Week 3: Kernel Density Estimation

MATH-517 Statistical Computation and Visualization

Linda Mhalla

2023-10-06

Section 1

Univariate Density Estimation

The problem

Setup: $X_1, \ldots, X_n$ is a random sample from a distribution F with continuous density $f(x)$

Goal: Estimate f non-parametrically, i.e., without assuming a particular form

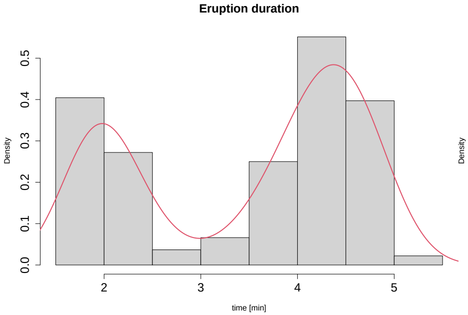
The **histogram** is the simplest form of density estimation. It requires a specification of

- *origin* and *binwidth*, or
- *breaks:* more general, but non-equidistant binning is bad anyway, so think only about origin and bindwidth

Running Ex.: Yellowstone's Old Faithful geyser - `faithful` data:

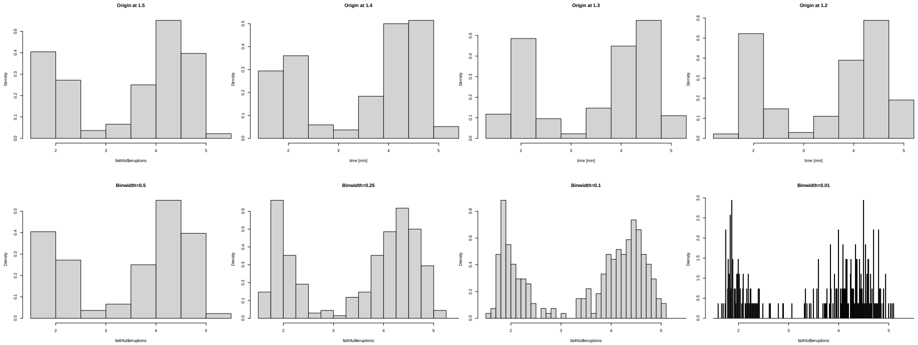
- `waiting` - time between eruptions
- `eruptions` - duration of the eruptions

Basic estimator: Histogram



(equally spaced) `breaks` specified, so a rule of thumb used to choose origin and binwidth

Histogram: Change in Origin and Binwidth

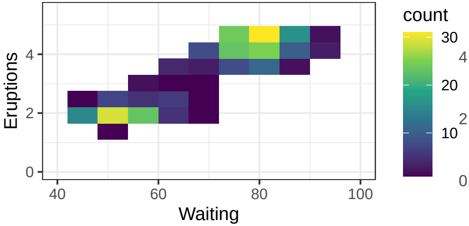


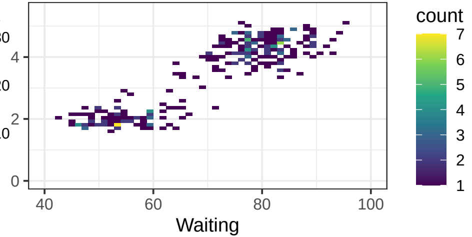
$\Rightarrow$ density estimate depends on the starting position and width of the bins

Issues with Histogram

Histogram is great for visualization, but fails as a density estimator

- *origin* is completely arbitrary
- *binwidth* relates to smoothness of f, but histogram cannot be smooth. The discontinuities of the estimate are not due to the underlying density but to bins' locations and widths
- *curse of dimensionality*: number of bins grows exponentially with the number of dimensions



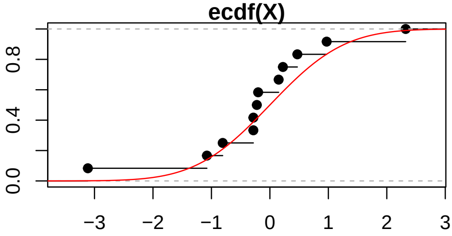


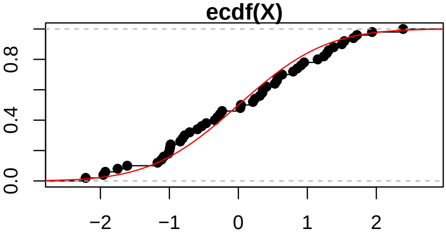
Let us now address these issues by a naive version of kernel density estimation

