KERNEL DENSITY ESTIMATION (See chapter 1 of Tsybakov 2008)

Let $X_1, \dots, X_n$ be a r.s. with cdf F.

If the cdf F has a continuous derivative F', then the corresponding pdf is $f = F'$. In this case

$$f(x) = \lim_{h \to 0} \frac{F(x+h) - F(x-h)}{2h} \quad \text{for all } x \in \mathbb{R}.$$

This suggests the estimator of $f(x)$ given by

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

for some small value of h, where $\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}(X_i \le x)$.

We may rewrite $\hat{f}_n(x)$ as

$$\begin{aligned}
\hat{f}_n(x) &= \frac{1}{nh} \sum_{i=1}^n \frac{1}{2}\left[\mathbb{1}(X_i \le x+h) - \mathbb{1}(X_i \le x-h)\right] \\
&= \frac{1}{nh} \sum_{i=1}^n \frac{1}{2} \mathbb{1}(x-h < X_i \le x+h) \\
&= \frac{1}{nh} \sum_{i=1}^n \frac{1}{2} \mathbb{1}\left(-1 < \frac{X_i - x}{h} \le 1\right) \\
&= \frac{1}{nh} \sum_{i=1}^n K_0\left(\frac{X_i - x}{h}\right),
\end{aligned}$$

where $K_0(u) = \frac{1}{2} \mathbb{1}(-1 < u \le 1)$.

This is called the Rosenblatt estimator of f.

Exercise: Check whether $\hat{f}_n$ is a legitimate pdf.

Solution: We have $\hat{f}_n(x) \geq 0 \;\forall\, x \in \mathbb{R}$, since $K_0(u) \geq 0 \;\forall\, u \in \mathbb{R}$.

We have

$$\int_{\mathbb{R}} \hat{f}_n(x)\, dx = \int_{\mathbb{R}} \frac{1}{nh} \sum_{i=1}^{n} K_0\left(\frac{X_i - x}{h}\right) dx$$

$u = \frac{X_i - x}{h}$ $\quad dx = -h\,du$

$x = X_i - hu$

$$= -\frac{1}{n} \sum_{i=1}^{n} \int_{\infty}^{-\infty} K_0(u)\, du$$

$$= \frac{1}{n} \sum_{i=1}^{n} \underbrace{\int_{-\infty}^{\infty} \frac{1}{2} \mathbb{1}(-1 < u \leq 1)\, du}_{=1}$$

$$= 1.$$

We can generalize the Rosenblatt estimator by choosing other K:

$$K(u) = (1 - |u|)\, \mathbb{1}(|u| \leq 1) \quad [\text{Triangular}]$$

$$K(u) = \frac{3}{4}(1 - u^2)\, \mathbb{1}(|u| \leq 1) \quad [\text{Epanechnikov}]$$

$$K(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2} \quad [\text{Gaussian}]$$

Then we have the so-called Kernel density estimator (KDE)

$$\hat{f}_n(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right) \quad \text{for } x \in \mathbb{R}.$$

The function K is called the Kernel and h the bandwidth.

For $\hat{f}_n$ to be a legitimate density, we require

(K0) $K(u) \geq 0 \quad \forall \; u \in \mathbb{R}$.

(K1*) $\int_{\mathbb{R}} K(u)\, du = 1$.

<u>Exercise</u>: Generate data and plot KDEs along with true density. Try different kernels and bandwidths.

<u>Mean squared error of KDE at a point x_0 (upper bound):</u>

<u>Variance</u>: Let $\sigma_n^2(x_0) = \text{Var}\, \hat{f}_n(x_0)$ for $x_0 \in \mathbb{R}$.

Make the assumptions

(F1) $\exists \; f_{max} > 0$ s.t. $f(x) \leq f_{max} \quad \forall \; x \in \mathbb{R}$.

(K2) $\int_{\mathbb{R}} K^2(u)\, du \leq \kappa^2 < \infty$.

<u>Result</u>: Under (F1) and (K2) we have

$$\sigma_n^2(x_0) \leq \frac{1}{nh} f_{max} \cdot \kappa^2$$

for each $x_0 \in \mathbb{R}$.

