KERNEL DENSITY ESTIMATION

ETHAN LIGON

1. Introduction

In general, we're interested in estimating things like:

- $\mathbb{E}(y|x)$ (Conditional expectations)
- $f(y|x)$ (Conditional pdf)
- Extends to estimating any (smooth?) function.

(1) Note
$$\mathbb{E}(y|x = x) = \int y f(y|x) dy,$$
So if we can estimate $f(y|x)$ we can compute expectations.

2. Linear Model

For the linear model we've assumed $y = \alpha + \beta x + u$, with $\mathbb{E}(u|x) = 0$, so that
$$\begin{aligned}\mathbb{E}(y|x) &= \mathbb{E}(\alpha + \beta x + u|x)\\ &= \alpha + \beta x,\end{aligned}$$
so that conditional moments are linear functions of the conditioning variables. This leads us to focus on estimating the vector of *parameters* (α, β).

3. Non-linear Model

In contrast with what we've seen so far in this course, which focused on linear estimation, now we escape our strai(gh)t-jackets! We will aim at estimating
$$\mathbb{E}(y|x) = m(x),$$
where m is a nicely behaved (e.g., smooth, continuous, bounded) but possibly very non-linear function.

(1) Today Focus on estimating *unconditional* density $f(x)$. Our approach will be **fully non-parametric**, and will allow us to construct **arbitrarily nonlinear** densities.

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4. Construction of Estimator

Suppose we have a random sample $\{X_1, X_2, \ldots, X_n\}$.

(1) Empirical Distribution Function (EDF)

$$\hat{F}(x) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}(X_i \leq x)$$

We *might* think of taking the derivative of the EDF wrt x, but this would just give us a set of mass points located at the points in the sample.

5. Density estimator

Instead, *assume* density exists, and recall

$$f(x) = \lim_{h\to 0} \frac{F(x+h) - F(x-h)}{2h}$$

Then by analogy:

$$\hat{f}(x) = \frac{\hat{F}(x+h) - \hat{F}(x-h)}{2h}.$$

Note this holds h fixed!

(1) Construction of Estimator

$$\hat{f}(x) = \frac{\hat{F}(x+h) - \hat{F}(x-h)}{2h}$$

$$= \frac{1}{2nh}\sum_{i=1}^{n} \mathbb{1}(x - h < X_i \leq x + h)$$

$$= \frac{1}{2nh}\sum_{i=1}^{n} \mathbb{1}\left(\frac{|X_i - x|}{h} \leq 1\right)$$

or

$$\hat{f}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{X_i - x}{h}\right)$$

where

$$k(u) = \begin{cases} 1/2 & |u| \leq 1 \\ 0 & \text{otherwise.} \end{cases}$$

The function k is an example of a *kernel*. Note that it integrates to one.

6. Kernels

Lots of possible kernels. Only strict requirement is that $k(u)$ integrate to one. But there are other desirable properties:

Non-negativity: $k(u) \geq 0$ for all u. (In this case we can interpret k as a probability density function.)
Boundedness: $\int |u|^r k(u) du < \infty$ for all positive integers r.
Symmetry: $k(u) = k(-u)$. (Note that boundedness & symmetry imply $\int uk(u)du = 0$.)
Normalized: $\int u^2 k(u) du = 1$
Differentiable: $\hat{f}$ will inherit differentiability of kernel, and often one prefers "smooth" estimates.

7. Menagerie of Kernels

See Hansen (2022) for a list of common kernels. In practice you'll most often meet:

Rectangular:

$$k(u) = \begin{cases} \frac{1}{2\sqrt{3}} & \text{if } |u| < \sqrt{3} \\ 0 & \text{otherwise.} \end{cases}$$

Gaussian:

$$k(u) = \frac{1}{2\pi} \exp\left(-\frac{u^2}{2}\right)$$

Epanechnikov:

$$k(u) = \begin{cases} \frac{3}{4\sqrt{5}} \left(1 - \frac{u^2}{5}\right) & \text{if } |u| < \sqrt{5}; \\ 0 & \text{otherwise.} \end{cases}$$

