

1 Basic concepts

1.1 Parametric vs Nonparametric models

A statistical model postulates a family of possible data generating mechanisms. Examples include:

- (i) Let $X_1, \dots, X_n \sim^{\text{iid}} \Gamma(m, \theta)$ where m is known and $\theta \in (0, \infty) := \Theta$;
- (ii) Let $Y_i = \alpha + \beta x_i + \varepsilon_i$ for $i \in [n] := \{1, \dots, n\}$, where x_1, \dots, x_n and $\varepsilon_1, \dots, \varepsilon_n \sim^{\text{iid}} \mathcal{N}(0, \sigma^2)$. Here the unknown parameter is $\theta = (\alpha, \beta, \sigma^2) \in \mathbb{R} \times \mathbb{R} \times (0, \infty) := \Theta$.

If the parameter space Θ is finite-dimensional, we speak of a *parametric model*. When the model is correctly specified, i.e there exists $\theta_0 \in \Theta$ for which the data were generated from the distribution with parameter θ_0 , typically we can use the MLE $\hat{\theta}_n$ to estimate θ_0 , and expect $n^{1/2}(\hat{\theta}_n - \theta_0)$ to converge to a non-degenerate limiting distribution. On the other hand, when the model is misspecified, inferences may be very misleading.

Examples of nonparametric models include:

- (i) Let $X_1, \dots, X_n \sim^{\text{iid}} F$ for some unknown distribution function F ;
- (ii) Let $X_1, \dots, X_n \sim^{\text{iid}} f$ for some density f belonging to some unknown smoothness class;
- (iii) Let $Y_i = m(x_i) + \varepsilon_i$ for $i \in [n]$, where x_1, \dots, x_n are known, m belongs to some unknown smoothness class and $\varepsilon_1, \dots, \varepsilon_n$ are iid with $\mathbb{E}(\varepsilon_1) = 0$, $\text{Var}(\varepsilon_1) = \sigma^2$.

Such infinite-dimensional models are much less vulnerable to model misspecification. Typically however, we will pay a price in terms of a slower rate of convergence.

1.2 Estimating an arbitrary distribution function

Let \mathcal{F} denote the set of all distribution functions on \mathbb{R} . The *empirical distribution function* \mathbb{F}_n of real-valued random variables X_1, \dots, X_n is defined by

$$\mathbb{F}_n(x) = \mathbb{F}_n(x, X_1, \dots, X_n) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{X_i \leq x\}.$$

Theorem (Glivenko-Cantelli Theorem). *Let $X_1, \dots, X_n \sim^{\text{iid}} F \in \mathcal{F}$ and let \mathbb{F}_n denote the empirical distribution function of X_1, \dots, X_n . Then*

$$\sup_{x \in \mathbb{R}} |\mathbb{F}_n(x) - F(x)| \xrightarrow{a.s.} 0 \text{ as } n \rightarrow \infty.$$

Proof. Let $\varepsilon > 0$ and $k := \lceil \frac{1}{\varepsilon} \rceil$. Let $x_0 = -\infty$, $x_i = \inf\{x \in \mathbb{R} : F(x) \geq i/k\}$ for $i \in [k-1]$ and $x_k = \infty$. Writing $F(x-)$ for $\lim_{y \uparrow x} F(y)$, note that for $i \in [k]$

$$F(x_i-) - F(x_{i-1}) \leq \frac{i}{k} - \frac{i-1}{k} = \frac{1}{k} \leq \varepsilon.$$

Now define the event

$$\Omega_{n,\varepsilon} = \left\{ \max_{i \in [k]} \sup_{m \geq n} |\mathbb{F}_m(x_i) - F(x_i)| \leq \varepsilon \right\} \cap \left\{ \max_{i \in [k]} \sup_{m \geq n} |\mathbb{F}_m(x_i-) - F(x_i-)| \leq \varepsilon \right\}$$

Noting that both $\mathbb{F}_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{X_i \leq x\}$ and $\mathbb{F}_n(x-) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{X_i < x\}$ are both sample averages of i.i.d random variables, we have by a union bound and the SLLN that

$$\begin{aligned} & \mathbb{P}_F(\Omega_{n,\varepsilon}^c) \\ & \leq \sum_{i=1}^k \mathbb{P}_F \left(\sup_{m \geq n} |\mathbb{F}_m(x_i) - F(x_i)| > \varepsilon \right) + \sum_{i=1}^k \mathbb{P}_F \left(\sup_{m \geq n} |\mathbb{F}_m(x_i-) - F(x_i-)| > \varepsilon \right) \\ & \xrightarrow{a.s.} 0. \end{aligned}$$

Now let $x \in \mathbb{R}$ and find $i_* \in [k]$ such that $x \in [x_{i_*-1}, x_{i_*})$. Then for any $n_0 \in \mathbb{N}$ and $n \geq n_0$,

$$\begin{aligned} \mathbb{F}_n(x) - F(x) & \leq \mathbb{F}_n(x_{i_*-}) - F(x_{i_*-1}) \\ & = \mathbb{F}_n(x_{i_*-}) - F(x_{i_*-}) + F(x_{i_*-}) - F(x_{i_*-1}) \\ & \leq \max_{i \in [k]} \sup_{m \geq n_0} |\mathbb{F}_m(x_i-) - F(x_i-)| + \varepsilon. \end{aligned}$$

We also have

$$\begin{aligned} F(x) - \mathbb{F}_n(x) & \leq F(x_{i_*-}) - \mathbb{F}_n(x_{i_*-1}) \\ & = F(x_{i_*-}) - F(x_{i_*-1}) + F(x_{i_*-1}) - \mathbb{F}_n(x_{i_*-1}) \\ & \leq \varepsilon + \max_{i \in [k]} \sup_{m \geq n_0} |\mathbb{F}_m(x_i) - F(x_i)|. \end{aligned}$$

It follows that

$$\mathbb{P}_F \left(\sup_{n \geq n_0} \sup_{x \in \mathbb{R}} |\mathbb{F}_n(x) - F(x)| > 2\varepsilon \right) \leq \mathbb{P}_F(\Omega_{n_0,\varepsilon}^c) \rightarrow 0 \text{ as } n_0 \rightarrow \infty.$$

Since $\varepsilon > 0$ was arbitrary, we conclude that

$$\begin{aligned} \mathbb{P}_F \left(\sup_{x \in \mathbb{R}} |\mathbb{F}_n(x) - F(x)| \rightarrow 0 \right) & = \mathbb{P}_F \left(\bigcap_{L=1}^{\infty} \bigcup_{n_0=1}^{\infty} \left\{ \sup_{n \geq n_0} \sup_{x \in \mathbb{R}} |\mathbb{F}_n(x) - F(x)| \leq \frac{1}{L} \right\} \right) \\ & = \lim_{L \rightarrow \infty} \lim_{n_0 \rightarrow \infty} \mathbb{P}_F \left(\sup_{n \geq n_0} \sup_{x \in \mathbb{R}} |\mathbb{F}_n(x) - F(x)| \leq \frac{1}{K} \right) \\ & = 1. \end{aligned}$$

□

In fact, we can say much more:

Theorem (Dvoretzky-Kiefer-Wolfowitz Theorem). *Under the conditions of the previous theorem, for every $\varepsilon > 0$,*

$$\mathbb{P}_F \left(\sup_{x \in \mathbb{R}} |\mathbb{F}_n(x) - F(x)| > \varepsilon \right) \leq 2e^{-2n\varepsilon^2}.$$

Proof. Not given. □

Corollary (Uniform Glivenko-Cantelli). *Under the conditions of the Glivenko-Cantelli Theorem,*

$$\sup_{F \in \mathcal{F}} \mathbb{P}_F \left(\sup_{m \geq n} \sup_{x \in \mathbb{R}} |\mathbb{F}_m(x) - F(x)| > \varepsilon \right) \rightarrow 0 \text{ as } n \rightarrow \infty.$$