Proof: For a point $x_0 \in \mathbb{R}$ we have

$$\begin{aligned}
\mathrm{Var}\left[K\left(\frac{X_1 - x_0}{h}\right)\right] &= \mathbb{E}\left[K^2\left(\frac{X_1 - x_0}{h}\right)\right] - \left[\mathbb{E}\, K\left(\frac{X_1 - x_0}{h}\right)\right]^2 \\
&\leq \mathbb{E}\left[K^2\left(\frac{X_1 - x_0}{h}\right)\right] \\
&= \int_{\mathbb{R}} K^2\left(\frac{x - x_0}{h}\right) f(x)\, dx \\
&\leq f_{max} \int_{\mathbb{R}} K^2\left(\frac{x - x_0}{h}\right) dx \\
&= f_{max} \cdot h \cdot \int_{\mathbb{R}} K^2(u)\, du \\
&\leq h \cdot f_{max} \cdot \kappa^2 .
\end{aligned}$$

Now we have

$$\begin{aligned}
\mathrm{Var}\, \hat{f}_n(x_0) &= \frac{1}{n^2 h^2} \sum_{i=1}^{n} \mathrm{Var}\left[K\left(\frac{X_i - x_0}{h}\right)\right] \\
&\leq \frac{1}{n^2 h^2} \sum_{i=1}^{n} h \cdot f_{max} \cdot \kappa^2 \\
&= \frac{1}{nh} \cdot f_{max} \cdot \kappa^2 .
\end{aligned}$$

$\square$

Bias: Let $b_n(x_0) = \mathbb{E}\, \hat{f}_n(x_0) - f(x_0)$ for some $x_0 \in \mathbb{R}$.

Trickier than the variance, must consider wiggliness of f.

Defn: Let T be an interval in $\mathbb{R}$ and $L > 0$. The Lipschitz class of functions Lipschitz(L) on T is the set of functions $f: T \to \mathbb{R}$ satisfying

$$|f(x) - f(x')| \leq L\,|x - x'| \quad \forall \; x, x' \in T.$$

Let the set of pdfs that belong to Lipschitz (L) on $\mathbb{R}$ be denoted by

$$\mathcal{P}_{\mathcal{L}}(L) = \left\{ f : f \geq 0, \int_{\mathbb{R}} f(x)\,dx = 1, \; f \in \text{Lipschitz}(L) \text{ on } \mathbb{R} \right\}$$

We require another assumption on K, which we will later expand on:

$$(K3^*) \quad \int_{\mathbb{R}} |u|\,|K(u)|\,du \leq K_1 < \infty$$

Result: Under $(K1^*)$ and $(K3^*)$, and if $f \in \mathcal{P}_{\mathcal{L}}(L)$, then

$$|b(x_0)| = h \cdot L \cdot K_1$$

for each $x_0 \in \mathbb{R}$.

Proof: We have

$$\mathbb{E}\hat{f}_n(x_0) - f(x_0) = \frac{1}{nh} \sum_{i=1}^{n} \left[\mathbb{E}\, K\left(\frac{X_i - x_0}{h}\right) \right] - f(x_0),$$

$$= \frac{1}{h} \mathbb{E}\, K\left(\frac{X_1 - x_0}{h}\right) - f(x_0)$$

$$= \frac{1}{h} \int_{\mathbb{R}} K\left(\frac{x - x_0}{h}\right) f(x)\,dx - f(x_0)$$

$$u = \frac{x - x_0}{h}, \quad x = x_0 + uh, \quad dx = h\,du$$

$$= \int_{\mathbb{R}} K(u)\, f(x_0 + uh)\, du - f(x_0)$$

by $(K1^*)$

$$= \int_{\mathbb{R}} K(u) \left[f(x_0 + uh) - f(x_0) \right] du .$$

So we have

$$|b_n(x_0)| \le \int_{\mathbb{R}} K(u) \left| f(x_0 + uh) - f(x_0) \right| du$$

by $(F2^*)$

$$\le \int_{\mathbb{R}} |K(u)|\, L\, |uh|\, du$$

$$= L \cdot h \int_{\mathbb{R}} |u| \, |K(u)|\, du$$

by $(K3^*)$

$$\le L \cdot h \cdot K_1 . \qquad \square$$

Putting the bias and variance together we get the following result:

Result: Under $(K1^*)$, $(K2)$, $(K3^*)$, $(F1)$, and if $f \in \mathcal{P}_{\mathcal{L}}(L)$, then

$$MSE\ \hat{f}_n(x_0) \le h^2 \cdot L^2 \cdot K_1^2 + \frac{1}{nh} \cdot f_{max} \cdot K^2 .$$

for each point $x_0 \in \mathbb{R}$.

Optimal h: To minimize $MSE\ \hat{f}_n(x_0)$ in the setting of the previous result, we would choose

$$h_{opt} = n^{-1/3}\, C_1 \qquad \left(f \in \mathcal{P}_{\mathcal{L}}(L) \right)$$

where C_1 depends on unknown constants.

