

## Lec 7: Density estimation

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## Preliminary

- Small  $O$  and big  $O$

- Density estimation

- Performance of estimate

- Cross validation

## Density estimation

- Histogram

- Naive density estimator

- Kernel estimation

- If  $X_n \rightarrow 0$  in probability, then we write  $X_n = o_p(1)$ . The expression  $O_p(1)$  denotes a sequence that is bounded in probability, say, write  $X_n = O_p(1)$ : for all  $\epsilon > 0$ , there exists some  $M > 0$  such that

$$P(|X_n| \geq M) < \epsilon$$

- More generally, for a given sequence of random variables  $R_n$ :

$X_n = o_p(R_n)$  means  $X_n = Y_n R_n$  and  $Y_n \rightarrow 0$  in probability;

$X_n = O_p(R_n)$  means  $X_n = Y_n R_n$  and  $Y_n = O_p(1)$

- This expresses that the sequence  $X_n$  converges in probability to zero or is bounded in probability "at the rate  $R_n$ ".
- Obviously,  $X_n = o_p(R_n)$  implies that  $X_n = O_p(R_n)$ .

## Results on $o_p$ and $O_p$

- For some sequence  $a_n$ , if  $a_n X_n \rightarrow 0$  in probability, then we write  $X_n = o_p(a_n^{-1})$ ; if  $a_n X_n = O_p(1)$ , then we write  $X_n = O_p(a_n^{-1})$ .
- There are many rules of calculus with  $o$  and  $O$  symbols, which we will apply without comment. For instance,

$$o_p(1) + o_p(1) = o_p(1), o_p(1) + O_p(1) = O_p(1),$$

$$O_p(1)o_p(1) = o_p(1), (1 + o_p(1))^{-1} = O_p(1),$$

$$O_p(R_n) = R_n O_p(1), o_p(R_n) = R_n o_p(1), o_p(O_p(1)) = o_p(1).$$

- Particularly, if  $X_n \rightsquigarrow F$ , then  $X_n = O_p(1)$ ,  $X_n + o_p(1) \rightsquigarrow F$ ,  $X_n \cdot o_p(1) = o_p(1)$ .

## Density estimation

- Let  $X_1, \dots, X_n$  be a sample from a distribution  $F$  with density  $f$ . The goal of nonparametric density estimation is to estimate  $f$  with as few assumptions about  $f$  as possible.
- Density estimation used for: regression, classification, clustering and unsupervised prediction. For example, if  $\hat{f}(x, y)$  is an estimate of  $f(x, y)$  then we get the following estimate of the regression function:

$$\hat{m}(x) = \hat{E}[Y|x] = \int y \hat{f}(y|x) dy$$

where  $\hat{f}(y|x) = \hat{f}(x, y) / \hat{f}_X(x)$ .

## Bart Simpson density

Consider the density

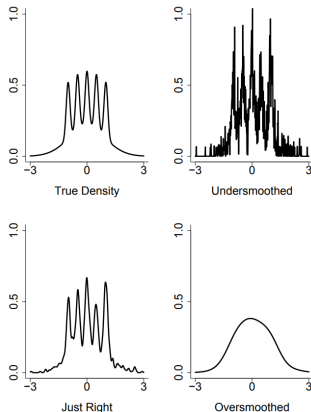
$$f(x) = \frac{1}{2}\phi(x; 0, 1) + \frac{1}{10} \sum_{j=0}^4 \phi(x; j/2 - 1, 1/10)$$

where  $\phi(x; \mu, \sigma)$  denotes a Normal density with mean  $\mu$  and standard deviation  $\sigma$ . Such density is called "the claw" or "Bart Simpson" density.



- Based on 1,000 draws from  $f$ , we computed a kernel density estimator, which depends on a tuning parameter called the bandwidth.

## Density estimation



Top left: true density. The other plots are kernel estimators based on  $n = 1,000$  draws.

Bottom left: bandwidth  $h = 0.05$  chosen by leave-one-out cross-validation.

Top right: bandwidth  $h/10$ .

Bottom right: bandwidth  $10h$ .

## Error for Density Estimates

Our first step is to get clear on what we mean by a “good” density estimate. There are three leading ideas:

- $\int [\hat{f}(x) - f(x)]^2 dx$  should be small: the squared deviation from the true density should be small, averaging evenly over all space.
- $\int |\hat{f}(x) - f(x)| dx$  should be small: minimize the average absolute, rather than squared, deviation.
- $\int f(x) \log \frac{f(x)}{\hat{f}_n(x)} dx$  should be small: the average log-likelihood ratio should be kept low.