Proof. By a union bound and the DKW inequality,

$$\begin{aligned} \sup_{F \in \mathcal{F}} \mathbb{P}_F \left(\sup_{m \geq n} \sup_{x \in \mathbb{R}} |\mathbb{F}_m(x) - F(x)| > \varepsilon \right) &\leq \sup_{F \in \mathcal{F}} \sum_{m \geq n} \mathbb{P}_F \left(\sup_{x \in \mathbb{R}} |\mathbb{F}_m(x) - F(x)| > \varepsilon \right) \\ &\leq 2 \sum_{m \geq n} e^{-2m\varepsilon^2} \\ &= \frac{2e^{-2n\varepsilon^2}}{1 - e^{-2\varepsilon^2}} \rightarrow 0 \text{ as } n \rightarrow \infty. \end{aligned}$$

□

As another application of the DKW inequality, consider the problem of finding a confidence bound for F . Given $\alpha \in (0, 1)$, set $\varepsilon_n = \varepsilon_n(\alpha) := \left\{ \frac{1}{2n} \log \left(\frac{2}{\alpha} \right) \right\}^{1/2}$. Then, by the DKW Theorem,

$$\mathbb{P}_F (\max\{0, \mathbb{F}_n(x) - \varepsilon_n\} \leq F(x) \leq \min\{\mathbb{F}_n(x) + \varepsilon_n, 1\} \quad \forall x \in \mathbb{R}) \geq 1 - \alpha.$$

In fact, let $U_1, \dots, U_n \sim^{\text{iid}} \mathcal{U}[0, 1]$ and let \mathbb{G}_n denote their empirical distribution. Define the *quantile function* $F^{-1} : (0, 1] \rightarrow (-\infty, \infty]$ by $F^{-1}(p) := \inf\{x \in \mathbb{R} : F(x) \geq p\}$ (i.e the *generalised inverse*). Since F is increasing and right-continuous, we have $\{x \in \mathbb{R} : F(x) \geq p\} = [F^{-1}(p), \infty)$, so $\{U_i \leq F(x)\} = \{F^{-1}(U_i) \leq x\}$. Hence

$$\begin{aligned} \mathbb{G}_n(F(x)) &= \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{U_i \leq F(x)\} = \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{F^{-1}(U_i) \leq x\} \stackrel{d}{=} \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{X_i \leq x\} \\ &= \mathbb{F}_n(x). \end{aligned}$$

So

$$\sup_{x \in \mathbb{R}} |\mathbb{F}_n(x) - F(x)| \stackrel{d}{=} \sup_{x \in \mathbb{R}} |\mathbb{G}_n(F(x)) - F(x)| \leq \sup_{t \in [0, 1]} |\mathbb{G}_n(t) - t|$$

with equality if F is continuous. Thus if F is continuous, the distribution of $\sup_{x \in \mathbb{R}} |\mathbb{F}_n(x) - F(x)|$ does not depend on F !

Other generalisations of the Glivenko-Cantelli Theorem include Uniform Laws of Large Numbers (ULLN). Let X_1, X_2, \dots, X_n be iid, taking values in some measurable space $(\mathcal{X}, \mathcal{A})$, and let \mathcal{G} denote a family of real-valued measurable functions on \mathcal{X} . We say \mathcal{G} satisfies a ULLN if

$$\sup_{g \in \mathcal{G}} \left| \frac{1}{n} \sum_{i=1}^n g(X_i) - \mathbb{E}g(X) \right| \xrightarrow{a.s.} 0.$$

Remark. \mathcal{G} may be uncountable, so this random variable could be non measurable. But we can get around this by working with an outer probability $\mathbb{P}^*(A) = \inf\{\mathbb{P}(B) : B \in \mathcal{F}, B \supseteq A\}$.

Thus, in the Glivenko-Cantelli Theorem we proved that $\{\mathbb{1}\{\cdot \leq x\} : x \in \mathbb{R}\}$ satisfies a ULLN. In general, proving a ULLN requires control of the ‘size’ of \mathcal{G} , which can be measured for instance through its metric entropy (see van de Geer, 2000).

1.3 Concentration Inequalities

Definition. A random variable X is *sub-Gaussian with variance parameter σ^2* if

$$\mathbb{E}(e^{tX}) \leq e^{t^2\sigma^2/2} \quad \forall t \in \mathbb{R}.$$

Remark. It can be shown (see Example Sheet) that any such random variable must satisfy $\mathbb{E}(X) = 0$ and $\text{Var}(X) \leq \sigma^2$. Note also that we have equality in the definition if $X \sim \mathcal{N}(0, \sigma^2)$.

Here are some characterisations of sub-Gaussianity:

Proposition.

- (a) If X is sub-Gaussian with variance parameter σ^2 , then

$$\max \{\mathbb{P}(X \geq x), \mathbb{P}(X \leq -x)\} \leq e^{-\frac{x^2}{2\sigma^2}} \quad (*)$$

for every $x \geq 0$.

- (b) If X satisfies $(*)$, then for every $q \in \mathbb{N}$,

$$\mathbb{E}(X^{2q}) < 2q!(2\sigma^2)^q \leq q!(4\sigma^2)^q.$$

- (c) Suppose that $\mathbb{E}(X) = 0$ and $\mathbb{E}(X^{2q}) \leq q!C^{2q}$ for every $q \in \mathbb{N}$. Then X is sub-Gaussian with variance parameter $4C^2$.

Proof.

- (a) By Markov's inequality (i.e Chernoff's bound)

$$\mathbb{P}(X \geq x) \leq \inf_{t \geq 0} e^{-tX} \mathbb{E}(e^{tX}) \leq \inf_{t \geq 0} e^{-tx + t^2\sigma^2/2} = e^{-\frac{x^2}{2\sigma^2}}$$

for every $x \geq 0$, since the infimum is attained at $t = \frac{x}{\sigma^2}$. The bound for $\mathbb{P}(X \leq -x)$ is similar (since $-X$ is also σ^2 -sub-Gaussian).

- (b) We have

$$\begin{aligned} \mathbb{E}(X^{2q}) &= \int_0^\infty \mathbb{P}(X^{2q} \geq x) dx = 2q \int_0^\infty y^{2q-1} \mathbb{P}(|X| \geq y) dy \\ &\leq 4q \int_0^\infty y^{2q-1} e^{-\frac{y^2}{2\sigma^2}} dy \\ &= 2q(2\sigma^2)^q \int_0^\infty t^{q-1} e^{-t} dt \quad (t = \frac{y^2}{2\sigma^2}) \\ &= 2q!(2\sigma^2)^q \end{aligned}$$

for $q \in \mathbb{N}$.

- (c) Let X' denote an independent copy of X . Then $X - X'$ has a symmetric distribution, so for every $t \in \mathbb{R}$,

$$\begin{aligned} \mathbb{E}(e^{t(X-X')}) &= \frac{1}{2} \left(\mathbb{E}(e^{t(X-X')}) + \mathbb{E}(e^{-t(X-X')}) \right) \\ &= \mathbb{E}(\cosh(t(X - X'))) \\ &= \sum_{q \geq 0} \frac{t^{2q} \mathbb{E}[(X - X')^{2q}]}{(2q)!} \end{aligned}$$

where the final step follows from Fubini's theorem, since the terms in the Taylor series of $x \mapsto \cosh(x)$ are non-negative. Moreover, $\mathbb{E}(e^{-tX}) \geq 1$ by Jensen's inequality. Hence by applying the inequality $(a+b)^r \leq \max(1, 2^{r-1})(a^r + b^r)$ for every $a, b, r \geq 0$ we have for every $t \in \mathbb{R}$

$$\begin{aligned}
\mathbb{E}(e^{tX}) &\leq \mathbb{E}(e^{-tX})\mathbb{E}(e^{tX}) = \mathbb{E}(e^{t(X-X')}) = \sum_{q \geq 0} \frac{t^{2q} \mathbb{E}[(X - X')^{2q}]}{(2q)!} \\
&\leq \sum_{q \geq 0} \frac{t^{2q} \mathbb{E}[(|X| + |X'|)^{2q}]}{(2q)!} \\
&\leq \sum_{q \geq 0} \frac{2^{2q-1} t^{2q} (\mathbb{E}(X^{2q}) + \mathbb{E}(X'^{2q}))}{(2q)!} \\
&\leq \sum_{q \geq 0} \frac{(2tC)^{2q} q!}{(2q)!} \\
&= \sum_{q \geq 0} \frac{(2tC)^{2q}}{\prod_{j=1}^q (q+j)} \\
&\leq \sum_{q \geq 0} \frac{(2tC)^{2q}}{\prod_{j=1}^q (2j)} \\
&= \sum_{q \geq 0} \frac{2^q (tC)^{2q}}{q!} = e^{2t^2 C^2}.
\end{aligned}$$

