell \geqslant 0} a_\ell x^\ell$ a power series with radius of convergence r.
By stability under sum and product, we have that

$$\sum_{\ell=0}^{L} a_\ell K^\ell$$

Proof IV

is PDS, and

$$\lim_{L \to +\infty} \sum_{\ell=0}^{L} a_\ell K^\ell = \sum_{\ell \geqslant 0} a_\ell K^\ell$$

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

More properties on kernels

Theorem (Cauchy-Schwarz)

The following inequality holds for k, k' two PDS kernels

$$k(x, x')^2 \leqslant k(x, x)k(x', x')$$

for any $x, x' \in \mathcal{X}$.

It is called the *Cauchy-Schwarz inequality* for PSD kernels.

Proof

Take $x, x' \in \mathcal{X}$ and consider the Gram matrix

$$G = \begin{bmatrix} k(x,x) & k(x,x') \\ k(x',x) & k(x',x') \end{bmatrix}.$$

Since k is PDS, then $G \succcurlyeq 0$, which entails that

$$0 \leqslant \det G = k(x,x)k(x',x') - k(x,x')^2.$$

Sufficient condition for the reproducing property

Theorem (Reproducing Kernel Hilbert Space (RKHS))

Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a PDS kernel. Then, there is a Hilbert space $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ endowed with an inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and a mapping $\varphi : \mathcal{X} \to \mathcal{H}$ such that

$$k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$$

and such that the ***reproducing property*** *holds:*

$$h(x) = \langle h, k(x, \cdot) \rangle_{\mathcal{H}}$$

for any $h \in \mathcal{H}$ and $x \in \mathcal{X}$.

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for any $h \in \mathcal{H}$ and $x \in \mathcal{X}$.

We say that $\mathcal{H}$ is a reproducting kernel Hilbert space associated to the kernel k.

Some vocabulary

- Note that

$$\text{RKHS} \Rightarrow \text{Hilbert space}, \qquad \text{BUT} \qquad \text{Hilbert space} \not\Rightarrow \text{RKHS}$$

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- $\mathcal{H}$ is endowed with an inner product $\langle h, h' \rangle_{\mathcal{H}}$ for $h, h' \in \mathcal{H}$ and a norm $\|h\|_{\mathcal{H}} = \sqrt{\langle h, h \rangle_{\mathcal{H}}}$

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- $\mathcal{H}$ is endowed with an inner product $\langle h, h' \rangle_{\mathcal{H}}$ for $h, h' \in \mathcal{H}$ and a norm $\|h\|_{\mathcal{H}} = \sqrt{\langle h, h \rangle_{\mathcal{H}}}$
- The feature space might not be unique in general

Some examples of RKHS

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2. the space $L^2(\mathbb{R})$ is not a RKHS.
3. the space of $\mathcal{F} = \left\{ f : f(0) = 0, f \text{ absolutely continuous}, f, f' \in L^2(\mathbb{R}) \right\}$ is a RKHS with $k(x, x') = e^{-|x-x'|}$.

In summary

- Choose a kernel k you think relevant
- If it's PDS, then there is a mapping φ and a RKHS $\mathcal{H}$ for it

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- Choose a kernel k you think relevant
- If it's PDS, then there is a mapping φ and a RKHS $\mathcal{H}$ for it
- Feature engineering becomes kernel engineering with kernel methods
- Any linear algorithm based on computing inner products can be extended into a non-linear version by replacing the inner products by a kernel function $\rightsquigarrow$ kernel trick

$$k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$$

Normalized kernel

Definition

The **normalized kernel** k' associated to a kernel k is given by

$$k'(x, x') = \frac{k(x, x')}{\sqrt{k(x, x)k(x', x')}}$$

if $k(x, x)k(x', x') > 0$ and $k(x, x') = 0$ otherwise.

Theorem

If k is a PDS kernel, its normalized kernel k' is PDS.