- Option (1) is reminiscent of the MSE criterion we've used in regression.
- Option (2) looks at what's called the L1 or **total variation** distance between the true and the estimated density. It has the nice property that  $\frac{1}{2} \int |f(x) - \hat{f}_n(x)| dx$  is exactly the maximum error in our estimate of the probability of *any set*. Unfortunately it's a bit tricky to work with, so we'll skip it here.
- Finally, minimizing the log-likelihood ratio is intimately connected to maximizing the likelihood. This is not a good loss function to use for nonparametric density estimation. The reason is that the Kullback-Leibler loss is completely dominated by the tails of the densities.

we will give more attention to minimizing (1), because it's mathematically tractable.

- Given the sample  $X_1, \dots, X_n$ , our goal is to estimate  $f$  nonparametrically. Finding the best estimator  $\hat{f}_n$  in some sense is equivalent to finding the optimal smoothing parameter  $h$ .
- Notice that the **Risk/Integrated Mean Square Error (IMSE,MISE)**:

$$\begin{aligned} R(\hat{f}_n, f) &= \int E(\hat{f}_n(x) - f(x))^2 \\ &= \int E(\hat{f}_n(x) - E\hat{f}_n(x) + E\hat{f}_n(x) - f(x))^2 \\ &= \int \text{Var}(\hat{f}_n(x))dx + \int (E\hat{f}_n(x) - f(x))^2 dx \end{aligned}$$

- One can find an optimal estimator that minimizes the risk function:

$$\hat{f}_n^*(x) = \arg \min R(\hat{f}_n, f)$$

## Cross validation

- Use leave-one-out cross validation to estimate the risk function.
- One can express the loss function as a function of the smoothing parameter  $h$

$$\begin{aligned} ISE(h) &= \int (\hat{f}_n(x) - f(x))^2 dx \\ &= \underbrace{\int (\hat{f}_n(x))^2 dx - 2 \int \hat{f}_n(x) f(x) dx}_{J(h)} + \int f^2(x) dx \end{aligned}$$

- **(Least-Square) Cross-validation estimator** (LSCV) of the risk function  $J(h)$  (up to constant)

$$cv(h) = \int \hat{f}_n^2(x) dx - \frac{2}{n} \sum_{i=1}^n \hat{f}_{n,-i}(X_i)$$

where  $\hat{f}_{n,-i}$  is the density estimator obtained after removing  $i$ th observation.

- **Biased Cross-Validation (BCV)** The difference between the LSCV and the biased cross-validation method is the fact that here, minimization is based on the AMISE (discussed later).
- **(Pseudo)-Likelihood Cross-Validation (LCV)** The LCV-selector was maybe the first commonly used automatic bandwidth selector because it is based on a basic statistic concept, the maximum-likelihood optimization. The criterion to maximize is

$$LCV(h) = \frac{1}{n} \prod_{i=1}^n \hat{f}_{n,-i}(X_i)$$

## Histogram

- The oldest density estimator is the histogram.
- Without loss of generality, we assume that the support of  $f$  is  $[0,1]$ . Divide the support into  $m$  equally sized bins

$$B_1 = \left[0, \frac{1}{m}\right), B_2 = \left[\frac{1}{m}, \frac{2}{m}\right), \dots, B_m = \left[\frac{m-1}{m}, 1\right]$$

- Let  $h = \frac{1}{m}$ ,  $p_j = \int_{B_j} f(x)dx$  and  $Y_j = \sum_{i=1}^n I(X_i \in B_j)$
- The histogram estimator is defined by

$$\hat{f}_n(x) = \sum_{j=1}^m \frac{\hat{p}_j}{h} I(x \in B_j)$$

where  $\hat{p}_j = \frac{Y_j}{n}$ .

## Theorem

Suppose that  $f'$  is absolutely continuous and  $\|f'(x)\|^2 < \infty$ , then

$$R(\hat{f}_n, f) = \frac{h^2}{12} \|f'\|^2 + \frac{1}{nh} + o(h^2) + O\left(\frac{1}{n}\right)$$

The optimal bandwidth is

$$h_{opt} = \frac{1}{n^{1/3}} \left( \frac{6}{\|f'\|^2} \right)^{1/3} = kn^{-1/3}$$

with the optimal bandwidth,

$$R(\hat{f}_n, f) \approx \frac{C}{n^{2/3}}$$

where  $\|g\|^2 = \int (g(x))^2 dx$ ,  $C = (\frac{3}{4})^{2/3} \|f'\|^{2/3}$ .

