MLCC 2015 - Regularization Network II: Kernels

Francesca Odone

23 June, 2015

About this class

- Extend our model to deal with non linear problems
- Formulate the Representer Theorem
- Introduce kernel functions (+ examples)

Linear model...

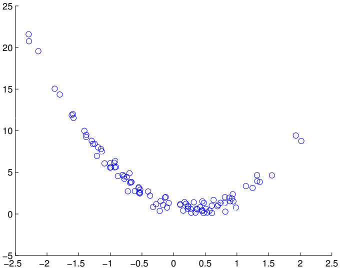
- Data set $S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ with $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$
- $\hat{X} = (x_1, \ldots, x_n)^\top \in \mathbb{R}^{n \times d}$ and $\hat{y} = (y_1, \ldots, y_n)^\top$.
- Linear model $w \in \mathbb{R}^d$: $y = w^\top x$
- $$\min_{w \in \mathbb{R}^d} \ell(y_i, f_w(x_i)) + \lambda \|w\|^2$$

Linear model...

- Data set $S = \{(x_1, y_1), \dots, (x_n, y_n)\}$ with $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$
- Linear model $w \in \mathbb{R}^d$

$$y = w^\top x$$

Example $d = 1$ and S as in the plot.



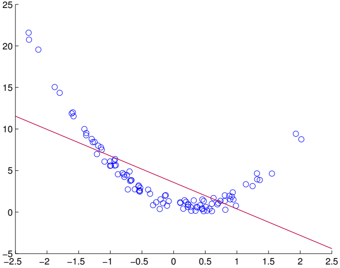
with $w = (\hat{X}^\top \hat{X} + \lambda n I)^{-1} \hat{X}^\top \hat{y}$ for a given $\lambda \geq 0$ (RLS).

Linear model...

- Data set $S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ with $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$
- Linear model $w \in \mathbb{R}^d$

$$y = w^\top x$$

Example $d = 1$ and S as in the plot.



with $w = (\hat{X}^\top \hat{X} + \lambda n I)^{-1} \hat{X}^\top \hat{y}$ for a given $\lambda \geq 0$ (RLS).

… and beyond

What if we want to learn a more general model?

$$y = w_1 x^2 + w_2 x + w_3$$

... and beyond

What if we want to learn a more general model?

$$y = w_1 x^2 + w_2 x + w_3$$

It is again a linear model! But in a different space ($\mathbb{R}^3$ instead of $\mathbb{R}$)

$$y = w^\top \phi(x)$$

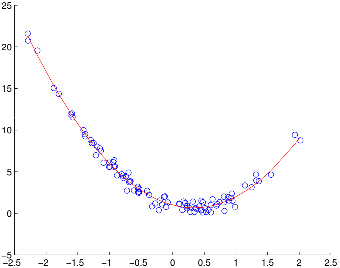
... and beyond

What if we want to learn a more general model?

$$y = w_1 x^2 + w_2 x + w_3$$

It is again a linear model! But in a different space ($\mathbb{R}^3$ instead of $\mathbb{R}$)

$$y = w^\top \phi(x)$$



with $\phi(x) = (x^2, x, 1)^\top$ and $w = (w_1, w_2, w_3)$

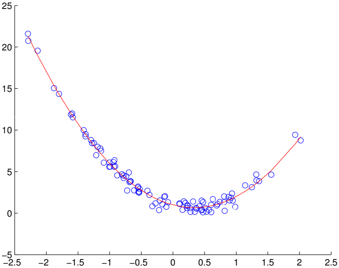
... and beyond

What if we want to learn a more general model?

$$y = w_1 x^2 + w_2 x + w_3$$

It is again a linear model! But in a different space ($\mathbb{R}^3$ instead of $\mathbb{R}$)

$$y = w^\top \phi(x)$$



with $\phi(x) = (x^2, x, 1)^\top$ and $w = (w_1, w_2, w_3)$

Generalized linear models

- Let define $\varphi_j(x) : \mathbb{R}^d \to \mathbb{R}$ with $j \in \{1, \dots, D\}$ (in general with $D >> d$)
- $\phi : \mathbb{R}^d \to \mathbb{R}^D$ is named *feature map* with $\phi(x) = (\varphi_1(x), \dots, \varphi_D(x))^\top$.
- $w \in \mathbb{R}^D$.