□

Theorem (Hoeffding's inequality). *Let X_1, \dots, X_n be independent sub-Gaussian random variables with X_i having sub-Gaussian parameter σ_i^2 for $i \in [n]$. Then $\bar{X} := n^{-1} \sum_{i=1}^n X_i$ is sub-Gaussian with variance parameter $\frac{\bar{\sigma}^2}{n}$, where $\bar{\sigma}^2 = n^{-1} \sum_{i=1}^n \sigma_i^2$. In particular,*

$$\mathbb{P}(\bar{X} \geq x) \leq e^{-\frac{nx^2}{2\bar{\sigma}^2}}$$

for every $x \geq 0$.

Proof. For every $t \in \mathbb{R}$,

$$\mathbb{E}(e^{t\bar{X}}) = \prod_{i=1}^n \mathbb{E}(e^{\frac{t}{n} X_i}) \leq \prod_{i=1}^n e^{\frac{t^2 \sigma_i^2}{2n^2}} = e^{\frac{t^2 \bar{\sigma}^2}{n}}.$$

The second claim then follows from part (a) of the previous proposition. □

Remark. It is often convenient to state the conclusion of Hoeffding's inequality as an upper bound on the $(1 - \delta)$ th quantile of the distribution of \bar{X} : for every $\delta \in [0, 1]$

$$\mathbb{P}\left(\bar{X} \geq \frac{2^{1/2} \bar{\sigma} \log^{1/2}(1/\delta)}{n^{1/2}}\right) \leq \delta.$$

Remark. Since we have the same bound on $\mathbb{P}(\bar{X} \leq -x)$ we have that

$$\mathbb{P}(|X| \geq x) \leq 2e^{-\frac{nx^2}{2\sigma^2}}$$

for every $x \geq 0$. Often, Hoeffding's inequality is stated in this (weaker) way.

Lemma (Hoeffding's Lemma). *Let X be a mean 0 bounded random variable taking values in $[a, b]$. Then X is sub-Gaussian with variance parameter $(b - a)^2/4$.*

Proof. Example Sheet 1. □

Corollary. *Let X_1, \dots, X_n be independent with $\mathbb{E}(X_i) = \mu_i$ and X_i taking values in $[a_i, b_i]$ for $i \in [n]$. Writing $\bar{X} := n^{-1} \sum_{i=1}^n X_i$ and $\bar{\mu} = n^{-1} \sum_{i=1}^n \mu_i$, we have*

$$\mathbb{P}(\bar{X} - \bar{\mu} \geq x) \leq \exp\left(-\frac{2n^2x^2}{\sum_{i=1}^n (b_i - a_i)^2}\right)$$

for every $x \geq 0$.

Proof. By Hoeffding's Lemma and Hoeffding's inequality, $\bar{X} - \bar{\mu}$ is sub-Gaussian with variance parameter $\sum_{i=1}^n \frac{(b_i - a_i)^2}{4n^2}$. □

The bound in the previous corollary may be loose when the variance of X_i is small by comparison with $(b_i - a_i)^2$. This happens for instance when $X_i \sim \text{Bernoulli}(p_i)$ with p_i close to 0 or 1. In such circumstances, Bennett's inequality (which applies when the random variables have a bounded right tail) or Bernstein's inequality (which applied under a weaker integrability condition) may be preferred.

Theorem (Bennett's inequality). *Let X_1, \dots, X_n be independent with $\mathbb{E}X_i = 0$ and $X_i \leq b$ for some $b > 0$ and all $i \in [n]$. Write $S = \sum_{i=1}^n X_i$ and assume that $\nu = n^{-1} \sum_{i=1}^n \text{Var}(X_i) \in (0, \infty)$, and define $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ by $\varphi(u) = e^u - 1 - u$. Then, for every $t \geq 0$*

$$\log \mathbb{E}(e^{tS}) \leq \frac{n\nu}{b^2} \varphi(bt).$$

Hence, defining $h : [0, \infty) \rightarrow [0, \infty)$ by $h(u) = (1+u) \log(1+u) - u$, we have for every $x \geq 0$ that

$$\mathbb{P}\left(\frac{S}{n} \geq x\right) \leq \exp\left(-\frac{n\nu}{b^2} h\left(\frac{bx}{2}\right)\right).$$

Proof. Define $g : \mathbb{R} \rightarrow \mathbb{R}$ by

$$g(u) = \begin{cases} \frac{\varphi(u)}{u^2} & \text{if } u \neq 0 \\ \frac{1}{2} & \text{if } u = 0 \end{cases}.$$

We claim that g is increasing. To see this, define $G : \mathbb{R} \rightarrow \mathbb{R}$ by

$$G(u) = \int_0^1 e^{su} ds = \begin{cases} \frac{e^u - 1}{u} & \text{if } u \neq 0 \\ 1 & \text{if } u = 0 \end{cases}.$$

Then G is convex, because if $\lambda \in (0, 1)$ and $u, v \in \mathbb{R}$ we have

$$\begin{aligned} G(\lambda u + (1-\lambda)v) &= \int_0^1 e^{s(\lambda u + (1-\lambda)v)} ds \\ &\leq \lambda \int_0^1 e^{su} ds + (1-\lambda) \int_0^1 e^{sv} ds \\ &= \lambda G(u) + (1-\lambda)G(v) \end{aligned}$$

by convexity of $u \mapsto e^{su}$. Hence

$$g(u) = \begin{cases} \frac{G(u) - G(0)}{u} & \text{if } u \neq 0 \\ G'(0) & \text{if } u = 0 \end{cases}$$

is increasing, as required.

It follows that for every $t \geq 0$,

$$e^{tX_i} - 1 - tX_i \leq X_i^2 \frac{e^{bt} - 1 - bt}{b^2} = X_i^2 \frac{\varphi(bt)}{b^2}.$$

Hence for every $t \geq 0$

$$\begin{aligned} \mathbb{E}(e^{tS}) &= \sum_{i=1}^n \log \mathbb{E}(e^{tX_i}) \leq \sum_{i=1}^n \log \left(1 + \frac{\mathbb{E}(X_i^2) \varphi(bt)}{b^2}\right) \\ &\leq n \log \left(1 + \frac{\nu}{b^2} \varphi(bt)\right) \quad (\text{Jensen}) \\ &\leq \frac{n\nu}{b^2} \varphi(bt) \end{aligned}$$

where the final inequality uses the fact $\log(1+x) \leq x$ for $x > -1$.