ECDF

Let $\widehat{F}$ denote the empirical (cumulative) distribution function (ECDF) of the data $\{X_i\}_{i=1}^n$, i.e.,

$$\widehat{F}_n(x) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{[X_i \leq x]}$$





Naive Density Estimator

- The ECDF $\widehat{F}_n(x)$ is an estimator of F
  - by Glivenko-Cantelli theorem uniformly almost surely consistent:

$$\sup_x |\widehat{F}(x) - F(x)| \overset{a.s.}{\to} 0$$

- Note that f is the derivative F. However, plugging $\widehat{F}_n(x)$ results in a sum of point masses at the observations as $\widehat{F}_n$ is discrete
- But,

$$f(x) = \lim_{h \to 0_+} \frac{F(x+h) - F(x-h)}{2h}$$

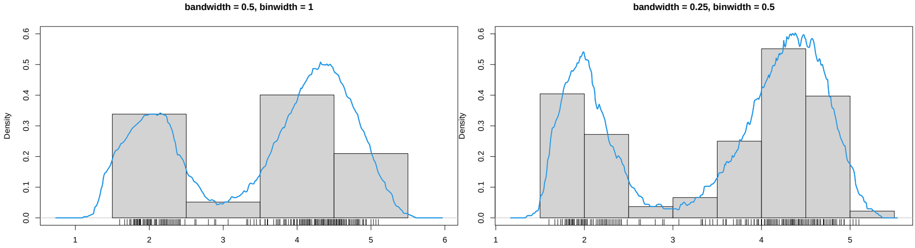
and we can fix $h = h_n$ small and depending on n, and plug it in:

$$\hat{f}(x) = \frac{\widehat{F}_n(x+h_n) - \widehat{F}_n(x-h_n)}{2h_n} = \frac{1}{2h_n} \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{[X_i \in (x-h_n, x+h_n]]}$$

$\Rightarrow$ This is called the naive density estimator

Naive Density Estimator

- The naive DE $\hat{f}$ is a step function with jumps at the points $X_i \pm h$, and thus discontinuous
- $\hat{f}$ is the sum of boxcar functions centered at the observations with width $2h$ and area $1/n \Rightarrow$ this is equivalent to the notion of moving histogram with binwidth$=2h$
  - aggregate data in intervals of the form $(x-h, x+h)$ and approximate the density at x by the relative frequency in $(x-h, x+h)$
  - *origin* does not matter anymore



Consistency

Theorem If $h = h_n \to 0$ and $nh_n \to \infty$ as $n \to \infty$, then, for any t,

$$\hat{f}_n(t) \xrightarrow{p} f(t),$$

as $n \to \infty$. Thus, $\hat{f}_n$ is a consistent estimator

For instance, since

$$\hat{f}(x) = \frac{1}{2nh_n} \sum_{i=1}^{n} \overbrace{\mathbb{1}_{\left[X_i \in (x-h_n, x+h_n]\right]}}^{Ber\left(F(x+h_n)-F(x-h_n)\right)}$$

- $\mathbb{E}\hat{f}(x) = \frac{F(x+h_n)-F(x-h_n)}{2h_n} \to f(x)$ as $h_n \to 0_+$, when $n \to \infty$
- $\mathrm{var}\{\hat{f}(x)\} = \frac{1}{4nh_n^2}\{F(x+h_n) - F(x-h_n)\}\{1 - F(x+h_n) + F(x-h_n)\}$