Proof

Let $x_1, \dots, x_n \in \mathcal{X}$ and $c \in \mathbb{R}^n$. If $k(x_i, x_i) = 0$ or $k(x_j, x_j) = 0$ then $k(x_i, x_j) = 0$ using Cauchy-Schwarz, so $k'(x_i, x_j) = 0$.
So, we can assume $k(x_i, x_i) > 0$ for all $i = 1, \dots, n$ and write the following:

$$\sum_{1 \leqslant i,j \leqslant n} \frac{c_i c_j k(x_i, x_j)}{\sqrt{k(x_i, x_i) k(x_j, x_j)}} = \sum_{1 \leqslant i,j \leqslant n} \frac{c_i c_j \langle \varphi(x_i), \varphi(x_j) \rangle}{\|\varphi(x_i)\| \, \|\varphi(x_j)\|}$$

$$= \left\| \sum_{i=1}^{n} \frac{c_i \varphi(x_i)}{\|\varphi(x_i)\|} \right\|^2 \geqslant 0$$

which proves the theorem.

A few remarks

Remark

- *We have that $k(x, x')$ is the cosine of the angle between $\varphi(x)$ and $\varphi(x')$ if k is a normalized kernel (if none is zero).*
- *Once again, $k(x, x')$ is a similarity measure between x and x'*

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- *Once again,* $k(x, x')$ *is a similarity measure between* x *and* x'

Remark

If k *is a normalized kernel, then*

$$\|\varphi(x)\|_{\mathcal{H}} = \langle \varphi(x), \varphi(x) \rangle_{\mathcal{H}} = k(x, x) = 1$$

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

Some famous kernels

The polynomial kernel.

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

$$K(x, x') = (\langle x, x' \rangle + c)^q.$$

It is a PDS kernel,

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It is a PDS kernel, since it is the power of the PDS kernel $(x, x') \mapsto \langle x, x' \rangle + b$.

We already computed its mapping $\varphi(x)$: it contains all the monomials of degree less than q of the coordinates of x.

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The Gaussian or the Radial Basis Function (RBF) kernel.

For $\gamma > 0$ it is given by

$$k(x, x') = \exp(-\gamma \left\| x - x' \right\|_2^2)$$

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Proposition

The RBF kernel is a PDS and normalized kernel.

By far, the RBF kernel is the most widely used: uses as a similarity measure the Euclidean norm

Proof

First remark that

$$\exp(-\gamma \left\|x - x'\right\|_2^2) = \frac{\exp(2\gamma\langle x, x'\rangle)}{\exp(\gamma \left\|x\right\|^2)\exp(\gamma \left\|x'\right\|^2)}$$
$$= \frac{k'(x, x')}{\sqrt{k'(x, x)k'(x', x')}}$$

with $k'(x, x') = \exp(2\gamma\langle x, x'\rangle)$ and that k' is PDS since

$$k'(x, x') = \sum_{n \geqslant 0} \frac{(2\gamma\langle x, x'\rangle)^n}{n!}$$

namely a series of the PDS kernel $(x, x') \mapsto 2\gamma\langle x, x'\rangle$.

Some famous kernels

The tanh kernel or the sigmoid kernel.

$$k'(x, x') = \tanh(a\langle x, x'\rangle + c) = \frac{e^{a\langle x,x'\rangle + c} - e^{-a\langle x,x'\rangle - c}}{e^{a\langle x,x'\rangle + c} + e^{-a\langle x,x'\rangle - c}}$$

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

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<u>Exercise</u>: compute its mapping.

Kernel-based algorithms?

Question

How to use kernels for classification and regression?

Kernel-based algorithms?

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How to use kernels for classification and regression?

Recall the linear SVM

Figure: SVM: hard and soft margins

Recall the linear SVM

Linear SVM

- Back to the primal problem

$$\min_{w\in\mathbb{R}^d, b\in\mathbb{R}, s\in\mathbb{R}^n} \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^n s_i$$

$$\text{s.t.} \quad y_i(\langle x_i, w\rangle + b) \geqslant 1 - s_i \ \text{ and } \ s_i \geqslant 0 \ \text{ for all } \ i = 1, \ldots, n$$

- or equivalently

$$\text{argmin}_{w\in\mathbb{R}^d, b\in\mathbb{R}} \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^n \ell(y_i, \langle x_i, w\rangle + b)$$

  where $\ell(y, y') = \max(0, 1 - yy') = (1 - yy')_+$ is the hinge loss.

