Kernel Methods

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Contents

Bring in the feature map to kernelization

A kernelized objective

- Previously, we took the following optimization problem:

$$w^* \in \underset{w \in \mathcal{H}}{\arg\min}\, R\left(\|w\|\right) + L\left(\langle w, x_1 \rangle, \ldots, \langle w, x_n \rangle\right)$$

and kernelized it as

$$\alpha^* \in \underset{\alpha \in \mathbf{R}^n}{\arg\min}\, R\left(\sqrt{\alpha^T K \alpha}\right) + L\left(K\alpha\right),$$

where

$$K = \begin{pmatrix} \langle x_1, x_1 \rangle & \cdots & \langle x_1, x_n \rangle \\ \vdots & \ddots & \ldots \\ \langle x_n, x_1 \rangle & \cdots & \langle x_n, x_n \rangle \end{pmatrix} \quad \text{and} \quad k_x = \begin{pmatrix} \langle x_1, x \rangle \\ \vdots \\ \langle x_n, x \rangle \end{pmatrix}$$

- But computing K and k_x can be computationally hard for large feature spaces.
- To address this issue, we'll take a step back, and explicitly talk about feature maps.

The Input Space $\mathcal{X}$

- Our general learning theory setup: no assumptions about $\mathcal{X}$
- But $\mathcal{X} = \mathbf{R}^d$ for the specific methods we've developed:
    - Ridge regression
    - Lasso regression
    - Support Vector Machines
- Our hypothesis space for these was all affine functions on $\mathbf{R}^d$:

$$\mathcal{F} = \left\{ x \mapsto w^T x + b \mid w \in \mathbf{R}^d, b \in \mathbf{R} \right\}.$$

- What if we want to do prediction on inputs not natively in $\mathbf{R}^d$?

Linear Models with Explicit Feature Map

- **Input space**: $\mathcal{X}$
- **Feature space**: $\mathcal{H}$ (a Hilbert space, i.e. an inner product space with projections, e.g. $\mathbf{R}^d$)
- **Feature map**: $\psi : \mathcal{X} \to \mathcal{H}$
- Hypothesis space of affine functions on feature space:

$$\mathcal{F} = \{x \mapsto \langle w, \psi(x) \rangle + b \mid w \in \mathcal{H}, b \in \mathbf{R}\}.$$

Kernelized objective with feature map

- Optimization problem with explicit feature map:

$$w^* \in \underset{w \in \mathcal{H}}{\arg\min}\, R\left(\|w\|\right) + L\left(\langle w, \psi\left(x_1\right)\rangle, \ldots, \langle w, \psi\left(x_n\right)\rangle\right)$$

and kernelized it as

$$\alpha^* \in \underset{\alpha \in \mathbf{R}^n}{\arg\min}\, R\left(\sqrt{\alpha^T K \alpha}\right) + L\left(K\alpha\right),$$

where

$$K = \begin{pmatrix} \langle \psi\left(x_1\right), \psi\left(x_1\right)\rangle & \cdots & \langle \psi\left(x_1\right), \psi\left(x_n\right)\rangle \\ \vdots & \ddots & \cdots \\ \langle \psi\left(x_n\right), \psi\left(x_1\right)\rangle & \cdots & \langle \psi\left(x_n\right), \psi\left(x_n\right)\rangle \end{pmatrix} \quad \text{and} \quad k_x = \begin{pmatrix} \langle \psi\left(x_1\right), \psi\left(x\right)\rangle \\ \vdots \\ \langle \psi\left(x_n\right), \psi\left(x\right)\rangle \end{pmatrix}$$

The Kernel Function

The Kernel Function

- **Input space**: $\mathcal{X}$
- **Feature space**: $\mathcal{H}$ (a Hilbert space, i.e. an inner product space with projections, e.g. $\mathbf{R}^d$)
- **Feature map**: $\psi : \mathcal{X} \to \mathcal{H}$
- The **kernel function** corresponding to ψ in $\mathcal{H}$ is

$$k(x, x') = \left\langle \psi(x), \psi(x') \right\rangle,$$

where $\langle \cdot, \cdot \rangle$ is the inner product associated with $\mathcal{H}$.

