Nonparametrics & Bayes

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Non-parametrics

- Bayesian Statistics
 - Interval estimates

Some more set-up



- If we'd still like to estimate a parameter, can use the plug-in principle:
- Let $\nu = \nu(F)$ be a parameter of interest.
- We can use $\widehat{\nu} = \nu(\widehat{F}_n)$ as an estimator of $\nu(F)$, i.e. we plug in \widehat{F}_n in $\nu(F)$.
- ullet This is a "flipped" view of viewing u as a function of F.
- Only sort of parameter we can consider, since no parametric model assumed!
- For the first two moments we get

$$\mu(F) = \int_{-\infty}^{\infty} y \ d\widehat{F}_n(y) = \frac{1}{n} \sum_i Y_i = \overline{Y}$$
 (1)

$$\sigma^{2}(F) = \int_{-\infty}^{\infty} \{y - \mu(F)\}^{2} d\widehat{F}_{n}(y) = \frac{1}{n} \sum_{i} \{Y_{i} - \mu(F)\}^{2}$$
$$= \frac{1}{n} \sum_{i} \{Y_{i} - \overline{Y}\}^{2}.$$
 (2)



Observations:

- No matter what the true distribution is, the same parameter is always estimated by the same statistic when using plug-in estimation.
- Consequence: plug-in estimator may be inefficient in some cases, e.g.
 - \hookrightarrow if F is Gaussian, then plug-in estimator of mean is same as MLE...
 - \hookrightarrow but if F is Laplace, MLE of mean is median, not mean...
- Stylised fact: if parametric model can be assumed, MLE preferable.
- Provided mapping $F \mapsto \nu(F)$ is "well behaved", corresponding plug-in estimator will be consistent
 - \hookrightarrow E.g. $F \mapsto \int_{-\infty}^{+\infty} h(x) dF(x)$ for h such that $\mathbb{E}[h(Y)] < \infty$.
- Why care about parameters anyway if we can estimate CDF?
 - \hookrightarrow Parameters usually interpretable, CDFs are harder to appreciate visually.
- Densities are more easily interpreted also defined as functional of CDF!
- ullet The density f (when it exists) at $x_0\in\mathbb{R}$ is $u(F):=rac{d}{dx}F(x)ig|_{x=x_0}$
- Caution: mapping $F \mapsto \nu(F)$ not a "well behaved" mapping in general...



Let's focus on estimating the density f(x) of a continuous distribution F,

$$F(t) = \int_{-\infty}^{t} f(x) dx,$$

using the plug-in principle. Write $u_x(F) = \frac{d}{dt} F(t) \big|_{t=x} = f(x)$.

- ullet Need to take $\hat{F}_n\mapsto
 u_x(\hat{F}_n)$ not a "well-behaved" mapping:
 - If $x \notin \{Y_1, ..., Y_n\}$ estimator $\nu_x(\hat{F}_n)$ is zero.
 - If $x \in \{Y_1,...,Y_n\}$ estimator is undefined!
- ullet Problem is that estimator requires differentiation of a function \hat{F}_n with jumps
- ullet We will need a "smoother" estimate of F to plug in instead of \hat{F}_n , e.g.

$$ilde{F}_n(x) \coloneqq \int_{-\infty}^{\infty} \Phi\left(rac{x-y}{h}
ight) d\hat{F}_n(y) = rac{1}{n} \sum_{i=1}^n \Phi\left(rac{x-Y_i}{h}
ight)$$

for Φ a standard normal CDF and h > 0 a smoothing parameter.

 Transforms flat steps with hard corners to inclined steps with smooth corners (buffs the edges)



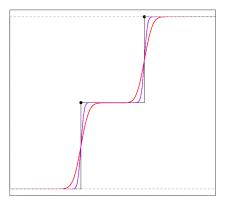


Figure: Empirical distribution function (black) for a size n=2 sample, and "smoothed" approximations by convolution with $\Phi\left(\frac{u}{h}\right)$ for h=0.3 (red) and h=0.2 (purple).