Why??

$$\frac{\partial}{\partial h}\left(\text{bound on MSE } \hat{f}_n(x_0)\right) = 2h \cdot L^2 \cdot K_1^2 - \frac{1}{nh^2} \cdot f_{max} \cdot K^2 = 0$$

$$\Longleftrightarrow \quad 2h^3 \cdot L^2 \cdot K_1^2 = \frac{f_{max} K^2}{n}$$

$$\Longleftrightarrow \quad h = n^{-1/3} \underbrace{\left(\frac{f_{max} \cdot K^2}{L^2 \cdot K_1^2 \cdot 2}\right)^{1/3}}_{C_1}$$

Optimal order of MSE $\hat{f}_n(x_0)$: Plugging in $h_{opt} = n^{-1/3} C_1$ gives

$$\text{MSE } \hat{f}_n(x) \leq n^{-2/3} C_1^* . \quad \left(f \in \mathcal{P}_{\mathcal{L}}(L)\right)$$

We now introduce a more general class of functions than Lipschitz.

Defn: Let T be an interval in $\mathbb{R}$, β a positive integer, and $L > 0$. The Hölder class $\mathcal{H}(\beta, L)$ on T is the set of $\ell = \beta - 1$ times differentiable functions $f: T \to \mathbb{R}$ of which the derivative $f^{(\ell)}$ satisfies

$$\left| f^{(\ell)}(x) - f^{(\ell)}(x') \right| \leq L \left| x - x' \right| \qquad \forall \; x, x' \in T .$$

* Can define Hölder classes for non-integer β, but we ignore these.

For $\beta = 2$, the condition is $\left| f^{(1)}(x) - f^{(1)}(x') \right| \leq L \left| x - x' \right|$.

Exercise: Determine if $f \in \mathcal{H}(\beta, L)$ for some β, L or if $f \in \text{Lipschitz}(L)$.

(a) $f(x) = x^2$ (b) $f(x) = 1/x$ (c) $f(x) = \log x$

(d) $f(x) = e^x$ (e) $f(x) = e^{-x} \mathbb{1}(x > 0)$

Let the set of all pdfs belonging to $\mathcal{H}(\beta, L)$ on $\mathbb{R}$ be represented by

$$\mathcal{P}_{\mathcal{H}}(\beta, L) = \left\{ f : f \geq 1, \int_{\mathbb{R}} f(x)\,dx, \quad f \in \mathcal{H}(\beta, L) \text{ on } \mathbb{R} \right\}.$$

To consider estimating $f \in \mathcal{P}_{\mathcal{H}}(\beta, L)$, we must expand $(K1^*)$. We will need a new definition:

<u>Defn:</u> Let $\ell \geq 1$ be an integer. We call $K : \mathbb{R} \to \mathbb{R}$ a kernel of order ℓ if the functions $u \mapsto u^j K(u)$, $j = 0, 1, \dots, \ell$ are integrable and satisfy

$$\int_{\mathbb{R}} K(u)\,du = 1, \qquad \int_{\mathbb{R}} u^j K(u)\,du = 0, \quad j = 1, \dots, \ell.$$

In the following we will use the assumptions

(K1) K is a kernel of order ℓ

(K3) $\displaystyle\int_{\mathbb{R}} |u|^\beta |K(u)|\,du \leq \kappa_\beta < \infty$

with ℓ and β taken from the relevant Hölder class.

We now revisit the bias:

<u>Result:</u> Under (K1) and (K3) and if $f \in \mathcal{P}_{\mathcal{H}}(\beta, L)$ on $\mathbb{R}$, we have

$$|b_n(x_0)| \leq h^\beta \cdot \frac{L \cdot \kappa_\beta}{\ell!}$$

for each $x_0 \in \mathbb{R}$.

<u>Proof:</u> Following our previous work, we can write

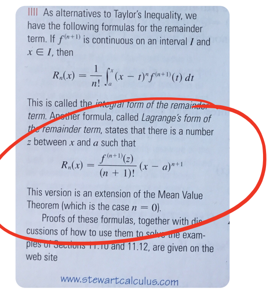
$$\mathbb{E}\hat{f}_n(x_0) - f(x_0) = \frac{1}{nh} \sum_{i=1}^{n} \left[\mathbb{E}\, K\left(\frac{X_i - x_0}{h}\right) \right] - f(x_0),$$

$$\vdots$$

$$= \int_{\mathbb{R}} K(u) \left[f(x_0 + uh) - f(x_0) \right] du.$$

Now we write $f(x_0 + uh)$ via Taylor expansion as

$$f(x_0 + uh) = f(x_0) + \sum_{j=1}^{\ell-1} \frac{f^{(j)}(x_0)(uh)^j}{j!} + \frac{f^{(\ell)}(x_0 + \tau u h)\,(uh)^\ell}{\ell!}$$


