S&DS 365 / 665

Intermediate Machine Learning

Mercer Kernels

September 10

Yale

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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 25 (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 $\int uK(u)\,du = 0$

Variance

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

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

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

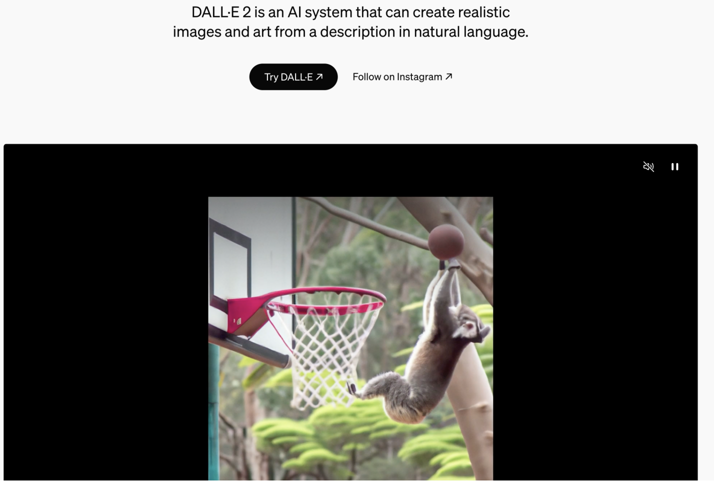
Generative models

- The KDE is a *generative model*
- We can sample from the density to “generate” a new data point
- What is an algorithm for sampling from the estimated distribution?

Generative models

1. Sample an index i uniformly from 1 to n
2. Sample a point x from a Gaussian with mean X_i and variance h^2

Generative models



Generative models

As we'll see later in the course, Transformers can be naturally seen as a form of kernel smoothing and kernel density estimation.

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

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

where penalty($\widehat{\text{m}}$) 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?

A kernel is a bivariate function $K(x, x')$. We think of this as a measure of “similarity” between points x and x'.

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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

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

is positive semidefinite (no negative eigenvalues)

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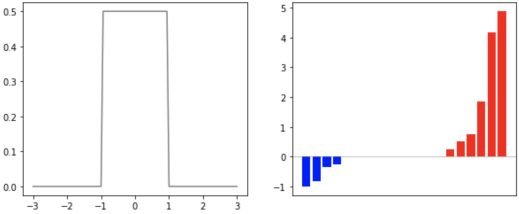
This property has many important (and beautiful!) mathematical consequences. It is a characterization of Mercer kernels.

Which of the kernels we used for smoothing are Mercer?

(demo)

```
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

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

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

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

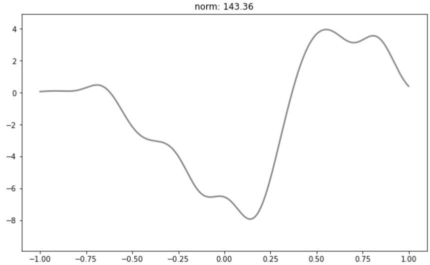
The norm is

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

What do the functions look like?

(demo)

```
plot_function(x, f, norm, sleeptime=1)
```



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!

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

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 *penalize* functions for being too rough

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

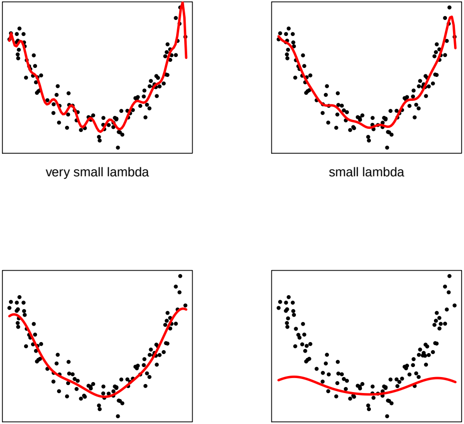
Smoothing Kernels *Versus* Mercer Kernels

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
  - Can define similarity functions that are kernels for all kinds of data — graphs, molecules, text documents
  - Gaussian processes
  - 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