At the level of density, this yields the "smoothed plug-in estimator"

$$\hat{f}(x) = \frac{d}{dx}\tilde{F}_n(x) = \frac{d}{dx}\frac{1}{n}\sum_{i=1}^n \Phi\left(\frac{x-Y_i}{h}\right) = \frac{1}{n}\sum_{i=1}^n \frac{1}{h}\varphi\left(\frac{x-Y_i}{h}\right)$$

for $\varphi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$ the standard normal density.

- Much more important is the choice of h > 0 called a bandwidth or smoothing parameter.

Definition (Kernel Density Estimator)

Let $Y_1, \ldots, Y_n \stackrel{ind}{\sim} f$, where f is a probability density function. A Kernel Density Estimator (KDE) \hat{f} of f is a random density function defined as

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

for $K : \mathbb{R} \to \mathbb{R}$ a kernel and h > 0 a bandwidth or smoothing parameter.



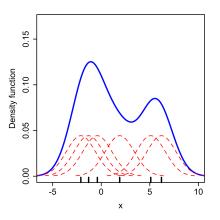


Figure: Schematic Illustration of a kernel density estimator



Only problem: how should we choose arbitrary tuning parameter h > 0?

← Can have decisive effect on quality of estimator.

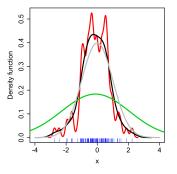


Figure: Effect of bandwidth choice on KDE of standard normal density, n=100. True density in gray.KDE with: h=0.05 in red, h=0.337 in black, h=2 in green.



To select h, need to understand its effect on KDE.

In short, it regulates the bias-variance tradeoff:

- Large h: gives "flattened" estimator (higher bias) but quite stable to small perturbations of the sample values (low variance).
- Small h: gives "wiggly" estimator (lower bias) but overly sensitive to small perturbations of the sample values (high variance).

What bias and variance? Those corresponding to integrated mean squared error:

$$ext{IMSE}(\hat{f},f) = \int_{\mathbb{R}} \mathbb{E} \Big(\hat{f}(x) - f(x)\Big)^2 dx.$$

$$\mathrm{IMSE}(\hat{f},f) = \underbrace{\int_{\mathbb{R}} \Big(\mathbb{E}\left[\hat{f}(x)\right] - f(x)\Big)^2 dx}_{\text{integrated squared bias}} + \underbrace{\int_{\mathbb{R}} \mathbb{E}\Big\{\hat{f}(x) - \mathbb{E}\left[\hat{f}(x)\right]\Big\}^2 dx}_{\text{integrated variance}}$$

To get a useful expression for this we resort to asymptotics.



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Theorem (Asymptotic Risk of KDE)

Let $f \in C^3$ be a probability density and $K \in C^2$ a kernel function satisfying

$$\int_{\mathbb{R}} \left(f''(x)\right)^2 dx < \infty \quad \int_{\mathbb{R}} \left|f'''(x)\right| dx < \infty \quad \& \quad \int_{\mathbb{R}} \left(K''(x)\right)^2 dx < \infty.$$

If \hat{f}_n is the KDE of f with iid sample size n, kernel K and bandwidth h,

$$\mathrm{IMSE}(\hat{f},f) = \frac{h^4}{4} \int_{\mathbb{R}} \left(f''(x) \right)^2 dx + \frac{1}{nh} \int_{\mathbb{R}} K^2(x) dx + o\left(h^4 + \frac{1}{nh}\right).$$

as h o 0.

Conclusions:

- For consistency, need $h \to 0$ but $nh \to \infty$ as $n \to \infty$.
- Optimal choice of h will unfortunately depend on (unknown) f''
- ullet For the record, optimal h is given (after some calculations) by

$$h^* = \left\{rac{1}{n}\!\int_{\mathbb{R}} K^2(x) dx \middle/ \int_{\mathbb{R}} \left(f''(x)
ight)^2 dx
ight\}^{1/5}$$

- Plugging in the optimal bandwidth yields the a risk of asymptotic order $n^{-4/5}$
- \bullet Compare this to parametric model optimal rate of n^{-1}
- Asymptotic bias proportional to curvature of f.