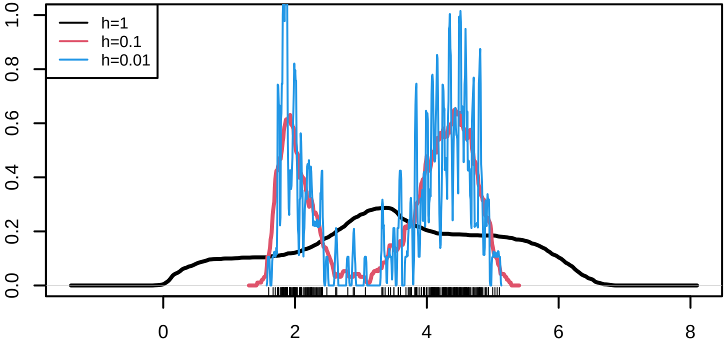
$$= \frac{F(x+h_n)-F(x-h_n)}{2h_n} \frac{1-F(x+h_n)+F(x-h_n)}{2nh_n} \to 0$$

as $h_n \to 0$ and $nh_n \to \infty$, when $n \to \infty$

Smoothness of the Naive DE

Smoothness of $\hat{f}$ depends on the *bandwidth* h (small h produces more wiggly/rough estimates), often called the *smoothing parameter*

- the bandwidth h is a *tuning parameter* and needs to be chosen somehow in practice
  - h small $\rightarrow$ wiggly estimator
  - h large $\rightarrow$ smooth estimator



Naive DE Rewritten

The naive DE can be written as

$$\hat{f}(x) = \frac{1}{2nh_n}\sum_{i=1}^{n} \mathbb{1}_{\left[X_i \in (x-h_n, x+h_n]\right]} = \frac{1}{2nh_n}\sum_{i=1}^{n} \mathbb{1}_{\left[-1 < \frac{X_i - x}{h_n} \leq 1\right]}$$
$$= \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h_n} K\left(\frac{x - X_i}{h_n}\right)$$

where $K(t) = \frac{1}{2}\mathbb{1}_{\{-1<t\leq 1\}}$ is the density of $U[-1, 1]$.

- Since $\int_{-\infty}^{+\infty} K(t)dt = 1$, we have that

$$\int_{-\infty}^{+\infty} \hat{f}(x)dx = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h_n}\int_{-\infty}^{+\infty} K\left(\frac{x - X_i}{h_n}\right) dx = 1$$

- Since $K(x) \geq 0$, then $\hat{f}(x) \geq 0$ for all x.

$\Rightarrow$ $\hat{f}(x)$ is a probability density function

Next step: replace $K(x)$ by another probability density, maybe one giving more weight to points closer to x ?

KDE - Definition and Properties

Definition. KDE of f based on $X_1, \dots, X_N$ is

$$\hat{f}(x) = \frac{1}{nh_n} \sum_{i=1}^{n} K\left(\frac{X_i - x}{h_n}\right),$$

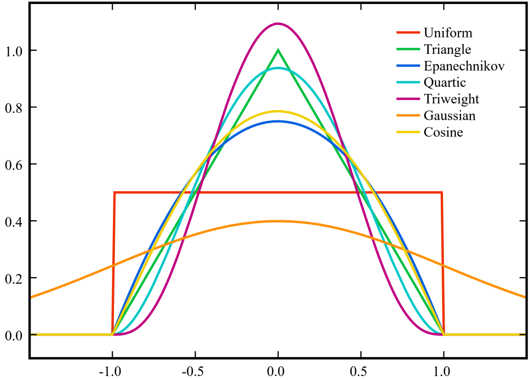
where the **kernel** $K(\cdot)$ satisfies:

1. $K(x) \geq 0$ for all $x \in \mathbb{R}$
2. $K(-x) = K(x)$ for all $x \in \mathbb{R}$
3. $\int_{\mathbb{R}} K(x)dx = 1$
4. $\lim_{|x|\to\infty} |x|K(x) = 0$
5. $\sup_x |K(x)| < \infty$

- $K(\cdot)$ is usually taken to be a density, and the assumptions
  - 1-3 hold if it is symmetric
  - 4 holds if it has a finite absolute moment
  - 5 holds if it is uniformly bounded
- if $h_n \to 0$ and $nh_n \to \infty$ (as $n \to \infty$), we have pointwise consistency
  - we will show this in a bit
  - also uniform consistency, but tricky to show