*Proof.* For any  $x, u \in B_j$ ,

$$f(u) = f(x) + (u - x)f'(x) + \frac{(u - x)^2}{2}f''(\tilde{x})$$

for some  $\tilde{x}$  between  $x$  and  $u$ . Hence,

$$\begin{aligned} p_j &= \int_{B_j} f(u) du \\ &= \int_{B_j} \left( f(x) + (u - x)f'(x) + \frac{(u - x)^2}{2}f''(\tilde{x}) \right) du \\ &= f(x)h + hf'(x) \left( h(j - \frac{1}{2}) - x \right) + O(h^3). \end{aligned}$$

Therefore, the bias of  $\hat{f}_n(x)$  is

$$\begin{aligned}b(x) &= E(\hat{f}_n(x) - f(x)) = \frac{p_j}{h} - f(x) \\&= \frac{1}{h} \left( f(x)h + hf'(x) \left( h(j - 1/2) - x \right) + O(h^3) \right) - f(x) \\&= f'(x) \left( h(j - 1/2) - x \right) + O(h^2)\end{aligned}$$

By the mean value theorem, for some  $\tilde{x} \in B_j$ ,

$$\begin{aligned}\int_{B_j} b^2(x) dx &= \int_{B_j} (f'(x))^2 \left( h(j - 1/2) - x \right)^2 dx + O(h^4) \\&= (f'(\tilde{x}))^2 \int_{B_j} \left( h(j - 1/2) - x \right)^2 dx + O(h^4) \\&= (f'(\tilde{x}))^2 \frac{h^3}{12} + O(h^4).\end{aligned}$$



Hence,

$$\begin{aligned}\int_0^1 b^2(x)dx &= \sum_{j=1}^m \int_{B_j} b^2(x)dx \\ &= \sum_{j=1}^m (f'(\tilde{x}))^2 \frac{h^3}{12} + O(h^3) \\ &= \frac{h^2}{12} \|f'(x)\|^2 + o(h^2)\end{aligned}$$

For the variance of  $\hat{f}_n$ :

$$v(x) = \text{Var}(\hat{f}_n(x)) = \frac{1}{h^2} \text{Var}(\hat{p}_j) = \frac{p_j(1-p_j)}{nh^2}$$

By the mean value theorem, for some  $x_j \in B_j$ ,

$$p_j = \int_{B_j} f(x)dx = hf(x_j).$$

Therefore,

$$\begin{aligned}\int_0^1 v(x)dx &= \sum_{j=1}^m \int_{B_j} v(x)dx = \sum_{j=1}^m \int_{B_j} \frac{p_j(1-p_j)}{nh^2} dx \\&= \frac{1}{nh^2} \sum_{j=1}^m \int_{B_j} p_j dx - \frac{1}{nh^2} \sum_{j=1}^m \int_{B_j} p_j^2 dx \\&= \frac{1}{nh} - \frac{1}{nh} \sum_{j=1}^m p_j^2 = \frac{1}{nh} - \frac{1}{nh} \sum_{j=1}^m h^2 f^2(x_j) \\&= \frac{1}{nh} - \frac{1}{n} (\|f\|^2 + o(1)) = \frac{1}{nh} + O\left(\frac{1}{n}\right).\end{aligned}$$

This completes the proof.

Now, note that if we minimize the asymptotic integrated squared error,

$$AMISE(h) = \frac{h^2}{12} \|f'\|^2 + \frac{1}{nh}$$

we obtain the optimal bandwidth  $h_{opt} = cn^{-1/3}$ .

- if  $X \sim N(\mu, \sigma^2)$ , then we have Scott's  $c \approx 3.5\sigma$
- Freedman and Diaconis proposed a robust estimator of  $\sigma$  by using the interquartile range  $IQR$ , then  $h^* = 2IQRn^{-1/3}$ .

- the **R** *hist* command uses  $h = 1/(\log_2(n) + 1)$  which R calls Sturges rule and is sometimes also called Doane's Rule.
- Since the number of bars in a histogram is  $k = O(h^{-1})$ , we have  $k = O(\log_2(n) + 1)$  bars while for optimal method we have  $k = O(c^{-1}n^{1/3})$ .
- So the number of bars increases much faster for optimal choice. For  $n < 500$  it doesn't matter much but for  $n$  larger than 500 it does matter.
- R allows the user to specify one of these alternative rules by specifying `breaks = "Scott"` for the rule  $k = 3.5\hat{\sigma}n^{-1/3}$  or `breaks = "FD"` for the rule  $k = 2IQRn^{-1/3}$ .

## Theorem

*The cross-validation estimator of risk for the histogram is*

$$cv(h) = \frac{2}{h(n-1)} - \frac{n+1}{h(n-1)} \sum_{j=1}^m \hat{p}_j^2$$

- It turns out that if we pick  $h$  by cross-validation, then we attain this optimal rate in the large-sample limit.
- By contrast, if we knew the correct parametric form and just had to estimate the parameters, we'd typically get an error decay of  $O(n^{-1})$ .
- This is substantially faster than histograms, so it would be nice if we could make up some of the gap, without having to rely on parametric assumptions.

