Foundations of Machine Learning

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Week 5 Lab: Concept Check Exercises

Kernels

Kernel Learning Objectives

- Explain how explicit feature maps can be used to extend the expressivity of linear models.
- Explain potential issues explicitly computing large feature spaces.
- State and explain the definition of a 'kernelized' method.
- Explain why the SVM dual is kernelized, while the primal is not (ignoring the representer theorem).
- Give the relationship between a feature map and kernel function.
- Explain the computational benefits of kernelization based on costs of optimizing over $\mathbb{R}^n$ vs $\mathbb{R}^d$.
- Be able to apply the kernel trick using the kernel matrix K.
- Be able to apply the elements of our proof of the representer theorem (ex: projections decrease norms) to prove related theorems.
- Compare using the representer theorem and duality to kernelized SVM.
- Describe common kernels (RBF/polynomial) and their properties (i.e. equivalent feature maps, computational benefits relative to explicit computation (if possible),...).
- Describe some general recipes for deriving "new" kernel function.

Kernel Concept Check Questions

1. Fix $n > 0$. For $x, y \in \{1, 2, \ldots, n\}$ define $k(x, y) = \min(x, y)$. Give an explicit feature map $\varphi : \{1, 2, \ldots, n\}$ to $\mathbb{R}^D$ (for some D) such that $k(x, y) = \varphi(x)^T \varphi(y)$.

   Solution. Define $\varphi(x) = (\mathbf{1}(x \leq 1), \mathbf{1}(x \leq 2), \ldots, \mathbf{1}(x \leq n))$. Then $\varphi(x)^T \varphi(y) = \min(x, y)$.

2. Show that $k(x, y) = (x^T y)^4$ is a positive semidefinite kernel on $\mathbb{R}^d \times \mathbb{R}^d$.

   Solution. $k_1(x, y) = x^T y$ is a psd kernel, since $x^T y$ is an inner product on $\mathbb{R}^d$. Using the product rule for psd kernels, we see that

   $$k(x, y) = k_1(x, y)k_1(x, y)k_1(x, y)k_1(x, y) = k_1(x, y)^4$$

   is psd as well.

3. Let $A \in \mathbb{R}^{d \times d}$ be a positive semidefinite matrix. Prove that $k(x, y) = x^T A y$ is a positive semidefinite kernel.

   Solution. Fix $x_1, \ldots, x_n \in \mathbb{R}^d$ and let X denote the matrix that has x_i^T as its ith row. Then note that $(XAX^T)_{ij} = x_i^T A x_j = k(x_i, x_j)$. Thus we are done if we can show XAX^T is positive semidefinite. But note that, for any $\alpha \in \mathbb{R}^n$,

   $$\alpha^T XAX^T \alpha = (X^T \alpha)^T A (X^T \alpha) \geq 0,$$

   since A is positive semidefinite.

4. Consider the objective function

   $$J(w) = \|Xw - y\|_1 + \lambda \|w\|_2^2.$$

   Assume we have a positive semidefinite kernel k.

   (a) What is the kernelized version of this objective?

   (b) Given a new test point x, find the predicted value.

   Solution.

   (a) $J(\alpha) = \|K\alpha - y\|_1 + \lambda \alpha^T K \alpha$, where $K_{ij} = k(x_i, x_j)$. Here x_i^T is the ith row of X.

   (b) $f_\alpha(x) = \sum_{i=1}^n \alpha_i k(x_i, x)$.

5. Show that the standard 2-norm on $\mathbb{R}^n$ satisfies the parallelogram law.

   Solution.

   $$\begin{aligned} \|x - y\|_2^2 + \|x + y\|_2^2 &= (\|x\|_2^2 - 2x^T y + \|y\|_2^2) + (\|x\|_2^2 + 2x^T y + \|y\|_2^2) \\ &= 2\|x\|_2^2 + 2\|y\|_2^2. \end{aligned}$$

6. Suppose you are given an training set of distinct points $x_1, x_2, \ldots, x_n \in \mathbb{R}^n$ and labels $y_1, \ldots, y_n \in \{-1, +1\}$. Show that by properly selecting σ you can achieve perfect $0-1$ loss on the training data using a linear decision function and the RBF kernel.

   Solution. By selecting σ sufficiently small (say, much smaller than $\min_{i \neq j} \|x_i - x_j\|_2$) we can use $\alpha_i = y_i$ and get very pointy spikes at each data point. [Note: This is not possible if any repeated points have different labels, which is not unusual in real data.]

7. Suppose you are performing standard ridge regression, which you have kernelized using the RBF kernel. Prove that any decision function $f_\alpha(x)$ learned on a training set must satisfy $f_\alpha(x) \to 0$ as $\|x\|_2 \to \infty$.

   Solution. Since $f_\alpha(x) = \sum_{i=1}^n \alpha_i k(x_i, x)$ we have

$$\lim_{\|x\|_2 \to \infty} f_\alpha(x) = \lim_{\|x\|_2 \to \infty} \sum_{i=1}^n \alpha_i \exp\left(-\frac{\|x_i - x\|_2^2}{2\sigma^2}\right) = \sum_{i=1}^n \alpha_i \lim_{\|x\|_2 \to \infty} \exp\left(-\frac{\|x_i - x\|_2^2}{2\sigma^2}\right) = 0.$$

8. Consider the standard (unregularized) linear regression problem where we minimize $L(w) = \|Xw - y\|_2^2$ for some $X \in \mathbb{R}^{n \times m}$ and $y \in \mathbb{R}^n$. Assume $m > n$.

   (a) Let w^* be one minimizer of the loss function L above. Give an infinite set of minimizers of the loss function.

   (b) What property defines the minimizer given by the representer theorem (in terms of X)?

   Solution.

   (a) $\{w^* + v \mid v \in \text{null}(X)\}$. Using the standard inner product on $\mathbb{R}^n$, we can also write $\text{null}(X)$ as the set of all vectors orthogonal to the row space of X.

   (b) w^* lies in the row space of X.