Kernel Methods

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Setup and Motivation

The Input Space $\mathcal{X}$

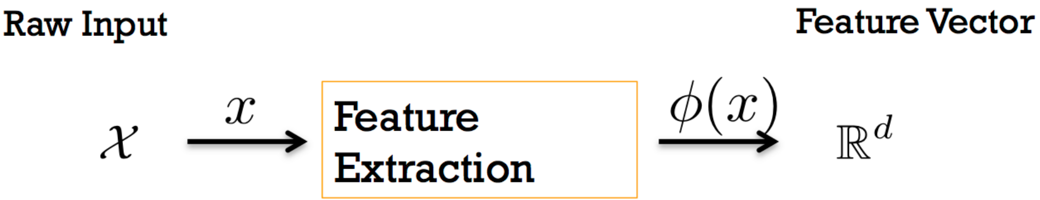
- Our general learning theory setup: no assumptions about $\mathcal{X}$
- But $\mathcal{X} = \mathbf{R}^d$ for the specific methods we've developed:
  - Ridge regression
  - Lasso regression
  - Support Vector Machines
- Our hypothesis space for these was all affine functions on $\mathbf{R}^d$:

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

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

Definition

Mapping an input from $\mathcal{X}$ to a vector in $\mathbf{R}^d$ is called **feature extraction** or **featurization**.

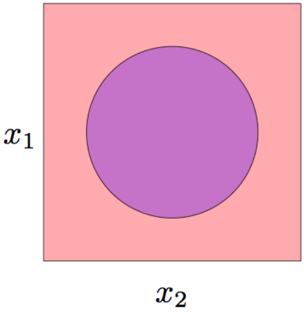


Linear Models with Explicit Feature Map

- Input space: $\mathcal{X}$ (no assumptions)
- Introduce **feature map** $\psi : \mathcal{X} \to \mathbf{R}^d$
- The feature map maps into the **feature space** $\mathbf{R}^d$.
- Hypothesis space of affine functions on feature space:

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

Geometric Example: Two class problem, nonlinear boundary



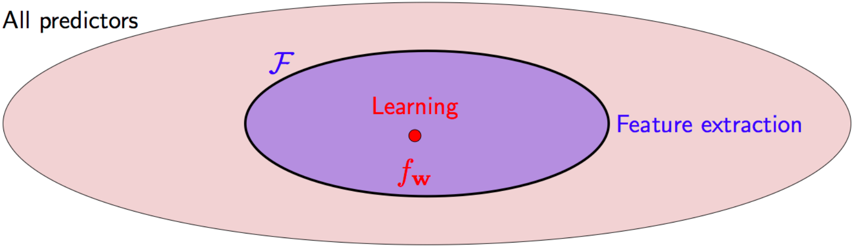
- With linear feature map $\phi(x) = (x_1, x_2)$ and linear models, can't separate regions
- With appropriate nonlinearity $\phi(x) = \left(x_1, x_2, x_1^2 + x_2^2\right)$, piece of cake.
- Video: http://youtu.be/3liCbRZPrZA

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

Expressivity of Hypothesis Space

- Consider a linear hypothesis space with a feature map $\phi : \mathcal{X} \to \mathbf{R}^d$:

$$\mathcal{F} = \{f(x) = w^T \phi(x)\}$$



Question: does $\mathcal{F}$ contain a good predictor?

We can grow the linear hypothesis space $\mathcal{F}$ by adding more features.

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

Linear Models Need Big Feature Spaces

- To get **expressive** hypothesis spaces using linear models,
  - need high-dimensional feature spaces
- Suppose we start with $x=(1,x_1,\ldots,x_d)\in\mathbf{R}^{d+1}=\mathcal{X}$.
- We want to add all monomials up to degree M: $x_1^{p_1}\cdots x_d^{p_d}$, with $p_1+\cdots+p_d\leqslant M$.
- How many features will we end up with?
- $\binom{M+d}{M}$ ("flower shop probem" from combinatorics)
- For $d=40$ and $M=8$, we get 377348994 features.
- That will make some extremely large matrices...

Big Feature Spaces

Very large feature spaces have two problems:

1. Overfitting
2. Memory and computational costs

- Overfitting we handle with regularization.
- "Kernel methods" can (sometimes) help with memory and computational costs.