- Label prediction given by

$$y = \text{sign}(\langle x, w\rangle + b)$$

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Kernel SVM

Principle

- Replace x_i by $\varphi(x_i)$. In the primal this leads to

$$\text{argmin}_{w\in\mathbb{R}^d, b\in\mathbb{R}} \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^{n}\ell(y_i, \langle\varphi(x_i), w\rangle + b)$$

- Label prediction is given by

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

Problem

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

Linear SVM

Dual problem

$$\max_{\alpha \in \mathbb{R}^n} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$$

subject to $\quad 0 \leqslant \alpha_i \leqslant C \;$ and $\; \sum_{i=1}^{n} \alpha_i y_i = 0 \;$ for all $\; i = 1, \ldots, n$

and the label prediction using dual variables

$$x \mapsto \operatorname{sign}(\langle w, x \rangle + b) = \operatorname{sign}\left(\sum_{i=1}^{n} \alpha_i y_i \langle x, x_i \rangle + b \right)$$

depends only on the features x_i via their inner products $\langle x_i, x_j \rangle$

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Remark (Fundamental remark)

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

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Given some kernel k, let's replace the "raw" inner products $\langle x_i, x_j \rangle$ by the "new" inner products $k(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j) \rangle$

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The kernel trick

To train the SVM with a kernel, you don't need to know or compute the $\varphi(x_i)$!

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Take-home message: kernel trick

- Kernel + SVM = ♡
- But do it in the dual problem only!

Kernel SVM

Dual problem

$$\max_{\alpha \in \mathbb{R}^n} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j k(x_i, x_j)$$

$$\text{subject to} \quad 0 \leqslant \alpha_i \leqslant C \quad \text{and} \quad \sum_{i=1}^{n} \alpha_i y_i = 0 \quad \text{for all} \quad i = 1, \ldots, n$$

Label prediction

The label prediction using dual variables

$$x \mapsto \operatorname{sign}\left(\sum_{i=1}^{n} \alpha_i y_i k(x, x_i) + b\right)$$

with the intercept given by

$$b = y_i - \sum_{j=1}^{n} \alpha_j y_j k(x_j, x_i)$$

for any i such that $0 < \alpha_i < C$ (support vector) (cf previous lecture)

Kernel & support vectors

This proves that the hypothesis solution writes

$$h(x) = \text{sign}\Big(\sum_{i:\alpha_i \neq 0} \alpha_i y_i k(x, x_i) + b \Big),$$

namely a combination of functions $k(x_i, \cdot)$ where x_i are the support vectors.

For the RBF kernel

The decision function is

$$x \mapsto \sum_{i:\alpha_i \neq 0} \alpha_i y_i \exp\big(-\gamma \, \|x - x_i\|_2^2 \big) + b$$

It is a mixture of Gaussian "densities". Let's recall that the x_i with $\alpha_i \neq 0$ are the support vectors

Kernel and regression

The kernel trick is not only for the SVM!

Theorem ((Kimeldorf & Wahba 1971, Schölkopf et al. 2001))

If k is a PDS kernel and $\mathcal{H}$ its corresponding RKHS, for any increasing function g and any function $L : \mathbb{R}^n \to \mathbb{R}$, the optimization problem

$$\min_{h \in \mathcal{H}} g(\|h\|_{\mathcal{H}}) + L(h(x_1), \ldots, h(x_n))$$

admits only solutions of the form

$$h^\star = \sum_{i=1}^{n} \alpha_i k(x_i, \cdot).$$

This theorem is called the representer theorem.

The representer theorem

It means that in the case of a penalization increasing with $\| \cdot \|_{\mathcal{H}}$, any optimal solution $h^\star$ lives in a finite dimensional vector space of $\mathcal{H}$, even if $\mathcal{H}$ is infinite-dimensional!

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 $\varphi : \mathcal{X} \to \mathcal{H}$ with PDS kernel k

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- Kernel Ridge regression considers the problem

$$\min_w \left\{ \sum_{i=1}^n \ell(y_i, \langle w, \varphi(x_i) \rangle) + \frac{\lambda}{2} \|w\|_2^2 \right\}$$

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

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- Can be written as

$$\min_w F(x) \quad \text{with} \quad F(w) = \|y - Xw\|_2^2 + \lambda \|w\|_2^2$$

with X the matrix with rows containing the $\varphi(x_i)$ and $y = [y_1 \cdots y_n] \in \mathbb{R}^n$

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- Note that $X^\top X + \lambda \mathrm{Id}$ is always invertible. Thus kernel ridge admits a closed-form solution.
- Requires to solve a $D \times D$ linear system, where D is the dimension of $\mathcal{H}$
- What if D is large ?

