MATH5714 Linear Regression, Robustness and Smoothing

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Contents

Preface

From previous modules we know how to fit a regression line through points $(x_1, y_1), \dots, (x_n, y_n) \in \mathbb{R}^2$. The underlying model here is described by the equation

$$y_i = \alpha + \beta x_i + \varepsilon_i$$

for all $i \in \{1, 2, \dots, n\}$, and the aim is to find values for the intercept α and the slope β such that the residuals ε_i are as small as possible. This procedure, linear regression, and its extensions are discussed in the level 3 component of the module.

In the level 5 component of this module, we will discuss "smoothing" which is a technique which can be used when linear models are no longer appropriate for the data. An example of such a situation is illustrated in figure 1.

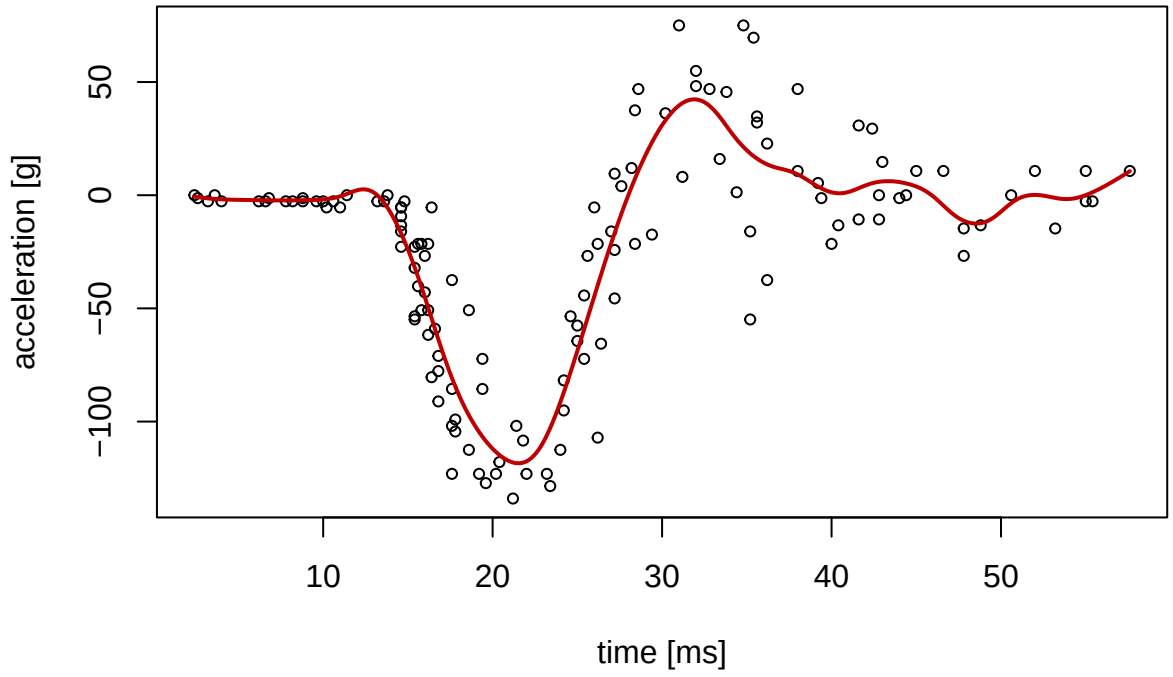


Figure 1: An illustration of a data set where a linear (straight line) model is not appropriate. The data represents a series of measurements of head acceleration in a simulated motorcycle accident, used to test crash helmets (the `mcycle` dataset from the `MASS` R package).

1 Kernel Density Estimation

In this section we discuss the topic of "Kernel Density Estimation". Here we suppose we are given data $x_1, \dots, x_n \in \mathbb{R}^d$ from an unknown probability density, say f. Our objective is to estimate the density f. This section lays the foundations for many of the following topics.

1.1 Histograms

1.1.1 Probability Densities

Before we consider how to estimate a density, let just remember what a density is. A random variable $X \in \mathbb{R}$ has **density** $f \colon \mathbb{R} \to [0, \infty)$ if

$$P(X \in [a, b]) = \int_a^b f(x)\, dx$$

for all $a, b \in \mathbb{R}$ with $a < b$. Densities are sometimes also called "probability densities" or even "probability density functions".

A density f is large in regions where X is very likely to take values, and small in regions where X is less likely to take values. If $f(x) = 0$ for all x in a region, that means that X never takes values there. Graphically, the integral $\int_a^b f(x)\, dx$ can be interpreted as the area under the graph of f. This is illustrated in figure 2.