|||| As alternatives to Taylor's Inequality, we have the following formulas for the remainder term. If $f^{(n+1)}$ is continuous on an interval I and $x \in I$, then

$$R_n(x) = \frac{1}{n!}\int_a^x (x-t)^n f^{(n+1)}(t)\,dt$$

This is called the *integral form of the remainder term.* Another formula, called *Lagrange's form of the remainder term,* states that there is a number z between x and a such that

$$R_n(x) = \frac{f^{(n+1)}(z)}{(n+1)!}(x-a)^{n+1}$$

This version is an extension of the Mean Value Theorem (which is the case $n = 0$).

Proofs of these formulas, together with discussions of how to use them to solve the examples of Sections 11.10 and 11.12, are given on the web site

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for some $0 \leq \tau \leq 1$. Note that

$$\int_{\mathbb{R}} K(u) \sum_{j=1}^{\ell-1} f^{(j)}(x_0)(uh)^j \, du = 0,$$

since K, by (K1) is a kernel of order ℓ. This gives

$$b_n(x_0) = \int_{\mathbb{R}} K(u) \frac{f^{(\ell)}(x_0 + \tau u h)\,(uh)^\ell}{\ell!} \, du$$

by (K1)

$$= \frac{h^\ell}{\ell!} \int_{\mathbb{R}} u^\ell K(u) \left[f^{(\ell)}(x_0 + \tau u h) - f^{(\ell)}(x_0) \right] du .$$

So we have

$$|b_n(x_0)| \leq \frac{h^\ell}{\ell!} \int_{\mathbb{R}} |u|^\ell K(u) \left| f^{(\ell)}(x_0 + \tau u h) - f^{(\ell)}(x_0) \right| du$$

$$\leq \frac{h^\ell}{\ell!} \int_{\mathbb{R}} |u|^\ell |K(u)| \, L \, |\tau u h| \, du$$

$(\beta = \ell + 1)$

$$\leq \frac{h^\beta}{\ell!} \cdot L \int_{\mathbb{R}} |u|^\beta |K(u)| \, du$$

$$\leq \frac{h^\beta}{\ell!} \cdot L \cdot K_\beta . \qquad \square$$

The variance depends only on f_{max} and K^2 from (F1), (K2).

Result: Under (K1), (K2), (K3), (F1), and if $f \in \mathcal{P}_{H}(\beta, L)$, then

$$\text{MSE}\ \hat{f}_n(x_0) \le h^{2\beta}\left(\frac{L \cdot K_\beta}{\ell!}\right)^2 + \frac{1}{nh} f_{max} \cdot K^2$$

for each point $x_0 \in \mathbb{R}$.

Optimal h: To minimize $\text{MSE}\ \hat{f}_n(x_0)$ in the setting of the previous result, we would choose

$$h_{opt} = n^{-\frac{1}{2\beta+1}} C_2, \qquad \left(f \in \mathcal{P}_{H}(\beta, L)\right)$$

where C_2 depends on unknown constants.

Why??

$$\frac{\partial}{\partial h}\left(\text{Bound on MSE}\ \hat{f}_n(x_0)\right) = 2\beta h^{2\beta-1}\left(\frac{L \cdot K_\beta}{\ell!}\right)^2 - \frac{1}{nh^2} f_{max} \cdot K^2 = 0$$

$$\Leftrightarrow \quad h^{2\beta+1} = \frac{1}{n} \frac{f_{max} \cdot K^2}{2\beta\,(L \cdot K_\beta / \ell!)^2}$$

$$\Leftrightarrow \quad h = n^{-\frac{1}{2\beta+1}} \underbrace{\left[\frac{f_{max} \cdot K^2}{2\beta\,(L \cdot K_\beta / \ell!)^2}\right]^{\frac{1}{2\beta+1}}}_{C_2}.$$

Optimal order of $\text{MSE}\ \hat{f}_n(x_0)$: Plugging h_{opt} into the MSE bound gives

$$\text{MSE}\ \hat{f}_n(x_0) \le n^{-\frac{2\beta}{2\beta+1}} C_2^*. \qquad \left(f \in \mathcal{P}_{H}(\beta, L)\right)$$

Exercise: Suppose f is $2\times$ differentiable with a bounded second derivative. What is h_{opt} and the resulting bound on MSE $\hat{f}_n(x_0)$?

