S&DS 365 / 665

Intermediate Machine Learning

Mercer Kernels

September 14

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 28 (two weeks)
- Topics: Lasso, smoothing, Mercer kernels, some neural nets

Topics for today

- Mercer kernels

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

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

where $\mathrm{penalty}(\widehat{\mathrm{m}})$ 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

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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)

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

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

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

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The norm is

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

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

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Exercise: Verify this identity!

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What do the functions look like?

(demo)

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!

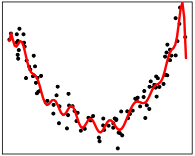
Smoothing Kernels *Versus* Mercer Kernels

Smoothing kernels: bandwidth h controls the amount of smoothing.

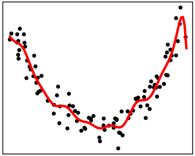
Mercer kernels: norm $\|f\|_K$ controls the amount of smoothing.

In practice these two methods give answers that are very similar.

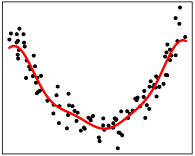
Mercer Kernels: Examples



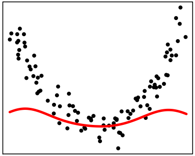
very small lambda



small lambda



medium lambda



large lambda

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

$$\begin{aligned} \langle f, g \rangle_K &= \sum_r \sum_s \alpha_r \beta_s K(z_r, y_s) \\ &= \sum_r \alpha_r g(z_r) \\ &= \sum_s \beta_s f(y_s) \end{aligned}$$

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