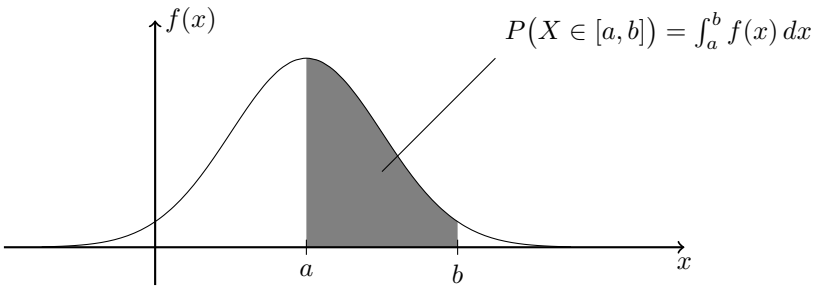


Figure 2: An illustration of how the area under the graph of a density can be interpreted as a probability.

A function f is the density of some random variable X, if and only if $f \geq 0$ and

$$\int_{-\infty}^{\infty} f(x)\, dx = 1.$$

1.1.2 Histograms

In the univariate case, *i.e.* for $d = 1$, a commonly used technique to approximate density of a sample is to plot a histogram. To illustrate this, we use the `faithful` dataset built in R, which contains waiting times between eruptions and the duration of the eruption for the Old Faithful geyser in the Yellowstone National Park. (You can type `help(faithful)` in R to learn more about this data set.) Here we focus on the waiting times only. A simple histogram for this dataset is shown in figure 3.

```
x <- faithful$waiting
hist(x, probability = TRUE,
     main = NULL, xlab = "time between eruptions [mins]")
```

The histograms splits the range of the data into "buckets", and for every bucket $[a, b]$ it shows a bar where the height is proportional the number of samples in the bucket. I am ignoring the case that a sample may fall exactly on the boundary between two buckets here; in reality all but one buckets need to be half-open intervals, for example $[40, 45]$, $(45, 50]$, ..., $(95, 100]$.

As we have seen, the area under the graph of the density f over the interval $[a, b]$ corresponds to the probability $P(X \in [a, b])$. For the histogram to approximate the density, we need to scale the height

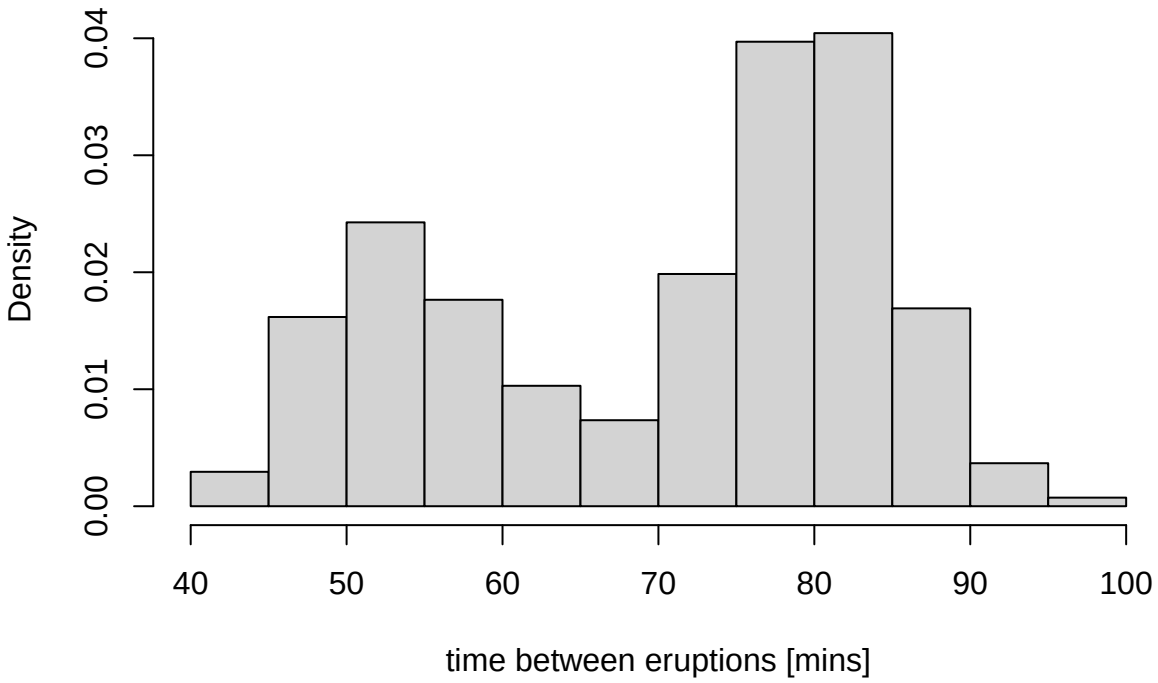


Figure 3: This figure shows how a histogram can be used to approximate a probability density. From the plot one can see that the density of the waiting times distribution seems to be bi-modal with peaks around 53 and 80 minutes.