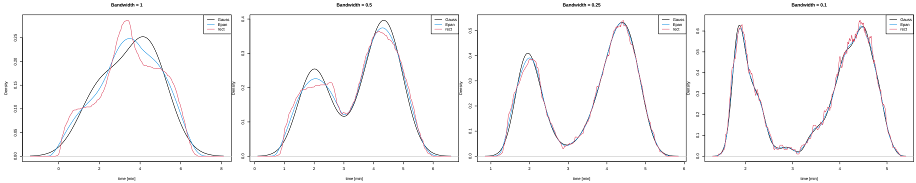
Common Kernels

Kernel Name	Formula
Epanechnikov	$K(x) \propto (1 - x^2)\mathbb{1}_{[\lvert x\rvert \leq 1]}$
Tricube (a.k.a. Triweight)	$K(x) \propto (1 - \lvert x\rvert^3)^3\mathbb{1}_{[\lvert x\rvert \leq 1]}$
Gaussian	$K(x) \propto \exp(-x^2/2)$
...	...



Bandwidth > Kernel

- While there is improvement when using non-rectangular kernels, the choice of the bandwidth is more important than that of the kernel
- A good choice is one that makes the estimate asymptotically converge quite rapidly in some well-chosen norm



Bias-Variance Trade-off

Goal: choose the tuning parameter h so that the mean squared error of the estimator is minimized:

$$\underbrace{\mathbb{E}[\{\hat{f}(x) - f(x)\}^2]}_{MSE\{\hat{f}(x)\}} = \mathbb{E}[\{\hat{f}(x) \pm \mathbb{E}\hat{f}(x) - f(x)\}^2]$$

$$= \underbrace{\{\mathbb{E}\hat{f}(x) - f(x)\}^2}_{bias^2} + \underbrace{\mathrm{var}\{\hat{f}(x)\}}_{variance}$$

Blackboard calculations (available in the lecture notes) give

$$\mathrm{bias}\{\hat{f}(x)\} = \frac{1}{2} h_n^2 f''(x) \int z^2 K(z) dz + o(h_n^2)$$

$$\mathrm{var}\{\hat{f}(x)\} = \frac{1}{nh_n} f(x) \int \{K(z)\}^2 dz + o\left(\frac{1}{nh_n}\right)$$

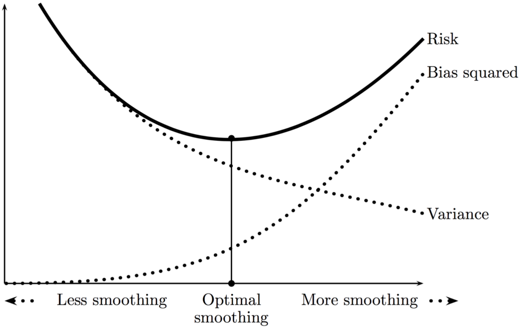
This shows consistency for $h_n \to 0$ and $nh_n \to \infty$ and the trade-off:

- small $h \Rightarrow$ small bias but large variance
- large $h \Rightarrow$ large bias but small variance

Bias-Variance Trade-off

The bias-variance trade-off is common when it comes to smoothing:

- In KDE, the smoothing is determined by the bandwidth
- Smoother estimates result in smaller variance but higher bias



Source: Wassermann (2006)

Optimal Bandwidth

Plugging this back in the MSE formula ignoring the *little-o* terms, differentiating the MSE w.r.t. h and setting it to zero leads to asymptotically optimal bandwidth choice:

$$h_{opt}(x) = n^{-1/5} \left(\frac{f(x) \int K(z)^2 dz}{\big[f''(x)\big]^2 \big[\int z^2 K(z) dz\big]^2} \right)^{1/5}$$

- $h_{opt}(x) \asymp n^{-1/5}$ ($h_{opt}(x)$ is of the order $n^{-1/5}$) and with this choice $MSE \asymp variance = \mathcal{O}(n^{-4/5})$
  - optimal non-parametric convergence rate
  - slower than the MSE of a MLE ($\mathcal{O}(n^{-1})$): price to pay for non-parametric approach
- $h_{opt}(x)$ is a local choice - depends on x. A global choice can be obtained by minimizing the MISE (to follow)

Optimal Kernel

The optimal bandwidth results in

$$MSE_{h_{opt}} = c(n, f) \left[\underbrace{\int x^2 K(z) dz \left\{ \int K^2(z) dz \right\}^2}_{A} \right]^{2/5},$$

where $c(n, f)$ is constant and depends only on n and f.

