The Representer Theorem

Theorem 4 *Given: a p.d. kernel* k *on* $\mathcal{X} \times \mathcal{X}$, *a training set* $(x_1, y_1), \ldots, (x_m, y_m) \in \mathcal{X} \times \mathbb{R}$, *a strictly monotonic increasing real-valued function* Ω *on* $[0, \infty[$, *and an arbitrary cost function* $c : (\mathcal{X} \times \mathbb{R}^2)^m \to \mathbb{R} \cup \{\infty\}$

Any $f \in \mathcal{F}$ *minimizing the regularized risk functional*

$$c\left((x_1, y_1, f(x_1)), \ldots, (x_m, y_m, f(x_m))\right) + \Omega\left(\|f\|\right) \tag{3}$$

admits a representation of the form

$$f(.) = \sum_{i=1}^{m} \alpha_i k(x_i, .).$$

Mercer's Theorem

If k is a continuous kernel of a positive definite integral operator on $L_2(\mathcal{X})$ (where $\mathcal{X}$ is some compact space),

$$\int_{\mathcal{X}} k(x, x') f(x) f(x') \, dx \, dx' \geq 0,$$

it can be expanded as

$$k(x, x') = \sum_{i=1}^{\infty} \lambda_i \psi_i(x) \psi_i(x')$$

using eigenfunctions ψ_i and eigenvalues $\lambda_i \geq 0$ [41].

The Mercer Feature Map

In that case

$$\Phi(x) := \begin{pmatrix} \sqrt{\lambda_1}\psi_1(x) \\ \sqrt{\lambda_2}\psi_2(x) \\ \vdots \end{pmatrix}$$

satisfies $\langle \Phi(x), \Phi(x') \rangle = k(x, x')$.

Proof:

$$\langle \Phi(x), \Phi(x') \rangle = \left\langle \begin{pmatrix} \sqrt{\lambda_1}\psi_1(x) \\ \sqrt{\lambda_2}\psi_2(x) \\ \vdots \end{pmatrix}, \begin{pmatrix} \sqrt{\lambda_1}\psi_1(x') \\ \sqrt{\lambda_2}\psi_2(x') \\ \vdots \end{pmatrix} \right\rangle$$

$$= \sum_{i=1}^{\infty} \lambda_i \psi_i(x) \psi_i(x') = k(x, x')$$

Positive Definite Kernels

It can be shown that (modulo some details) the admissible class of kernels coincides with the one of positive definite (pd) kernels: kernels which are symmetric, and for

- any set of training points $x_1, \ldots, x_m \in \mathcal{X}$ and
- any $a_1, \ldots, a_m \in \mathbb{R}$

satisfy

$$\sum_{i,j} a_i a_j K_{ij} \geq 0, \quad \text{where } K_{ij} := k(x_i, x_j).$$

Elementary Properties of PD Kernels

Kernels from Feature Maps.
If Φ maps $\mathcal{X}$ into a dot product space $\mathcal{H}$, then $\langle \Phi(x), \Phi(x') \rangle$ is a pd kernel on $\mathcal{X} \times \mathcal{X}$.

Positivity on the Diagonal.
$k(x, x) \geq 0$ for all $x \in \mathcal{X}$

Cauchy-Schwarz Inequality.
$k(x, x')^2 \leq k(x, x)k(x', x')$ (Hint: compute the determinant of the Gram matrix)

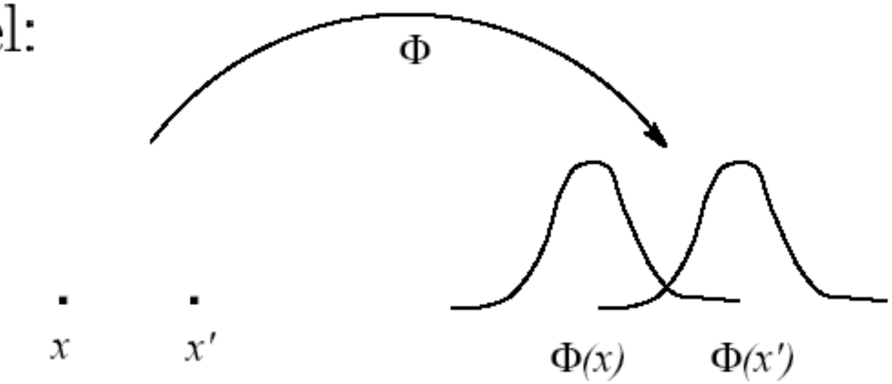
Vanishing Diagonals.
$k(x, x) = 0$ for all $x \in \mathcal{X} \Longrightarrow k(x, x') = 0$ for all $x, x' \in \mathcal{X}$