Solution: We have $f \in \mathcal{P}_H(2, L)$ for some L, so

$$h_{opt} \asymp n^{-\frac{1}{5}} \qquad \text{and} \qquad \text{MSE}\, \hat{f}_n(x_0) \asymp n^{-\frac{4}{5}}$$

We now present a summarizing theorem for this section

Theorem 1: Under (K1), (K2), and (K3), if $h = \alpha n^{-\frac{1}{2\beta+1}}$ for some $\alpha \geqslant 0$, then for all $n \geqslant 1$, we have

$$\sup_{x_0 \in \mathbb{R}} \ \sup_{f \in \mathcal{P}_H(\beta, L)} \mathbb{E}_f\left[\left(\hat{f}_n(x_0) - f(x_0)\right)^2\right] \leq C\, n^{-\frac{2\beta}{2\beta+1}}$$

where $C > 0$ depends only on β, L, α, and the kernel $K(\cdot)$.

This bounds MSE $\hat{f}_n(x_0)$ uniformly over the class of densities $\mathcal{P}_H(\beta, L)$.

Remark: Where did assumption (F1) go? We can show that $\exists\, f_{max}$ s.t.

$$\sup_{x_0 \in \mathbb{R}} \ \sup_{f \in \mathcal{P}_H(\beta, L)} f(x_0) \leq f_{max} < \infty, \qquad \text{[see Tsyb. pg 9]}$$

so (F1) is redundant if $f \in \mathcal{P}_H(\beta, L)$.

Mean integrated squared error of KDE (upper bound):

Instead of looking at a single point x_0, look at entire $\mathbb{R}$.

Defn: The mean integrated squared error (MISE) of $\hat{f}_n$ is defined as

$$\text{MISE } \hat{f}_n = \mathbb{E} \int_{\mathbb{R}} [\hat{f}_n(x) - f(x)]^2 \, dx \, .$$

We have the following decomposition:

$$\begin{aligned}
\text{MISE } \hat{f}_n &= \mathbb{E} \int_{\mathbb{R}} [\hat{f}_n(x) - f(x)]^2 \, dx \\
&\overset{\text{(Fubini-Tonelli)}}{=} \int_{\mathbb{R}} \mathbb{E} [\hat{f}_n(x) - f(x)]^2 \, dx \\
&= \int_{\mathbb{R}} \text{MSE } \hat{f}_n(x) \, dx \\
&= \underbrace{\int_{\mathbb{R}} b^2(x) \, dx}_{\text{bias term}} + \underbrace{\int_{\mathbb{R}} \sigma^2(x) \, dx}_{\text{variance term}}
\end{aligned}$$

Result: Under (K2) we have

$$\int_{\mathbb{R}} \sigma^2(x) \, dx \le \frac{1}{nh} K^2 .$$

Proof:

$$\sigma^2(x) = \text{Var } \hat{f}_n(x)$$

$$
\begin{aligned}
&= \operatorname{Var}\left(\frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right)\right) \\
&= \frac{1}{nh^2}\operatorname{Var}\left(K\left(\frac{X_1 - x}{h}\right)\right) \\
&= \frac{1}{nh^2}\left[\mathbb{E}\, K^2\left(\frac{X_1 - x}{h}\right) - \left(\mathbb{E}\, K\left(\frac{X_1 - x}{h}\right)\right)^2\right] \\
&\le \frac{1}{nh^2}\,\mathbb{E}\, K^2\left(\frac{X_1 - x}{h}\right) \\
&= \frac{1}{nh^2}\int_{\mathbb{R}} K^2\left(\frac{z - x}{h}\right) f(z)\, dz \\
&= \frac{1}{nh}\int_{\mathbb{R}} K^2(u)\, f(x + uh)\, du
\end{aligned}
$$

Now we have

$$
\begin{aligned}
\int_{\mathbb{R}} \sigma^2(x)\, dx &\le \frac{1}{nh}\int_{\mathbb{R}}\int_{\mathbb{R}} K^2(u)\, f(x + uh)\, du\, dx \\
&= \frac{1}{nh}\int_{\mathbb{R}} K^2(u)\underbrace{\left[\int_{\mathbb{R}} f(x + uh)\, dx\right]}_{=1} du \\
&= \frac{1}{nh} K^2. \qquad \square
\end{aligned}
$$

The bias, as before, is much trickier, as we must consider the smoothness of the function.