Kernel Methods: Motivation

Review: Linear SVM and Dual

- The [featurized] SVM prediction function is the solution to

$$\min_{w\in\mathbf{R}^d,b\in\mathbf{R}} \frac{1}{2}\|w\|^2+\frac{c}{n}\sum_{i=1}^{n}\left(1-y_i\left[w^T\psi(x_i)+b\right]\right)_+ .$$

- Found it is equivalent to solve the dual problem to get α^*:

$$\begin{aligned}
\sup_{\alpha} \quad & \sum_{i=1}^{n}\alpha_i-\frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j \psi(x_j)^T\psi(x_i) \\
\text{s.t.} \quad & \sum_{i=1}^{n}\alpha_i y_i=0 \\
& \alpha_i\in\left[0,\frac{c}{n}\right] \quad i=1,\ldots,n.
\end{aligned}$$

- Notice: $\psi(x)$'s only show up as inner products with other x's.

Some Methods Can Be "Kernelized"

Definition

A method is **kernelized** if inputs only appear inside inner products: $\langle \psi(x), \psi(y) \rangle$ for $x, y \in \mathcal{X}$.

- The **kernel function** corresponding to ψ and inner product $\langle \cdot, \cdot \rangle$ is

$$k(x, y) = \langle \psi(x), \psi(y) \rangle .$$

- Why introduce this new notation $k(x, y)$?
- Turns out, we can often evaluate $k(x, y)$ directly,
  - without explicilty computing $\psi(x)$ and $\psi(y)$.
- For large feature spaces, can be much faster.

Kernel Evaluation Can Be Fast

Example

Quadratic feature map

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

has dimension $O(d^2)$, but for any $x^{(1)}, x^{(2)} \in \mathbf{R}^d$

$$k(x^{(1)}, x^{(2)}) = \left\langle \phi(x^{(1)}), \phi(x^{(2)}) \right\rangle = \left\langle x^{(1)}, x^{(2)} \right\rangle + \left\langle x^{(1)}, x^{(2)} \right\rangle^2$$

- Naively explicit computation of $k(w, x)$: $O(d^2)$
- Implicit computation of $k(w, x)$: $O(d)$

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 **Mercer kernels,** which correspond to inner products in some feature space.
  - Has many mathematical benefits.

What are the Benefits of Kernelization?

1. Computational (e.g. when feature space dimension d larger than sample size n).
2. Access to infinite-dimensional feature spaces.
3. Allows thinking in terms of "similarity" rather than features.

Example: SVM

SVM Dual

- Recall the SVM dual optimization problem

$$
\begin{aligned}
\sup_{\alpha} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_j^T x_i \\
\text{s.t.} \quad & \sum_{i=1}^{n} \alpha_i y_i = 0 \\
& \alpha_i \in \left[0, \frac{c}{n}\right] \quad i = 1, \ldots, n.
\end{aligned}
$$

- Can replace $x_j^T x_i$ by an arbitrary kernel $k(x_j, x_i)$.
- What kernel are we currently using?

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:

$$k(x_1, x_2) = x_1^T x_2$$

The Kernel Matrix (or the Gram Matrix)

Definition

For a set of $\{x_1, \ldots, x_n\}$ and an inner product $\langle \cdot, \cdot \rangle$ on the set, the **kernel matrix** or the **Gram matrix** is defined as

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

Then for the standard Euclidean inner product $\langle x_i, x_j \rangle = x_i^T x_j$, we have

$$K = XX^T$$

SVM Dual with Kernel Matrix

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

- Once our algorithm works with kernel matrices, we can change kernel just by changing the matrix.
- Size of matrix: $n \times n$, where n is the number of data points.
- Recall with ridge regression, we worked with $X^T X$, which is $d \times d$, where d is feature space dimension.

Some Nonlinear Kernels

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:

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

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

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

- 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:
$$k(w,x) = (1 + \langle w, x \rangle)^M$$
- 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.

Radial Basis Function (RBF) / Gaussian Kernel

- Input space $\mathcal{X} = \mathbf{R}^d$. $\forall w, x \in \mathbf{R}^d$,

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

  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.

Kernel Trick: Overview

The "Kernel Trick"

1. Given a kernelized ML algorithm.
2. Can swap out the inner product for a new kernel function.
3. New kernel may correspond to a high dimensional feature space.
4. Once kernel matrix is computed, computational cost depends on number of data points, rather than the dimension of feature space.

Swapping out a linear kernel for a new kernel is called the **kernel trick**.