Hence, by a Chernoff bound

$$\mathbb{P}\left(\frac{S}{n} \geq x\right) = \mathbb{P}(S \geq nx) \leq \inf_{t \geq 0} e^{-ntx + \frac{n\nu}{b^2} \varphi(bt)}.$$

But if $f(t) = -tx + \frac{\nu}{b^2} \varphi(bt)$ then $f'(t) = -x + \frac{\nu}{b} (e^{bt} - 1)$, so its infimum is attained at $t^* = \frac{1}{b} \log\left(1 + \frac{bx}{\nu}\right) \geq 0$, and

$$\begin{aligned} \mathbb{P}\left(\frac{S}{n} \geq x\right) &\leq \exp\left[-\frac{nx}{b} \log\left(1 + \frac{bx}{\nu}\right) + \frac{n\nu}{b^2} \left\{\left(1 + \frac{bx}{\nu}\right) - 1 - \log\left(1 + \frac{bx}{\nu}\right)\right\}\right] \\ &\leq \exp\left[-\frac{n\nu}{b^2} \left\{\left(1 + \frac{bx}{\nu}\right) \log\left(1 + \frac{bx}{\nu}\right) - \frac{bx}{\nu}\right\}\right] \\ &= \exp\left\{-\frac{n\nu}{b^2} h\left(\frac{bx}{\nu}\right)\right\} \end{aligned}$$

for every $x \geq 0$, as required. \square

Before we can state Bernstein's inequality, we first introduce the notion of sub-Gamma random variables.

Definition. A random variable X with $\mathbb{E}X = 0$ is *sub-Gamma in the right tail* with variance factor $\sigma^2 > 0$ and scale parameter $c > 0$ if

$$\log \mathbb{E}(e^{tX}) \leq \frac{\sigma^2 t^2}{2(1 - ct)}$$

for all $t \in [0, 1/c)$.

Proposition.

- (a) Let X be sub-Gamma in the right tail with variance parameter σ^2 and scale parameter c . Then

$$\mathbb{P}(X \geq x) \leq e^{-\frac{x^2}{2(\sigma^2 + cx)}}$$

for $x \geq 0$.

- (b) Let X be a random variable with $\mathbb{E}X = 0$, $\text{Var}(X) \leq \sigma^2$ and $\mathbb{E}(X_+^q) \leq \frac{q!}{2} \sigma^2 c^{q-2}$ for all integers $q \geq 3$. Then X is sub-Gamma in the right tail with variance factor σ^2 and scale parameter c .

Proof.

- (a) By a Chernoff bound, for all $x \geq 0$ we have

$$\mathbb{P}(X \geq x) \leq \inf_{t \in [0, 1/c)} e^{-tx + \frac{\sigma^2 t^2}{2(1 - ct)}} \leq e^{-\frac{x^2}{2(\sigma^2 + cx)}}$$

where the final inequality follows by setting $t = \frac{x}{\sigma^2 + cx} \in [0, 1/c)$.

- (b) Recall from the proof of the previous theorem (Bennett's inequality) that $\varphi(u) \leq u^2/2$ for $u \leq 0$. It follows that

$$\varphi(u) = e^u - 1 - u \leq \frac{u^2}{2} + \sum_{q \geq 3} \frac{u^q}{q!} \text{ for all } u \in \mathbb{R}.$$

Hence, for $t \in [0, 1/c)$, by Fubini's theorem

$$\begin{aligned} \log \mathbb{E}(e^{tX}) &\leq \mathbb{E}(e^{tX}) - 1 = \mathbb{E}\varphi(tX) && (\text{since } \mathbb{E}X = 0) \\ &= \frac{t^2}{2} \mathbb{E}(X^2) + \sum_{q \geq 3} \frac{t^q \mathbb{E}(X_+^q)}{q!} \\ &\leq \frac{\sigma^2}{2} \sum_{q \geq 2} t^q c^{q-2} \\ &= \frac{\sigma^2 t^2}{2(1 - ct)} \end{aligned}$$

as required. □

Finally, we are in a position to state Bernstein's inequality.

Theorem (Bernstein's Inequality). *Let X_1, \dots, X_n be independent, mean 0 random variables with $\frac{1}{n} \sum_{i=1}^n \text{Var}(X_i) \leq \sigma^2$ and $\frac{1}{n} \sum_{i=1}^n \mathbb{E}[(X_i)_+^q] \leq \frac{q!}{2} \sigma^2 c^{q-2}$ for some $\sigma, c > 0$. Then $S = \sum_{i=1}^n X_i$ is sub-Gamma in the right tail with variance factor $n\sigma^2$ and scale parameter c . In particular, writing $\bar{X} = n^{-1} \sum_{i=1}^n X_i$, we have for every $x \geq 0$ that*

$$\mathbb{P}(\bar{X} \geq x) \leq \exp\left(-\frac{nx^2}{2(\sigma^2 + cx)}\right).$$

Proof. As in the proof of (b) of the previous proposition, for every $t \in [0, 1/c)$,

$$\begin{aligned} \log \mathbb{E}(e^{tS}) &\leq \sum_{i=1}^n \left[\frac{t^2}{2} \mathbb{E}(X_i^2) + \sum_{q \geq 3} \frac{t^q}{q!} \mathbb{E}[(X_i)_+^q] \right] \\ &\leq \frac{n\sigma^2}{2} \sum_{q \geq 2} t^q c^{q-2} && (\text{Fubini}) \\ &= \frac{n\sigma^2}{2(1 - ct)} \end{aligned}$$

as required. By part (a) of the previous proposition, for every $x \geq 0$ we have

$$\mathbb{P}(\bar{X} \geq x) = \mathbb{P}(S \geq nx) \leq \exp\left(-\frac{nx^2}{2(\sigma^2 + cx)}\right)$$

as required. □

Remark. If in addition we have $X_i \leq b$ for some $b > 0$ and all $i \in [n]$, then for every integer $q \geq 3$,

$$\frac{1}{n} \sum_{i=1}^n \mathbb{E}[(X_i)_+^q] \leq \frac{b^{q-2}}{n} \sum_{i=1}^n \mathbb{E}[X_i^2] \leq \sigma^2 b^{q-2} \leq \frac{q!}{2} \sigma^2 \left(\frac{b}{3}\right)^{q-3}.$$

Thus we can take $c = b/3$. In that case, Bernstein's inequality can be deduced from Bennett's inequality, since

$$h(u) \geq \frac{u^2}{2(1 + u/3)}$$

for all $u > 0$; see Example Sheet.

2 Kernel density estimation

2.1 Introduction

Let X_1, \dots, X_n be independent, real-valued random variables with density f . The oldest, and most commonly used non-parametric density estimator is the *histogram*, usually formed by dividing the real lines into equal-sized intervals, known as *bins*.

If I_x denotes the bin for which $x \in \mathbb{R}$ belongs, and $b > 0$ denotes the *binwidth*, then the histogram density estimator of f is $\hat{f}_n^H = \hat{f}_{n,b}^H$, where

$$\hat{f}_n^H(x) = \frac{1}{nb} \sum_{i=1}^n \mathbb{1}\{i \in I_x\}.$$

Drawbacks of histograms include:

- Difficulties of choosing the binwidth and the positioning of the bin edges;
- Suboptimal theoretic performance;
- Difficulties of graphical display in the multivariate case.

2.2 The univariate kernel density estimator

A *kernel* is a Borel-measurable function $k : \mathbb{R} \rightarrow \mathbb{R}$ satisfying $\int_{-\infty}^{\infty} k(x) dx = 1$.

A *univariate kernel density estimator* of f is of the form $\hat{f}_n = \hat{f}_{n,h,k}$, where

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

where k is a kernel and $h > 0$ is called the *bandwidth*. It is convenient to define the *scaled kernel* $k_h(\cdot) := h^{-1}k(\cdot/h)$, so that

$$\hat{f}_n(x) = \frac{1}{n} \sum_{i=1}^n k_h(x - X_i).$$

Typically in practice, k is chosen to be non-negative (though see later discussion), which ensures that k (and hence \hat{f}_n) is a density; often k is chosen to be symmetric about 0.

The main intuition is that, perhaps surprisingly, the choice of kernel is much less important than the choice of bandwidth.