Proof (*).

Using the fact that the observations are iid, we can write $\mathbb{E}\left[f_n(x)
ight]$ as

$$\frac{1}{h}\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[K\left(\frac{x-Y_{i}}{h}\right)\right] = \frac{1}{h}\int_{\mathbb{R}}K\left(\frac{x-t}{h}\right)f(t)dt = \int_{\mathbb{R}}K(y)f(x-hy)dy$$

by change of variables y = (x - t)/h. Now Taylor expanding f yields

$$f(x-hy) = f(x) - hyf'(x) + rac{1}{2}h^2y^2f''(x) + o(h^2)$$
 as $h o 0$.

Plugging into the equation for the expectation, we get that $\mathbb{E}[f_n(x)]$ equals

$$f(x)\underbrace{\int_{\mathbb{R}}K(y)dy}_{=1}-hf'(x)\underbrace{\int_{\mathbb{R}}yK(y)dy}_{=0}+\frac{1}{2}h^2f''(x)\underbrace{\int_{\mathbb{R}}y^2K(y)dy}_{=1}+o(h^2)$$

as $h \to 0$ by the kernel properties of K. In summary the pointwise bias is

$$\mathbb{E}\left[\hat{f}_n(x)
ight] - f(x) = rac{1}{2}h^2f''(x) + o(h^2), \quad ext{as } h o 0.$$



The pointwise variance $\mathrm{var}[\hat{f_n}(x)]$, on the other hand, equals (by iid assumption)

$$\frac{1}{n^2h^2}\sum_{i=1}^n \operatorname{var}\left[K\left(\frac{x-Y_i}{h}\right)\right] = \frac{1}{nh^2}\left(\mathbb{E}\left[K^2\left(\frac{x-Y_1}{h}\right)\right] - \mathbb{E}^2\left[K\left(\frac{x-Y_1}{h}\right)\right]\right)$$

and by similar manipulations as earlier, and the expression for $\mathbb{E}\left[\hat{f}_n(x)
ight]$, we get

$$\operatorname{var}[\hat{f_n}(x)] = \underbrace{\frac{1}{nh}\int_{\mathbb{R}}K^2(y)f(x-hy)dy}_{A} - \underbrace{\frac{1}{nh^2}\mathbb{E}^2[\hat{f_n}(x)]}_{B}$$

Now observe that as as $h \to 0$, we have

$$B = \frac{1}{nh^2}(f(x) + \frac{1}{2}h^2f''(x) + o(h^2))^2 = \frac{1}{nh^2}[f(x) + o(h)]^2 = o\left(\frac{1}{n}\right).$$

On the other hand, Taylor expanding f(x-hy)=f(x)+o(1) as h o 0, we have

$$A = \frac{1}{nh} \int_{\mathbb{R}} K^2(y) [f(x) + o(1)] dy = \frac{1}{nh} f(x) \int_{\mathbb{R}} K^2(y) dy + o\left(\frac{1}{nh}\right)$$

since $\frac{1}{nh}o(1) = o\left(\frac{1}{nh}\right)$



Putting A and B together gives

$$\operatorname{var}[\hat{f}_n(x)] = \frac{1}{nh} \int_{\mathbb{R}} K^2(y) dy + o\left(\frac{f(x)}{nh}\right) - o\left(\frac{1}{n}\right) = \frac{f(x)}{nh} \int_{\mathbb{R}} K^2(y) dy + o\left(\frac{1}{nh}\right)$$

Summing pointwise squared-bias and variance, the pointwise MSE is given by

$$MSE(\hat{f}_n(x), f(x)) = \frac{1}{4}h^4(f''(x))^2 + \frac{f(x)}{nh} \int_{\mathbb{R}} K^2(y) dy + o\left(h^4 + \frac{1}{nh}\right)$$

Finally, integrating over $\mathbb R$ and re-arranging yields the sought form

$$\mathrm{IMSE}(\hat{f},f) = \tfrac{1}{nh} \int_{\mathbb{R}} K^2(x) dx + \tfrac{h^4}{4} \int_{\mathbb{R}} \left(f''(x)\right)^2 dx + o\left(h^4 + \tfrac{1}{nh}\right).$$



Can we do better than $n^{-4/5}$ by more smoothness assumptions?