Inner Product Spaces and Projections (Hilbert Spaces)

Inner Product Space (or "Pre-Hilbert" Spaces)

An **inner product space** (over reals) is a vector space $\mathcal{V}$ and an **inner product**, which is a mapping

$$\langle \cdot, \cdot \rangle : \mathcal{V} \times \mathcal{V} \to \mathbf{R}$$

that has the following properties $\forall x, y, z \in \mathcal{V}$ and $a, b \in \mathbf{R}$:

- Symmetry: $\langle x, y \rangle = \langle y, x \rangle$
- Linearity: $\langle ax + by, z \rangle = a \langle x, z \rangle + b \langle y, z \rangle$
- Positive-definiteness: $\langle x, x \rangle \geqslant 0$ and $\langle x, x \rangle = 0 \iff x = 0$.

Norm from Inner Product

For an inner product space, we define a norm as

$$\|x\| = \sqrt{\langle x, x \rangle}.$$

Example

$\mathbf{R}^d$ with standard Euclidean inner product is an inner product space:

$$\langle x, y \rangle := x^T y \qquad \forall x, y \in \mathbf{R}^d.$$

Norm is

$$\|x\| = \sqrt{x^T x}.$$

What norms can we get from an inner product?

Theorem (Parallelogram Law)

A norm $\|v\|$ can be generated by an inner product on $\mathcal{V}$ iff $\forall x, y \in \mathcal{V}$

$$2\|x\|^2 + 2\|y\|^2 = \|x+y\|^2 + \|x-y\|^2,$$

*and if it can, the inner product is given by the **polarization identity***

$$\langle x, y \rangle = \frac{\|x\|^2 + \|y\|^2 - \|x-y\|^2}{2}.$$

Example

ℓ_1 norm on $\mathbf{R}^d$ is NOT generated by an inner product. [Exercise]

Is ℓ_2 norm on $\mathbf{R}^d$ generated by an inner product?

Pythagorean Theroem

Definition

Two vectors are **orthogonal** if $\langle x, y\rangle = 0$. We denote this by $x \perp y$.

Definition

x is orthogonal to a set S, i.e. $x \perp S$, if $x \perp s$ for all $x \in S$.

Theorem (Pythagorean Theorem)

If $x \perp y$, *then* $\|x+y\|^2 = \|x\|^2 + \|y\|^2$.

Proof.

We have

$$\begin{aligned}
\|x+y\|^2 &= \langle x+y, x+y\rangle \\
&= \langle x,x\rangle + \langle x,y\rangle + \langle y,x\rangle + \langle y,y\rangle \\
&= \|x\|^2 + \|y\|^2
\end{aligned}$$

Projection onto a Plane (Rough Definition)

- Choose some $x \in \mathcal{V}$.
- Let M be a subspace of inner product space $\mathcal{V}$.
- Then m_0 is the **projection of** x **onto** M**,**
    - if $m_0 \in M$ and is the closest point to x in M.
- In math: For all $m \in M$,

$$\|x - m_0\| \leqslant \|x - m\|.$$

Hilbert Space

- Projections exist for all finite-dimensional inner product spaces.
- We want to allow infinite-dimensional spaces.
- Need an extra condition called **completeness**.
- A space is **complete** if all Cauchy sequences in the space converge.

Definition

A **Hilbert space** is a complete inner product space.

Example

Any finite dimensional inner product space is a Hilbert space.

The Projection Theorem

Theorem (Classical Projection Theorem)

- *$\mathcal{H}$ a Hilbert space*
- *M a closed subspace of $\mathcal{H}$ (picture a hyperplane through the origin)*
- *For any $x \in \mathcal{H}$, there **exists a unique** $m_0 \in M$ for which*

$$\|x - m_0\| \leqslant \|x - m\| \; \forall m \in M.$$

- *This m_0 is called the **[orthogonal] projection of** x **onto** M.*
- *Furthermore, $m_0 \in M$ is the projection of x onto M iff*

$$x - m_0 \perp M.$$

Projection Reduces Norm

Theorem

Let M be a closed subspace of $\mathcal{H}$. For any $x \in \mathcal{H}$, let $m_0 = \text{Proj}_M x$ be the projection of x onto M. Then

$$\|m_0\| \leqslant \|x\|,$$

with equality only when $m_0 = x$.