## Naive density estimator

- Since

$$f(x) = \lim_{h \rightarrow 0} \frac{F(x+h) - F(x-h)}{2h} = \lim_{h \rightarrow 0} \frac{1}{2h} P(x-h < X \leq x+h)$$

- One could imagine estimating  $f$  by picking a small value of  $h$  and taking

$$\begin{aligned}\hat{f}_h(x) &= \frac{1}{2h} [\hat{F}_n(x+h) - \hat{F}_n(x-h)] \\ &= \frac{1}{2hn} \sum_{i=1}^n I(x-h < X_i \leq x+h) \\ &= \frac{1}{n} \sum_{i=1}^n \frac{1}{h} K\left(\frac{X_i - x}{h}\right)\end{aligned}$$

where  $K(x) = \frac{1}{2}I(-1 < x \leq 1)$ .

- This is the *naive density estimate*.

## Theorem

If  $h = h_n \rightarrow 0$  and  $nh_n \rightarrow \infty$ , as  $n \rightarrow \infty$ , then, for any  $x$ ,

$$\hat{f}_h \rightarrow f(x) \text{ in } P$$

- $\hat{f}_h$  is a probability density function.

- The fact that

$$n(\hat{F}_n(x+h) - \hat{F}_n(x-h)) \sim B(n, F(x+h) - F(x-h))$$

leads to

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

$$Var(\hat{f}_h) = \frac{(F(x+h) - F(x-h))(1 - F(x+h) + F(x-h))}{4nh^2}$$

- It amounts to estimating  $f(x)$  by a superposition (sum) of boxcar functions centered at the observations, each with width  $2h$  and area  $1/n$ .
- This sum is also blocky and discontinuous, but it avoids one of the arbitrary choices in constructing a histogram: the choice of locations of the bins.
- As  $h \rightarrow 0$ , the naive estimate converges weakly to the sum of point masses at the data; for  $h > 0$ , the naive estimator smooths the data.
- The tuning parameter  $h$  is analogous to the bin width in a histogram. Larger values of  $h$  give smoother density estimates. Whether "smoother" means "better" depends on the true density  $f$ ; generally, there is a tradeoff between bias and variance: increasing the smoothness increases the bias but decreases the variance.



## Kernel estimation

- Obviously, whenever  $K(x)$  is itself a probability density function, then  $\hat{f}_K$  is a probability density function.
- Using a smoother kernel function  $K$ , such as a Gaussian density, leads to a smoother estimate  $\hat{f}_K$ .
- Estimates that are linear combinations of such kernel functions centered at the data are called **kernel density estimates**. We denote the kernel density estimate with bandwidth (smoothing parameter)  $h$  by

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

Is  $\hat{f}_h(x)$  a legitimate density function? It needs to satisfy:

(1) nonnegative

(2) integrate to one

Easy to do: Require the Kernel function,  $K(\cdot)$  to satisfy:

- $K(u) \geq 0$  for all  $u$
- $\int K(u)du = 1$

Additionally, the kernel  $K$  is also assumed to satisfy

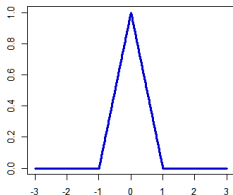
$$K(u) = K(-u), \int uK(u)du = 0$$

$$0 < \kappa_{21} = \int u^2 K(u)du < \infty, \kappa_{02} = \|K\|^2 = \int K^2(u)du < \infty$$

where  $\kappa_{ij} = \int u^i K^j(u)du$ .

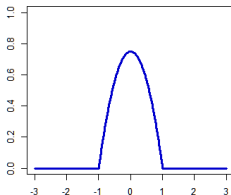
# Popular kernels

Triangle



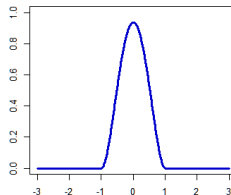
$$K(u) = (1 - |u|)I(|u| \leq 1)$$

Epanechnikov



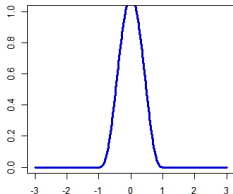
$$K(u) = \frac{3}{4}(1 - u^2)I(|u| \leq 1)$$

Quartic (biweight)



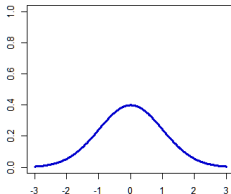
$$K(u) = \frac{15}{16}(1 - u^2)^2I(|u| \leq 1)$$

Triweight



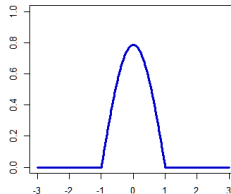
$$K(u) = \frac{35}{32}(1 - u^2)^3I(|u| \leq 1)$$

Gaussian



$$K(u) = (2\pi)^{-1/2}\exp(-\frac{1}{2}u^2)$$

Cosin



$$K(u) = \frac{\pi}{4}\cos(\frac{\pi u}{2})I(|u| \leq 1)$$

To see the performance of the estimator, consider the bias and the mean square error of  $\hat{f}_h(x)$  for fixed  $x$ .