Generalized linear model

$$y = w^\top \phi(x) = \sum_{j=1}^{D} w_j \varphi_j(x)$$

How to compute a linear model (Least squares)

Let define $\hat{\Phi} = (\phi(x_1), \dots, \phi(x_n))^\top \in \mathbb{R}^D$.
$\hat{\Phi}$ in generalized linear models has the same role of $\hat{X}$ in the linear models

$$w = (\hat{\Phi}^\top \hat{\Phi} + \lambda n I)^{-1} \hat{\Phi}^\top \hat{y}$$

Can we do better? (from a computational point of view)

Note that $\hat{\Phi}^\top \hat{\Phi} \in \mathbb{R}^{D \times D}$

Can we do better? (from a computational point of view)

Note that $\hat{\Phi}^\top \hat{\Phi} \in \mathbb{R}^{D \times D}$ when D is huge, $\hat{\Phi}^\top \hat{\Phi}$ is not computable.
Can we do better?

Can we do better? (from a computational point of view)

Note that $\hat{\Phi}^\top \hat{\Phi} \in \mathbb{R}^{D \times D}$ when D is huge, $\hat{\Phi}^\top \hat{\Phi}$ is not computable.
Can we do better?

Representer Theorem (in the least squares context)
There exists a $c \in \mathbb{R}^n$ such that

$$w = \hat{\Phi}^\top c = \sum_{i=1}^n c_i \phi(x_i),$$

in particular $c = (\hat{\Phi}\hat{\Phi}^\top + \lambda n I)^{-1} \hat{y}$.
Note that $\hat{\Phi}\hat{\Phi}^\top \in \mathbb{R}^{n \times n}$.

Sketch of the Proof

- Let $\hat{\Phi} = U \Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n \times n}$, $V^\top V = I_{n \times n}$
- $\Sigma = \operatorname{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = (\hat{\Phi}^\top \hat{\Phi} + \lambda n I)^{-1} \hat{\Phi}^\top \hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = (V\Sigma U^\top U \Sigma V^\top + \lambda n I)^{-1} V \Sigma U^\top \hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = (V\Sigma^2 V^\top + \lambda n I)^{-1} V\Sigma U^\top \hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \dots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = V(\Sigma^2 + \lambda n I)^{-1}\Sigma U^\top \hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = V\Sigma(\Sigma^2 + \lambda n I)^{-1} U^\top \hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = V\Sigma U^\top U(\Sigma^2 + \lambda n I)^{-1} U^\top \hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = V\Sigma U^\top (U\Sigma^2 U^\top + \lambda n {\color{red}UU^\top})^{-1}\hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U \Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n \times n}$, $V^\top V = I_{n \times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = V \Sigma U^\top (U \Sigma V^\top \, V \Sigma U^\top + \lambda n I^\top)^{-1} \hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = \hat{\Phi}^\top(\hat{\Phi}\hat{\Phi}^\top + \lambda n I^\top)^{-1}\hat{y}$$

Sketch of the Proof

- Let $\hat{\Phi} = U\Sigma V^\top$ be the Singular Value Decomposition of $\hat{\Phi}$
- $U^\top U = I_{n\times n}$, $V^\top V = I_{n\times n}$
- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. (Note that $\Sigma = \Sigma^\top$)

$$w = \hat{\Phi}^\top c$$

with $c = (\hat{\Phi}\hat{\Phi}^\top + \lambda n I^\top)^{-1}\hat{y}$

Representer Theorem for general Loss Functions

For a given loss function $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, let the problem be

$$w^* = \arg\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \phi(x_i)^\top w) + \lambda \|w\|^2$$

The solution can always be written as $w^* = \hat{\Phi}^\top c$ for some coefficients vector $c = (c_1, \ldots, c_n)$

Representer Theorem for general Loss Functions

Let define the linear subspace $\hat{W}$ as $\hat{W} = \{\hat{\Phi}^\top c \mid c \in \mathbb{R}^n\}$.