The Kernel Function: Why do we need this?

- **Feature map**: $\psi : \mathcal{X} \to \mathcal{H}$
- The **kernel function** corresponding to ψ is

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

- Why introduce this new notation $k(x, x')$?
- We can often evaluate $k(x, x')$ without explicitly computing $\psi(x)$ and $\psi(x')$.
- For large feature spaces, can be much faster.

Kernel Evaluation Can Be Fast

Example

Quadratic feature map for $x = (x_1, \ldots, x_d) \in \mathbf{R}^d$.

$$\psi(x) = (x_1, \ldots, x_d, x_1^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_ix_j, \ldots \sqrt{2}x_{d-1}x_d)^T$$

has dimension $O(d^2)$, but for any $x, x' \in \mathbf{R}^d$ and the standard Euclidean dot products,

$$k(x, x') = \langle \psi(x), \psi(x') \rangle = \langle x, x' \rangle + \langle x, x' \rangle^2$$

- Explicit computation of $k(x, x')$: $O(d^2)$
- Implicit computation of $k(x, x')$: $O(d)$

Kernels as Similarity Scores

- Often useful to think of the kernel function as a **similarity score**.
- But this is not a mathematically precise statement.
- There are many ways to design a similarity score.
- We will use kernel functions that correspond to inner products in some feature space.
- These are called **Mercer kernels.**

What are the Benefits of Kernelization?

1. Computational (when optimizing over $\mathbf{R}^n$ is better than over $\mathbf{R}^d$)).
2. Can sometimes avoid any $O(d)$ operations
   - allows access to **infinite-dimensional feature spaces**.
3. Allows thinking in terms of "similarity" rather than features.

The Kernel Matrix

Definition

The **kernel matrix** for a kernel k on $x_1, \ldots, x_n \in \mathcal{X}$ is

$$K = \left(k(x_i, x_j)\right)_{i,j} = \begin{pmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & \ddots & \cdots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{pmatrix} \in \mathbf{R}^{n \times n}.$$

- In ML this is also called a **Gram matrix**, but traditionally (in linear algebra),
  - Gram matrices are defined without reference to a kernel or feature map.

The Kernel Matrix

- The kernel matrix summarizes all the information we need about the training inputs $x_1, \ldots, x_n$ to solve a kernelized optimization problem.
- e.g. in the kernelized SVM, we can replace $\psi(x_i)^T \psi(x_j)$ with K_{ij}:

$$\begin{array}{lll} \sup_{\alpha} & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j K_{ij} & \\ \text{s.t.} & \sum_{i=1}^{n} \alpha_i y_i = 0 \quad \text{and} \quad & \alpha_i \in \left[0, \frac{c}{n}\right] \; i = 1, \ldots, n. \end{array}$$

The "Kernel Trick"

1. Given a kernelized ML algorithm (i.e. all $\psi(x)$'s show up as $\langle \psi(x), \psi(x') \rangle$).
2. Can swap out the inner product for a new kernel function.
3. New kernel may correspond to a very high-dimensional feature space.
4. Once the kernel matrix is computed, the computational cost depends on number of data points, rather than the dimension of feature space.

The **trick** is that once you've implemented your method in terms of a kernel matrix, you can go from a kernel corresponding to a very small feature vector to a kernel corresponding to a very large (even infinite dimensional) feature vector, without changing your code, just by swapping one kernel matrix for another. Runtime is unaffected, after the kernel matrix is computed.

Our Plan

- Present our principal tool for kernelization: the **representer theorem**
- To keep things clean, we'll drop the explicit feature map until we need it: $\psi(x) = x$.
- Discuss specific cases of kernel ridge regression and kernel SVM
- Discuss several kernels, including the famous RBF kernel.
- Discuss how to create a kernel without an explicit feature map.

