

To understand bandwidth selection, let us analyze MISE. Suppose that  $K$  is a symmetric, continuous probability density function with mean 0 and variance  $0 < \sigma_K^2 < \infty$ . Let  $R(g) = \int g^2(z) dz$ . Recall that

$$\text{MISE} = \int \text{MSE}(\hat{f}(x)) dx = \int [\text{var}(\hat{f}(x)) + [\text{bias}(\hat{f}(x))]^2] dx$$

Now let  $h \rightarrow 0$  and  $nh \rightarrow \infty$  as  $n \rightarrow \infty$ .

Bias: Note  $E\{\hat{f}(x)\} = \frac{1}{h} \int K\left(\frac{x-u}{h}\right) f(u) du$

$$= \int K(t) f(x-ht) dt \quad (\text{change of variable})$$

and using Taylor's expansion,  $f(x-ht) = f(x) - ht f'(x) + \frac{h^2 t^2}{2} f''(x) + o(h^2)$ .

$$\Rightarrow E\{\hat{f}(x)\} = f(x) + \frac{h^2 \sigma_K^2}{2} f''(x) + o(h^2) \quad \text{because } K \text{ is symmetric about } 0.$$

$$\text{So, } [\text{bias}\{\hat{f}(x)\}]^2 = \frac{h^4 \sigma_K^4}{4} [f''(x)]^2 + o(h^4).$$

$$\Rightarrow \text{ISB} = \int [\text{bias}\{\hat{f}(x)\}]^2 dx = \frac{h^4 \sigma_K^4}{4} R(f'') + o(h^4).$$

Variance:  $\text{Var}\{\hat{f}(x)\} = \frac{1}{n} \text{Var}\left\{\frac{1}{h} K\left(\frac{x-x_i}{h}\right)\right\}$

change of variables  
(same as above)

$$= \frac{1}{nh} \int K(t)^2 f(x-ht) dt - \frac{1}{n} \left[ E\left\{\frac{1}{h} K\left(\frac{x-x_i}{h}\right)\right\} \right]^2$$

Taylor's expansion  
(same as above)

$$= \frac{1}{nh} \int K(t)^2 [f(x) + o(h)] dt - \frac{1}{n} [f(x) + o(h)]^2$$

$$= \frac{1}{nh} f(x) R(K) + o\left(\frac{1}{nh}\right).$$

$$\Rightarrow \text{IV} = \int \text{Var}\{\hat{f}(x)\} dx = \frac{R(K)}{nh} + o\left(\frac{1}{nh}\right).$$

$$\text{and } \text{MISE} = \frac{R(K)}{nh} + \frac{h^4 \sigma_K^4}{4} R(f'') + o\left(\frac{1}{nh} + h^4\right).$$

AMISE

To minimize AMISE with respect to  $h$ , seek value of  $h$  that avoids excessive bias and variance.

$$\text{optimal bandwidth } h_0 = \left( \frac{R(K)}{n \sigma_K^4 R(f'')} \right)^{1/5}$$

$$\Rightarrow \text{minimal AMISE: } \text{AMISE}_0 = \frac{5}{4} [\sigma_K R(K)]^{4/5} R(f'')^{1/5} n^{-4/5}$$

$$\text{Recall for histogram, } \text{AMISE}_0 = \left[ \frac{R(f')}{16} \right]^{1/3} n^{-2/3}$$

w/ kernel density estimator, getting closer to parametric of  $\frac{1}{n}$ .

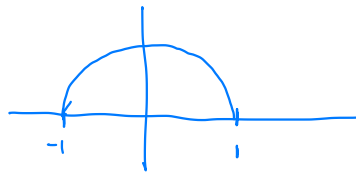
The term  $R(f'')$  measures the roughness of the true underlying density. In general, rougher densities are more difficult to estimate and require smaller bandwidth.

The term  $[\sigma_K R(K)]^{4/5}$  is a function of the kernel function  $K$ .

we could choose  $K$  to minimize  $[\sigma_K R(K)]^{4/5}$ :

If  $K$  restricted to be a proper density, minimizer is a scaled version of a quadratic density:

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



"Epanechnikov Kernel", more later.