### Theorem

*Let  $f$  be twice continuously differentiable in a neighborhood of  $x$ . Let the kernel  $K$  satisfy the above assumptions. If  $\lim_{n \rightarrow \infty} h = 0$ , then,*

$$E(\hat{f}_h(x) - f(x)) = \frac{1}{2}h_n^2 f''(x)\kappa_{21} + o(h^2)$$

*If in addition,  $\lim_{n \rightarrow \infty} nh = \infty$ , then*

$$\text{Var}(\hat{f}_h(x)) = \frac{1}{nh} f(x)\kappa_{02} + o\left(\frac{1}{nh}\right)$$

Thus,

$$\begin{aligned}MSE(\hat{f}_h(x)) &= E(\hat{f}_h(x) - f(x))^2 \\&= \underbrace{\frac{1}{4}h_n^4(f''(x))^2\kappa_{21}^2 + \frac{1}{nh}f(x)\kappa_{02}}_{AMSE} + o(h^4 + \frac{1}{nh})\end{aligned}$$

*Proof.* By Taylor expansion of  $f(x + uh)$  at  $x$ :

$$f(x + uh) = f(x) + f'(x)uh + \frac{1}{2}f''(x)(uh)^2 + o((uh)^2)$$

Therefore,

$$\begin{aligned} E\hat{f}_h(x) &= E\left[\frac{1}{n}\sum_{i=1}^n \frac{1}{h}K\left(\frac{X_i - x}{h}\right)\right] = \frac{1}{h}EK\left(\frac{X_1 - x}{h}\right) \\ &= \int K(u)f(x + uh)du \\ &= \int K(u)[f(x) + f'(x)uh + \frac{1}{2}f''(x)u^2h^2 + u^2o(h^2)]du \\ &= f(x) + \frac{1}{2}f''(x)\kappa_{21}h^2 + o(h^2) \end{aligned}$$

and

$$\begin{aligned} \text{Var}(\hat{f}_h(x)) &= \text{Var}\left[\frac{1}{n} \sum_{i=1}^n \frac{1}{h} K\left(\frac{X_i - x}{h}\right)\right] = \frac{1}{n} \text{Var}\left(\frac{1}{h} K\left(\frac{X_1 - x}{h}\right)\right) \\ &= \frac{1}{n} E\left[\frac{1}{h} K\left(\frac{X_1 - x}{h}\right)\right]^2 - \frac{1}{n} \left[E\frac{1}{h} K\left(\frac{X_1 - x}{h}\right)\right]^2 \\ &= \frac{1}{nh} \int K^2(u) f(x + uh) du - \frac{1}{n} \left(\int K(u) f(x + uh) du\right)^2 \\ &= \frac{1}{nh} \int K^2(u) f(x + uh) du - \frac{1}{n} \left(f(x) + \frac{1}{2} f''(x) \kappa_{21} h^2 + o(h^2)\right)^2 \\ &= \frac{f(x)}{nh} \kappa_{02} + o\left(\frac{1}{nh}\right) \end{aligned}$$

This completes the proof.

Observe that as  $h$  increases, the bias becomes large while the variance decreases. In order to find the optimal value of  $h$ , we minimize the AMSE. This leads to:

$$h_{opt1}(x) = \left( \frac{f(x)\kappa_{02}}{(f''(x))^2\kappa_{21}^2} \right)^{1/5} n^{-1/5}$$

It follows that the corresponding AMSE and variance are both of the order  $n^{-4/5}$ .



Observe that

$$MISE(\hat{f}_h) = \int MSE(\hat{f}_h(x))dx = \int E(\hat{f}_h(x) - f(x))^2 dx$$

It can be shown

$$MISE(\hat{f}_h) = \underbrace{\frac{\kappa_{02}}{nh} + \frac{1}{4}\|f''\|^2\kappa_{21}^2h^4}_{AMISE} + o(h^4 + \frac{1}{nh})$$

Thus  $MISE(\hat{f}_h) \rightarrow 0$  and further

$$ISE_h(\hat{f}_h) = \int (\hat{f}_h(x) - f(x))^2 dx \rightarrow 0.$$

Minimizing the AMISE leads to the following optimal bandwidth,

$$h_{opt2} = \left( \frac{\kappa_{02}}{\|f''\|^2 \kappa_{21}^2} \right)^{1/5} n^{-1/5}.$$

The resulting MISE is of the order  $n^{-4/5}$ .