The Feature Space for PD Kernels [4, 1, 48]

- define a feature map

$$\begin{aligned} \Phi : \mathcal{X} &\to \mathbb{R}^{\mathcal{X}} \\ x &\mapsto k(.,x). \end{aligned}$$

E.g., for the Gaussian kernel:



Next steps:

- turn $\Phi(\mathcal{X})$ into a linear space
- endow it with a dot product satisfying $\langle k(.,x_i), k(.,x_j) \rangle = k(x_i, x_j)$
- complete the space to get a *reproducing kernel Hilbert space*

Endow it With a Dot Product

$$\langle f, g \rangle := \sum_{i=1}^{m} \sum_{j=1}^{m'} \alpha_i \beta_j k(x_i, x'_j)$$
$$= \sum_{i=1}^{m} \alpha_i g(x_i) = \sum_{j=1}^{m'} \beta_j f(x'_j)$$

- This is well-defined, symmetric, and bilinear.
- It can be shown that it is also strictly positive definite (hence it is a dot product).
- Complete the space in the corresponding norm to get a Hilbert space $\mathcal{H}_k$.

The Reproducing Kernel Property

Two special cases:

- Assume

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

In this case, we have

$$\langle k(., x), g \rangle = g(x).$$

- If moreover

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

we have the kernel trick

$$\langle k(., x), k(., x') \rangle = k(x, x').$$

k is called a *reproducing kernel* for $\mathcal{H}_k$.

Turn it Into a Linear Space

Form linear combinations

$$f(.) = \sum_{i=1}^{m} \alpha_i k(., x_i),$$

$$g(.) = \sum_{j=1}^{m'} \beta_j k(., x'_j)$$

$(m, m' \in \mathbb{N},\ \alpha_i, \beta_j \in \mathbb{R},\ x_i, x'_j \in \mathcal{X})$.

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Kernels

Recall that the dot product has to satisfy

$$\langle k(x,.), k(x',.)\rangle = k(x,x').$$

For a Mercer kernel

$$k(x,x') = \sum_{j=1}^{N_F} \lambda_j \psi_j(x)\psi_j(x')$$

(with $\lambda_i > 0$ for all i, $N_F \in \mathbb{N} \cup \{\infty\}$, and $\langle \psi_i, \psi_j \rangle_{L_2(\mathcal{X})} = \delta_{ij}$), this can be achieved by choosing $\langle .,. \rangle$ such that

$$\langle \psi_i, \psi_j \rangle = \delta_{ij}/\lambda_i.$$

ctd.

To see this, compute

$$\begin{aligned}\langle k(x,.), k(x',.)\rangle &= \left\langle \sum_i \lambda_i \psi_i(x)\psi_i, \sum_j \lambda_j \psi_j(x')\psi_j \right\rangle \\ &= \sum_{i,j} \lambda_i \lambda_j \psi_i(x)\psi_j(x')\langle \psi_i, \psi_j\rangle \\ &= \sum_{i,j} \lambda_i \lambda_j \psi_i(x)\psi_j(x')\delta_{ij}/\lambda_i \\ &= \sum_i \lambda_i \psi_i(x)\psi_i(x') \\ &= k(x,x').\end{aligned}$$

Some Properties of Kernels [53]

If $k_1, k_2, \ldots$ are pd kernels, then so are

- αk_1, provided $\alpha \geq 0$
- $k_1 + k_2$
- $k_1 \cdot k_2$
- $k(x, x') := \lim_{n\to\infty} k_n(x, x')$, provided it exists
- $k(A, B) := \sum_{x\in A, x'\in B} k_1(x, x')$, where A, B are finite subsets of $\mathcal{X}$
  (using the feature map $\tilde{\Phi}(A) := \sum_{x\in A} \Phi(x)$)

Further operations to construct kernels from kernels: tensor products, direct sums, convolutions [28].

Computing Distances in Feature Spaces

Clearly, if k is positive definite, then there exists a map Φ such that

$$\|\Phi(x) - \Phi(x')\|^2 = k(x,x) + k(x',x') - 2k(x,x')$$

(it is the usual feature map).

This embedding is referred to as a *Hilbert space representation* as a distance. It turns out that this works for a larger class of kernels, called *conditionally positive definite*.

In fact, all algorithms that are translationally invariant (i.e. independent of the choice of the origin) in $\mathcal{H}$ work with cpd kernels [53].