Kernels

Linear Kernel

- Input space: $\mathcal{X} = \mathbf{R}^d$
- Feature space: $\mathcal{H} = \mathbf{R}^d$, with standard inner product
- Feature map

$$\psi(x) = x$$

- Kernel:

$$k(x, x') = x^T x'$$

Quadratic Kernel in $\mathbf{R}^d$

- Input space $\mathcal{X} = \mathbf{R}^d$
- Feature space: $\mathcal{H} = \mathbf{R}^D$, where $D = d + \binom{d}{2} \approx d^2/2$.
- Feature map:

$$\psi(x) = (x_1, \ldots, x_d, x_1^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_ix_j, \ldots \sqrt{2}x_{d-1}x_d)^T$$

- Then for $\forall x, x' \in \mathbf{R}^d$

$$\begin{aligned} k(x,x') &= \langle \psi(x), \psi(x') \rangle \\ &= \langle x, x' \rangle + \langle x, x' \rangle^2 \end{aligned}$$

- Computation for inner product with explicit mapping: $O(d^2)$
- Computation for implicit kernel calculation: $O(d)$.

Based on Guillaume Obozinski's Statistical Machine Learning course at Louvain, Feb 2014.

Polynomial Kernel in $\mathbf{R}^d$

- Input space $\mathcal{X} = \mathbf{R}^d$
- Kernel function:
$$k(x,x') = \left(1 + \langle x, x' \rangle\right)^M$$
- Corresponds to a feature map with all monomials up to degree M.
- For any M, computing the kernel has same computational cost
- Cost of explicit inner product computation grows rapidly in M.

The RBF Kernel

Radial Basis Function (RBF) / Gaussian Kernel

- Input space $\mathcal{X} = \mathbf{R}^d$

$$k(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right),$$

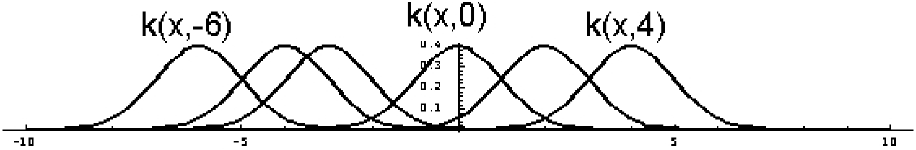
  where σ^2 is known as the bandwidth parameter.
- Does it act like a similarity score?
- Why "radial"?
- Have we departed from our "inner product of feature vector" recipe?
  - Yes and no: corresponds to an infinite dimensional feature vector
- Probably the most common nonlinear kernel.

RBF Basis

- Input space $\mathcal{X} = \mathbf{R}$
- Output space: $\mathcal{Y} = \mathbf{R}$
- RBF kernel $k(w,x) = \exp\left(-(w-x)^2\right)$.
- Suppose we have 6 training examples: $x_i \in \{-6,-4,-3,0,2,4\}$.
- If representer theorem applies, then

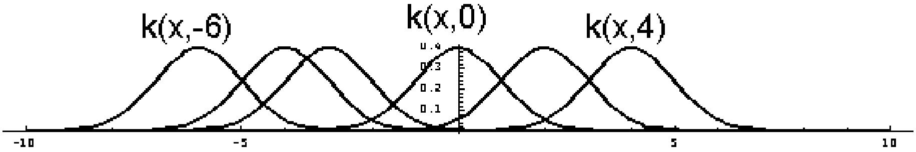
$$f(x) = \sum_{i=1}^{6} \alpha_i k(x_i, x).$$

- f is a linear combination of 6 basis functions of form $k(x_i,\cdot)$:

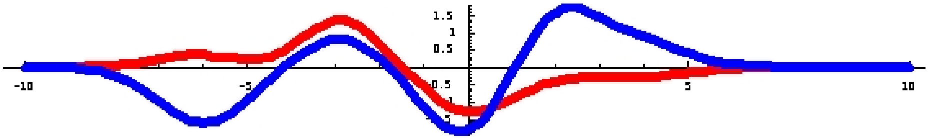


RBF Predictions

- Basis functions



- Predictions of the form $f(x) = \sum_{i=1}^{6} \alpha_i k(x_i, x)$:



- When kernelizing with RBF kernel, prediction functions always look this way.
- (Whether we get w from SVM, ridge regression, etc...)

RBF Feature Space: The Sequence Space ℓ_2

- To work with infinite dimensional feature vectors, we need a space with certain properties.
  - an inner product
  - a norm related to the inner product
  - projection theorem: $x = x_\perp + x_\|$ where $x_\| \in S = \text{span}(w_1, \ldots, w_n)$ and $\langle x_\perp, s \rangle = 0 \quad \forall s \in S$.
- Basically, we need a Hilbert space.

Definition

ℓ_2 is the space of all real-valued sequences: $(x_0, x_1, x_2, x_3, \ldots)$ with $\sum_{i=0}^{\infty} x_i^2 < \infty$.

Theorem

*With the the inner product $\langle x, x' \rangle = \sum_{i=0}^{\infty} x_i x_i'$, ℓ_2 is a **Hilbert space**.*

The Infinite Dimensional Feature Vector for RBF

- Consider RBF kernel (1-dim): $k(x,x') = \exp\left(-(x-x')^2/2\right)$
- We claim that $\psi : \mathbf{R} \to \ell_2$, defined by

$$[\psi(x)]_j = \frac{1}{\sqrt{j!}} e^{-x^2/2} x^j$$

gives the **"infinite-dimensional feature vector" corresponding to RBF kernel**.

- Is this mapping even well-defined? Is $\psi(x)$ even an element of ℓ_2?
- Yes:

$$\sum_{j=0}^{\infty} \frac{1}{j!} e^{-x^2} x^{2j} = e^{-x^2} \sum_{j=0}^{\infty} \frac{\left(x^2\right)^j}{j!} = 1 < \infty$$

.

The Infinite Dimensional Feature Vector for RBF

- Does feature vector $[\psi(x)]_n = \frac{1}{\sqrt{j!}} e^{-x^2/2} x^j$ actually correspond to the RBF kernel?
- Yes! Proof:

$$
\begin{aligned}
\left\langle \psi(x), \psi(x') \right\rangle &= \sum_{j=0}^{\infty} \frac{1}{j!} e^{-\left(x^2+(x')^2\right)/2} x^j \left(x'\right)^j \\
&= e^{-\left(x^2+(x')^2\right)/2} \sum_{j=0}^{\infty} \frac{(xx')^j}{j!} \\
&= \exp\left(-\left[x^2+\left(x'\right)^2\right]/2\right) \exp\left(xx'\right) \\
&= \exp\left(-\left[(x-x')^2/2\right]\right)
\end{aligned}
$$

QED

When is $k(x, x')$ a kernel function? (Mercer's Theorem)

How to Get Kernels?

1. Explicitly construct $\psi(x): \mathcal{X} \to \mathbf{R}^d$ and define $k(x, x') = \psi(x)^T \psi(x')$.
2. Directly define the kernel function $k(x, x')$, and verify it corresponds to $\langle \psi(x), \psi(x') \rangle$ for some ψ.