- Both locally and globally, the optimal bandwidth is of the order  $n^{-1/5}$ , and the convergence rate is  $n^{-4/5}$ .
- Bandwidth plays a more important role than the kernel. The choice of kernel does not effect the order of bandwidth or the rate of mean square convergence. Any kernel from a large class satisfying the assumptions can be used.

## Practical bandwidth choices

The theoretically optimal bandwidth,  $h_{opt2}$ , depends on the unknown density  $f$  through  $\|f''\|^2$ . The actual choice of  $h$  is a critical issue. There are different approaches to choose  $h$  in practice. Write  $h_{opt2} = n^{-1/5} \frac{C(K)}{\|f''\|^{2/5}}$ , where  $C(K)$  is the constant depending only on  $K$ .

- **Rule of thumb** Choose an auxiliary parametric family, say normal distributions, to choose  $h$ , not to estimate  $f$ .
  - ▶ We plug in the density of  $N(0, \sigma^2)$  into the formula of  $h_{opt2}$ , then

$$h_{opt} \approx 1.06 \hat{\sigma} n^{-1/5}$$

where  $\hat{\sigma}$  is the sample standard deviation.

- ▶ It is recommended to estimate  $\sigma$  with  $\min(\hat{\sigma}, R/1.35)$ , where  $\hat{\sigma}$  is the sample standard deviation and  $R$  is the sample interquantile range, that is  $R = \hat{F}_n^{-1}(0.75) - \hat{F}_n^{-1}(0.25)$  ( $\Phi^{-1}(0.75) - \Phi^{-1}(0.25) = 1.35$ ).

$$h_{opt} = 1.06 \min\left\{\hat{\sigma}, \frac{R}{1.35}\right\} n^{-1/5}$$

## Practical bandwidth choices

- **Cross-validation** Cross-validation score function:

$$cv(h) = \int \hat{f}_h^2(x) dx - \frac{2}{n} \sum_{i=1}^n \hat{f}_{h,-i}(X_i)$$

Since the first term

$$\begin{aligned} \int \hat{f}_h^2(x) dx &= \int \frac{1}{nh} \sum_{i=1}^n K\left(\frac{X_i - x}{h}\right) \frac{1}{nh} \sum_{j=1}^n K\left(\frac{X_j - x}{h}\right) dx \\ &= \frac{1}{n^2 h^2} \sum_{i=1}^n \sum_{j=1}^n \int K\left(\frac{X_i - x}{h}\right) K\left(\frac{X_j - x}{h}\right) dx \\ &= \frac{1}{n^2 h} \sum_{i=1}^n \sum_{j=1}^n \int K(u) K\left(u - \frac{X_i - X_j}{h}\right) du \\ &= \frac{1}{n^2 h} \sum_{i=1}^n \sum_{j=1}^n K * K\left(\frac{X_i - X_j}{h}\right) \end{aligned}$$

where  $K * K(v) = \int K(u)K(v-u)du$  is the convolution of kernel  $K$ .

For the second term,

$$\frac{2}{n} \sum_{i=1}^n \hat{f}_{h,-i}(X_i) = \frac{2}{n(n-1)h} \sum_{i=1}^n \sum_{j=1, j \neq i}^n K\left(\frac{X_i - X_j}{h}\right)$$

Therefore, the optimal  $h$  is  $\hat{h} = \arg \min_h cv(h)$ .

### Theorem (Stone's Theorem)

*Suppose  $f$  is bounded. Let  $\hat{f}_n$  denote the kernel estimator with bandwidth  $h$  and let  $h_*$  denote the bandwidth chosen by cross-validation. Then*

$$\frac{ISE_{h_*}(\hat{f}_{h_*})}{\inf_h ISE_h(\hat{f}_h)} \rightarrow 1, a.s.$$

- **Biased cross-validation.** This was proposed by Scott and George (1987), which has as its immediate target the AMISE. They proposed to estimate  $R(f'') = \|f''\|^2$  by

$$\hat{R}(f'') = \|\hat{f}_h''\|^2 - \frac{\|K''\|^2}{nh^5}$$

The biased cross-validation for bandwidth choice is

$$BCV(h) = \frac{\|K\|^2}{nh} + \frac{\kappa_{21}^2}{4n(n-1)h} \sum_{i=1}^n \sum_{j=1, j \neq i}^n K'' * K'' \left( \frac{X_j - X_i}{h} \right)$$

- There is another version of BCV by Jones and Kappenman (1991).
- Other variants include Maximum likelihood cross-validation, Complete cross-validation, Modified cross-validation, Trimmed cross-validation. (See R package **kedd**)

## Choosing the Kernel

- To discuss the choice of the kernel we will consider equivalent kernels, i.e. kernel functions that lead to exactly the same kernel density estimator.
- Consider a kernel function  $K(\cdot)$  and the following modification:

$$K_\delta(\cdot) = \frac{1}{\delta} K\left(\frac{\cdot}{\delta}\right)$$

- If  $h = \delta\tilde{h}$ , then the following two KDEs are equivalent:

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^n K_h(X_i - x) = \frac{1}{n} \sum_{i=1}^n K_{\tilde{h}\delta}(X_i - x) = \tilde{f}_{\tilde{h}\delta}(x)$$

This means, all rescaled versions  $K_\delta$  of a kernel function  $K$  are equivalent if the bandwidth is adjusted accordingly.