Theorem (Minimax Optimal Rates for KDE)

Let $\mathcal{F}(m,r)$ be the subset of m-differentiable densities with mth derivative in an L^2 ball of radius r,

$$\int_{\mathbb{R}} \left(f^{(m)}(x)
ight)^2 dx \leq r^2.$$

Then, given any KDE \hat{f}_n ,

$$\sup_{f\in\mathcal{F}(m,r)}\mathbb{E}\left\{\int_{\mathbb{R}}\left(\hat{f}_n(x)-f(x)\right)^2\,dx\right\}\geq Cn^{-\frac{2m}{2m+1}},$$

where the constant C > 0 depends only on m and c.

- The smoother the density the better the worst case rate.
- Can never beat n^{-1} , though.
- The price to pay for flexibility!



So how do we choose h in practice? Here's a couple of approches:

- Pilot estimator: use a parametric family (e.g. normal, or mixture) to obtain a
 preliminary estimator f, and plug this into the optimal bandwidth expression
 to select a bandwidth.
- Least squares cross-validation: try to construct an unbiased estimator of the IMSE after all, it is an expectation. Then choose h to minimise the estimated IMSE. Also known as unbiased risk estimation.

Let's consider the second approach in more detail. Notice that we can write

$$\begin{split} \mathit{IMSE}(\hat{f}_{\hbar},f) &= \int_{\mathbb{R}} \mathbb{E} \Big(\hat{f}_{\hbar}(x) - f(x) \Big)^2 dx = \mathbb{E} \left[\int_{\mathbb{R}} \big(\hat{f}_{\hbar}(x) - f(x) \big)^2 dx \right] \\ &= \underbrace{\mathbb{E} \left[\int_{\mathbb{R}} \hat{f}_{\hbar}^2(x) dx \right] - 2\mathbb{E} \left[\int_{\mathbb{R}} \hat{f}_{\hbar}(x) f(x) dx \right]}_{H(\hat{f}_{\hbar})} + \mathbb{E} \left[\int_{\mathbb{R}} f^2(x) dx \right]. \end{split}$$

where the last term does not vary with h.



How can we estimate $H(\hat{f}_h)$?

- ① Can easily estimate $\mathbb{E}\left[\int_{\mathbb{R}}\hat{f}_h^2(x)dx\right]$ by $\int_{\mathbb{R}}\hat{f}_h^2(x)dx$.
- 2 Other term trickier (depends on f!). Define the *leave-one-out* estimator

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

i.e. the kernel estimator leaving the ith observation out. Observe that

$$\mathbb{E}\Big[\hat{f}_{h,-i}(Y_i)\Big] = \frac{1}{n-1} \sum_{j \neq i} \mathbb{E}\left[\frac{1}{h}K\left(\frac{Y_i - Y_j}{h}\right)\right] = \mathbb{E}\left[\frac{1}{h}K\left(\frac{Y_1 - Y_2}{h}\right)\right] =$$

$$=\int_{\mathbb{R}}\int_{\mathbb{R}}\frac{1}{h}K\left(\frac{u-v}{h}\right)f(u)f(v)dudv=\int_{\mathbb{R}}\mathbb{E}\left[\frac{1}{h}K\left(\frac{Y_{1}-v}{h}\right)\right]f(v)dv=$$

$$= \int_{\mathbb{R}} \mathbb{E}\left[\frac{1}{nh} \sum_{k=1}^{n} K\left(\frac{Y_k - v}{h}\right)\right] f(v) dv = \mathbb{E}\left[\int_{\mathbb{R}} \underbrace{\frac{1}{nh} \sum_{k=1}^{n} K\left(\frac{Y_k - v}{h}\right)}_{=\hat{h}(v)} f(v) dv\right]$$

Thus $\{\hat{f}_{h,-i}(Y_i)\}_{i=1}^n$ are n variables with mean $\mathbb{E}\left[\int_{\mathbb{R}}\hat{f}_h(x)f(x)dx
ight]!$



Motivates definition of leave-one-out cross validation estimator

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

which by construction satisfies

$$\mathbb{E}[LSCV(h)] = H(\hat{f}_h).$$

Strategy: choose h by minimising LSCV(h). Does it work?