$h_{a,b}$ of the bucket $[a, b]$ so that the area in the histogram is also close to this probability. Since we don't know the probability $P(X \in [a, b])$ exactly, we have to approximate it as

$$P(X \in [a, b]) \approx \frac{n_{a,b}}{n},$$

where $n_{a,b}$ is the number of samples in the bucket $[a, b]$, and n is the total number of samples. So we need

$$\begin{aligned}(b-a) \cdot h_{a,b} &= \text{area of the histogram bar} \\ &\approx \text{area of the density} \\ &= P(X \in [a, b]) \\ &\approx \frac{n_{a,b}}{n}.\end{aligned}$$

and thus we choose

$$h_{a,b} = \frac{1}{(b-a)n} n_{a,b}.$$

As expected, the height of the bar for the bucket $[a, b]$ is proportional to the number $n_{a,b}$ of samples in the bucket.

1.1.3 Choice of Buckets

Histograms are only meaningful if the buckets are chosen well. If the buckets are too large, not much of the structure of f can be resolved. If the buckets are too small, the estimate $P(X \in [a, b]) \approx n_{a,b}/n$ will be poor and the histogram will no longer resemble the shape of f. This

```
set.seed(1)
x <- rnorm(50)
hist(x, probability = TRUE, main = NULL,
     breaks = seq(-2.5, 2.5, length.out = 500))
```

Finally, even if reasonable bucket sizes are chosen, the result can depend quite strongly on the exact locations of these buckets. To illustrate this effect, we consider a (dataset about the annual amount

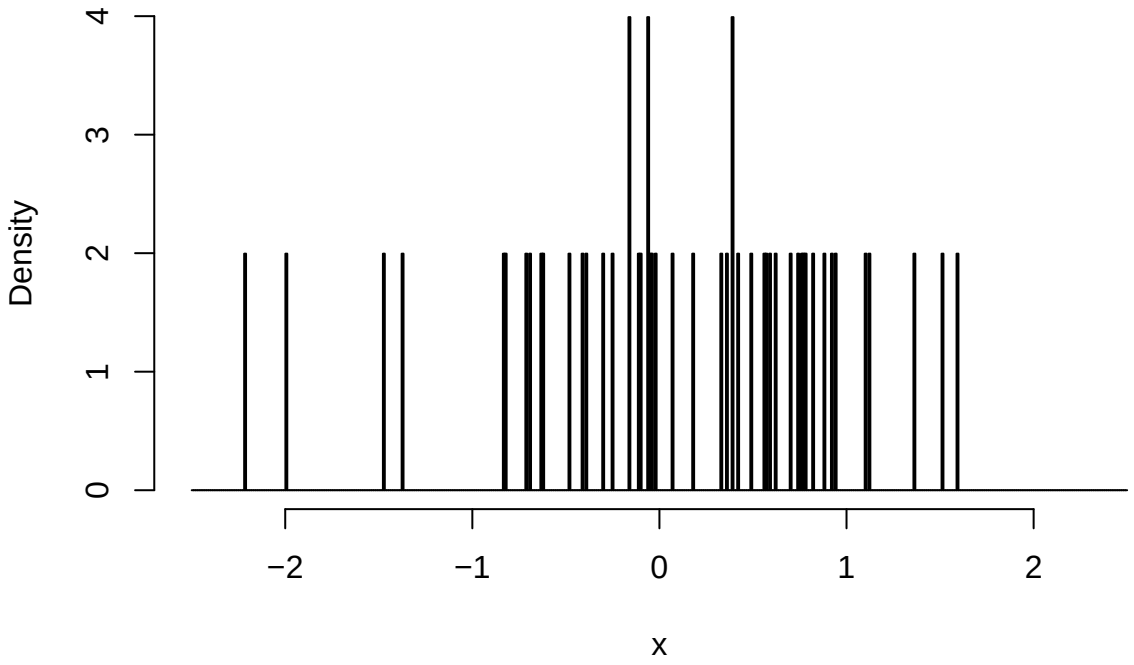


Figure 4: This figure shows how a histogram can be used to approximate a probability density. From the plot one can see that the density of the waiting times distribution seems to be bi-modal with peaks around 53 and 80 minutes.

