MLCC 2019
Regularization Network II: Kernels

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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 $w \in \mathbb{R}^d$: $y = w^\top x$
- Tikhonov regularization

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_w(x_i)) + \lambda \|w\|^2$$

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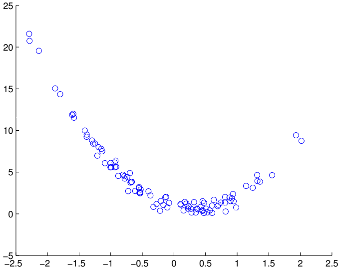
- Linear model $w \in \mathbb{R}^d$

$$f_w(x) = w^\top x$$

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



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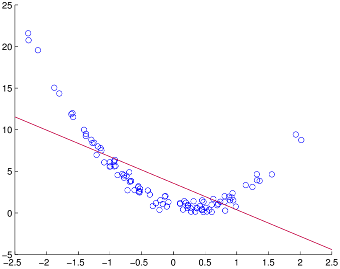

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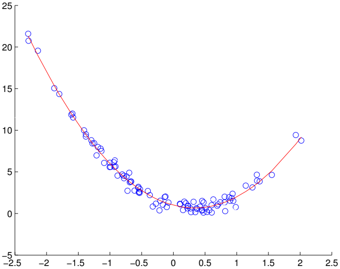

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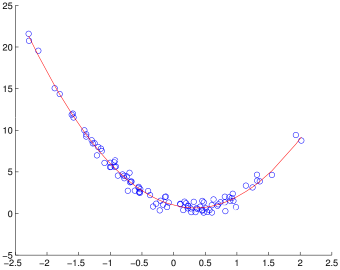
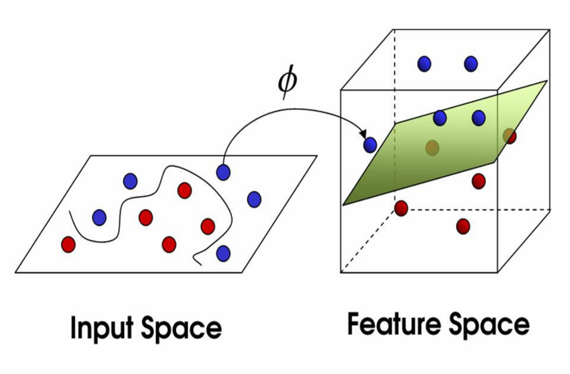


Geometric view

$$f(x) = w^\top \Phi(x)$$



Non linear models

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

Nonlinear model

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

How to compute a non linear model (least squares)

Let $\hat{\Phi} = (\phi(x_1), \dots, \phi(x_n))^\top \in \mathbb{R}^D$.

$\hat{\Phi}$ is the data matrix in the feature space (simply $\hat{X}$ if ϕ is the identity).

For RLS

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

Can we do better?
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Representer Theorem (in the least squares context)
If w solves RLS then

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

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

Sketch of the Proof

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

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

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 $c = (c_1, \ldots, c_n)$

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

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

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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

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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

$$f(x) = \phi(x)^\top \hat{\Phi}^\top c = \sum_{j=1}^{D} \varphi_j(x)\varphi_j(x_i)c_i$$

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

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In this way we have

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

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

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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

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

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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

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

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

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

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

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

Examples of Kernel: Gaussian Kernel

For $X = \mathbb{R}$ and $\gamma > 0$ consider

$$K(x, x') = e^{-|x-\bar{x}|^2\gamma}$$

Proof Let

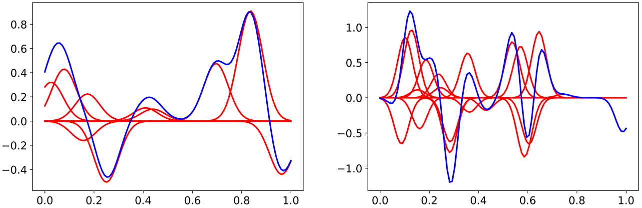
$$\varphi_j(x) = x^{j-1} e^{-x^2\gamma} \sqrt{\frac{(2\gamma)^{(j-1)}}{(j-1)!}}, \qquad j = 2, \ldots, \infty$$

with $\varphi_1(x) = 1$.
Then

$$\begin{aligned} \sum_{j=1}^{\infty} \varphi_j(x)\varphi_j(\bar{x}) &= \sum_{j=1}^{\infty} x^{j-1} e^{-x^2\gamma} \sqrt{\frac{(2\gamma)^{j-1}}{(j-1)!}} \bar{x}^{j-1} e^{-\bar{x}^2\gamma} \sqrt{\frac{(2\gamma)^{j-1}}{(j-1)!}} \\ &= e^{-x^2\gamma} e^{-\bar{x}^2\gamma} \sum_{j=1}^{\infty} \frac{(2\gamma)^{j-1}}{(j-1)!} (x\bar{x})^{j-1} = e^{-x^2\gamma} e^{-\bar{x}^2\gamma} e^{2x\bar{x}^2\gamma} \\ &= e^{-|x-\bar{x}|^2\gamma} \end{aligned}$$

A key result

Functions defind by Gaussian kernels with large and small widths.



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

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

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

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

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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.