8. Bias of $\hat{f}$

We're interested in $\mathbb{E}\hat{f}(x)$ (NB: this is for x *fixed*). In particular, we want to calculate

$$\text{Bias}(x) = \mathbb{E}\hat{f}(x) - f(x).$$

(1) Bias of $\hat{f}$ We have

$$\begin{aligned} \mathbb{E}\hat{f}(x) &= \mathbb{E}\left[\frac{1}{nh}\sum_i k\left(\frac{X_i - x}{h}\right)\right] \\ &= \mathbb{E}\left[\frac{1}{h}k\left(\frac{X - x}{h}\right)\right]. \end{aligned}$$

Our next step involves a change of variable: let $u = g(v) = (v - x)/h$, so that $g^{-1}(u) = x + hu$. Then

$$\mathbb{E}\hat{f}(x) = \int \frac{1}{h} k\left(\frac{v-x}{h}\right) f(v)dv \qquad \text{and using change-of-variable}$$
$$= \int k(u) f(x + hu) du,$$

which should remind you of convolutions of continuous random variables. Finally, a simple trick of adding and subtracting $f(x)$ gives us

$$\hat{f}(x) = f(x) + \int k(u)\left(f(x + hu) - f(x)\right) du,$$

so that the second term is the bias. Note that the bias disappears as $h \to 0$ (and recall our rule of thumb that larger bandwidths mean more bias and less variance).

9. Variance of $\hat{f}$

To calculate the variance of $\hat{f}(x)$ (again holding x fixed),

$$\mathrm{Var}(\hat{f}(x)) = \frac{1}{(nh)^2} \mathrm{Var}\left[\sum_i k\left(\frac{X_i - x}{h}\right)\right]$$
$$= \frac{1}{nh^2} \mathrm{Var}\left[k\left(\frac{X - x}{h}\right)\right].$$

10. Estimator of Variance

For a random sample, the quantities $k\left(\frac{X_i - x}{h}\right)$ are sometimes called the "kernel smooths"; note that there are just n of these, and our estimator $\hat{f}(x)$ is just the mean of these.

(1) Analogy So, we can estimate the sample variance of $\hat{f}$ by just computing the sample variance of the kernel smooths:

$$\widehat{\mathrm{Var}}(\hat{f}(x)) = \frac{1}{n}\left(\frac{1}{nh^2}\sum_i k\left(\frac{X_i - x}{h}\right)^2 - \hat{f}(x)^2\right).$$

11. MSE/IMSE

In general, estimates both biased and imprecise. Usual measure of this is the *Mean Squared Error*, or

$$\mathrm{MSE}(\hat{f}(x)) = \mathrm{Bias}(\hat{f}(x))^2 + \mathrm{Var}(\hat{f}(x)).$$

Note that the MSE is a *function of* x. To get a summary measure, consider the Integrated Mean Square Error, or

$$\mathrm{IMSE}(\hat{f}) = \int \mathrm{MSE}(\hat{f}(x))dx.$$

12. Bandwidths (asymptotics)

(1) Idea
- Smaller bandwidths allow for more complicated estimates.
- But sample size has to increase faster than bandwidth shrinks ("effective sample size" has to increase) for asymptotic arguments to work.
- OR: To estimate more complicated things, need more data!

13. Bandwidths (in practice)

We don't usually get sample sizes that go to infinity, instead we usually have n fixed. So:

- We need a single **fixed** bandwidth.
- We can see with a fixed bandwidth model is *misspecified*, and at best only an approximation to true density.
- Increasing complexity (smaller bandwidth) holding sample size fixed tends to:
  - Increase variance
  - Decrease bias

  To balance variance vs. bias, appeal to a particular loss function (often MSE).

14. Bandwidth choice

So how should we go about selecting a bandwidth? The choice is often much more important than the choice of kernel.

We've seen that the MSE (and IMSE) depend on h; how about choosing h to minimize IMSE?

(1) Silverman's rule of thumb Silverman assumed a Gaussian kernel and that the true f was Gaussian, so he was able to compute the IMSE and find the h that minimized it:

$$h^* \approx \hat{\sigma} 1.06/\sqrt[5]{n},$$

where $\hat{\sigma}^2$ is the sample variance.

(2) Take-away Silverman's rule of thumb is thought to be a decent choice for lots of problems. BUT: a much better general approach would be to construct an estimator of IMSE(h) —we'll later discuss how to use cross-validation to do exactly this.