Proof.

$$\begin{aligned}
\|x\|^2 &= \|m_0 + (x - m_0)\|^2 \text{ (note: } x - m_0 \perp m_0 \text{ by Projection theorem)} \\
&= \|m_0\|^2 + \|x - m_0\|^2 \text{ by Pythagorean theorem} \\
\|m_0\|^2 &= \|x\|^2 - \|x - m_0\|^2
\end{aligned}$$

If $\|x - m_0\|^2 = 0$, then $x = m_0$, by definition of norm. □

Representer Theorem

Generalize from SVM Objective

- Featurized SVM objective:

$$\min_{w \in \mathbf{R}^d} \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\left(1 - y_i\left[\langle w, \psi(x_i)\rangle\right]\right)_+ .$$

- **Generalized objective**:

$$\min_{w \in \mathcal{H}} R(\|w\|) + L(\langle w, \psi(x_1)\rangle, \ldots, \langle w, \psi(x_n)\rangle),$$

where

- $R : \mathbf{R}^{\geqslant 0} \to \mathbf{R}$ is nondecreasing (**Regularization term**)
- and $L : \mathbf{R}^n \to \mathbf{R}$ is arbitrary. (**Loss term**)

- **Generalized objective**:

$$\min_{w \in \mathcal{H}} R\left(\|w\|\right) + L\left(\langle w, \psi(x_1)\rangle, \ldots, \langle w, \psi(x_n)\rangle\right),$$

where

  - $w, \psi(x_1), \ldots, \psi(x_n) \in \mathcal{H}$ for some Hilbert space $\mathcal{H}$. (We typically have $\mathcal{H} = \mathbf{R}^d$.)
  - $\|\cdot\|$ is the norm corresponding to the inner product of $\mathcal{H}$. (i.e. $\|w\| = \sqrt{\langle w, w\rangle}$)
  - $R : \mathbf{R}^{\geqslant 0} \to \mathbf{R}$ is nondecreasing (**Regularization term**), and
  - $L : \mathbf{R}^n \to \mathbf{R}$ is arbitrary (**Loss term**).

Generalized Linear Objective Function

- **Generalized objective**:

$$\min_{w \in \mathcal{H}} R(\|w\|) + L(\langle w, \psi(x_1)\rangle, \ldots, \langle w, \psi(x_n)\rangle),$$

- Why "linear"? $\langle w, \psi(x_i)\rangle$ is a generalization of predictions $w^T\psi(x_i)$
  - a linear function of $\psi(x_i) \in \mathbf{R}^d$.
- Ridge regression and SVM are of this form.
- What if we penalize with $\lambda\|w\|_2$ instead of $\lambda\|w\|_2^2$? Yes!.
- What if we use lasso regression? No! ℓ_1 norm does not correspond to an inner product.

The Representer Theorem

Theorem (Representer Theorem)

Let

$$J(w) = R(\|w\|) + L(\langle w, \psi(x_1)\rangle, \ldots, \langle w, \psi(x_n)\rangle),$$

where

- $w, \psi(x_1), \ldots, \psi(x_n) \in \mathcal{H}$ *for some Hilbert space* $\mathcal{H}$. *(We typically have* $\mathcal{H} = \mathbf{R}^d$.*)*
- $\|\cdot\|$ *is the norm corresponding to the inner product of* $\mathcal{H}$. *(i.e.* $\|w\| = \sqrt{\langle w, w\rangle}$*)*
- $R : \mathbf{R}^{\geqslant 0} \to \mathbf{R}$ *is nondecreasing (**Regularization term**), and*
- $L : \mathbf{R}^n \to \mathbf{R}$ *is arbitrary (**Loss term**).*

If $J(w)$ *has a minimizer, then it has a minimizer of the form* $w^* = \sum_{i=1}^n \alpha_i \psi(x_i)$.
[If R *is strictly increasing, then all minimizers have this form. (Proof in homework.)]*

The Representer Theorem (Proof)

1. Let w^* be a minimizer.
2. Let $M = \text{span}\left(\psi(x_1), \ldots, \psi(x_n)\right)$. [the **"span of the data"**]
3. Let $w = \text{Proj}_M w^*$. So $\exists \alpha$ s.t. $w = \sum_{i=1}^n \alpha_i \psi(x_i)$.
4. Then $w^\perp := w^* - w$ is orthogonal to M.
5. Projections decrease norms: $\|w\| \leqslant \|w^*\|$.
6. Since R is nondecreasing, $R(\|w\|) \leqslant R(\|w^*\|)$.
7. By (4), $\langle w^*, \psi(x_i)\rangle = \left\langle w + w^\perp, \psi(x_i)\right\rangle = \langle w, \psi(x_i)\rangle$.
8. $L\left(\langle w^*, \psi(x_1)\rangle, \ldots, \langle w^*, \psi(x_n)\rangle\right) = L\left(\langle w, \psi(x_1)\rangle, \ldots, \langle w, \psi(x_n)\rangle\right)$
9. $J(w) \leqslant J(w^*)$.
10. Therefore $w = \sum_{i=1}^n \alpha_i \psi(x_i)$ is also a minimizer.