of snow)[https://teaching.seehuhn.de/data/buffalo/] falling in Buffalo, New York for different years. Figures 5 and 6 show that same data in two different ways, allowing to come to different conclusions about the distribution.

```
# downloaded from https://teaching.seehuhn.de/data/buffalo/
x <- read.csv("data/buffalo.csv")
snowfall <- x$snowfall
hist(snowfall, probability = TRUE,
     breaks = seq(24.30, 208.22, length.out = 20),
     main = NULL, xlab = "snowfall [in]")
```

```
hist(snowfall, probability = TRUE,
     breaks = seq(22.85, 204.92, length.out = 20),
     main = NULL, xlab = "snowfall [in]")
```

As a further illustration of the effect of bucket width, the code in figure 7 shows how histograms with different bucket widths can be generated in R. Here we simply specify numeric values for the `break` argument to `hist()`, which R uses as the *approximate* number of buckets in the plot.

```
par(mfrow = c(2,2))

for (breaks in c(80, 40, 20, 10)) {
  hist(snowfall,
       prob = TRUE,
       breaks = breaks,
       xlim = c(25,200),
       ylim = c(0, 0.03),
       xlab = paste("breaks =", breaks),
       main = NULL)
}
```

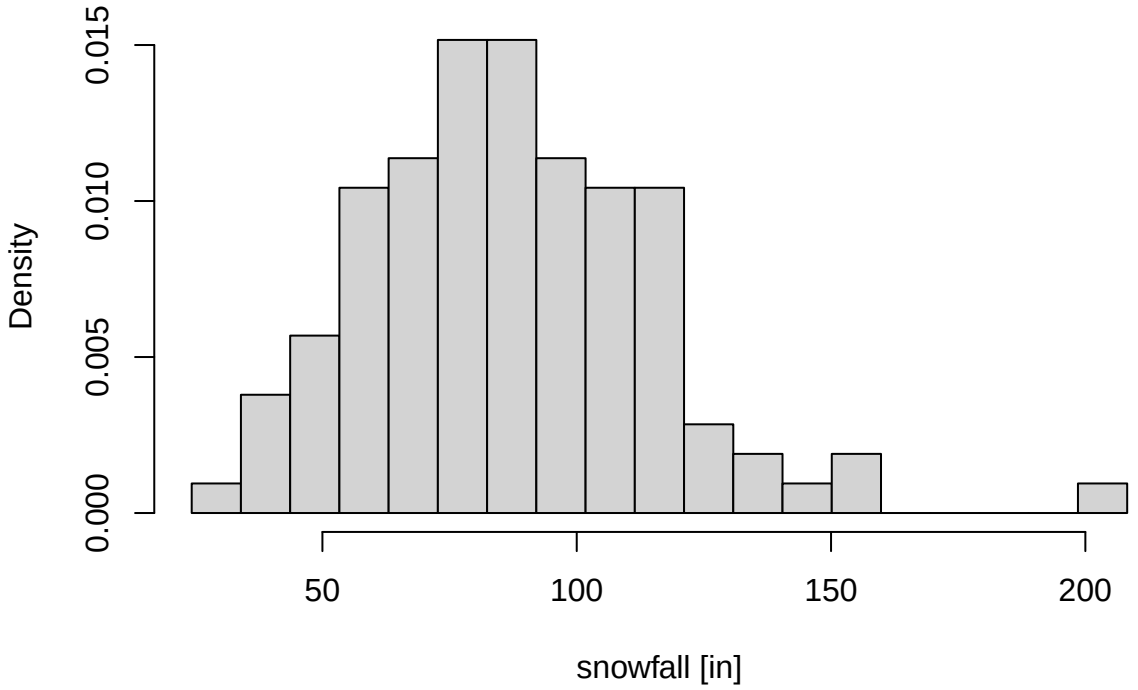


Figure 5: The annual amount of snowfall in Buffalo, New York, in inches. The histogram makes it plausible that there is one main peak in the distribution.