$\Rightarrow$ The optimal kernel is the one minimizing the term A.

It can easily be shown to be the Epanechnikov kernel!

Global Optimal Bandwidth

A common measure of performance of the estimator over all x is the Mean Integrated Squared Error (MISE):

$$\begin{aligned}
MISE(\hat{f}) &= \mathbb{E}\int \{\hat{f}(x) - f(x)\}^2 dx \\
&= \int \mathbb{E}\{\hat{f}(x) - f(x)\}^2 dx = \int MSE\{\hat{f}(x)\} dx
\end{aligned}$$

Minimizing the MISE yields the optimal bandwidth

$$\tilde{h}_{opt} = n^{-1/5}\left(\frac{\int K^2(z)dz}{\int \{f''(x)\}^2 dx \left[\int z^2 K(z)dz\right]^2}\right)^{1/5}$$

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

The Chicken and Egg problem

The theoretically optimal bandwidth $\tilde{h}_{opt} = n^{-1/5}(C(k)/\int\{f''(x)\}^2 dx)^{1/5}$ cannot be directly used as it depends on the unknown f. There are different approaches for the practical choice of h.

- **Reference method**: choose a parametric family for this formula
  - assume that f is the density of a $\mathcal{N}(\mu, \sigma^2)$ and then plug in its curvature $\frac{3}{8\sqrt{\pi}\sigma^5}$ into the formula of $\tilde{h}_{opt}$. This yields

    $$\tilde{h}_{opt} = n^{-1/5}\sigma C(k)^{1/5}(8\pi/3)^{1/5}$$

    which when combined with a normal kernel gives the famous rule of thumb $\hat{h}_{opt} = (4/3)^{1/5} n^{-1/5}\hat{\sigma}$
- **Two-step method**: f in the formula is estimated non-parametrically by a pilot fit
  - estimate f'' by kernel estimate with pilot bandwidth
  - plug this estimate into $\tilde{h}_{opt}$ to estimate the optimal bandwidth in the kernel estimation of f

Section 2

Multivariate Density Estimation

Multivariate Density estimator

In practice, data are often multivariate

Consider n i.i.d. realizations of a d-dimensional random vector $\mathbf{X}_i = (X_{i,1}, \ldots, X_{i,d})$ from unknown F. We wish to estimate f, the density of F

The multivariate kernel density estimator is defined as

$$\hat{f}_n(\mathbf{x}) = \frac{1}{nh^d} \sum_{i=1}^{n} K\left(\frac{\mathbf{x} - \mathbf{X}_i}{h}\right),$$

where the kernel $K(\cdot)$ is a d-dimensional density

Multivariate Kernel

In practice, K is often chosen as

- the product of univariate kernels: $K(\mathbf{x}) = \prod_{i=1}^{d} K_0(x_i)$
- ellipsoidal kernel
  - multivariate normal density: $(2\pi)^{-d/2} \exp(-\mathbf{x}\mathbf{x}^\top/2)$

  $\Rightarrow$ the matrix of bandwidths plays the role of the covariance-variance matrix

  - multivariate Epanechnikov: $\frac{d+2}{2c_d}(1-\mathbf{x}\mathbf{x}^\top)\mathbb{1}_{[-1,1]}(\mathbf{x}\mathbf{x}^\top)$, with c_d the volume of a d-dimensional unit ball ($c_1 = 1$, $c_2 = \pi$, $c_3 = 4\pi/3$)

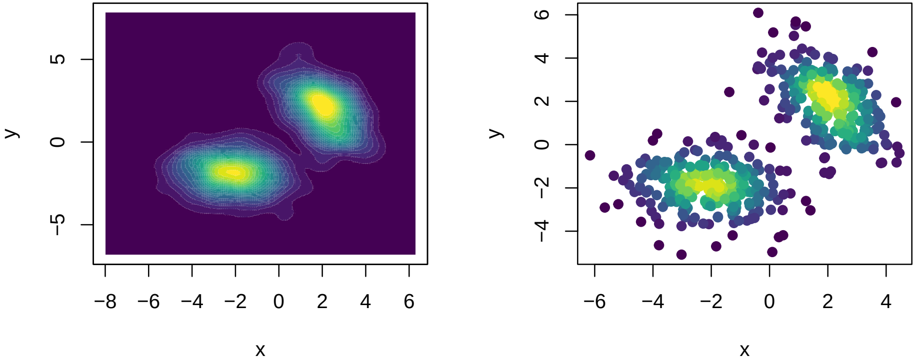
Degrees of smoothing are controlled by h and can be set different along the directions, i.e., under a product kernel, the KDE is