Theorem (Stone's Theorem)

In the same context, and under the same assumptions, let h_{CV} denote the bandwidth selected by cross-validation. Then,

$$rac{\displaystyle\int_{\mathbb{R}} \left(\hat{f}_{h_{CV}}(x) - f(x)
ight)^2 dx}{\displaystyle\inf_{h>0} \displaystyle\int_{\mathbb{R}} \left(\hat{f}_h(x) - f(x)
ight)^2 dx} \stackrel{a.s.}{\longrightarrow} 1,$$

provided that the true density f is bounded.



Conceptually, can generalise KDE very easily to higher dimensions.

- ullet Let ${Y}_1,...,{Y}_n\stackrel{\ddot{u}d}{\sim} f(y)$ be a sample in \mathbb{R}^d with density $f:\mathbb{R}^d o [0,+\infty)$
- Let $H \succeq 0$ be a $d \times d$ symmetric positive-definite bandwidth matrix.
- ullet Let K be a probability density on \mathbb{R}^d with mean 0 and covariance $I_{d imes d}.$
 - \hookrightarrow E.g. $K(x_1,...,x_n)=\prod_{j=1}^d \varphi(x_j)$ for φ the N(0,1) density.

We can define a d-dimensional KDE as

$$\widehat{f}(x) = rac{1}{n|H|^{1/2}} \sum_{i=1}^n K\left(H^{-1/2}(x-Y_i)
ight), \qquad x \in \mathbb{R}^d.$$

Once again choice of kernel is secondary but choice of H is paramount.

- Considerably harder: need to choose $d(d+1)/2 \sim d^2$ bandwidth parameters.
- Intuitively: $H = U \operatorname{diag}\{h_1,...,h_d\}U^{\top}$ for $U^{\top}U = I_{d\times d}$ and $h_i > 0$.
 - \hookrightarrow Choose d smoothing directions, and a bandwidth for each such direction.
- LSCV-type solutions exist for d moderate (computationally intensive).
- Visualisation challenging for d > 3.

Some more set-up



- We have assumed that there is some parameter θ with some unknown constant value.
- We could think of the unknown parameter θ as being a realisation from random variable Θ where Θ has some supposed distribution $p(\Theta = \theta)$.
- The previous approach is a special case of this method with $p(\Theta = \theta_0) = 1$ and $p(\Theta \neq \theta) = 0$.
- We write

$$p(\mathcal{D}, \theta) = p(\mathcal{D}|\theta)p(\theta) = p(\theta|\mathcal{D})p(\mathcal{D}),$$

where $\mathcal{D} = (X_1, \dots, X_n)$ and $p(\cdot)$ is either a pmf or pdf.

Some more Bayesian set-up



This gives us

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} \propto p(D|\theta)p(\theta)$$

Posterior = Likelihood × Prior.

• By Bayes' Theorem and note that p(D) is **not** a function of θ and it is given by

$$p(D) = \int_{\Theta} p(D|\theta)p(\theta)d\theta.$$

- We write the likelihood with a conditional sign rather than a semi-colon to reflect the fact that θ is a random variable rather than a constant.
- Using Bayes theorem allows us to determine a posterior distribution for Θ which gives us all the available information about it after we have seen the data, D.