2.3 Mean squared error of kernel estimators

If we think of $\hat{f}_n(x)$ as a point estimate of $f(x)$, then it is natural to try to choose h and k to minimise the *mean squared error* (MSE), defined by

$$\text{MSE}[\hat{f}_n(x)] = \mathbb{E}[(\hat{f}_n(x) - f(x))^2].$$

This is often preferred to alternatives, such as the mean absolute error, due to its appealing decomposition into variance and squared bias terms:

$$\begin{aligned} \text{MSE}(\hat{f}_n) &= \mathbb{E}[(\hat{f}_n(x) - \mathbb{E}[\hat{f}_n(x)])^2] + [\mathbb{E}(\hat{f}_n(x)) - f(x)]^2 \\ &= \text{Var}(\hat{f}_n(x)) + \text{Bias}^2 \hat{f}_n(x). \end{aligned}$$

The *convolution* of Borel-measurable functions $g_1, g_2 : \mathbb{R} \rightarrow \mathbb{R}$ is $g_1 * g_2$, where

$$(g_1 * g_2)(x) = \int_{\mathbb{R}} g_1(x - z)g_2(z)dz,$$

whenever this integral exists. We can now compute

$$\begin{aligned} \text{Bias} \hat{f}_n(x) &= \mathbb{E}[k_h(x - X_1)] - f(x) = \int_{-\infty}^{\infty} k_h(x - z)f(z)dz - f(x) \\ &= (k_h * f)(x) - f(x). \end{aligned}$$

Now, for $i \in [n]$, let $\xi_i = \xi_i(x) = k_h(x - X_i)$. Then ξ_1, \dots, ξ_n are iid, so

$$\begin{aligned} \text{Var} \hat{f}_n(x) &= \frac{1}{n} \text{Var}(\xi_1) = \frac{1}{n} [\mathbb{E}[\xi_1^2] - \mathbb{E}^2[\xi_1]] \\ &= \frac{1}{n} [(k_h^2 * f)(x) - (k_h * f)^2(x)]. \end{aligned}$$

Hence

$$\text{MSE}[\hat{f}_n(x)] = \frac{1}{n} [(k_h^2 * f)(x) - (k_h * f)^2(x)] + [(k_h * f)(x) - f(x)]^2.$$

Often however, we prefer to choose h and k based on how well \hat{f}_n estimates f as a function, as measured by the *mean integrated squared error* (MISE), defined by

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

Since the integrand is non-negative, we have by Fubini's theorem that

$$\begin{aligned} \text{MISE}(\hat{f}_n) &= \int_{\mathbb{R}} \text{MSE}(\hat{f}_n(x)) dx \\ &= \frac{1}{n} \int_{\mathbb{R}} \frac{1}{n} [(k_h^2 * f)(x) - (k_h * f)^2(x)] dx + \int_{\mathbb{R}} [(k_h * f)(x) - f(x)]^2 dx. \end{aligned}$$

Although this expression is exact, it depends on the bandwidth in a complicated way. So we therefore seek finite-sample bounds to clarify this dependence.

2.4 Bounds on the variance and bias

For a kernel k , we write $R(k) := \int_{\mathbb{R}} k^2(u) du$.

Proposition. Let \hat{f}_n denote a KDE with bandwidth h and kernel k constructed from $X_1, \dots, X_n \sim^{\text{iid}} f$. Then for every $x \in \mathbb{R}$,

$$\text{Var} \hat{f}_n(x) \leq \frac{1}{nh} R(k) \|f\|_{\infty}.$$

Proof. We have

$$\begin{aligned} \text{Var} \hat{f}_n(x) &= \frac{1}{n} \text{Var}(\xi_1) \\ &\leq \frac{1}{n} \mathbb{E}(\xi_1^2) \\ &\leq \frac{1}{nh^2} \int_{\mathbb{R}} k^2 \left(\frac{x-z}{h} \right) f(z) dz \\ &= \frac{1}{nh} \int_{\mathbb{R}} k^2(u) f(x - uh) du \quad (u = \frac{x-z}{h}) \\ &\leq \frac{1}{nh} R(k) \|f\|_{\infty}. \end{aligned}$$

□

To study the bias, we will need conditions on both f and k .

Definition. Let I be an interval, let $\beta, L > 0$ and let $m := \lceil \beta \rceil - 1$. The *Hölder class* $\mathcal{H}(\beta, L)$ on I is the set of m -times differentiable functions $f : I \rightarrow \mathbb{R}$ satisfying

$$|f^{(m)}(x) - f^{(m)}(x')| \leq L|x - x'|^{\beta-m}$$

for all $x, x' \in I$. Where I is unspecified we will take $I = \mathbb{R}$.

Example. For $\alpha \in (0, 1)$, the function $x \mapsto x^\alpha$ belongs to $\mathcal{H}(\beta, 1)$ on $[0, 1]$ for every $\beta \in (0, \alpha]$. Indeed, wlog suppose $0 \leq x' < x \leq 1$, and write $x' = \varepsilon x$ for some $\varepsilon \in (0, 1)$. Then

$$\frac{x^\alpha - (x')^\alpha}{x - x'} = \frac{x^\alpha(1 - \varepsilon^\alpha)}{x^\beta(1 - \varepsilon)^\beta} \leq \frac{1 - \varepsilon^\alpha}{(1 - \varepsilon)^\beta} \leq (1 - \beta) \leq 1.$$

On the other hand, by considering $x' = 0$, we see that this function does not belong to $\mathcal{H}(\beta, L)$ for any $\beta > 0$ and any $L > 0$.

The densities in $\mathcal{H}(\beta, L)$ are denoted $\mathcal{F}(\beta, L) := \{f \in \mathcal{H}(\beta, L) : \int_{\mathbb{R}} f = 1\}$.

Definition. For $\ell \in \mathbb{N}$, we say a kernel K is *of order ℓ* if $\int_{\mathbb{R}} u^j k(u) du$ for all $j \in [\ell - 1]$.

Most kernels used in practice are of order 2. Kernels of order $\ell \geq 3$ cannot be non-negative, because $\int_{\mathbb{R}} u^2 k(u) du = 0$. This means that the resulting KDE is not necessarily a density.

Proposition. Let $f \in \mathcal{F}(\beta, L)$ and assume that k is a kernel of order $\ell := \lceil \beta \rceil$ satisfying

$$\mu_\beta(k) := \int_{\mathbb{R}} |u|^\beta |k(u)| du < \infty.$$

If \hat{f}_n denotes the KDE with kernel K and bandwidth h based on $X_1, \dots, X_n \sim f$, then

$$|\text{Bias} \hat{f}_n(x)| \leq \frac{L}{(\ell - 1)!} \mu_\beta(k) h^\beta$$

for every $x \in \mathbb{R}$.

Proof. We have

$$\begin{aligned} \text{Bias} \hat{f}_n(x) &= \frac{1}{h} \int_{\mathbb{R}} k\left(\frac{x - z}{h}\right) f(z) dz - f(x) \\ &= \int_{\mathbb{R}} k(u) \{f(x - uh) - f(x)\} du. \quad (u = (x - z)/h) \end{aligned}$$

By a Taylor expansion with the mean value form of the remainder, with $m := \lceil \beta \rceil - 1$, there exists $\tau \in [0, 1]$ such that

$$f(x - uh) - f(x) = \sum_{r=1}^{m-1} \frac{(-uh)^r}{r!} f^{(r)}(x) + \frac{(-uh)^m}{m!} f^{(m)}(x - \tau uh).$$

Since k is a kernel of order $\ell = m + 1$, we find that

$$\begin{aligned} \text{Bias} \hat{f}_n(x) &= \frac{(-h)^m}{m!} \int_{\mathbb{R}} u^m k(u) f^{(m)}(x - \tau uh) du \\ &= \frac{(-h)^m}{m!} \int_{\mathbb{R}} u^m k(u) \{f^{(m)}(x - \tau uh) - f^{(m)}(x)\} du. \end{aligned}$$

We conclude that

$$|\text{Bias} \hat{f}_n(x)| \leq \frac{Lh^m}{m!} \int_{\mathbb{R}} |u|^m |k(u)| |\tau uh|^{\beta-m} du \leq \frac{L}{m!} \mu_{\beta}(k) h^{\beta}.$$

□

Observe that our upper bound on $\text{Var} \hat{f}_n(x)$ is decreasing in h , whereas the upper bound on the bias is increasing in h . This is a prototypical example of a bias-variance trade-off.