**3.1.1 Cross Validation** We want to evaluate quality of  $\hat{f}$  as an estimator of  $f$  without using data twice (once for fitting  $\hat{f}$  and once for evaluating).  
 $\Rightarrow$  again use  $\hat{f}_{-i}(x_i) = \frac{1}{h(n-1)} \sum_{j \neq i} K\left(\frac{x_i - x_j}{h}\right)$  and let  $\hat{Q}(h)$  be a function of  $\hat{f}_{-i}(x_i)$  that assesses quality of fit.  
 e.g. ISE from before.

If  $\hat{Q} = \text{ISE}$ , choose  $h$  to minimize  $R(\hat{f}) - \frac{2}{n} \sum_{i=1}^n \hat{f}_{-i}(x_i)$ .

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 could instead choose  $\hat{Q}(h)$  as the pseudolikelihood  $PL(h) = \prod_{i=1}^n \hat{f}_{-i}(x_i)$  and choose  $h$  to maximize!

Typically, will be undersmoothed  $\Rightarrow$  too bumpy.

### 3.1.2 Plug-in Methods

If the reference density  $f$  is Gaussian and a Gaussian kernel  $K$  is used,

$$h_0 = 1.059 \sigma n^{-1/5}$$

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sample variance or IQR.

this will probably oversmooth.

Empirical estimation of  $R(f'')$  may be a better option.

We could use a kernel density estimator for  $f''$ :

$$\begin{aligned} \hat{f}''(x) &= \frac{d^2}{dx^2} \left\{ \frac{1}{nh_0} \sum_{i=1}^n L\left(\frac{x-x_i}{h_0}\right) \right\} \\ &= \frac{1}{nh_0^3} \sum_{i=1}^n L''\left(\frac{x-x_i}{h_0}\right) \end{aligned}$$

where  $h_0 =$  bandwidth,  $L$  is a sufficiently differentiable kernel to estimate  $f''$ .

Note: estimating  $f$  and  $f''$  (or  $R(f'')$ ) will require different bandwidth.

If we use  $h_0, L$  to estimate  $R(f'')$  and  $h, K$  to estimate  $f$ , then AMISE of  $R(f'')$  is minimized when  $h_0 \propto n^{-1/5}$

$$\Rightarrow h_{0, \text{opt}} = C_1 (R(f''), R(f''')) C_2(L) h^{5/7}$$

$\curvearrowright$  use Gaussian plugin rule.

$\Rightarrow$  2 stage solution: (Sheather-Jones method).

① Use Gaussian plugin rule for  $h_0$  (the bandwidth used to estimate  $R(f'')$ ).

②  $h$  is calculated using  $h = \left( \frac{R(K)}{n \hat{\sigma}_K^4 \hat{R}(f'')} \right)^{1/5}$  used to produce the final kernel density estimate.  
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comes from ①.

## 3.2 Choice of Kernel

There are two choices we have to make to perform density estimation:

The kernel and the bandwidth.

The shape of the kernel is much less important.

Recall  $AMISE_0 = \frac{5}{4} [\sigma_K R(K)]^{4/5} R(f'')^{2/5} n^{-4/5}$

### 3.2.1 Epanechnikov Kernel

The *Epanechnikov kernel* results from choosing  $K$  to minimize  $[\sigma_K R(K)]^{4/5}$ , restricted to be a symmetric density with finite moments and variance equal to 1

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

$$\text{and } \sigma_K R(K) = \frac{3}{(5\sqrt{5})}$$

$\Rightarrow$  The ratio of  $\frac{\sigma_K R(K)}{3/(5\sqrt{5})}$  (\*) gives a measure of relative inefficiency of other kernel.

Kernel	Form	Inefficiency ratio (*)
Epanechnikov	$\frac{3}{4} (1-u^2) \mathbb{I}( u  \leq 1)$	1
Biweight	$\frac{15}{16} (1-u^2)^2 \mathbb{I}( u  \leq 1)$	1.0061
Triweight	$\frac{35}{32} (1-u^2)^3 \mathbb{I}( u  \leq 1)$	1.0135
Gaussian	$\frac{1}{\sqrt{2\pi}} \exp(-u^2/2)$	1.0513
Uniform	$\frac{1}{2} \mathbb{I}( u  \leq 1)$	1.0758

} kernel choice doesn't make much of a difference!

### 3.2.2 Canonical Kernels

Unfortunately a particular value of  $h$  corresponds to a different amount of smoothing depending on which kernel is being used.