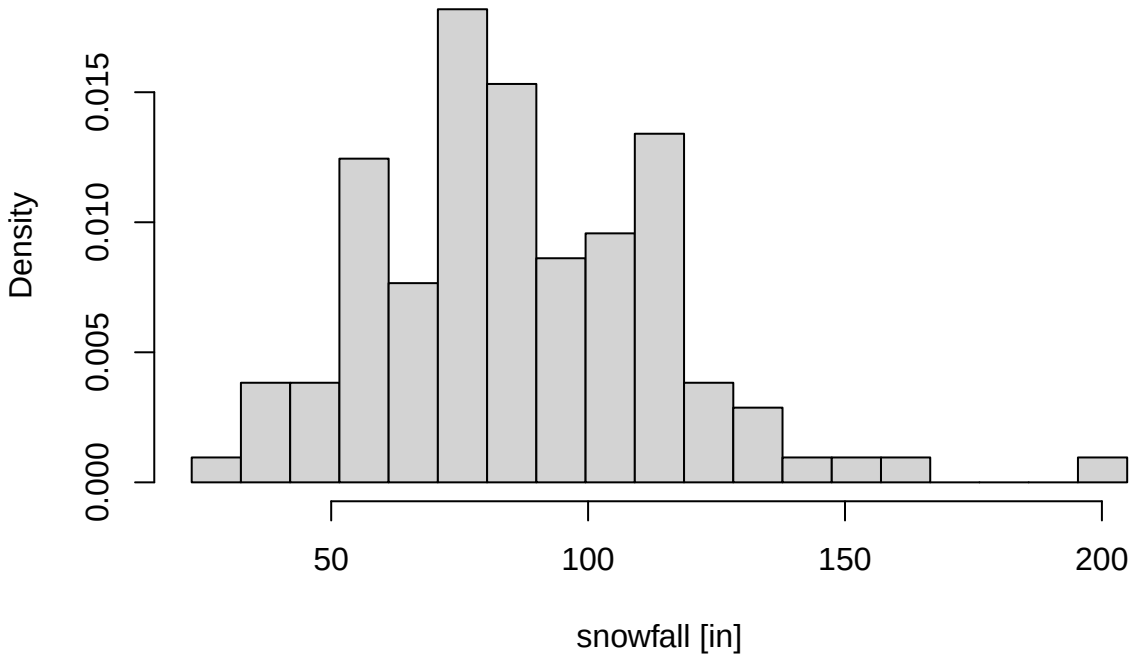


Figure 6: Continued from 5, this histogram shows the dataset in a way that three peaks are visible.

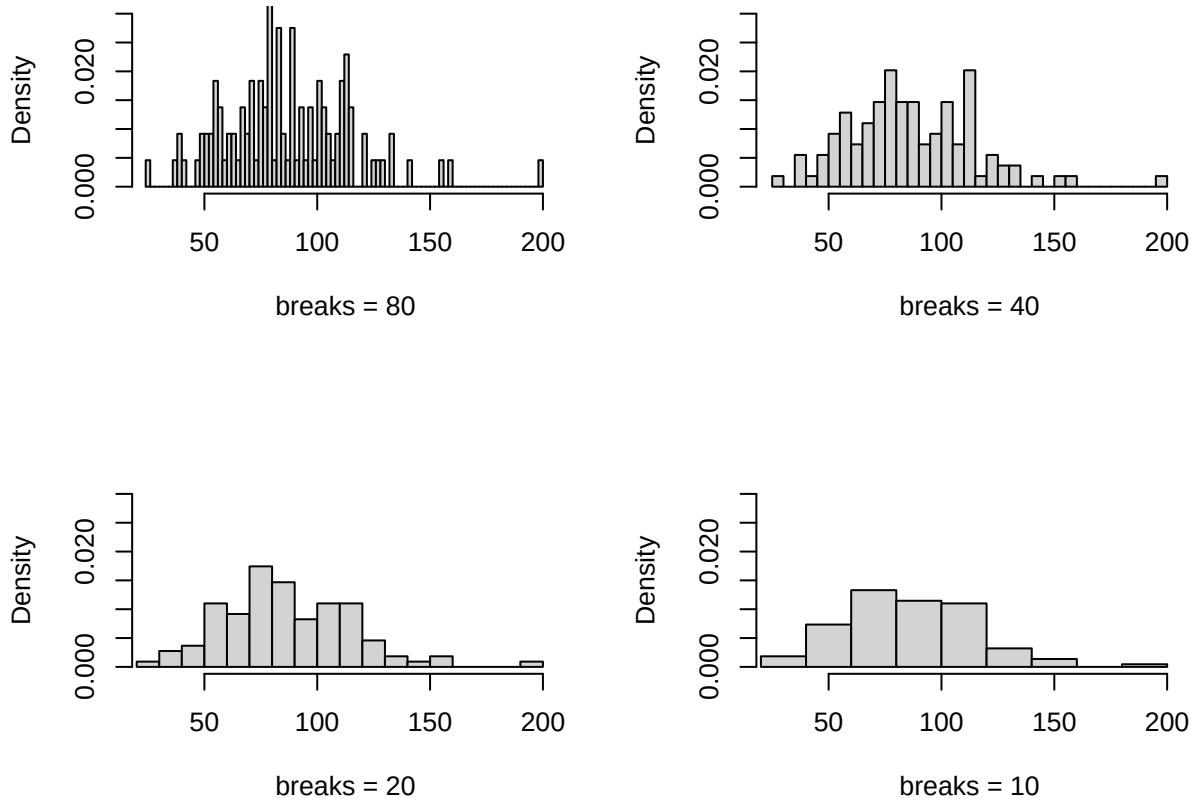


Figure 7: This figure illustrates how the bucket size in a histogram can be controlled in R.