Theorem. Assume that k is a kernel of order $\ell := \lceil \beta \rceil$ satisfying $\max\{R(k), \mu_{\beta}(k)\} < \infty$. Then there exists $C = C(\beta, k) > 0$ and $h_n^* = h_n^*(\beta, L, k) > 0$ such that the KDE $\hat{f}_{n, h_n^*, k}$ based on iid observations X_1, \dots, X_n satisfies

$$\sup_{x \in \mathbb{R}} \sup_{f \in \mathcal{F}(\beta, L)} \text{MSE}_f\{\hat{f}_{n, h_n^*, k}(x)\} \leq CL^{\frac{2}{\beta+1}} n^{-\frac{2\beta}{2\beta+1}}.$$

Proof. We first claim that there exists $C' = C'(\beta) > 0$ such that

$$\sup_{f \in \mathcal{F}(\beta, L)} \|f\|_{\infty} \leq C' \beta^{\frac{1}{\beta+1}}.$$

To see this, let k^* denote a bounded kernel of order $\ell := \lceil \beta \rceil$ satisfying $\mu_{\beta}(k^*) < \infty$. Then by the triangle inequality and the previous proposition, we have for every $x \in \mathbb{R}$ and $f \in \mathcal{F}(\beta, L)$ that

$$\begin{aligned} f(x) &\leq \inf_{h>0} \int_{\mathbb{R}} |k^*(x-z)| f(z) dz + \left| \int_{\mathbb{R}} k_h^*(x-z) f(z) dz - f(x) \right| \\ &\leq \inf_{h>0} \left\{ \frac{\|k^*\|_{\infty}}{h} + \frac{L}{(\ell-1)!} \mu_{\beta}(k^*) h^{\beta} \right\} \\ &\leq C' L^{\frac{1}{\beta+1}} \end{aligned}$$

which establishes our first claim. Moreover, the RHS of the upper bound

$$\text{MSE}\{\hat{f}_n(x)\} \leq \frac{C' L^{\frac{1}{\beta+1}}}{nh} R(k) + \frac{L^2}{[(\ell-1)!]^2} \mu_{\beta}^2(k) h^{2\beta}$$

is minimised at

$$h_n^* = h_n^*(\beta, L, K) := \left(\frac{C' R(k) [(\ell-1)!]^2}{2\beta \mu_{\beta}^2(k)} \right) L^{-\frac{1}{\beta+1}} n^{-\frac{1}{2\beta+1}}.$$

We conclude that

$$\text{MSE}(\hat{f}_{n, h_n^*, k}(x)) \leq \left(\frac{(C')^{2\beta} R(k)^{2\beta} \mu_{\beta}^2(k) (2\beta+1)^{2\beta+1}}{[(\ell-1)!]^2 (2\beta)^{2\beta}} \right) L^{\frac{2}{\beta+1}} n^{-\frac{2\beta}{2\beta+1}}.$$

□

2.5 Bounds on the Integrated Variance and Squared Bias

Proposition. Let \hat{f}_n denote the KDE with kernel k and bandwidth h based on iid observations X_1, \dots, X_n having an arbitrary distribution P on \mathbb{R} . Then

$$\int_{\mathbb{R}} \text{Var}(\hat{f}_n(x)) dx \leq \frac{R(k)}{nh}.$$

Proof. By the proof of the pointwise analogue and Fubini's theorem,

$$\begin{aligned} \int_{\mathbb{R}} \text{Var} \hat{f}_n(x) dx &\leq \frac{1}{nh^2} \int_{\mathbb{R}} \int_{\mathbb{R}} k^2 \left(\frac{x-z}{h} \right) dP(z) dx \\ &= \frac{1}{nh^2} \int_{\mathbb{R}} \int_{\mathbb{R}} k^2 \left(\frac{x-z}{h} \right) dx dP(z) \\ &\leq \frac{R(k)}{nh}. \end{aligned}$$

□

Definition. Fix $\beta, L > 0$ and let $m := \lceil \beta \rceil - 1$. The Nikol'ski class $\mathcal{N}(\beta, L)$ is the set of $(m - 1)$ -times differentiable $f : \mathbb{R} \rightarrow \mathbb{R}$ for which $f^{(m-1)}$ is locally absolutely continuous, with weak derivative $f^{(m)}$ satisfying

$$\left[\int_{\mathbb{R}} (f^{(m)}(x+t) - f^{(m)}(x))^2 dx \right]^{1/2} \leq L|t|^{\beta-m}$$

for $t \in \mathbb{R}$. The densities in $\mathcal{N}(\beta, L)$ are denoted as $\mathcal{F}_{\mathcal{N}}(\beta, L) = \{f \in \mathcal{N}(\beta, L) : f \geq 0, \int_{\mathbb{R}} f = 1\}$.

Theorem (Generalised Minkowski Inequality). *For $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ measurable*

$$\left[\int_{\mathbb{R}} \left\{ \int_{\mathbb{R}} f(x, y) dy \right\}^2 dx \right]^{1/2} \leq \int_{\mathbb{R}} \left\{ \int_{\mathbb{R}} f^2(x, y) dx \right\}^{1/2} dy.$$

Proof. Not given (see Part II Analysis of Functions). □

Proposition. Fix $\beta, L > 0$ and let k denote a kernel of order $\ell = \lceil \beta \rceil$. Then the kernel density estimator \hat{f}_n with kernel k and bandwidth $h > 0$ based on $X_1, \dots, X_n \sim f \in \mathcal{F}_{\mathcal{N}}(\beta, L)$ satisfies

$$\int_{\mathbb{R}} \text{Bias}^2 \hat{f}_n(x) dx \leq \frac{L^2}{[(\ell - 1)!]^2} \mu_{\beta}^2(k) h^{2\beta}.$$

Proof. First consider the case $m := \ell - 1 \geq 1$. Since $f^{(m-1)}$ is absolutely continuous on the line segment joining $x - uh$ and x , we have by a Taylor expansion with the integral form of remainder that for every $x, u \in \mathbb{R}$ and $h > 0$ we have

$$f(x - uh) - f(x) = \sum_{r=1}^{m-1} \frac{(-uh)^r}{r!} f^{(r)}(x) + \frac{(-uh)^m}{(m-1)!} \int_0^1 (1-\tau)^{m-1} f^{(m)}(x - \tau uh) d\tau.$$

Since the kernel is of order $\ell = m + 1$, we have from the proof of the pointwise bound that

$$\begin{aligned} \text{Bias} \hat{f}_n(x) &= \int_{\mathbb{R}} k(u) \frac{(-uh)^m}{(m-1)!} \int_0^1 (1-\tau)^{m-1} f^{(m)}(x - \tau uh) d\tau du \\ &= \int_{\mathbb{R}} k(u) \frac{(-uh)^m}{(m-1)!} \int_0^1 (1-\tau)^{m-1} (f^{(m)}(x - \tau uh) - f^{(m)}(x)) d\tau du. \end{aligned}$$