Let  $h_K$  and  $h_L$  denote the bandwidths that minimize AMISE when using symmetric kernel densities  $K$  and  $L$ . Then,

$$\frac{h_K}{h_L} = \frac{(R(K)/\sigma_K^4)^{1/5}}{(R(L)/\sigma_L^4)^{1/5}} = \frac{\delta(K)}{\delta(L)}$$

$\Rightarrow$  the change from bandwidth  $h$  for kernel  $K$  to a bandwidth that gives the same amount of smoothing for  $L$ , use bandwidth  $h \delta(L)/\delta(K)$ .

Epanechnikov:  $\delta(K) = 15^{1/5}$

Gaussian:  $\delta(K) = (\sqrt{2/\pi})^{1/5}$

Uniform:  $\delta(K) = (9/2)^{1/5}$

Suppose we rescale a kernel shape so that  $h = 1$  corresponds to a bandwidth of  $\delta(K)$ ,

The kernel density estimator can then be written as  $\hat{f}(x) = \frac{1}{n} \sum_{i=1}^n K_{h\delta(K)}(x-x_i)$

$$\text{where } K_{h\delta(K)}\left(\frac{z}{h\delta(K)}\right) = \frac{1}{h\delta(K)} K\left(\frac{z}{h\delta(K)}\right).$$

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called a "canonical kernel"

benefit: a single value of  $h$  can be used interchangeably for each canonical kernel without affecting the smoothing.

$\Rightarrow$  For a canonical kernel w/ bandwidth  $h$ ,

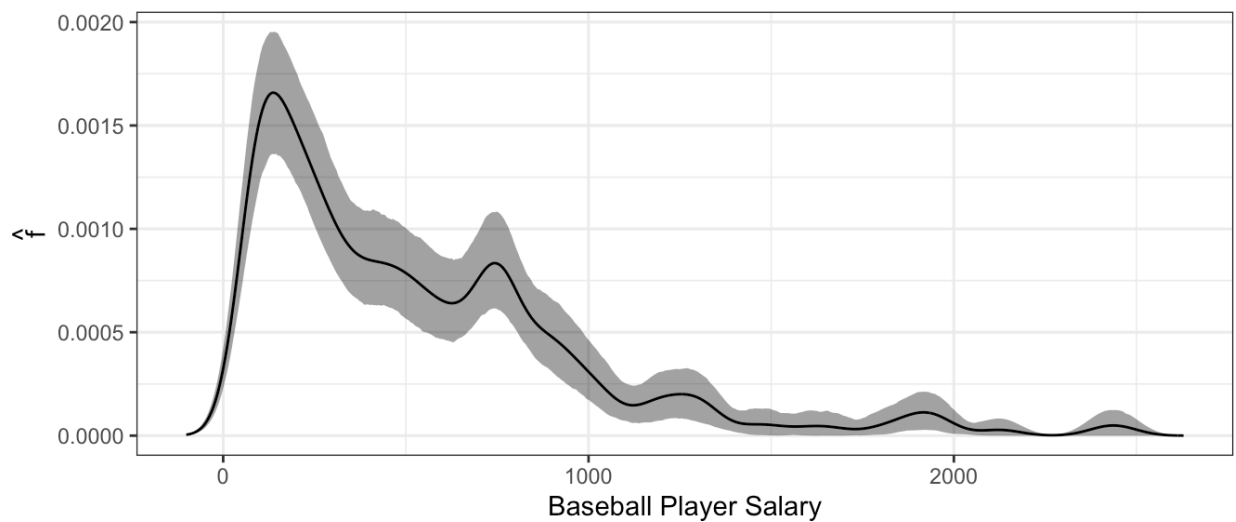
$$\text{AMISE}(h) = (\sigma_K R(f))^{4/5} \underbrace{\left( \frac{1}{nh} + \frac{h^4 R(f'')}{4} \right)}_{\text{bias/variance tradeoff}}$$

So, the Epanechnikov kernel is optimal for any degree of smoothing.

### 3.3 Bootstrapping and Variability Plot

repeat many times  
values of  $\hat{f}$   
recorded at a fixed  
grid of values.

- ① get bootstrap sample
- ② choose bandwidth for sample from ① using Sheather-Jones, density estimate obtained



Note this is NOT a 95% CI  
just representation of variability in process of estimating  $\hat{f}$ .

↳ not telling us  $P(\hat{f}(x)_{\text{lower}} \leq f(x) \leq \hat{f}(x)_{\text{upper}})$ . because bias  $\neq 0$ .