- Different values of  $\delta$  correspond to different members of an equivalence class of kernels.
- Recall the AMISE criterion, i.e.

$$AMISE = \frac{\|K\|^2}{nh} + \frac{h^4}{4} \|f''\|^2 \mu_2^2(K),$$

where  $\mu_2(K) = \kappa_{21}$ .

- We rewrite this formula for some equivalence class of kernel functions  $K_\delta$ :

$$AMISE(K_\delta) = \frac{\|K_\delta\|^2}{nh} + \frac{h^4}{4} \|f''\|^2 \mu_2^2(K_\delta)$$

- In each of the two components of this sum there is a term involving  $K_\delta$ . The idea for separating the problems of choosing  $h$  and  $K$  is to find  $\delta$  such that

$$\|K_\delta\|^2 = \mu_2^2(K_\delta)$$

This is fulfilled if

$$\delta_0 = \left( \frac{\|K\|^2}{\mu_2^2(K)} \right)^{1/5} = \left( \frac{\kappa_{02}}{\kappa_{21}^2} \right)^{1/5}$$

The value  $\delta_0$  is called the *canonical bandwidth* corresponding to the kernel function  $K$ .

- Let  $T(K) = \kappa_{02}/\delta_0$ , then

$$AMISE(h) = \left[ \frac{1}{nh} + \frac{h^4}{n} \|f''\|^2 \right] T(K)$$

- This has an interesting implication: Even though  $T(K)$  is not the same for different kernels, it does not matter for the asymptotic behavior of AMISE (since it is just a multiplicative constant).
- Hence, AMISE will be asymptotically equal for different equivalence classes if we use  $K_{\delta_0}$  to represent each class, and call it *canonical kernel* of an equivalent class.

Kernel	$\delta_0$
Uniform	$\left(\frac{9}{2}\right)^{1/5} \approx 1.3510$
Epanechnikov	$15^{1/5} \approx 1.7188$
Quartic	$35^{1/5} \approx 2.0362$
Triweight	$\left(\frac{9450}{143}\right)^{1/5} \approx 2.3122$
Gaussian	$\left(\frac{1}{4\pi}\right)^{1/10} \approx 0.7764$

- Suppose now that we have estimated an unknown density  $f$  using some kernel  $K^A$  and bandwidth  $h_A$ , what bandwidth  $h_B$  should we use in the estimation with kernel  $K^B$  when we want to get approximately the same degree of smoothness as we had in the case of  $K^A$  and  $h_A$ ?
- The answer is given by the following formula:

$$h_B = h_A \frac{\delta_0^B}{\delta_0^A}$$

- A question of immediate interest is to find the kernel that minimizes  $T(K)$ , Epanechnikov (1969, the person, not the kernel) has shown that under all nonnegative kernels with compact support, the kernel of the form

$$K(u) = \frac{3}{4} \frac{1}{15^{1/5}} \left( 1 - \left( \frac{u}{15^{1/5}} \right)^2 \right) I(|u| \leq 15^{1/5})$$

minimizes the function  $T(K)$ .

- Compare the values of  $T(K)$  of other kernels with the value of  $T(K)$  for the Epanechnikov kernel:

Kernel	$T(K)$	$T(K)/T(K_{Epa})$
Uniform	0.3701	1.0602
Triangle	0.3531	1.0114
Epanechnikov	0.3491	1.0000
Quartic	0.3507	1.0049
Triweight	0.3699	1.0595
Gaussian	0.3633	1.0408
Cosine	0.3494	1.0004

- After all, we can conclude that for practical purposes the choice of the kernel function is almost irrelevant for the efficiency of the estimate.

