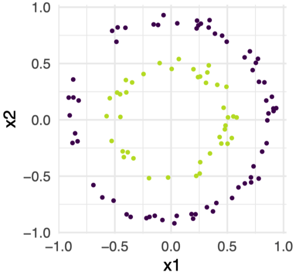
Introduction to Machine Learning

Reproducing Kernel Hilbert Space and Representer Theorem



Learning goals

- Know that for every kernel there is an associated feature map and space (Mercer's Theorem)
- Know that this feature map is not unique, and the reproducing kernel Hilbert space (RKHS) is a reference space
- Know the representation of the solution of a SVM is given by the representer theorem

KERNELS: MERCER'S THEOREM

- Kernels are symmetric, positive definite functions $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
- A kernel can be thought of as a shortcut computation for a two-step procedure: the feature map and the inner product.

Mercer's theorem says that for every kernel there exists an associated (well-behaved) feature space where the kernel acts as a dot-product.

- There exists a Hilbert space Φ of continuous functions $\mathcal{X} \to \mathbb{R}$ (think of it as a vector space with inner product where all operations are meaningful, including taking limits of sequences; this is non-trivial in the infinite-dimensional case)
- and a continuous "feature map" $\phi : \mathcal{X} \to \Phi$,
- so that the kernel computes the inner product of the features:

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle .$$

REPRODUCING KERNEL HILBERT SPACE

- There are many possible Hilbert spaces and feature maps for the same kernel, but they are all “equivalent” (isomorphic).
- It is often helpful to have a reference space for a kernel $k(\cdot,\cdot)$, called the **reproducing kernel Hilbert space (RKHS)**.
- The feature map of this space is

$$\phi : \mathcal{X} \to \mathcal{C}(\mathcal{X}) \,; \quad \mathbf{x} \mapsto k(\mathbf{x}, \cdot) \ ,$$

  where $\mathcal{C}(\mathcal{X})$ is the space of continuous functions $\mathcal{X} \to \mathbb{R}$. The "features" of the RKHS are the kernel functions evaluated at an **x**.
- The Hilbert space is the completion of the span of the features:

$$\Phi = \overline{\text{span}\{\phi(\mathbf{x}) \,|\, \mathbf{x} \in \mathcal{X}\}} \subset \mathcal{C}(\mathcal{X}) \ .$$

- The so-called **reproducing property** states:

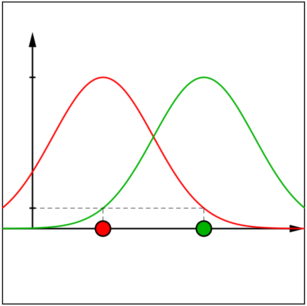
$$\langle k(\mathbf{x}, \cdot), k(\tilde{\boldsymbol{x}}, \cdot)\rangle = \langle \phi(\mathbf{x}), \phi(\tilde{\boldsymbol{x}})\rangle = k(\mathbf{x}, \tilde{\boldsymbol{x}}).$$

REPRODUCING KERNEL HILBERT SPACE

- The RKHS provides us with a useful interpretation:
  an input $\mathbf{x} \in \mathcal{X}$ mapped to the **basis function** $\phi(\mathbf{x}) = k(\mathbf{x}, \cdot)$.
- The kernel maps 2 points and computes the inner product:

$$\langle k(\mathbf{x}, \cdot), k(\tilde{\mathbf{x}}, \cdot) \rangle = k(\mathbf{x}, \tilde{\mathbf{x}}) \ .$$

- This is best illustrated with the Gaussian kernel.



REPRODUCING KERNEL HILBERT SPACE

- Caveat: Not all elements of the Hilbert space are of the form $k(\mathbf{x}, \cdot)$ for some $\mathbf{x} \in \mathcal{X}$!
- A general element in the span takes the form

$$\sum_{i=1}^{n} \alpha_i k\left(\mathbf{x}^{(i)}, \cdot\right) \in \Phi \ .$$

- A general element in the closure of the span takes the form

$$\sum_{i=1}^{\infty} \alpha_i k\left(\mathbf{x}^{(i)}, \cdot\right) \in \Phi \ .$$

  with $\sum_{i=1}^{\infty} \alpha_i^2 < \infty$.