Representer Theorem for general Loss Functions

Let define the linear subspace $\hat{W}$ as $\hat{W} = \{\hat{\Phi}^\top c \mid c \in \mathbb{R}^n\}$.
By definition of linear subspace we have that

$$w = \hat{w} \ + \ w_\perp \quad \text{for each } w \in \mathbb{R}^D$$

with $\hat{w} \in \hat{W}$ and $v^\top w_\perp = 0$ for each $v \in \hat{W}$.

Representer Theorem for general Loss Functions

Let define the linear subspace $\hat{W}$ as $\hat{W} = \{\hat{\Phi}^\top c \mid c \in \mathbb{R}^n\}$.
By definition of linear subspace we have that

$$w = \hat{w} \; + \; w_\perp \quad \text{for each } w \in \mathbb{R}^D$$

with $\hat{w} \in \hat{W}$ and $v^\top w_\perp = 0$ for each $v \in \hat{W}$.
Moreover note that for each $i \in \{1, \dots n,\}$ we have $\phi(x_i) \in \hat{W}$.

Representer Theorem for general Loss Functions

Let define the linear subspace $\hat{W}$ as $\hat{W} = \{\hat{\Phi}^\top c \mid c \in \mathbb{R}^n\}$.
By definition of linear subspace we have that

$$w = \hat{w} \; + \; w_\perp \quad \text{for each } w \in \mathbb{R}^D$$

with $\hat{w} \in \hat{W}$ and $v^\top w_\perp = 0$ for each $v \in \hat{W}$.
Moreover note that for each $i \in \{1, \dots n, \}$ we have $\phi(x_i) \in \hat{W}$.
Therefore for any x_i with $i \in \{1, \dots, n\}$

$$\phi(x_i)^\top w = \phi(x_i)^\top \hat{w} \; + \; \phi(x_i)^\top w_\perp$$

Representer Theorem for general Loss Functions

Let define the linear subspace $\hat{W}$ as $\hat{W} = \{\hat{\Phi}^\top c \mid c \in \mathbb{R}^n\}$.
By definition of linear subspace we have that

$$w = \hat{w} \, + \, w_\perp \quad \text{for each } w \in \mathbb{R}^D$$

with $\hat{w} \in \hat{W}$ and $v^\top w_\perp = 0$ for each $v \in \hat{W}$.
Moreover note that for each $i \in \{1, \dots n,\}$ we have $\phi(x_i) \in \hat{W}$.
Therefore for any x_i with $i \in \{1, \dots, n\}$

$$\phi(x_i)^\top w = \phi(x_i)^\top \hat{w} \, + \, \underbrace{\phi(x_i)^\top w_\perp}_{=0}$$

Representer Theorem for general Loss Functions

Let define the linear subspace $\hat{W}$ as $\hat{W} = \{\hat{\Phi}^\top c \mid c \in \mathbb{R}^n\}$.
By definition of linear subspace we have that

$$w = \hat{w} \ + \ w_\perp \quad \text{for each } w \in \mathbb{R}^D$$

with $\hat{w} \in \hat{W}$ and $v^\top w_\perp = 0$ for each $v \in \hat{W}$.
Moreover note that for each $i \in \{1, \dots n, \}$ we have $\phi(x_i) \in \hat{W}$.
Therefore for any x_i with $i \in \{1, \dots, n\}$

$$\phi(x_i)^\top w = \phi(x_i)^\top \hat{w}$$

Representer Theorem for general Loss Functions

Therefore the problem become

$$w^* = \arg\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} V(y_i, \phi(x_i)^\top \hat{w}) + \lambda \|w\|^2$$

Moreover, considering that $\hat{w}^\top w_\perp = 0$ we have

$$\|\hat{w}\| \leq \|\hat{w}\| + \|w_\perp\| = \|w\|$$

Representer Theorem for general Loss Functions

Therefore the problem become

$$w^* = \arg\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} V(y_i, \phi(x_i)^\top \hat{w}) + \lambda \|w\|^2$$

Moreover, considering that $\hat{w}^\top w_\perp = 0$ we have

$$\|\hat{w}\| \leq \|\hat{w}\| + \|w_\perp\| = \|w\|$$

Now let $w^* = \hat{w}^* + w_\perp^*$. The problem is minimized when $w_\perp^* = 0$.