1.2 Kernel Density Estimation

Kernel density estimation allows to estimate the density f for given data while avoiding some of the disadvantages of histograms. Again, we suppose that we are given data $x_1, \dots, x_n \in \mathbb{R}$ and that we want to estimate the density f.

1.2.1 Motivation

Similar to the argument in the previous subsection, for x in a "small" interval $[a, b]$ we can estimate $f(x)$ as

$$f(x) \approx \frac{1}{b-a} \int_a^b f(y)\, dy = \frac{1}{b-a} P(X \in [a, b]) \approx \frac{1}{b-a} \frac{n_{a,b}}{n},$$

where $n_{a,b}$ denotes the number of samples in the interval $[a, b]$. This equation contains two approximation. The first one, $f(x) \approx 1/(ba) \int_a^b f(y)\, dy$, is more accurate if the interval is small, because then f will be nearly constant over the interval. The second approximation will be more accurate if the interval is large, because then the interval $[a, b]$ covers more samples and the estimate of the probability is based on more data. We will later discuss in detail how these two concerns can be optimally balanced.

A mathematical "trick" to write more clearly how $n_{a,b}$ depends on the data is to write the value as

$$n_{a,b} = \sum_{i=1}^{n} I_{[a,b]}(x_i),$$

where

$$I_{[a,b]}(x) = \begin{cases} 1 & \text{if } x \in [a, b], \text{ and} \\ 0 & \text{otherwise.} \end{cases}$$

The function $I_{[a,b]}$ is called the **indicator function** of the set $[a, b]$.

Using the indicator function notation, the estimate for $f(x)$ can be written as

$$f(x) \approx \frac{1}{n(b-a)} n_{a,b} = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{b-a} I_{[a,b]}(x_i)$$

whenever $x \in [a, b]$ and when $b - a$ is "not too large and not too small". For symmetry we choose the interval $[a, b]$ centred around x, say $[a, b] = [x - h, x + h]$ where h can be chosen to control the width of the interval. In this case we have $b - a = x + h - x + h = 2h$ and thus

$$\begin{aligned} f(x) &\approx \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2h} I_{[x-h,x+h]}(x_i) \\ &= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2h} I_{[-h,+h]}(x_i - x) \\ &= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2h} I_{[-1,+1]}\Big(\frac{x_i - x}{h}\Big) \end{aligned}$$

for all $x \in \mathbb{R}$. This is an example of a kernel density estimate. The function $K(x) = 1/2\, I_{[-1,+1]}(x)$ on the right-hand side is called the kernel of the estimate, and the parameter h is called the **bandwidth** or the smoothing parameter.

1.2.2 Definition of a Kernel Density Estimator

The general kernel density estimate is a generalisation of the idea from the previous subsection. We first define the class of functions which we use to replace the function $1/2\, I_{[-1,+1]}$.

Definition 1.1. A **kernel** is a function $K \colon \mathbb{R} \to \mathbb{R}$ such that

- $\int_{-\infty}^{\infty} K(x)\, dx = 1$,
- $K(x) = K(-x)$ (i.e. K is *symmetric*) and
- $K(x) \geq 0$ (i.e. K is *positive*) for all $x \in \mathbb{R}$.

Of these three properties, the first one is the most important one. The second condition, symmetry, ensures that K is centred around 0 and the third definition, positivity, makes K a probability density. (While most authors list all three properties shown above, sometimes the third condition is omitted.)

It is easy to check that $K(x) = 1/2\, I_{[-1,+1]}(x)$ satisfies all three conditions of definition 1.1. This function K is sometimes called the "uniform kernel", because it is the density of the uniform distribution $\mathcal{U}[-1, +1]$.

Based on the concept of a kernel, we now can define what a Kernel Density Estimate is.

Definition 1.2. For a kernel K, bandwidth $h > 0$ and $x \in \mathbb{R}$, the **kernel density estimate** for $f(x)$ is given by

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^{n} K_h(x - x_i),$$

where K_h is given by

$$K_h(y) = \frac{1}{h} K(y/h)$$

for all $y \in \mathbb{R}$.

