S&DS 365 / 665

Intermediate Machine Learning

Syncing up in person

Monday, February 7

Yale

Topics for today

- Recap: Everything so far
- Explanations, derivations on board
- Kernel density estimation
- If time, begin neural networks

Notes

- Notes posted to course page
  `http://interml.ydata123.org`
- Bias-variance tradeoff for smoothing
- More material on Mercer kernels 

Nonparametric Regression

Given $(X_1, Y_1), \ldots, (X_n, Y_n)$ predict Y from X.

Assume only that $Y_i = m(X_i) + \epsilon_i$ where where $m(x)$ is a smooth function of x.

The most popular methods are *kernel methods*. However, there are two types of kernels:

1. Smoothing kernels
2. Mercer kernels

Smoothing kernels involve local averaging.
Mercer kernels involve regularization.

Smoothing Kernels

- Smoothing kernel estimator:

$$\widehat{m}_h(x) = \frac{\sum_{i=1}^n Y_i\, K_h(X_i, x)}{\sum_{i=1}^n K_h(X_i, x)}$$

where $K_h(x, z)$ is a *kernel* such as

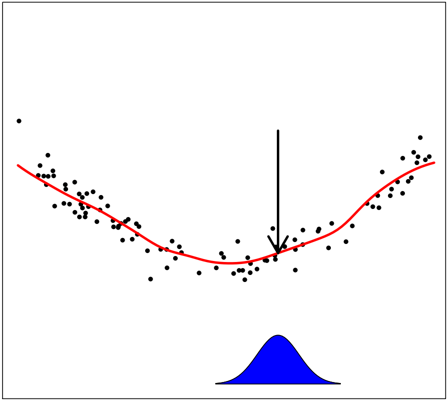
$$K_h(x, z) = \exp\left(-\frac{\|x - z\|^2}{2h^2}\right)$$

and $h > 0$ is called the *bandwidth*.

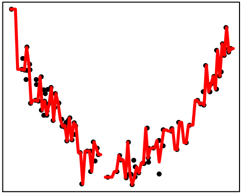
- $\widehat{m}_h(x)$ is just a local average of the Y_i's near x.

- The bandwidth h controls the bias-variance tradeoff:
Small h = large variance while *large h = large bias*.

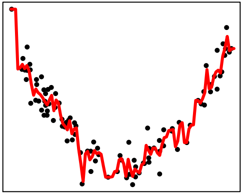
$\widehat{m}(x)$ is a local average



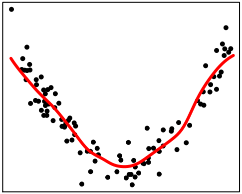
Effect of the bandwidth h



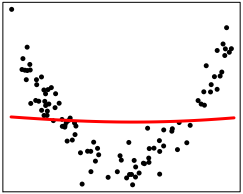
very small bandwidth



small bandwidth



medium bandwidth



large bandwidth

Smoothing Kernels

$$\text{Risk} = \mathbb{E}(Y - \widehat{m}_h(X))^2 = \text{bias}^2 + \text{variance} + \sigma^2.$$

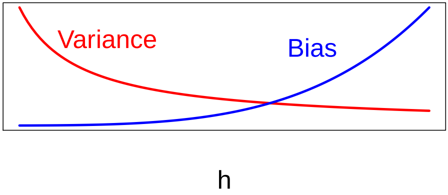
$$\text{bias}^2 \approx h^4,$$

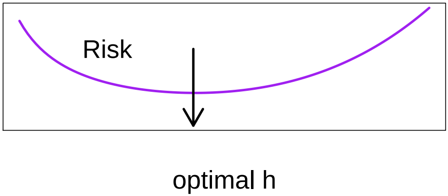
$$\text{variance} \approx \frac{1}{nh^p} \quad \text{where } p = \text{dimension of } X.$$

$\sigma^2 = \mathbb{E}(Y - m(X))^2$ is the unavoidable prediction error.

small h: low bias, high variance (undersmoothing)
large h: high bias, low variance (oversmoothing)

Risk Versus Bandwidth





Another Approach: Mercer Kernels

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 *Mercer Kernel* $K(x, x')$ is symmetric and positive definite:

$$\int\int f(x)f(x')K(x,x')\,dx\,dx' \geq 0 \quad \text{for all } f.$$

Example: $K(x, x') = e^{-||x-x'||^2/2}$.

Think of $K(x, x')$ as the *similarity* between x and x'. We will 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.

Mercer Kernels

Let

$$\mathcal{F} = \left\{ f(\cdot) = \sum_{j=1}^{k} \beta_j K(z_j, \cdot) \right\}$$

Define a norm: $\|f\|_K = \sum_j \sum_k \beta_j \beta_k K(z_j, z_k)$. $\|f\|_K$ *small means f smooth.*

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

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

$\mathcal{F}$ is a reproducing kernel Hilbert space (RKHS) because

$$\langle f, K(x, \cdot) \rangle = f(x)$$

Mercer Kernels

Check that this is well defined:

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

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

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

Nonparametric Regression: Mercer Kernels

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

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

Nonparametric Regression: Mercer Kernels

In more detail, we can write any $f \in \mathcal{H}_K$ as

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

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 $v = 0$.

Nonparametric Regression: Mercer Kernels

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: $\widehat{\alpha} = (\mathbb{K} + \lambda I)^{-1} Y$ and $\widehat{m}(x) = \sum_i \widehat{\alpha}_i K(X_i, x)$.

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.

