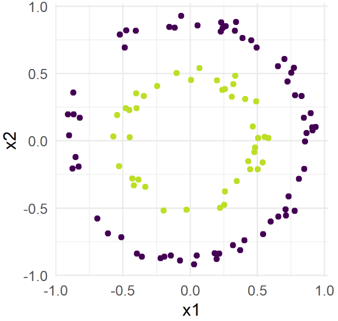
Introduction to Machine Learning

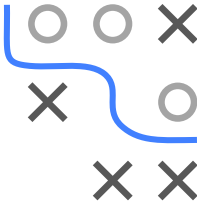
Nonlinear Support Vector Machines Reproducing Kernel Hilbert Space and Representer Theorem



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



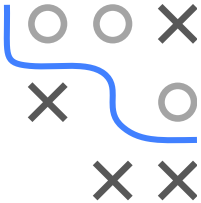
- Kernels are symmetric, positive definite functions $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
- A kernel can be thought of as a shortcut computation for a two-step procedure: the feature map and the inner product.

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 $\mathbf{x}$.
- 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:

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

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 $\boldsymbol{\theta} \in V = \operatorname{span}\left\{\phi\left(\mathbf{x}^{(1)}\right), \ldots, \phi\left(\mathbf{x}^{(n)}\right)\right\}$.

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, $\boldsymbol{\theta} = v \in V$.