Representer Theorem for general Loss Functions

Therefore the problem become

$$w^* = \arg\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} V(y_i, \phi(x_i)^\top \hat{w}) + \lambda \|w\|^2$$

Moreover, considering that $\hat{w}^\top w_\perp = 0$ we have

$$\|\hat{w}\| \leq \|\hat{w}\| + \|w_\perp\| = \|w\|$$

Now let $w^* = \hat{w}^* + w^*_\perp$. The problem is minimized when $w^*_\perp = 0$. That is

$$w^* = \hat{\Phi}^\top c$$

for some $c \in \mathbb{R}^n$.

Why we need Kernels...

Let analyze the RLS solution for the Generalized Linear model, we have

$$f(x) = \phi(x)^\top \hat{\Phi}^\top (\hat{\Phi}\hat{\Phi}^\top + \lambda n I)^{-1} \hat{y}$$

Why we need Kernels...

Let analyze the RLS solution for the Generalized Linear model, we have

$$f(x) = \phi(x)^\top \hat{\Phi}^\top (\hat{\Phi}\hat{\Phi}^\top + \lambda n I)^{-1} \hat{y}$$

Here $\phi(x)^\top \hat{\Phi}^\top$ is in $\mathbb{R}^n$ and is

$$\phi(x)^\top \hat{\Phi}^\top = (\phi(x)^\top \phi(x_1), \ldots, \phi(x)^\top \phi(x_n)),$$

Why we need Kernels...

Let analyze the RLS solution for the Generalized Linear model, we have

$$f(x) = \phi(x)^\top \hat{\Phi}^\top (\hat{\Phi}\hat{\Phi}^\top + \lambda n I)^{-1} \hat{y}$$

Here $\phi(x)^\top \hat{\Phi}^\top$ is in $\mathbb{R}^n$ and is

$$\phi(x)^\top \hat{\Phi}^\top = (\phi(x)^\top \phi(x_1), \dots, \phi(x)^\top \phi(x_n)),$$

moreover $\hat{\Phi}\hat{\Phi}^\top$ is in $\mathbb{R}^{n \times n}$ and is

$$(\hat{\Phi}\hat{\Phi}^\top)_{ij} = \phi(x_i)^\top \phi(x_j).$$

Why we need Kernels...

Let analyze the RLS solution for the Generalized Linear model, we have

$$f(x) = \phi(x)^\top \hat{\Phi}^\top (\hat{\Phi}\hat{\Phi}^\top + \lambda n I)^{-1} \hat{y}$$

Here $\phi(x)^\top \hat{\Phi}^\top$ is in $\mathbb{R}^n$ and is

$$\phi(x)^\top \hat{\Phi}^\top = (\phi(x)^\top \phi(x_1), \dots, \phi(x)^\top \phi(x_n)),$$

moreover $\hat{\Phi}\hat{\Phi}^\top$ is in $\mathbb{R}^{n \times n}$ and is

$$(\hat{\Phi}\hat{\Phi}^\top)_{ij} = \phi(x_i)^\top \phi(x_j).$$

$f(x)$ is expressed only by using inner products between feature vectors

Why we need Kernels...

Idea: In order to express $f(x)$ we need only $\phi(x)^\top \phi(x')$ for each couple $x, x' \in \mathbb{R}^d$.

Why we need Kernels...

Idea: In order to express $f(x)$ we need only $\phi(x)^\top \phi(x')$ for each couple $x, x' \in \mathbb{R}^d$. Therefore we define the *Kernel* as

$$K(x, x') = \phi(x)^\top \phi(x')$$

Why we need Kernels...

Idea: In order to express $f(x)$ we need only $\phi(x)^\top \phi(x')$ for each couple $x, x' \in \mathbb{R}^d$. Therefore we define the *Kernel* as

$$K(x, x') = \phi(x)^\top \phi(x')$$

In this way we have

$$f(x) = \hat{K}_x^\top (\hat{K} + \lambda n I)^{-1} \hat{y}$$

with $\hat{K}_x = (K(x, x_1), \dots, K(x, x_n)), \quad (\hat{K})_{ij} = K(x_i, x_j)$.