Some more Bayesian set-up



- We may want to report a single plausible value for Θ which summarises its posterior distribution.
- The "best" summary of the posterior, $\widetilde{\theta}$, needs a loss function, $L(\Theta, \widetilde{\theta})$, which ensures that the posterior density is concentrated near the point estimate, $\widetilde{\theta}$.
- \bullet We take $\widehat{\theta}$ as the value that minimises the expected posterior loss so that

$$E_{\Theta|D}\{L(\Theta,\tilde{\theta})|D\} = \int_{-\infty}^{\infty} L(\theta,\tilde{\theta})p(\theta|D)d\theta.$$

is a minimum.

• If $L(\theta, \tilde{\theta}) = (\theta - \tilde{\theta})^2$ we take $\tilde{\theta}$ to be the mean of the posterior distribution, $p(\theta|D)$.

Some Bayesian statistics



- If $L(\theta, \widetilde{\theta}) = |\theta \widetilde{\theta}|$ we find that $\widetilde{\theta}$ is the posterior median.
- If we take $L(\theta, \widetilde{\theta}) = 1$ if $\widetilde{\theta} \neq \theta$ and zero otherwise we take $\widetilde{\theta}$ as the point at the maximum of the density, i.e. the posterior mode.
- In Bayesian statistics all the information is contained in the posterior pdf $p(\theta|D)$.
- We may want an interval which will contain Θ with probability that include the most concentrated areas of $p(\theta|D)$.
- We can do this by determining the $100\gamma\%$ credible interval which is an interval which contains $100\gamma\%$ of the total density in the posterior distribution.

Some Bayesian statistics



• Let $\ell(x)$ and u(x) be some functions of the observed data then a $100\gamma\%$ credible interval satisfies

$$P(\ell(x) < \Theta < u(x)|D) = \int_{\ell x}^{u(x)} p(\theta|D)d\theta$$

= γ .

Further, we define the $100\gamma\%$ Highest Posterior Density (HPD) region to be the credible interval for which $u(x) - \ell(x)$ is a minimum.

Gaussian example



Assume that

$$Y_i|\mu \sim N(\mu, \sigma_0^2).$$

ullet We also put a prior distribution on μ of

$$\mu \mid \mu_0, \tau \sim N(\mu_0, \tau^2).$$

We can now from this calculate

$$p(\mu|Y) = \frac{p(Y|\mu)p(\mu)}{p(Y)} \propto p(Y|\mu)p(\mu)$$

$$\propto \frac{1}{(2\pi\sigma_0^2)^{n/2}} e^{-\frac{1}{2\sigma_0^2} \sum_{i=1}^n (Y_i - \mu)^2} \frac{1}{(2\pi\tau^2)^{1/2}} e^{-\frac{1}{2\tau^2} (\mu - \mu_0)^2}$$

$$\propto \exp\{-\frac{1}{2} \{\frac{n}{\sigma_0^2} + \frac{1}{\tau^2}\} \mu^2 + \{\frac{n\bar{Y}}{\sigma_0^2} + \frac{\mu_0}{\tau^2}\} \mu\}. \tag{3}$$

Gaussian example



ullet This is a Gaussian distribution on μ with a variance of

$$\frac{1}{\sigma_*^2} = \frac{n}{\sigma_0^2} + \frac{1}{\tau^2} = \frac{n\tau^2 + \sigma_0^2}{\sigma_0^2 \tau^2}.$$

This implies the posterior $\mu|Y \sim N(\mu_*, \sigma_*^2)$ with

$$\sigma_*^2 = \frac{\sigma_0^2 \tau^2}{n \tau^2 + \sigma_0^2},$$

and

$$\mu_* = \frac{\frac{n\bar{Y}}{\sigma_0^2} + \frac{\mu_0}{\tau^2}}{\frac{n}{\sigma_0^2} + \frac{1}{\tau^2}} = \frac{\frac{n}{\sigma_0^2}\bar{Y} + \frac{1}{\tau^2}\mu_0}{\frac{n}{\sigma_0^2} + \frac{1}{\tau^2}}.$$

• The latter is a convex combination of μ_0 and \bar{Y} . As $n \to \infty$ it becomes the sample mean.