REPRODUCING KERNEL HILBERT SPACE

What is $\langle f, g \rangle$ for two elements

$$f = \sum_{i=1}^{n} \alpha_i k\left(\mathbf{x}^{(i)}, \cdot\right), \qquad g = \sum_{j=1}^{m} \beta_j k\left(\mathbf{x}^{(j)}, \cdot\right) \ ?$$

We use the bilinearity of the inner product:

$$\begin{aligned}
\left\langle \sum_{i=1}^{n} \alpha_i k\left(\mathbf{x}^{(i)}, \cdot\right), \sum_{j=1}^{m} \beta_j k\left(\mathbf{x}^{(j)}, \cdot\right) \right\rangle &= \sum_{i=1}^{n} \alpha_i \left\langle k\left(\mathbf{x}^{(i)}, \cdot\right), \sum_{j=1}^{m} \beta_j k\left(\mathbf{x}^{(j)}, \cdot\right) \right\rangle \\
&= \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j \left\langle k\left(\mathbf{x}^{(i)}, \cdot\right), k\left(\mathbf{x}^{(j)}, \cdot\right) \right\rangle \\
&= \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)
\end{aligned}$$

The kernel defines the inner products of all elements in the span of the basis functions.

REPRESENTER THEOREM

The **representer theorem** tells us that the solution of a support vector machine problem

$$\begin{aligned} \min_{\boldsymbol{\theta},\theta_0,\zeta^{(i)}} \quad & \frac{1}{2}\boldsymbol{\theta}^\top\boldsymbol{\theta} + C\sum_{i=1}^{n}\zeta^{(i)} \\ \text{s.t.} \quad & y^{(i)}\left(\left\langle\boldsymbol{\theta},\phi\left(\mathbf{x}^{(i)}\right)\right\rangle + \theta_0\right) \geq 1-\zeta^{(i)} \quad \forall\, i \in \{1,\ldots,n\}, \\ \text{and} \quad & \zeta^{(i)} \geq 0 \quad \forall\, i \in \{1,\ldots,n\} \end{aligned}$$

can be written as

$$\boldsymbol{\theta} \;=\; \sum_{j=1}^{n}\beta_j\phi\left(\mathbf{x}^{(j)}\right)$$

for $\beta_j \in \mathbb{R}$.

REPRESENTER THEOREM

Theorem (Representer Theorem):
The solution $\boldsymbol{\theta}, \theta_0$ of the support vector machine optimization problem fulfills $\boldsymbol{\theta} \in V = \text{span}\left\{\phi\left(\mathbf{x}^{(1)}\right), \dots, \phi\left(\mathbf{x}^{(n)}\right)\right\}$.

Proof: Let $V^\perp$ denote the space orthogonal to V, so that $\Phi = V \oplus V^\perp$. The vector $\boldsymbol{\theta}$ has a unique decomposition into components $\boldsymbol{v} \in V$ and $\boldsymbol{v}^\perp \in V^\perp$, so that $\boldsymbol{v} + \boldsymbol{v}^\perp = \boldsymbol{\theta}$.

The regularizer becomes $\|\boldsymbol{\theta}\|^2 = \|\boldsymbol{v}\|^2 + \|\boldsymbol{v}^\perp\|^2$. The constraints $y^{(i)}\left(\left\langle\boldsymbol{\theta}, \phi\left(\mathbf{x}^{(i)}\right)\right\rangle + \theta_0\right) \geq 1 - \zeta^{(i)}$ do not depend on $\boldsymbol{v}^\perp$ at all:

$$\left\langle\boldsymbol{\theta}, \phi\left(\mathbf{x}^{(i)}\right)\right\rangle = \left\langle\boldsymbol{v}, \phi\left(\mathbf{x}^{(i)}\right)\right\rangle + \underbrace{\left\langle\boldsymbol{v}^\perp, \phi\left(\mathbf{x}^{(i)}\right)\right\rangle}_{=0} \quad \forall i \in \{1, 2, ..., n\}.$$

Thus, we have two independent optimization problems, namely the standard SVM problem for v and the unconstrained minimization problem of $\|v^\perp\|^2$ for $v^\perp$, with obvious solution $v^\perp = 0$. Thus, $\boldsymbol{\theta} = v \in V$.

REPRESENTER THEOREM

- Hence, we can restrict the SVM optimization problem to the **finite-dimensional** subspace $\text{span}\left\{\phi\left(\mathbf{x}^{(1)}\right), \ldots, \phi\left(\mathbf{x}^{(n)}\right)\right\}$. Its dimension grows with the size of the training set.
- More explicitly, we can assume the form

$$\boldsymbol{\theta} = \sum_{j=1}^{n} \beta_j \cdot \phi\left(\mathbf{x}^{(j)}\right)$$

  for the weight vector $\boldsymbol{\theta} \in \Phi$.
- The SVM prediction on $\mathbf{x} \in \mathcal{X}$ can be computed as

$$f(\mathbf{x}) = \sum_{j=1}^{n} \beta_j \left\langle \phi\left(\mathbf{x}^{(j)}\right), \phi(\mathbf{x}) \right\rangle + \theta_0 \ .$$

  It can be shown that the sum is **sparse**: $\beta_j = 0$ for non-support vectors.