Why we need Kernels...

Idea: In order to express $f(x)$ we need only $\phi(x)^\top \phi(x')$ for each couple $x, x' \in \mathbb{R}^d$. Therefore we define the *Kernel* as

$$K(x, x') = \phi(x)^\top \phi(x')$$

In this way we have

$$f(x) = \hat{K}_x^\top (\hat{K} + \lambda n I)^{-1} \hat{y}$$

with $\hat{K}_x = (K(x, x_1), \ldots, K(x, x_n)), \quad (\hat{K})_{ij} = K(x_i, x_j)$.
We don't have to define an explicit ϕ, we need only to define a Kernel K

Why we need Kernels...

Idea: In order to express $f(x)$ we need only $\phi(x)^\top \phi(x')$ for each couple $x, x' \in \mathbb{R}^d$. Therefore we define the *Kernel* as

$$K(x, x') = \phi(x)^\top \phi(x')$$

In this way we have

$$f(x) = \hat{K}_x^\top (\hat{K} + \lambda n I)^{-1} \hat{y}$$

with $\hat{K}_x = (K(x, x_1), \ldots, K(x, x_n)), \quad (\hat{K})_{ij} = K(x_i, x_j)$.
We don't have to define an explicit ϕ, we need only to define a Kernel K
The same holds for general loss functions indeed

$$f(x) = \phi(x)^\top w^* = \phi(x)^\top \hat{\Phi}^\top c = \hat{K}_x^\top c = \sum_{i=1}^{n} c_i K(x, x_i).$$

Examples of Kernel: Linear Kernel

For $x, z \in \mathbb{R}^d$

$$K(x, z) = x^\top z$$

Proof

$$K(x, z) = \phi(x)^\top \phi(z)$$

with $\phi : \mathbb{R}^d \to \mathbb{R}^d$ defined as

$$\phi(x) = x.$$

Examples of Kernel: Affine Kernel

For $x, z \in \mathbb{R}^d$

$$K(x, z) = x^\top z + \alpha^2$$

Proof

$$K(x, z) = \phi(x)^\top \phi(z)$$

with $\phi : \mathbb{R}^d \to \mathbb{R}^{d+1}$ defined as

$$\phi(x) = (x, \alpha).$$

Examples of Kernel: Polynomial Kernel of degree p

For $p \in \mathbb{N}$

$$K(x, z) = (xz + 1)^p \quad \text{with } x, z \in \mathbb{R}$$

Proof

$$(xz + 1)^p = \sum_{k=0}^{p} q_{p,k} (xz)^k = \phi(x)^\top \phi(z)$$

with $q_{p,k} = \frac{p!}{k!(p-k)!}$ and $\phi : \mathbb{R} \to \mathbb{R}^{p+1}$ defined as

$$\phi(x) = (\sqrt{q_{p,0}}, \sqrt{q_{p,1}}x, \sqrt{q_{p,2}}x^2, \ldots, \sqrt{q_{p,k}}x^k, \ldots, \sqrt{q_{p,p}}x^p)$$

Examples of Kernel: Polynomial Kernel of degree p

For $p \in \mathbb{N}$

$$K(x, z) = (xz + 1)^p \quad \text{with } x, z \in \mathbb{R}$$

Proof

$$(xz + 1)^p = \sum_{k=0}^{p} q_{p,k} (xz)^k = \phi(x)^\top \phi(z)$$

with $q_{p,k} = \frac{p!}{k!(p-k)!}$ and $\phi : \mathbb{R} \to \mathbb{R}^{p+1}$ defined as

$$\phi(x) = (\sqrt{q_{p,0}}, \sqrt{q_{p,1}} x, \sqrt{q_{p,2}} x^2, \ldots, \sqrt{q_{p,k}} x^k, \ldots, \sqrt{q_{p,p}} x^p)$$