We find that we need another function class to describe smoothness under the L_2-norm:

<u>**Defn:**</u> For $\beta > 0$ an integer and $L > 0$ the Nikol'ski class of functions $\mathcal{N}(\beta, L)$ is the set of functions $f : \mathbb{R} \to \mathbb{R}$ of which the derivatives $f^{(\ell)}$ of order $\ell = \beta - 1$ exist and satisfy

$$\left(\int_{\mathbb{R}} \left[f^{(\ell)}(x+t) - f^{(\ell)}(x) \right]^2 dx \right)^{1/2} \le L |t| \qquad \forall\, t \in \mathbb{R}.$$

Let the set of densities $f \in \mathcal{N}(\beta, L)$ be represented by

$$\mathcal{P}_{\mathcal{N}}(\beta, L) = \left\{ f \in \mathcal{N}(\beta, L) : \quad f \ge 0, \quad \int_{\mathbb{R}} f(x)\, dx = 1 \right\}$$

<u>**Result:**</u> Under (K1) and (K3), if $f \in \mathcal{P}_{\mathcal{N}}(\beta, L)$, then

$$\int_{\mathbb{R}} b^2(x)\, dx \le h^{2\beta} \left(\frac{L \cdot K_\beta}{\ell!} \right)^2.$$

In order to prove the result, we need this inequality:

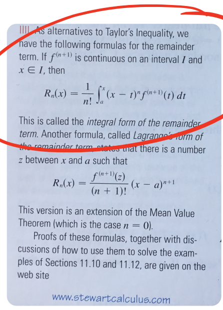
<u>**Generalized Minkowski inequality:**</u> For any Borel function on $\mathbb{R} \times \mathbb{R}$, we have

$$\left[\int_{\mathbb{R}} \left(\int_{\mathbb{R}} g(u,x)\, du \right)^2 dx \right]^{1/2} \le \int_{\mathbb{R}} \left(\int_{\mathbb{R}} g^2(u,x)\, dx \right)^{1/2} du.$$

Proof of bound on the bias term:

First consider the Taylor expansion

$$f(x+uh) = f(x) + \sum_{j=1}^{\ell-1} \frac{f^{(j)}(x)\,(uh)^j}{j!} + \underbrace{\frac{1}{(\ell-1)!}\int_x^{x+uh} (x+uh-t)^{\ell-1} f^{(\ell)}(t)\,dt}_{= \frac{(uh)^\ell}{(\ell-1)!}\int_0^1 (1-\tau)^{\ell-1} f^{(\ell)}(x+\tau uh)\,d\tau}$$


As alternatives to Taylor's Inequality, we have the following formulas for the remainder term. If $f^{(n+1)}$ is continuous on an interval I and $x \in I$, then

$$R_n(x) = \frac{1}{n!}\int_a^x (x-t)^n f^{(n+1)}(t)\,dt$$

This is called the *integral form of the remainder term*. Another formula, called *Lagrange's form of the remainder term*, states that there is a number z between x and a such that

$$R_n(x) = \frac{f^{(n+1)}(z)}{(n+1)!}(x-a)^{n+1}$$

This version is an extension of the Mean Value Theorem (which is the case $n = 0$).

Proofs of these formulas, together with discussions of how to use them to solve the examples of Sections 11.10 and 11.12, are given on the web site

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Now we write

$$b(x) = \mathbb{E}\,\frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right) - f(x)$$

$$= \frac{1}{h}\,\mathbb{E}\,K\left(\frac{X_1 - x}{h}\right) - f(x)$$

$$= \frac{1}{h}\int_{\mathbb{R}} K\left(\frac{z-x}{h}\right) f(z) - f(x)$$

$$= \int_{\mathbb{R}} K(u)\, f(x+uh)\,du - f(x)$$

$$= \int_{\mathbb{R}} K(u)\left[f(x+uh) - f(x)\right] du$$

$$= \int_{\mathbb{R}} K(u)\left[\sum_{j=1}^{\ell-1} \frac{f^{(j)}(x)\,(uh)^j}{j!} + \frac{1}{(\ell-1)!}\int_0^1 (uh)^{\ell-1} (1-\tau)^{\ell-1} f^{(\ell)}(x+\tau uh)\,d\tau\right] du$$

K a kernel of order ℓ

$$= \int_{\mathbb{R}} K(u)\,\frac{(uh)^\ell}{(\ell-1)!}\int_0^1 (1-\tau)^{\ell-1} f^{(\ell)}(x+\tau uh)\,d\tau\,du.$$

$$= \int_{\mathbb{R}} K(u) \frac{(uh)^{\ell}}{(\ell-1)!} \int_0^1 (1-\tau)^{\ell-1} \left[f^{(\ell)}(x+\tau uh) - f^{(\ell)}(x) \right] d\tau \, du$$

Can subtract because kernel of order ℓ.