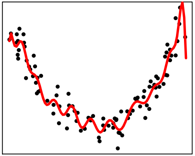
Smoothing Kernels *Versus* Mercer Kernels

Smoothing kernels: the bandwidth h controls the amount of smoothing.

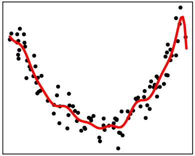
Mercer kernels: norm $\|f\|_K$ controls the amount of smoothing.

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

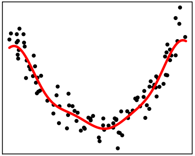
Mercer Kernels: Examples



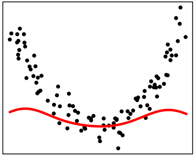
very small lambda



small lambda



medium lambda



large lambda

Multiple Regression

Both methods extend easily to the case where X has dimension $p > 1$. For example, just use

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

However, this is hard to interpret and is subject to the curse of dimensionality. This means that the *statistical performance* and the *computational complexity* degrade as dimension p increases.

An alternative is to use something less nonparametric such as additive model where we restrict $m(x_1, \ldots, x_p)$ to be of the form:

$$m(x_1, \ldots, x_p) = \beta_0 + \sum_j m_j(x_j).$$

Additive Models

Model: $m(x) = \beta_0 + \sum_{j=1}^{p} m_j(x_j)$.

We can take $\widehat{\beta}_0 = \overline{Y}$ and we will ignore β_0 from now on.

We want to minimize

$$\sum_{i=1}^{n} \left(Y_i - (m_1(X_{i1}) + \cdots + m_p(X_{ip})) \right)^2$$

subject to m_j smooth.

Additive models: Backfitting Algorithm

Input: Data (X_i, Y_i)

Iterate until convergence:

For each $j = 1, \ldots, p$:

Compute residual: $R_j = Y - \sum_{k \neq j} \widehat{m}_k(X_k)$

Smooth $\widehat{m}_j = \mathcal{S}_j R_j$

Output: Estimator $\widehat{m}(X_i) = \sum_j \widehat{m}_j(X_{ij})$.

Here, $\mathcal{S}_j R$ is any 1-dimensional nonparametric regression smoother

But what if p is large?

Sparse Additive Models

Additive Model: $Y_i = \sum_{j=1}^{p} m_j(X_{ij}) + \varepsilon_i, \quad i = 1, \ldots, n$

High dimensional: $n \ll p$, with most $m_j = 0$.

Optimization:

$$
\begin{aligned}
\text{minimize} \quad & \mathbb{E}\left(Y - \textstyle\sum_j m_j(X_j)\right)^2 \\
\text{subject to} \quad & \sum_{j=1}^{p} \sqrt{\mathbb{E}(m_j^2)} \leq L_n \\
& \mathbb{E}(m_j) = 0
\end{aligned}
$$

This generalizes the lasso!

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https://rss.onlinelibrary.wiley.com/doi/abs/10.1111/j.1467-9868.2009.00718.x

Sparse Backfitting Algorithm

Input: Data (X_i, Y_i), regularization parameter λ.

Iterate until convergence:

For each $j = 1, \ldots, p$:

Compute residual: $R_j = Y - \sum_{k \neq j} \widehat{m}_k(X_k)$

Smooth $\widehat{m}_j = \mathcal{S}_j R_j$

Estimate norm: $s_j = \sqrt{\mathbb{E}(\widehat{m}_j^2)}$

Soft-threshold: $\widehat{m}_j \leftarrow \left[1 - \frac{\lambda}{\widehat{s}_j}\right]_+ \widehat{m}_j$

Output: Estimator $\widehat{m}(X_i) = \sum_j \widehat{m}_j(X_{ij})$.

This generalizes coordinate descent algorithm from last time.

Kernel density estimation

To estimate a density, use the same idea behind kernel smoothing:

$$\widehat{f}(x) = \frac{1}{n}\sum_{i=1}^{n} K_h(X_i, x)$$
$$= \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h} K\left(\frac{X_i - x}{h}\right)$$

We require that $\int K(u)\,du = 1$ and $K \geq 0$ is symmetric around zero (an even function).

This places a “bump” around each data point.

Kernel density estimation

In p dimensions:

$$\widehat{f}(x) = \frac{1}{n}\sum_{i=1}^{n} K_h(X_i, x)$$
$$= \frac{1}{n\,h^p}\sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right)$$

We require that $\int K(u)\,du = 1$ and K is symmetric around zero.

This places a "bump" around each data point.

Kernel density estimation

The bias-variance tradeoff:

$$\text{bias}^2(x) \approx h^4$$
$$\text{var}(x) \approx \frac{1}{n\,h^p}$$

Note that the variance scales according to the expected number of data points in a cube of side length h in p-dimensions.

We'll go through the calculation of this on the board.

Back to regression

Using a kernel density estimator, the "plug-in" regression estimate gives us back the kernel smoother:

$$
\begin{aligned}
\widehat{m}(x) &= \int y\,\widehat{f}(y \mid x)\,dy \\
&= \frac{\int y\,\widehat{f}(x, y)\,dy}{\widehat{f}(x)} \\
&= \frac{\sum_i Y_i K_h(X_i, x)}{\sum_i K_h(X_i, x)}
\end{aligned}
$$

Summary

- Smoothing methods compute local averages, weighting points by a kernel
- Shape of the kernel doesn't matter
- Mercer kernels using penalization rather than smoothing
- Defining property: Matrix $\mathbb{K}$ is always positive-definite (non-negative eigenvalues)
- Equivalent to a type of ridge regression in function space
- The curse of dimensionality limits use of both approaches to low dimensions
- A compromise between nonparametric and linear models is to use additive models