S&DS 365 / 665
Intermediate Machine Learning

Mercer Kernels

September 11

Yale

Please note

- Materials posted to `http://interml.ydata123.org`
- Readings from "Probabilistic Machine Learning: An Introduction"
- `https://probml.github.io/pml-book/book1.html`

Some reminders

- Assn 1 posted today
- Due at midnight, September 27 (two weeks)
- Topics: Lasso, smoothing, Mercer kernels, leave-one-out

Topics for today

- Calculation from last class
- Mercer kernels

Bias-variance for density estimation

Recall from last class: We derived an expression for the squared bias of kernel density estimation using a Taylor expansion

The calculation is very similar for the variance

Bias

Recall:

$$
\begin{aligned}
\mathbb{E}\widehat{f}(x) &= \frac{1}{nh^p} \sum_{i=1}^{n} \mathbb{E}K\left(\frac{X_i - x}{h}\right) \\
&= \frac{1}{h^p} \int K\left(\frac{u - x}{h}\right) f(u)\, du \\
&= \int K(v)\, f(x + hv)\, dv \\
&= \int K(v)\left(f(x) + hv^T \nabla f(x) + \frac{1}{2}h^2 v^T \nabla^2 f(x)v + o(h^2)\right) dv \\
&= f(x) + C(x)h^2 + o(h^2)
\end{aligned}
$$

using $\int K(u)\, du = 1$ and $\int u K(u)\, du = 0$

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Variance

By a similar argument, using $\text{Var}(X) \leq \mathbb{E}X^2$

$$
\begin{aligned}
\mathbb{E}\widehat{f}(x)^2 &\leq C_2 \frac{1}{n^2 h^{2p}} \sum_{i=1}^{n} \mathbb{E}K\left(\frac{X_i - x}{h}\right)^2 \\
&= C_2 \frac{1}{nh^{2p}} \int K\left(\frac{u - x}{h}\right)^2 f(u)\, du \\
&= C_2 \frac{f(x)}{nh^p} \int K(v)^2\, dv + o\left(\frac{1}{nh^p}\right) \\
&= C_2 \frac{f(x)}{nh^p} + o\left(\frac{1}{nh^p}\right)
\end{aligned}
$$

assuming $nh^p \to \infty$.

Risk

This gives

$$\text{bias}^2 \approx h^4$$

$$\text{var} \approx \frac{1}{nh^p}$$

On the assignment, you'll work with these expressions to reason about the smallest possible risk and the curse of dimensionality

Mercer Kernels: The big picture 🖼️

Instead of using local smoothing, we can optimize the fit to the data subject to regularization (penalization). Choose $\widehat{m}$ to minimize

$$\sum_i (Y_i - \widehat{m}(X_i))^2 + \lambda \, \text{penalty}(\widehat{m})$$

where penalty($\widehat{m}$) is a *roughness penalty*.

λ is a parameter that controls the amount of smoothing.

How do we construct a penalty that measures roughness? One approach is: *Mercer Kernels* and *RKHS = Reproducing Kernel Hilbert Spaces.*

What is a Mercer Kernel?

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A Mercer kernel has a special property: For any set of points $x_1, \ldots, x_n$ the $n \times n$ matrix

$$\mathbb{K} = \begin{bmatrix} K(x_i, x_j) \end{bmatrix}$$

is positive semidefinite (no negative eigenvalues)

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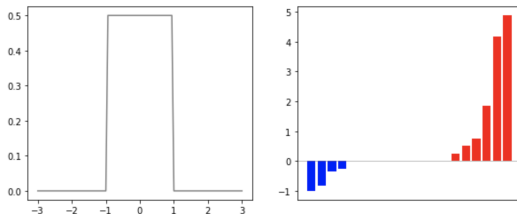
$$\mathbb{K} = \left[K(x_i, x_j) \right]$$

is positive semidefinite (no negative eigenvalues)

This property has many important (and beautiful!) mathematical consequences. It is a characterization of Mercer kernels.

Which of the kernels we used for smoothing are Mercer?
(demo)


```
In [8]: plot_eigenvalues(boxcar, 20)
```

Mercer Kernels: Key example

A Gaussian gives us a Mercer kernel:

$$K(x, x') = e^{-\frac{\|x - x'\|^2}{2h^2}}$$

Note: Here we fix the bandwidth h.