Kernel trick & regression

Let's use the kernel trick, as we did for SVM

- Representer theorem says that we can find α such that

$$h(x) = \langle w, \varphi(x) \rangle = \sum_{i=1}^{n} \alpha_i k(x_i, x) = \sum_{i=1}^{n} \alpha_i \langle \varphi(x_i), \varphi(x) \rangle$$

  for any $x \in \mathcal{X}$
- This means that

$$w = X^\top \alpha$$

New trick

Now use this trick

For any matrix X, we have

$$(X^\top X + \lambda \mathrm{Id})^{-1} X^\top = X^\top (X X^\top + \lambda \mathrm{Id})^{-1}$$

This entails

$$w = (X^\top X + \lambda \mathrm{Id})^{-1} X^\top y = X^\top (X X^\top + \lambda \mathrm{Id})^{-1} y$$

which gives (note that $(XX^\top)_{i,j} = \langle \varphi(x_i), \varphi(x_j) \rangle = k(x_i, x_j)$)

$$\alpha = (K + \lambda \mathrm{Id})^{-1} y$$

Proof of the trick

Note that

$$(X^\top X + \lambda \mathrm{Id}) X^\top = X^\top (X X^\top + \lambda \mathrm{Id}).$$

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

$$X^\top = (X^\top X + \lambda \mathrm{Id})^{-1} X^\top (X X^\top + \lambda \mathrm{Id}).$$

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

$$(X X^\top + \lambda \mathrm{Id})^{-1} X^\top = (X^\top X + \lambda \mathrm{Id})^{-1} X^\top$$

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

Another way for Kernel Ridge regression

An alternative formulation of

$$\min_{w} \sum_{i=1}^{n} (y_i - \langle w, \varphi(x_i) \rangle)^2 + \lambda \|w\|_2^2$$

is the **constrained version**, given by

$$\min_{w} \sum_{i=1}^{n} (y_i - \langle w, \varphi(x_i) \rangle)^2 \ \text{ subject to } \ \|w\|_2^2 \leqslant r^2$$

and also

$$\min_{w} \sum_{i=1}^{n} s_i^2 \ \text{ subject to } \ \|w\|_2^2 \leqslant r^2 \ \text{ and } \ s_i = y_i - \langle w, \varphi(x_i) \rangle$$

Then, using the Lagrangian

$$L(w, s, \alpha, \lambda) = \min_w \sum_{i=1}^{n} s_i^2 + \min_w \sum_{i=1}^{n} \alpha_i (y_i - s_i - \langle w, \varphi(x_i) \rangle) \\ + \lambda(\|w\|_2^2 - r^2)$$

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KKT conditions

$$\nabla_w L = -\sum_{i=1}^{n} \alpha_i \varphi(x_i) + 2\lambda w \Rightarrow w = \frac{1}{2\lambda} \sum_{i=1}^{n} \alpha_i \varphi(x_i)$$

$$\nabla_{s_i} L = 2s_i - \alpha_i \Rightarrow s_i = \alpha_i / 2$$

and the slackness complementary conditions:

$$\alpha_i (y_i - s_i - \langle w, \varphi(x_i) \rangle) = 0 \quad \text{and} \quad \lambda(\|w\|_2^2 - r^2) = 0$$

Plugging the expressions of w and s_i in functions of α in L gives after some algebra the dual objective

$$D(\alpha) = -\lambda \sum_{i=1}^{n} \alpha_i^2 + 2 \sum_{i=1}^{n} \alpha_i y_i \\ - \sum_{1 \leqslant i,j \leqslant n} \alpha_i \alpha_j \langle \varphi(x_i), \varphi(x_j) \rangle - \lambda r^2$$

(where we replaced $2\lambda\alpha_i$ by α_i)

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$$\begin{aligned} D(\alpha) &= -\lambda \|\alpha\|_2^2 + 2\langle \alpha, y \rangle - \alpha^\top X X^\top \alpha \\ &= 2\langle \alpha, y \rangle - \alpha^\top (K + \lambda \mathrm{Id}) \alpha \end{aligned}$$

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\end{aligned}
$$

with optimum achieved for

$$
\alpha = (K + \lambda \mathrm{Id})^{-1} y
$$

what we already got.

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Conclusion on kernels

- 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 !)