$$\hat{f}_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h_1} K_0\left(\frac{x_1 - X_{i,1}}{h_1}\right) \times \cdots \times \frac{1}{h_d} K_0\left(\frac{x_d - X_{i,d}}{h_d}\right)$$

$\Rightarrow$ if margins are standardized (on the same scale), set $h = h_1 = \ldots = h_d$

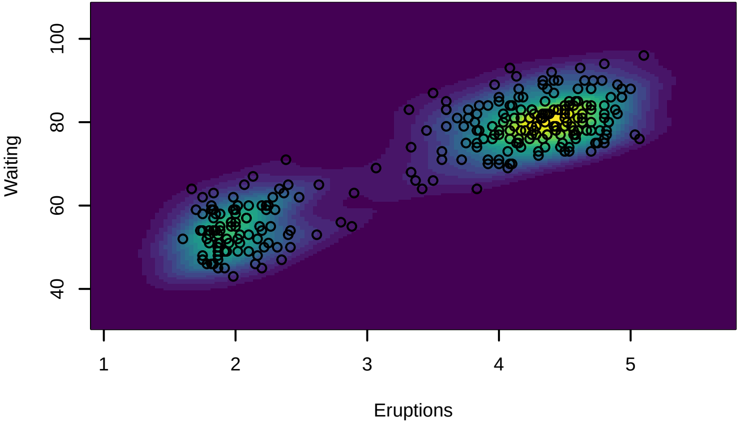
Multivariate KDE

- Mixture of bivariate normal



Multivariate KDE

- Faithful dataset



Curse of dimensionality

- KD estimation is typically restricted to $d = 2$
- Unless sample size is very large, neighbourhoods will be sparsely populated with data points (in higher dimensions)

For instance,

- If you have n data points uniformly distributed on the interval $[0, 1]$, how many data points are there in the interval $[0, 0.1]$?

Around $n/10$

- If you have n data points uniformly distributed on the 10-dimensional unit cube $[0, 1]^{10}$, how many are there in the cube $[0, 0.1]^{10}$?

Around $0.1^{10}n$

$\Rightarrow$ estimation gets harder very quickly as dimension increases

Curse of dimensionality

Under some smoothing conditions on f, the best possible MSE rate (the one obtained with optimal choice of bandwidth) is $O(n^{-4/(d+4)})$. That is, $MSE_{h_{opt}} \approx cn^{-4/(d+4)}$ and $n \approx (c/MSE_{h_{opt}})^{d/4}$

$\Rightarrow$ sample size grows exponentially with dimension

$n^{-4/(d+4)}$	$d=1$	$d=2$	$d=5$
$n=100$	0.025	0.046	0.129
$n=1000$	0.004	0.010	0.046
$n=10000$	6.3×10^{-4}	2.1×10^{-3}	1.6×10^{-2}

Thus, for $d=5$, the rate with $n=10000$ is the same than for $d=2$ with 10 times less data ...

Summary - Overall

Motivation:

1. On Week 2, we introduced the histogram as a data exploratory tool and noticed its limitations
2. Histogram is a poor estimator of density, because it
   - is never smooth and requires a choice of *origin*
3. Today, we introduced naive KDE by generalizing histogram to its *origin*-free version
4. Then, we generalized naive KDE by allowing for better kernels
5. Now we have a decent nonparametric density estimation tool: KDE
   - in exploratory analysis, histograms often overlaid with KDEs

Main takeaways:

7. Asymptotic properties analyzed using Taylor expansions
   - suggest a way to choose *bandwidth*
   - the bias-variance trade-off made explicit
8. Multivariate extension works well in low dimensions

Assignment 2 and Exercise

Go to Assignment 2 for details.

Go to Exercise 2 for details.