What is a Mercer Kernel?

A *Mercer kernel* $K(x, x')$ is symmetric and positive semidefinite bivariate function:

$$\int \int f(x)f(x')K(x, x')\,dx\,dx' \geq 0$$

for all (univariate) functions f.

Basis functions

We can create a set of *basis functions* based on K.

Fix z and think of $K(z, x)$ as a function of x. That is,

$$K(z, x) = K_z(x)$$

is a function of the second argument, with the first argument fixed.

Defining a norm from the kernel

Because of the positive semidefinite property, we can create an *inner product* and *norm* over the span of these functions

If $f(x) = \sum_r \alpha_r K_{z_r}(x)$, $g(x) = \sum_s \beta_s K_{y_s}(x)$, the inner product is

$$\langle f, g \rangle_K = \sum_r \sum_s \alpha_r \beta_s K(z_r, y_s)$$
$$= \alpha^T \mathbb{K} \beta$$

where $\mathbb{K} = [K(z_r, y_s)]$

Defining a norm from the kernel
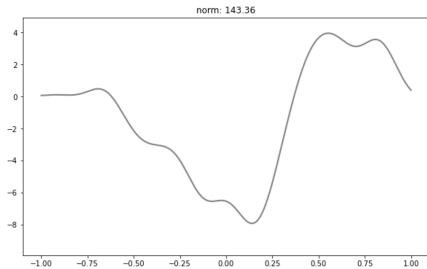
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The norm is

$$\|f\|_K^2 = \langle f, f \rangle_K = \sum_r \sum_s \alpha_r \alpha_s K(z_r, z_s)$$
$$= \alpha^T \mathbb{K} \alpha \geq 0$$

What do the functions look like?
(demo)

Defining a Hilbert space from the kernel

This gives us an infinite dimensional space of functions with a geometry — a notion of angle from the inner product $\langle \cdot, \cdot \rangle_K$

Technically speaking, we define the Hilbert space by "completing" the functions to include the limits of all Cauchy sequences with respect to the norm.

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It is called a *Reproducing Kernel Hilbert Space* (RKHS) because

$$\langle f, K_x(\cdot) \rangle_K = f(x)$$

That is, the kernel "reproduces" the values of the functions through the inner products

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Exercise: Verify this identity!

Nonparametric regression using Mercer kernels

The norm gives us a way to penalize functions for being too complex.

We carry out least squares regression subject to this penalty:

Minimize

$$\sum_{i=1}^{n} (Y_i - m(X_i))^2 + \lambda \|m\|_K^2.$$

over the RKHS of functions

Dilemma?

How do we carry out this penalized regression? It looks complicated!

Or maybe intractable...

Linear algebra to the rescue!

Representer Theorem

Let $\widehat{m}$ minimize

$$J(m) = \sum_{i=1}^{n}(Y_i - m(X_i))^2 + \lambda\|m\|_K^2.$$

Then

$$\widehat{m}(x) = \sum_{i=1}^{n} \alpha_i\, K(X_i, x)$$

for some $\alpha_1, \ldots, \alpha_n$.

So, we only need to find the coefficients

$$\alpha = (\alpha_1, \ldots, \alpha_n).$$

Mercer kernel regression

Plug $\widehat{m}(x) = \sum_{i=1}^{n} \alpha_i K(X_i, x)$ into J:

$$J(\alpha) = \| Y - \mathbb{K}\alpha \|^2 + \lambda \alpha^T \mathbb{K} \alpha$$

where $\mathbb{K}_{jk} = K(X_j, X_k)$

Now we find α to minimize J. We get (Assn 1):

$$\widehat{\alpha} = (\mathbb{K} + \lambda I)^{-1} Y$$

$$\widehat{m}(x) = \sum_i \widehat{\alpha}_i K(X_i, x)$$

Mercer kernel regression

The estimator depends on the amount of regularization λ.

Again, there is a bias-variance tradeoff.

We choose λ by cross-validation. This is like the bandwidth in smoothing kernel regression.

Takeaways

- Mercer kernels have a special property: When restricted to a finite sample they give positive semidefinite matrices

- This allows us to define an inner product and a norm

- We use the norm to do *penalization* of the functions

The underlying math is rich—see the notes if you want to learn more!