Q.E.D.

Using Representer Theorem to Kernelize

Kernelized Predictions

- Consider $w = \sum_{i=1}^{n} \alpha_i \psi(x_i)$. (As representer theorem implies.)
- How do we make predictions for a given $x \in \mathcal{X}$?

$$
\begin{aligned}
f(x) = \langle w, \psi(x) \rangle &= \left\langle \sum_{i=1}^{n} \alpha_i \psi(x_i), \psi(x) \right\rangle \\
&= \sum_{i=1}^{n} \alpha_i \langle \psi(x_i), \psi(x) \rangle \\
&= \sum_{i=1}^{n} \alpha_i k(x_i, x)
\end{aligned}
$$

Note: $f(x)$ is a linear combination of $k(x_1, x), \ldots, k(x_n, x)$, all considered as functions of x.

Kernelized Regularization

- Consider $w=\sum_{i=1}^{n}\alpha_i\psi(x_i)$.
- What does $R(\|w\|)$ look like?

$$\begin{aligned}
\|w\|^2 &= \langle w,w\rangle \\
&= \left\langle \sum_{i=1}^{n}\alpha_i\psi(x_i), \sum_{j=1}^{n}\alpha_j\psi(x_j)\right\rangle \\
&= \sum_{i,j=1}^{n}\alpha_i\alpha_j\langle\psi(x_i),\psi(x_j)\rangle \\
&= \sum_{i,j=1}^{n}\alpha_i\alpha_j k(x_i,x_j)
\end{aligned}$$

(You should recognize the last expression as a quadratic form.)

The Kernel Matrix (a.k.a. Gram Matrix)

Definition

The **kernel matrix** or **Gram matrix** for a kernel k on a set $\{x_1,\ldots,x_n\}$ is

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

Kernelized Regularization: Matrix Form

- Consider $w = \sum_{i=1}^{n} \alpha_i \psi(x_i)$.
- What does $R(\|w\|)$ look like?

$$\begin{aligned}\|w\|^2 &= \sum_{i,j=1}^{n} \alpha_i \alpha_j k(x_i, x_j) \\ &= \alpha^T K \alpha\end{aligned}$$

- So $R(\|w\|) = R\left(\sqrt{\alpha^T K \alpha}\right)$.

Kernelized Predictions

- Write $f_\alpha(x) = \sum_{i=1}^n \alpha_i k(x, x_i)$. (Switched from $k(x_i, x)$ by symmetry of inner product.)
- Predictions on the training points have a particularly simple form:

$$
\begin{aligned}
\begin{pmatrix} f_\alpha(x_1) \\ \vdots \\ f_\alpha(x_n) \end{pmatrix} &= \begin{pmatrix} \alpha_1 k(x_1, x_1) + \cdots + \alpha_n k(x_1, x_n) \\ \vdots \\ \alpha_1 k(x_n, x_1) + \cdots + \alpha_n k(x_n, x_n) \end{pmatrix} \\
&= \begin{pmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & \ddots & \cdots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} \\
&= K\alpha
\end{aligned}
$$

Kernelized Objective

- Substituting

$$w = \sum_{i=1}^{n} \alpha_i \psi(x_i)$$

into generalized objective, we get

$$\min_{\alpha \in \mathbf{R}^n} R\left(\sqrt{\alpha^T K \alpha}\right) + L(K\alpha).$$

- No direct access to $\psi(x_i)$.
- All references are via kernel matrix K.
- This is the **kernelized objective function.**

- The SVM objective:

$$\min_{w \in \mathcal{H}} \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\left(1 - y_i\left[\langle w, \psi(x_i)\rangle\right]\right)_+ .$$

- Kernelizing yields

$$\min_{\alpha \in \mathbf{R}^n} \frac{1}{2}\alpha^T K \alpha + \frac{c}{n}\sum_{i=1}^{n}\left(1 - y_i\left(K\alpha\right)_i\right)_+$$

- Ridge Regression:

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2 + \lambda \|w\|^2$$

- Featurized Ridge Regression

$$\min_{w \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \left(\langle w, \psi(x_i) \rangle - y_i\right)^2 + \lambda \|w\|^2$$

- Kernelized Ridge Regression

$$\min_{\alpha \in \mathbf{R}^n} \frac{1}{n} \|K\alpha - y\|^2 + \lambda \alpha^T K \alpha,$$

where $y = (y_1, \ldots, y_n)^T$.