Now we get a bound on $\int b^2(x)\,dx$ by using Minkowski's 2x and the smoothness class:

$$\int_{\mathbb{R}} b^2(x)\,dx \le \int_{\mathbb{R}} \Bigg[\int_{\mathbb{R}} \underbrace{K(u) \frac{(uh)^{\ell}}{(\ell-1)!} \int_0^1 (1-\tau)^{\ell-1} \left| f(x+\tau uh) - f(x) \right| d\tau \, du}_{g(u,x)\,du} \Bigg]^2 dx$$

$$\le \left[\int_{\mathbb{R}} \left(\int_{\mathbb{R}} \underbrace{\left[K(u) \frac{(uh)^{\ell}}{(\ell-1)!} \int_0^1 (1-\tau)^{\ell-1} \left| f(x+\tau uh) - f(x) \right| d\tau \right]^2 dx}_{g^2(u,x)\,dx} \right)^{1/2} du \right]^2$$

$$= \left[\int_{\mathbb{R}} \left(|K(u)| \frac{|uh|^{\ell}}{(\ell-1)!} \int_{\mathbb{R}} \left[\int_0^1 \underbrace{(1-\tau)^{\ell-1} \left| f(x+\tau uh) - f(x) \right| d\tau}_{g(\tau,x)\,d\tau} \right]^2 dx \right)^{1/2} du \right]^2$$

$$\le \left[\int_{\mathbb{R}} \left(|K(u)| \frac{|uh|^{\ell}}{(\ell-1)!} \int_0^1 \left[\int_{\mathbb{R}} \underbrace{(1-\tau)^{2(\ell-1)} \left| f(x+\tau uh) - f(x) \right|^2 dx}_{g^2(\tau,x)\,dx} \right]^{1/2} d\tau \, du \right]^2$$

$$\le \left[\int_{\mathbb{R}} \left(|K(u)| \frac{|uh|^{\ell}}{(\ell-1)!} \int_0^1 |1-\tau|^{(\ell-1)} \left[\int_{\mathbb{R}} \left| f(x+\tau uh) - f(x) \right|^2 dx \right]^{1/2} d\tau \, du \right]^2$$

$$\leq \left[\int_{\mathbb{R}} \left(|K(u)| \frac{|uh|^{\ell}}{(\ell-1)!} \underbrace{\int_0^1 (1-\tau)^{(\ell-1)} d\tau}_{\frac{1}{\ell}} \; L \, \underbrace{|\tau u h|}_{\leq 1} \; du \right] \right]^2$$

$(\beta = \ell + 1)$

$$\leq h^{2\beta} \frac{L^2}{\ell!} \left[\int_{\mathbb{R}} |u|^{\beta} |K(u)| \, du \right]^2 .$$

$\square$

Result: Under (K1), (K2), and (K3), if $f \in \mathcal{P}_{\mathcal{N}}(\beta, L)$, we have

$$\text{MISE } \hat{f}_n \leq h^{2\beta} \left(\frac{L \cdot K_\beta}{\ell!} \right)^2 + \frac{1}{nh} K^2 .$$

We can also state a uniform result:

Theorem 2: Under (K1), (K2), and (K3), if $h = \alpha n^{-\frac{1}{2\beta+1}}$ for some $\alpha > 0$, then for all $n \geq 1$,

$$\sup_{f \in \mathcal{P}_{\mathcal{N}}} \mathbb{E}_f \int_{\mathbb{R}} [\hat{f}_n(x) - f(x)]^2 dx \leq C n^{-\frac{2\beta}{2\beta+1}} ,$$

where $C > 0$ depends only on β, L, α and the kernel $K(\cdot)$.

Data-based bandwidth selection:

A "plug-in" method: the Sheather–Jones method uses the following result:

Theorem 3: If K is a kernel of order 1 s.t.

$$K^2 = \int_{\mathbb{R}} K^2(u)\,du < \infty, \quad \int_{\mathbb{R}} u^2 |K(u)|\,du < \infty, \quad \sigma_K^2 = \int_{\mathbb{R}} u^2 K(u)\,du < \infty$$

and f is differentiable on $\mathbb{R}$ with f' a.c. on $\mathbb{R}$ and with

$$\|f''\|_2^2 = \int_{\mathbb{R}} [f''(x)]^2\,dx < \infty,$$

then

$$\text{MISE}\,\hat{f}_n = \left[h^4 \left(\frac{\|f''\|_2 \cdot \sigma_K^2}{2} \right)^2 + \frac{1}{nh} K^2 \right] \Big(1 + \underbrace{o(1)}_{\to 0 \text{ as } h \to 0} \Big)$$

as $n \to \infty$, $h \to 0$.

See pg. 192 of Tsybakov for a proof.

The proof of the above result is more tedious than the proof of the MISE result under the Nikol'ski class.

The above result is also not a uniform result over any class of functions, but rather assumes a single, fixed density f.