## Confidence intervals and confidence bands

- Suppose that  $f''$  exists and  $h = cn^{-1/5}$ . Then

$$n^{2/5}(\hat{f}_h - f(x)) \rightsquigarrow N\left(\underbrace{\frac{c^2}{2}f''(x)\kappa_{21}}_{b_x}, \underbrace{\frac{1}{c}f(x)\kappa_{02}}_{v_x^2}\right)$$

- We then get

$$\begin{aligned}1 - \alpha &\approx P(b_x - z_{1-\alpha/2}v_x \leq n^{2/5}(\hat{f}_h(x) - f(x)) \leq b_x + z_{1-\alpha/2}v_x) \\&= P(\hat{f}_h(x) - n^{-2/5}(b_x + z_{1-\alpha/2}v_x) \\&\leq f(x) \leq \hat{f}_h(x) + n^{-2/5}(b_x - z_{1-\alpha/2}v_x))\end{aligned}$$

- Using  $h = cn^{-1/5}$  we get the asymptotic confidence interval for  $f(x)$ :

$$\left[ \hat{f}_h(x) - \frac{h^2}{2}f''(x)\kappa_{21} - z_{1-\alpha/2}\sqrt{\frac{f(x)\kappa_{02}}{nh}}, \right. \\ \left. \hat{f}_h(x) - \frac{h^2}{2}f''(x)\kappa_{21} + z_{1-\alpha/2}\sqrt{\frac{f(x)\kappa_{02}}{nh}} \right]$$

- Unfortunately, the interval boundaries still depend on  $f(x)$  and  $f''(x)$ . If  $h$  is small relative to  $n^{-1/5}$  we can neglect the second term of each boundary. Replacing  $f(x)$  with  $\hat{f}_h(x)$  gives an approximate confidence interval that is applicable in practice.

$$\left[ \hat{f}_h(x) - z_{1-\alpha/2} \sqrt{\frac{\hat{f}_h(x) \kappa_{02}}{nh}}, \right. \\ \left. \hat{f}_h(x) + z_{1-\alpha/2} \sqrt{\frac{\hat{f}_h(x) \kappa_{02}}{nh}} \right]$$

- Confidence bands for  $f$  have only been derived under some rather restrictive assumptions.

- Suppose that  $f$  is a density on  $[0, 1]$  and given that certain regularity conditions are satisfied, then for  $h = n^{-\delta}$ ,  $\delta \in (1/5, 1/2)$ , and for all  $x \in [0, 1]$  the following formula has been derived by Bickel & Rosenblatt (1973)

$$\begin{aligned} \lim_{n \rightarrow \infty} P\left(\hat{f}_h(x) - \left\{\frac{\hat{f}_h(x)\kappa_{02}}{nh}\right\}^{1/2} \left\{\frac{z}{(2\delta \log n)^{1/2}} + d_n\right\}^{1/2} \leq f(x) \right. \\ \left. \leq \hat{f}_h(x) + \left\{\frac{\hat{f}_h(x)\kappa_{02}}{nh}\right\}^{1/2} \left\{\frac{z}{(2\delta \log n)^{1/2}} + d_n\right\}^{1/2}\right) \\ = \exp\{-2\exp(-z)\}, \end{aligned}$$

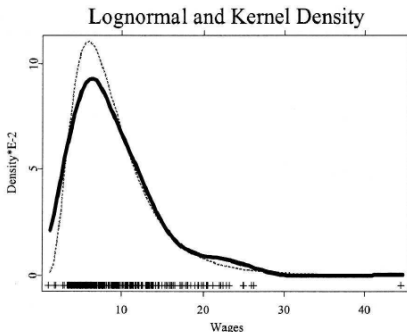
where  $d_n = (2\delta \log n)^{1/2} + (2\delta \log n)^{-1/2} \log\left(\frac{1}{2\pi} \frac{\|K'\|}{\|K\|}\right)$ .

- A confidence band for a given significance level  $\alpha$  can be found by searching the value of  $z$  that satisfies  $\exp\{-2\exp(-z)\} = 1 - \alpha$ . If  $\alpha = 0.05$ , then  $z \approx 3.663$ .



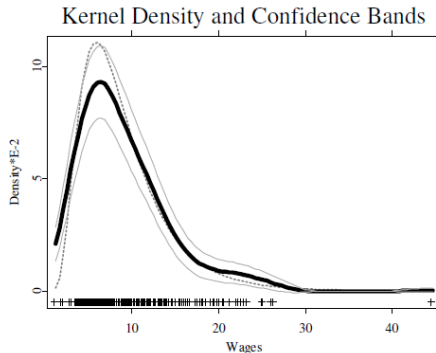
## What can we use the confidence intervals for $\hat{f}_h(x)$ in practice?

In the following example we check if a parametric estimate can describe the data



Sample of 534 randomly selected U.S workers average hourly earnings from May 1985. (Nonpar.: thick solid line, Lognormal: thin line)

Compute the 95% confidence bands around the nonpar. estimate



Lognormal density exceeds the upper limit of the confidence band in the mode- reject the lognormal distribution as "true", even though the lognormal distribution fit the shape quite well.

**Checking whether the parametric density does not exceed the conf. bands is a very conservative test-not the best way to check it.**