For $x, z \in \mathbb{R}^d$ it is defined as

$$K(x, z) = (x^\top z + 1)^p$$

Examples of Kernel: Polynomial Kernel of any degree

For $x, z \in [0,1]$ and $0 < \alpha < 1$

$$K(x,z) = \frac{1}{1 - \alpha^2 xz}$$

Proof

$$\frac{1}{1 - \alpha xz} = \sum_{k=0}^{\infty} (\alpha^2 xz)^k = \phi(x)^\top \phi(z)$$

with $\phi : \mathbb{R} \to \mathbb{R}^{\mathbb{N}}$ defined as

$$\phi(x) = (1, \alpha x, \alpha^2 x^2, \alpha^3 x^3, \dots)$$

Examples of Kernel: Polynomial Kernel of any degree

For $x, z \in [0,1]$ and $0 < \alpha < 1$

$$K(x,z) = \frac{1}{1 - \alpha^2 xz}$$

Proof

$$\frac{1}{1 - \alpha xz} = \sum_{k=0}^{\infty} (\alpha^2 xz)^k = \phi(x)^\top \phi(z)$$

with $\phi : \mathbb{R} \to \mathbb{R}^{\mathbb{N}}$ defined as

$$\phi(x) = (1, \alpha x, \alpha^2 x^2, \alpha^3 x^3, \dots)$$

ϕ is infinite dimensional, but $\phi(x)^\top \phi(x')$ is computed in constant time!!

Examples of Kernel: Polynomial Kernel of any degree

For $x, z \in [0, 1]$ and $0 < \alpha < 1$

$$K(x, z) = \frac{1}{1 - \alpha^2 xz}$$

Proof

$$\frac{1}{1 - \alpha xz} = \sum_{k=0}^{\infty} (\alpha^2 xz)^k = \phi(x)^\top \phi(z)$$

with $\phi : \mathbb{R} \to \mathbb{R}^{\mathbb{N}}$ defined as

$$\phi(x) = (1, \alpha x, \alpha^2 x^2, \alpha^3 x^3, \dots)$$

ϕ is infinite dimensional, but $\phi(x)^\top \phi(x')$ is computed in constant time!!
For $x, z \in \mathbb{R}^d$ it is defined as

$$K(x, z) = \frac{1}{1 - \alpha^2 x^\top z}$$

Kernel - Characterization

$K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a *Kernel* if it behaves like an inner product that is

1. it is symmetric

$$K(x, z) = K(z, x) \quad \text{for all } x, z \in \mathbb{R}^d$$

2. it is positive definite (p.d.).

Kernel - Characterization

$K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a *Kernel* if it behaves like an inner product that is

1. it is symmetric

$$K(x, z) = K(z, x) \quad \text{for all } x, z \in \mathbb{R}^d$$

2. it is positive definite (p.d.). For any $n \in \mathbb{N}$ and $x_1, \ldots, x_n \in \mathbb{R}^d$ define $\hat{K}$ as $(\hat{K})_{ij} = K(x_i, x_j)$.

Kernel - Characterization

$K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a *Kernel* if it behaves like an inner product that is

1. it is symmetric

$$K(x, z) = K(z, x) \quad \text{for all } x, z \in \mathbb{R}^d$$

2. it is positive definite (p.d.). For any $n \in \mathbb{N}$ and $x_1, \dots, x_n \in \mathbb{R}^d$ define $\hat{K}$ as $(\hat{K})_{ij} = K(x_i, x_j)$.

$$K \text{ is p.d.} \quad \text{iff} \quad \hat{K} \text{ is p.d. for any } n \in \mathbb{N}, x_1, \dots, x_n \in \mathbb{R}^d$$

The first is easy to check, the second is quite difficult!