For $K(x) = 1/2\, I_{[-1,+1]}(x)$ this definition recovers the approximation we discussed in the previous section. In later sections we will see how the kernel K can be chosen for the estimator $\hat{f}$ to have "good" properties. As a simple example we note that if K is continuous, then the rescaled kernel K_h and thus also the estimate f_h are continuous functions.

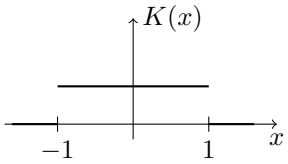
Similar to the bucket width in histograms, the bandwidth parameter h controls how smooth the density estimate $\hat{f}_h$ is, as a function of x.

1.2.3 Kernels

There are many different kernels in use. Some examples are listed below. A more exhautive list can, for example, be found on Wikipedia.

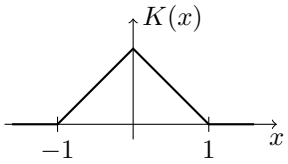
1.2.3.1 Uniform Kernel

$$K(x) = \begin{cases} 1/2 & \text{if } -1 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}$$



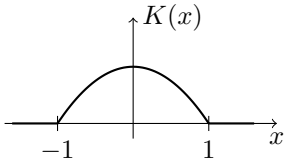
1.2.3.2 Triangular Kernel

$$K(x) = \begin{cases} 1 - |x| & \text{if } -1 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}$$



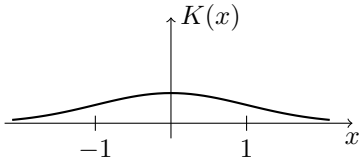
1.2.3.3 Epanechnikov Kernel

$$K(x) = \begin{cases} \frac{3}{4}(1 - x^2) & \text{if } -1 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}$$



1.2.3.4 Gaussian Kernel

$$K(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$$



1.3 Kernel Density Estimation in R

Kernel density estimates can be computed in R using the built-in `density()` function. If `x` is a vector containing the data, then `density(x)` computes a basic kernel density estimate, using the Gaussian kernel. The function has a number of optional arguments, which can be used to control details of the estimate:

- `bw = ...` can be used to control the bandwidth h. If no numeric value is given, a heuristic is used. Note that for some kernels, `bw` differs from our h by a constant factor. The value `bw=1` always corresponds to the case where the probability distribution with density K_h has variance 1.
- `kernel = ...` can be used to choose the kernel. Choices incluse `"rectangular"` (the uniform kernel), `"triangular"`, `"epanechnikov"` and `"gaussian"`.

Details about how to call `density()` can be found by using the command `help(density)` in R.

The return value of `density` is an R object which contains information about the kernel density estimate.

```
m <- density(snowfall)
str(m)
```

```
## List of 7
##  $ x         : num [1:512] -4.17 -3.72 -3.26 -2.81 -2.35 ...
##  $ y         : num [1:512] 4.32e-06 4.98e-06 5.73e-06 6.56e-06 7.48e-06 ...
##  $ bw        : num 9.72
##  $ n         : int 109
##  $ call      : language density.default(x = snowfall)
##  $ data.name: chr "snowfall"
##  $ has.na    : logi FALSE
##  - attr(*, "class")= chr "density"
```

The field `$x` and `$y` contain the x and y coordinates, respectively, of points on the $x \mapsto \widehat{f}_h(x)$ curve, which approximates f. The field `$bw` shows the numeric value for the bandwidth chosen by the heuristic. The returned object can also directly be used as an argument to `plot()` and `lines()`, to add the graph of $\widehat{f}_h$ to a plot. The commands in figure 8 show how the command `density()` can be used and illustrate the effect of the bandwidth parameter.

```
par(mfrow = c(2,2))

for (bw in c(1, 2, 4, 8)) {
  plot(density(snowfall, bw = bw, kernel = "triangular", n = 1000),
    xlim = c(25,200),
    ylim = c(0, 0.03),
    xlab = paste("bandwidth =", bw),
    main = NA)
}
```