Hence by two applications of the Generalised Minkowski Inequality

$$\begin{aligned}
& \int_{\mathbb{R}} \text{Bias}^2 \hat{f}_n(x) dx \\
&= \int_{\mathbb{R}} \left\{ \int_{\mathbb{R}} k(u) \frac{(-uh)^m}{(m-1)!} \int_0^1 (1-\tau)^{m-1} (f^{(m)}(x-\tau uh) - f^{(m)}(x)) d\tau du \right\}^2 dx \\
&\leq \left(\int_{\mathbb{R}} |k(u)| \frac{|uh|^m}{(m-1)!} \left[\int_{\mathbb{R}} \left\{ \int_0^1 (1-\tau)^{m-1} (f^{(m)}(x-\tau uh) - f^{(m)}(x)) d\tau \right\}^2 dx \right]^{1/2} du \right)^2 \\
&\leq \left[\int_{\mathbb{R}} |k(u)| \frac{|uh|^m}{(m-1)!} \int_0^1 (1-\tau)^{m-1} \left\{ \int_{\mathbb{R}} (f^{(m)}(x-\tau uh) - f^{(m)}(x))^2 dx \right\}^{1/2} d\tau du \right]^2 \\
&\leq \left[\int_{\mathbb{R}} |k(u)| \frac{|uh|^m}{(m-1)!} \int_0^1 (1-\tau)^{m-1} L |uh|^{\beta-m} d\tau du \right]^2 \\
&= \frac{L^2}{(m!)^2} \mu_{\beta}^2(k) h^{2\beta}.
\end{aligned}$$

When $m = 0$ we can proceed directly via one application of the Generalised Minkowski Inequality:

$$\begin{aligned}
\int_{\mathbb{R}} \text{Bias}^2 \hat{f}_n(x) dx &= \int_{\mathbb{R}} \left\{ \int_{\mathbb{R}} k(u) (f(x-uh) - f(x)) du \right\}^2 dx \\
&\leq \left[\int_{\mathbb{R}} |k(u)| \left\{ \int_{\mathbb{R}} (f(x-uh) - f(x))^2 dx \right\}^{1/2} du \right]^2 \\
&\leq L^2 \mu_{\beta}^2(k) h^{2\beta}.
\end{aligned}$$

□

Putting our results together, we have the following:

Theorem. Fix $\beta, L > 0$ and let k be a kernel of order $\ell = \lceil \beta \rceil$. Then the KDE \hat{f}_n with kernel k and bandwidth $h > 0$ based on $X_1, \dots, X_n \sim^{iid} f \in \mathcal{F}_{\mathcal{N}}(\beta, L)$ satisfies

$$\text{MISE}(\hat{f}_n) \leq \frac{R(k)}{nh} + \frac{L^2}{[(\ell-1)!]^2} \mu_{\beta}^2(k) h^{2\beta}.$$

In particular, if $\max\{R(k), \mu_{\beta}(k)\} < \infty$, then there exist $h_n^{**} = h_n^{**}(\beta, L, K) > 0$ and $C = C(\beta, K) > 0$ such that

$$\text{MISE}(\hat{f}_{n, h_n^{**}, k}) \leq CL^{\frac{2}{2\beta+1}} n^{-\frac{2\beta}{2\beta+1}}.$$

Proof. The first part follows from previous propositions. For the second part, the upper bound on the MISE is minimised by setting

$$h_n^{**} := \left(\frac{R(k)[(\ell-1)!]^2}{(2\beta)\mu_{\beta}^2(k)} \right)^{\frac{1}{2\beta+1}} L^{-\frac{2}{2\beta+1}} n^{-\frac{1}{2\beta+1}}.$$

This gives

$$\text{MISE}(\hat{f}_{n,h_n^{**},k}) \leq \left(\frac{R(k)^{2\beta} \mu_\beta^2(k) (2\beta+1)^{2\beta+1}}{[(\ell-1)!]^2 (2\beta)^{2\beta}} \right)^{\frac{1}{2\beta+1}} L^{\frac{2}{2\beta+1}} n^{-\frac{2\beta}{2\beta+1}}.$$

□

2.6 Bandwidth Selection

The choice of h_n^{**} in the previous theorem is not completely practical because typically we do not know β or L . Here we present two bandwidth selection algorithms, one based on least squares cross-validation, and the other based on Lepski's method.

2.6.1 Least squares cross-validation

Recall that provided all the terms are finite

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

Since the last term does not depend on h , it suffices to minimise the sum of the first two terms on the RHS. This depends on the unknown f , but an unbiased estimator for $n \geq 2$ is given by

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

where $\hat{f}_{n,-i}(x) = \hat{f}_{n,h,k,-i}(x) := \frac{1}{n-1} \sum_{j \neq i} k_h(x - x_j)$. The least squares cross-validation bandwidth selector minimises $\text{LSCV}(h)$.

2.7 Lepski's method

Lepski's method is a very general approach to choosing tuning parameters in an adaptive way. We present here a version of the method, tailored to the problem of estimating a density f at the point $x \in \mathbb{R}$.

Recall that if $f \in \mathcal{F}(\beta, L)$ where β and L are known, then the optimal bandwidth h_n^* is of the form $C_{\beta, L, k} n^{-\frac{1}{2\beta+1}}$. Suppose now that L is unknown and we only have an upper bound ℓ on β . Lepski's method chooses a bandwidth \hat{h} adaptively from a pre-defined geometric sequence \mathcal{H}_n of candidates. These extend from order n^{-1} up to order $n^{-\frac{1}{2\ell+1}}$, up to logarithmic factors, so contain the optimal bandwidth h_n^* when n is large. The procedure constructs confidence intervals $\hat{I}_{n,h}$ for $\mathbb{E}\hat{f}_{n,h,k}(x)$ for $h \in \mathcal{H}_n$, whose widths are data-driven proxies for the standard deviation of $\hat{f}_{n,h,k}(x)$. The required bias-variance tradeoff is achieved by choosing \hat{h} to be the largest $h \in \mathcal{H}_n$ for which the intersection of $\hat{I}_{n,\tilde{h}}$ for $\tilde{h} \in \mathcal{H}_n \cap (0, h]$ is non-empty.

More precisely, for $\ell \in \mathbb{N}$, let k denote a bounded kernel of order ℓ that vanishes outside $[-1, 1]$. Let $\Gamma := \frac{\|k\|_\infty^2}{9R(k)}$ and for $\delta \in (0, 1]$, let

$$\mathcal{H}_{n,\delta} = \left\{ \frac{2^j \Gamma}{n} \log \left(\frac{2 \left\lceil \frac{2\ell}{2\ell+1} \log_2(4n) \right\rceil}{\delta} \right) : j = 1, \dots, \left\lceil \frac{2\ell}{2\ell+1} \log_2(4n) \right\rceil \right\}.$$

Now let $\hat{f}_\infty := \max\{|\hat{f}_{n,h_{\max},k}(x)|, 0\} + 1$, where $h_{\max} := \max(\mathcal{H}_{n,\delta})$, and

$$\hat{\sigma}_{n,h,\delta} := \left(\frac{32\hat{f}_\infty R(k) \log \left(\frac{2|\mathcal{H}_{n,\delta}|}{\delta} \right)}{nh} \right)^{1/2}$$

and

$$\hat{I}_{n,h,\delta} := [\hat{f}_{n,h,k}(x) - \hat{\sigma}_{n,h,\delta} \hat{f}_{n,h,j}(x) + \hat{\sigma}_{n,h,\delta}].$$

The Lepski choice of bandwidth is then

$$\hat{h}_\delta := \max \left\{ h \in \mathcal{H}_{n,\delta} : \bigcap_{\tilde{h} \in \mathcal{H}_{n,\delta} \cap (0, h]} \hat{I}_{n,\tilde{h},\delta} \neq \emptyset \right\}.$$

Theorem. Let $X_1, \dots, X_n \sim^{iid} f \in \mathcal{F}(\beta, L)$ with $\beta \in (0, \ell]$. Then there exists $C = C(\beta, L, k) > 0$ such that for every $\delta \in [n^{-3}, 1]$, we have with probability at least $1 - \delta$ that

$$|\hat{f}_{n,\hat{h}_\delta,k}(x) - f(x)| \leq C \left(\frac{\log \left(\frac{\log(4n)}{\delta} \right)}{n} \right)^{\frac{\beta}{2\beta+1}}.$$