Exercise: Get an expression for the optimal bandwidth using Thm 3.

Solution: We have

$$\frac{\partial}{\partial h}\Big(\text{Dominating term of MISE} \Big) = h^3 \cdot \|f''\|_2^2 \cdot \sigma_K^4 - \frac{1}{nh} K^2 = 0$$

So the MISE-minimizing choice of h is

$$h_{opt} = n^{-\frac{1}{5}} \left(\frac{K^2}{\|f''\|_2^2 \cdot \sigma_K^4} \right)^{1/5}.$$

The SJ method "plugs in" an estimator of $\|f''\|_2^2$. Hence "plug-in" method. See option bw="SJ" of the density() function in R.

A Crossvalidation Method:

The idea is to estimate from the data the MISE of $\hat{f}_n$ at given bandwidth values and then to choose h which minimizes it.

Consider

$$\begin{aligned} MISE_h \hat{f}_n &= \mathbb{E}_f \int_{\mathbb{R}} [\hat{f}_n(x) - f(x)]^2 \, dx \\ &= \mathbb{E}_f \int_{\mathbb{R}} \hat{f}_n^2(x) \, dx \quad - 2\, \mathbb{E}_f \int_{\mathbb{R}} \hat{f}_n(x) f(x) \, dx \; - \; \int_{\mathbb{R}} f^2(x) \, dx \end{aligned}$$

Let

$$A_n = \mathbb{E}_f \int_{\mathbb{R}} \hat{f}_n^2(x) \, dx .$$

$$B_n = \mathbb{E}_f \int_{\mathbb{R}} \hat{f}_n(x) f(x) \, dx$$

Note that $\int_{\mathbb{R}} \hat{f}_n^2(x) \, dx$ is, trivially, an unbiased estimator of A_n.

Now, an unbiased estimator of B_n can be constructed as

$$\hat{B}_n = \frac{1}{n} \sum_{i=1}^{n} \hat{f}_{n,-i}(X_i),$$

where

"Leave-one-out" crossvalidation.

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

is the KDE of f computed after removing obs i from the data.

We see that

$$\mathbb{E}_f \hat{B} = \mathbb{E}_f \frac{1}{n} \sum_{i=1}^{n} \hat{f}_{n,-i}(X_i)$$

$$= \mathbb{E}_f f_{n,-1}(X_1)$$

$$= \mathbb{E}_f \left[\frac{1}{(n-1)h} \sum_{j \neq 1} K\left(\frac{X_j - X_1}{h}\right) \right]$$

$$= \frac{1}{h} \mathbb{E}_f K\left(\frac{X_2 - X_1}{h}\right)$$

$$= \frac{1}{h} \int_{\mathbb{R}} \int_{\mathbb{R}} K\left(\frac{z-x}{h}\right) f(z) f(x)\, dz\, dx$$

We also have

$$B_n = \mathbb{E}_f \int_{\mathbb{R}} \hat{f}_n(x) f(x)\, dx$$

$$= \mathbb{E}_f \int_{\mathbb{R}} \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right) f(x)\, dx$$

$$= \frac{1}{h} \int_{\mathbb{R}} \mathbb{E}_f K\left(\frac{X_i - x}{h}\right) f(x)\, dx$$

$$= \frac{1}{h} \int_{\mathbb{R}} \int_{\mathbb{R}} K\left(\frac{z-x}{h}\right) f(x)\, dx\ f(z)\, dz,$$

so that $\mathbb{E}\hat{B}_n = B_n$.

Since $\underset{h>0}{\operatorname{argmin}}\ MISE_h\ \hat{f}_n = \underset{h>0}{\operatorname{argmin}}\ A_n - 2B_n$, choose

$$h_{CV} = \underset{h>0}{\operatorname{argmin}}\ CV(h),$$

where

$$CV(h) = \int_{\mathbb{R}} \hat{f}_n^2(x)\,dx - \frac{2}{n}\sum_{i=1}^{n} \hat{f}_{n,-i}(X_i).$$

Some assumptions implicit in our work are given in the following proposition:

__Result:__ Assume that $K:\mathbb{R}\to\mathbb{R}$ and f satisfy

$$\int_{\mathbb{R}} f^2(x)\,dx < \infty \quad \text{and} \quad \int_{\mathbb{R}}\int_{\mathbb{R}} \left|K\left(\frac{z-x}{h}\right)\right| f(z)\,dz\, f(x)\,dx$$

for all $h>0$. Then

$$\mathbb{E}\,CV(h) = MISE_h\ \hat{f}_n - \int_{\mathbb{R}} f^2(x)\,dx.$$