Kernel properties

Let $K_1 : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}, K_2 : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}, K_3 : \mathbb{R}^t \times \mathbb{R}^t$ be Kernels and $x, x' \in \mathbb{R}^d$, $z, z' \in \mathbb{R}^t$ and $\alpha, \beta > 0$ then the following are Kernels too

1. $\alpha K_1(x, x') + \beta K_2(x, x')$
2. $K_1(x, x') K_2(x, x')$
3. $p(K_1(x, x'))$ for any p a function whose polynomial expansion has only non-negative coefficients
4. $f(x) K_1(x, x') f(x')$ for any $f : \mathbb{R}^d \to \mathbb{R}$
5. $\frac{K_1(x,x')}{\sqrt{K_1(x,x) K_1(x',x')}}$
6. $K_3(\psi(x), \psi(x))$ for any $\psi : \mathbb{R}^d \to \mathbb{R}^t$
7. $\alpha K_1(x, x') + \beta K_3(z, z')$
8. $K_1(x, x') K_3(z, z')$

Gaussian Kernel

Let $x, x' \in \mathbb{R}^d$ and $\sigma > 0$, the gaussian kernel is

$$K(x, x') = e^{-\frac{1}{2\sigma^2}\|x-x'\|^2}$$

Gaussian Kernel

Let $x, x' \in \mathbb{R}^d$ and $\sigma > 0$, the gaussian kernel is

$$K(x, x') = e^{-\frac{1}{2\sigma^2}\|x-x'\|^2}$$

Proof $K_1(x, x') = \frac{x^\top x'}{2\sigma^2}$ is a Kernel by Point 1

Gaussian Kernel

Let $x, x' \in \mathbb{R}^d$ and $\sigma > 0$, the gaussian kernel is

$$K(x, x') = e^{-\frac{1}{2\sigma^2}\|x-x'\|^2}$$

Proof $K_1(x, x') = \frac{x^\top x'}{2\sigma^2}$ is a Kernel by Point 1
Let $e^t = \sum_{k=1}^{\infty} \frac{t^k}{k!}$ has polynomial expansion with positive coefficients therefore the following is a Kernel (Point 3)

$$K_2(x, x') = e^{K_1(x,x')} = e^{\frac{x^\top x'}{2\sigma^2}}$$

is a Kernel.

Gaussian Kernel

Let $x, x' \in \mathbb{R}^d$ and $\sigma > 0$, the gaussian kernel is

$$K(x, x') = e^{-\frac{1}{2\sigma^2}\|x-x'\|^2}$$

Proof $K_1(x, x') = \frac{x^\top x'}{2\sigma^2}$ is a Kernel by Point 1
Let $e^t = \sum_{k=1}^{\infty} \frac{t^k}{k!}$ has polynomial expansion with positive coefficients therefore the following is a Kernel (Point 3)

$$K_2(x, x') = e^{K_1(x,x')} = e^{\frac{x^\top x'}{2\sigma^2}}$$

is a Kernel.
Let define $f(x) = e^{-\frac{x^\top x}{2\sigma^2}}$ then the following is a Kernel (Point 4)

$$K_3(x, x') = f(x) K_2(x, x') f(x')$$

Gaussian Kernel

Let $x, x' \in \mathbb{R}^d$ and $\sigma > 0$, the gaussian kernel is

$$K(x, x') = e^{-\frac{1}{2\sigma^2}\|x-x'\|^2}$$

Proof $K_1(x, x') = \frac{x^\top x'}{2\sigma^2}$ is a Kernel by Point 1
Let $e^t = \sum_{k=1}^{\infty} \frac{t^k}{k!}$ has polynomial expansion with positive coefficients therefore the following is a Kernel (Point 3)

$$K_2(x, x') = e^{K_1(x,x')} = e^{\frac{x^\top x'}{2\sigma^2}}$$

is a Kernel.
Let define $f(x) = e^{-\frac{x^\top x}{2\sigma^2}}$ then the following is a Kernel (Point 4)

$$K_3(x, x') = f(x)K_2(x, x')f(x')$$

But $K_3 = K$ indeed

$$K_3(x, x') = f(x)e^{\frac{x^\top x'}{\sigma^2}}f(x') = e^{-\frac{x^\top x + x'^\top x' - 2x^\top x'}{2\sigma^2}} = e^{\frac{-\|x-x'\|^2}{2\sigma^2}} = K(x, x')$$

Wrapping up

In this class we discussed how to deal with high dimensional non linear problems (feature maps and kernels). We also introduced the Represented Theorem.

Next class

Beyond prediction, we will focus more on data exploration and learning of interpretable models.