Prediction Functions with RBF Kernel

Radial Basis Function (RBF) / Gaussian Kernel

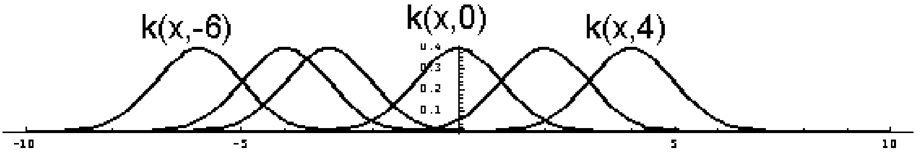
- Input space $\mathcal{X} = \mathbf{R}^d$
$$k(w,x) = \exp\left(-\frac{\|w-x\|^2}{2\sigma^2}\right),$$
where σ^2 is known as the bandwidth parameter.
- Does it act like a similarity score?
- Why "radial"?
- Have we departed from our "inner product of feature vector" recipe?
    - Yes and no: corresponds 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

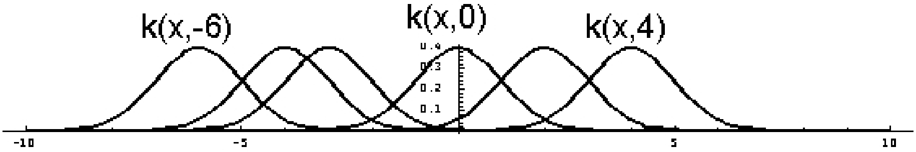
$$f(x) = \sum_{i=1}^{6} \alpha_i k(x_i, x).$$

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

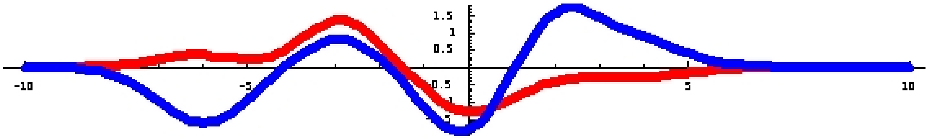


RBF Predictions

- 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: $x = x_\perp + x_\parallel$ where $x_\parallel \in S = \text{span}(w_1, \ldots, w_n)$ 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): $k(w,x) = \exp\left(-(w-x)^2/2\right)$
- We claim that $\psi : \mathbf{R} \to \ell_2$ defined by

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

  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:

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

.

The Infinite Dimensional Feature Vector for RBF

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

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

QED

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

How to Get Kernels?

1. Explicitly construct $\psi(x) : \mathcal{X} \to \mathbf{R}^d$ and define $k(x,w) = \psi(x)^T \psi(w)$.
2. Directly define the kernel function $k(x,w)$, and verify it corresponds to $\langle \psi(x), \psi(w) \rangle$ 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 M to be positive semidefinite:

- *M has a "square root", i.e. there exists R s.t. $M = R^T R$.*
- *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 $k(w,x)$ *can be expressed as an inner product*

$$k(w,x) = \langle \psi(w), \psi(x) \rangle$$

for some ψ *if and only if* $k(w,x)$ *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:

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

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

Details on New Kernels from Old

Additive Closure

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

$$k_1(w,x) + k_2(w,x)$$

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

Closure under Hadamard Products

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

$$k_1(w,x)k_2(w,x)$$

  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...

- Then

$$
\begin{aligned}
\langle \phi(x), \phi(w) \rangle &= \sum_{i,j} \phi(x)\phi(w) \\
&= \sum_{i,j} \left[\phi_1(x)\left[\phi_2(x)\right]^T\right]_{ij} \left[\phi_1(w)\left[\phi_2(w)\right]^T\right]_{ij} \\
&= \sum_{i,j} \left[\phi_1(x)\right]_i \left[\phi_2(x)\right]_j \left[\phi_1(w)\right]_i \left[\phi_2(w)\right]_j \\
&= \left(\sum_i \left[\phi_1(x)\right]_i \left[\phi_1(w)\right]_i\right) \left(\sum_j \left[\phi_2(x)\right]_j \left[\phi_2(w)\right]_j\right) \\
&= k_1(w,x)k_2(w,x)
\end{aligned}
$$