Smoothing Kernels *Versus* **Mercer Kernels**

Smoothing kernels: bandwidth h controls the amount of smoothing.
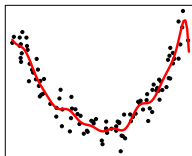
Mercer kernels: norm $\|f\|_K$ controls the amount of smoothing.

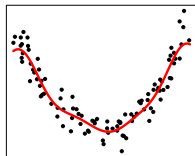*In practice these two methods give answers that are very similar.*
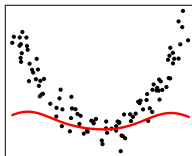
Mercer Kernels: Examples

very small lambda

small lambda

medium lambda

large lambda
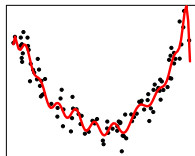
Kernels from features—and vice-versa

If $x \to \varphi(x) \in \mathbb{R}^d$ is a feature mapping, we can define a Mercer kernel by

$$K(x, x') = \varphi(x)^T \varphi(x')$$

Conversely, for any Mercer kernel we can derive the corresponding feature map (from the spectral theorem)

See the slides at the end

The importance of being Kernelist

- Mercer kernels play a central role in machine learning

- Why? We can define similarity functions that are kernels for all kinds of data — graphs, molecules, text documents

- Mercer kernels are also important for modern understanding of deep neural networks

Summary for today

- Smoothing methods compute local averages, weighting points by a kernel. The details of the kernel don't matter much

- Mercer kernels using penalization rather than smoothing

- Defining property: Matrix $\mathbb{K}$ is always positive semidefinite

- Equivalent to a type of ridge regression in function space

- The curse of dimensionality limits use of both approaches

Some technical details (optional)

Defining the inner product

Check that it is well defined:

If $f = \sum_r \alpha_r K(z_r, \cdot)$, $g = \sum_s \beta_s K(y_s, \cdot)$, the inner product is

$$\langle f, g \rangle_K = \sum_r \sum_s \alpha_r \beta_s K(z_r, y_s)$$
$$= \sum_r \alpha_r g(z_r)$$
$$= \sum_s \beta_s f(y_s)$$

using the reproducing property $\langle f, K(x, \cdot) \rangle = f(x)$

Representer theorem: Proof sketch

We can write any $f \in \mathcal{H}_K$ as

$$f(x) = \sum_i \alpha_i K(X_i, x) + v(x)$$

where v is orthogonal to the span of the functions $K(X_i, \cdot)$

By the reproducing property, $f(X_i)$ does not depend on v, and

$$\|f\|_K^2 = \alpha^T \mathbb{K} \alpha + \|v\|_K^2.$$

So, it must be that the minimizing function has $v = 0$

Feature maps

If *M* is symmetric, positive semidefinite matrix, can write

$$M = U^T \Lambda U$$

where *U* is an orthogonal matrix. Can rewrite this as

$$M = \Phi^T \Phi$$

where

$$\Phi = \sqrt{\Lambda} U$$

This transformation allows us to define *features* or *feature maps* for Mercer kernels

Features for Mercer kernels

Eigen-decomposition: $\{\psi_j\}$, $\{\lambda_j\}$ where

$$\int K(x, y)\psi_j(y)dy = \lambda_j \psi_j(x) \quad (K\psi_j = \lambda_j \psi_j)$$

The spectral theorem (see previous slide for finite dimensional case) tells us that

$$K(x, y) = \sum_{j=1}^{\infty} \lambda_j \psi_j(x)\psi_j(y)$$

We can think of the kernel in terms of the *feature map*

$$x \longrightarrow \Phi(x) = (\sqrt{\lambda_1}\psi_1(x), \sqrt{\lambda_2}\psi_2(x), \ldots)$$

Features for Mercer kernels (continued)

Since ψ_j forms an orthonormal basis, can write any function f as

$$f(x) = \sum_{r=1}^{\infty} a_r \psi_r(x)$$

By construction of the RKHS, can also write it as

$$f(x) = \sum_j \alpha_j K(x_j, x)$$

It follows that

$$\|f\|_K^2 = \sum_{r=1}^{\infty} \frac{a_r^2}{\lambda_r}$$

The functions that are smooth in the RKHS assign small weight to eigenfunctions with small eigenvalues