In particular, taking $\hat{h} = \hat{h}_{n^{-3}}$, there exists $C' = C'(\beta, L, k) > 0$ such that for every $n \in \mathbb{N}$,

$$\text{MSE}(\hat{f}_{n,\hat{h},k}(x)) \leq C' \left(\frac{\log(en)}{n} \right)^{\frac{2\beta}{2\beta+1}}.$$

Proof. For $i \in [n]$, let $Z_{i,h} = k_h(x - X_i) - \mathbb{E}k_h(x - X_i)$. Then for every $h \in (0, h_{\max}]$

$$\begin{aligned} \text{Var}(Z_{1,h}) &\leq \mathbb{E}k_h^2(x - X_1) \\ &= \frac{1}{h^2} \int_{\mathbb{R}} k^2\left(\frac{x-z}{h}\right) f(z) dz \\ &= \frac{1}{h} \int_{-1}^1 k^2(u) f(x - uh) du \quad (u = (x-z)/h) \\ &\leq \frac{R(k)}{h} \sup_{|t| \leq h_{\max}} f(x+t) \\ &:= \frac{R(k)}{h} f_{\infty}. \end{aligned}$$

Moreover, $|Z_{1,h}| \leq \frac{2\|k\|_{\infty}}{h}$, so by the version of Bernstein's inequality from Example Sheet 1 with $\sigma^2 = R(k)f_{\infty}/h$ and $c = 2\|k\|_{\infty}/(3h)$, we have for every $\eta \in (0, 1]$, $h \in (0, h_{\max}]$ and $n \in \mathbb{N}$ that

$$\mathbb{P} \left(|\hat{f}_{n,h,k}(x) - \mathbb{E}\hat{f}_{n,h,k}(x)| \leq \left(\frac{2f_{\infty}R(k)\log(2/\eta)}{nh} \right)^{1/2} + \frac{2\|k\|_{\infty}}{3nh} \log(2/\eta) \right) \geq 1 - \eta.$$

Hence, by a union bound, if we define the event $\Omega_0 = \Omega(n, \delta)$ by

$$\begin{aligned} \Omega_0 &:= \{ |\hat{f}_{n,h,k}(x) - \mathbb{E}\hat{f}_{n,h,k}(x)| \\ &\leq \left(\frac{2f_{\infty}R(k)\log(2|\mathcal{H}_{n,\delta}|/\delta)}{nh} \right)^{1/2} + \frac{2\|k\|_{\infty}}{3nh} \log(2|\mathcal{H}_{n,\delta}|/\delta) \quad \forall h \in \mathcal{H}_{n,\delta} \} \end{aligned}$$

then $\mathbb{P}(\Omega_0^c) \leq \delta$. Moreover (see Example Sheet 2), there exist $n_0 = n_0(\beta, L, k) \in \mathbb{N}$ and $A = A(\beta, L) > 0$ such that for $n \geq n_0$ and $\delta \in [n^{-3}, 1]$, we have on Ω_0 that $f_{\infty} \leq \hat{f}_{\infty} \leq A$.

It follows that for $n \geq n_0$ and $\delta \in [n^{-3}, 1]$, on Ω_0 , for every $h \in \mathcal{H}_{n,\delta}$,

$$\begin{aligned} |\hat{f}_{n,h,k}(x) - \mathbb{E}\hat{f}_{n,h,k}(x)| &\leq \left(\frac{2f_{\infty}R(k)\log\left(\frac{2|\mathcal{H}_{n,\delta}|}{\delta}\right)}{ng} \right)^{1/2} + \frac{2\|k\|_{\infty}}{3nh} \log(2|\mathcal{H}_{n,\delta}|/\delta) \\ &= 2 \left(\frac{2\hat{f}_{\infty}R(k)\log\left(\frac{2|\mathcal{H}_{n,\delta}|}{\delta}\right)}{ng} \right)^{1/2} \\ &:= \frac{\hat{\sigma}_{n,h,\delta}}{2} \end{aligned}$$

where we have used the definitions of $h_{\min} := \min(\mathcal{H}_{n,\delta})$ and Γ , as well as $\hat{f}_\infty \geq 1$. Now let

$$h_{\text{opt}} = \left(D_{\beta,L,k}^2 \frac{\log(2|\mathcal{H}_{n,\delta}|/\delta)}{n} \right)^{\frac{1}{2\beta+1}}$$

where

$$D_{\beta,L,k} := \frac{(\lceil \beta \rceil - 1)! \sqrt{8R(k)}}{L\mu_\beta(k)}.$$

Then by a previous proposition and the fact that $\hat{f}_\infty \geq 1$, we have for $h \in (0, h_{\text{opt}}]$ the bias bound

$$\begin{aligned} |bbE\hat{f}_{n,h,k}(x) - f(x)| &\leq \frac{L}{(\lceil \beta \rceil - 1)!} \mu_\beta(k) h^\beta \\ &\leq 2 \left(\frac{2\hat{f}_\infty R(k) \log(2|\mathcal{H}_{n,\delta}|/\delta)}{nh} \right)^{1/2} \\ &= \frac{\hat{\sigma}_{n,h,\delta}}{2}. \end{aligned}$$

Moreover, there exists $n_1 = n_1(\beta, L, k) \in \mathbb{N}$ such that for $n \geq n_1$,

$$h_{\min} = \frac{2\Gamma}{n} \log(2|\mathcal{H}_{n,\delta}|/n) \leq h_{\text{opt}} \leq \frac{4^{\frac{2\ell}{2\ell+1}} \Gamma}{2n^{\frac{1}{2\ell+1}}} \log(2|\mathcal{H}_{n,\delta}|/\delta) \leq h_{\max}$$

where we have used the fact that $|\mathcal{H}_{n,\delta}| = \lfloor \frac{2\ell}{2\ell+1} \log_2(4n) \rfloor \geq \frac{2\ell}{2\ell+1} \log(4n) - 1$. tHUS $\tilde{h}_{\text{opt}} := \max(\mathcal{H}_{n,\delta} \cap (0, h_{\text{opt}}]) \geq h_{\text{opt}}/2$. It follows by (*) and (**) that for $n \geq \max(n_0, n_1)$ and $\delta \in [n^{-3}, 1]$, we have on Ω_0 that

$$|\hat{f}_{n,h,k}(x) - f(x)| \leq \hat{\sigma}_{n,h,\delta} \quad \forall h \in \mathcal{H}_{n,\delta} \cap (0, \tilde{h}_{\text{opt}}],$$

and we deduce that $f(x) \in \bigcap_{h \in \mathcal{H}_{n,\delta} \cap (0, \tilde{h}_{\text{opt}}]} \hat{I}_{n,h,\delta}$, so $\hat{h}_\delta \geq \tilde{h}_{\text{opt}} \geq \frac{h_{\text{opt}}}{2}$. Moreover, $\hat{I}_{n,\hat{h}_\delta,\delta} \cap \hat{I}_{n,\tilde{h}_{\text{opt}},\delta} \neq \emptyset$, by definition of \hat{h}_δ . We conclude that for $n \geq \max(n_0, n_1)$, $\delta \in [n^{-3}, 1]$ and on Ω_0 ,

$$\begin{aligned} |\hat{f}_{n,\hat{h}_\delta,k}(x) - f(x)| &\leq |\hat{f}_{n,\hat{h}_\delta,k}(x) - \hat{f}_{n,\tilde{h}_{\text{opt}},k}(x)| + |\hat{f}_{n,\tilde{h}_{\text{opt}},k}(x) - f(x)| \\ &\leq \hat{\sigma}_{n,\hat{h}_\delta,\delta} + \hat{\sigma}_{n,\tilde{h}_{\text{opt}},\delta} + \hat{\sigma}_{n,\tilde{h}_{\text{opt}},\delta} \\ &\leq 3\hat{\sigma}_{n,\tilde{h}_{\text{opt}},\delta} \end{aligned}$$

□