There are many theorems to help us with the second approach

Positive Semidefinite Matrices

Definition

A real, symmetric matrix $M \in \mathbf{R}^{n \times n}$ is **positive semidefinite (psd)** if for any $x \in \mathbf{R}^n$,

$$x^T M x \geqslant 0.$$

Theorem

The following conditions are each necessary and sufficient for a symmetric matrix M to be positive semidefinite:

- *M has can be factorized as $M = R^T R$, for some matrix R.*
- *All eigenvalues of M are greater than or equal to 0.*

Positive Semidefinite Function

Definition

A symmetric kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbf{R}$ is **positive semidefinite (psd)** if for any finite set $\{x_1, \ldots, x_n\} \in \mathcal{X}$, the kernel matrix on this set

$$K = \left(k(x_i, x_j)\right)_{i,j} = \begin{pmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & \ddots & \cdots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{pmatrix}$$

is a positive semidefinite matrix.

Mercer's Theorem

Theorem

A symmetric function $k(x,x')$ can be expressed as an inner product

$$k(x,x') = \left\langle \psi(x), \psi(x') \right\rangle$$

for some ψ if and only if $k(x,x')$ is ***positive semidefinite.***

Generating New Kernels from Old

- Suppose $k, k_1, k_2 : \mathcal{X} \times \mathcal{X} \to \mathbf{R}$ are psd kernels. Then so are the following:

$$
\begin{aligned}
k_{\text{new}}(x,x') &= k_1(x,x') + k_2(x,x') \\
k_{\text{new}}(x,x') &= \alpha k(x,x') \\
k_{\text{new}}(x,x') &= f(x)f(x') \text{ for any function } f(\cdot) \\
k_{\text{new}}(x,x') &= k_1(x,x')k_2(x,x')
\end{aligned}
$$

- See Appendix for details.
- Lots more theorems to help you construct new kernels from old...

Details on New Kernels from Old [Optional]

Additive Closure

- Suppose k_1 and k_2 are psd kernels with feature maps ϕ_1 and ϕ_2, respectively.
- Then
$$k_1(x,x') + k_2(x,x')$$
is a psd kernel.
- Proof: Concatenate the feature vectors to get
$$\phi(x) = (\phi_1(x), \phi_2(x)).$$
Then ϕ is a feature map for $k_1 + k_2$.

Closure under Positive Scaling

- Suppose k is a psd kernel with feature maps ϕ.
- Then for any $\alpha > 0$,

$$\alpha k$$

  is a psd kernel.
- Proof: Note that

$$\phi(x) = \sqrt{\alpha}\phi(x)$$

  is a feature map for αk.

Scalar Function Gives a Kernel

- For any function $f(x)$,
$$k(x,x') = f(x)f(x')$$
is a kernel.
- Proof: Let $f(x)$ be the feature mapping. (It maps into a 1-dimensional feature space.)
$$\langle f(x), f(x') \rangle = f(x)f(x') = k(x,x').$$

Closure under Hadamard Products

- Suppose k_1 and k_2 are psd kernels with feature maps ϕ_1 and ϕ_2, respectively.
- Then

$$k_1(x,x')k_2(x,x')$$

  is a psd kernel.
- Proof: Take the outer product of the feature vectors:

$$\phi(x) = \phi_1(x)\left[\phi_2(x)\right]^T.$$

  Note that $\phi(x)$ is a matrix.
- Continued...

Closure under Hadamard Products

- Then

$$
\begin{aligned}
\left\langle \phi(x), \phi(x') \right\rangle &= \sum_{i,j} \phi(x)\phi(x') \\
&= \sum_{i,j} \left[\phi_1(x) \left[\phi_2(x)\right]^T \right]_{ij} \left[\phi_1(x') \left[\phi_2(x')\right]^T \right]_{ij} \\
&= \sum_{i,j} \left[\phi_1(x)\right]_i \left[\phi_2(x)\right]_j \left[\phi_1(x')\right]_i \left[\phi_2(x')\right]_j \\
&= \left(\sum_i \left[\phi_1(x)\right]_i \left[\phi_1(x')\right]_i \right) \left(\sum_j \left[\phi_2(x)\right]_j \left[\phi_2(x')\right]_j \right) \\
&= k_1(x,x')k_2(x,x')
\end{aligned}
$$