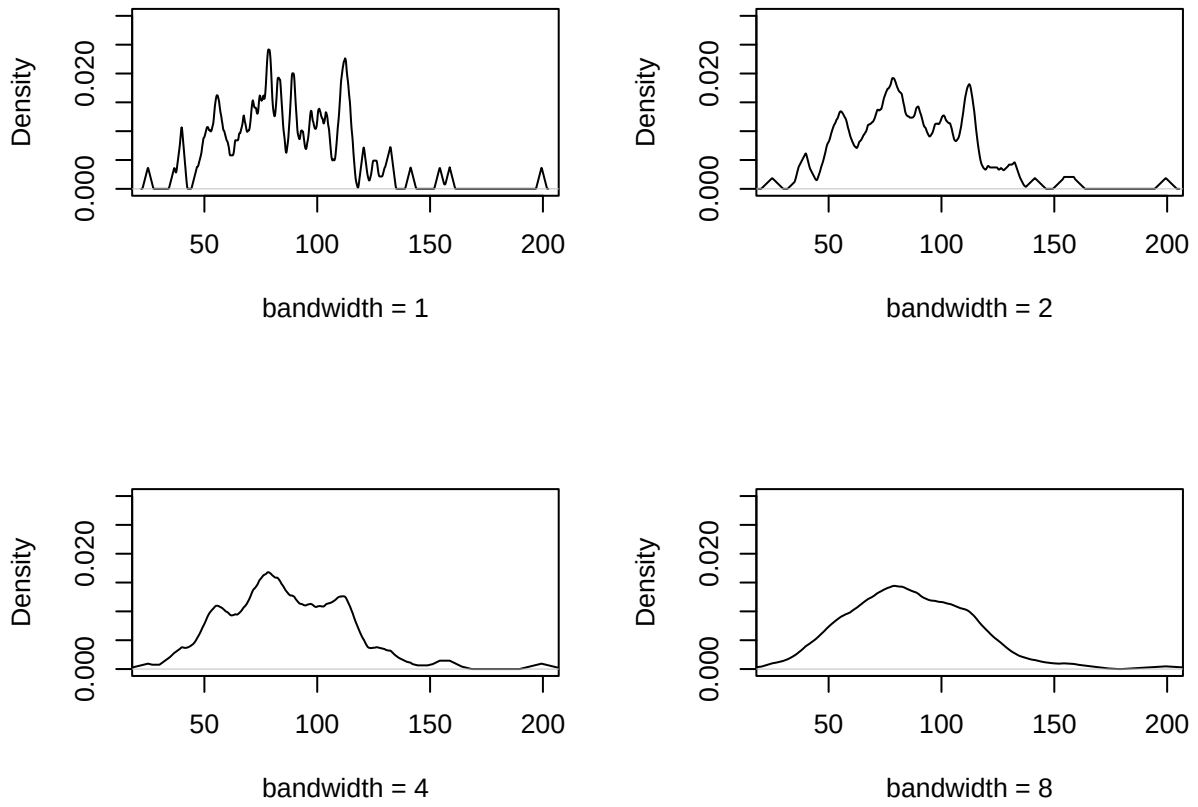


Figure 8: This figure illustrates how the bandwidth of a kernel density estimate can be controlled in R.

Summary

- Histograms can be scaled so that they approximate densities.
- Some care is needed when choosing buckets for a histogram.
- Kernel density estimates can be used to estimate densities from data.
- A variety of different kernel functions are commonly used.

2 The Bias of Kernel Density Estimates

In the previous section we introduced the kernel density estimate

$$\hat{f}_h(x) = \frac{1}{n}\sum_{i=1}^{n} K_h(x - x_i) \tag{1}$$

for estimating the density f, and we argued that $\hat{f}_h(x) \approx f(x)$. The aim of the current section is to quantify the error of this approximation and to understand how this error depends on the true density f and on the bandwidth $h > 0$.

2.1 A Statistical Model

As usual, we will make a statistical model for the data $x_1, \dots, x_n$, and then use this model to analyse how well the estimator performs. The statistical model we will consider here is extremely simple: we model the x_i using random variables

$$X_1, \dots, X_n \sim f, \tag{2}$$

which we assume to be independent and identically distributed (i.i.d.). Here, the notation $X \sim f$, where f is a probability density, simply denotes that the random variable X has density f.

It is important to not confuse x (the point where we are evaluating the densities during our analysis) with the data x_i. A statistical model describes the data, so here we get random variables $X_1, \dots, x_n$ to describe the behaviour of $x_1, \dots, x_n$, but it does not descibe x. The number x is not part of the data, so will never be modelled by a random variable.

While the model is very simple, for example it is much simpler than the model we use in the level 3 part of the module for linear regression, the associated parameter estimation problem is more challenging. The only "parameter" in this model is the function $f\colon \mathbb{R} \to \mathbb{R}$ instead of just a vector of numbers. The space of all possible density functions f is infinite dimensional, so this is a more challenging estimation problem then the one we consider, for example, for linear regression. Since f is not a "parameter" in the usual sense, sometimes this problem is called a "non-parametric" estimation problem.

Our estimate for the density f is the function $\hat{f}_h\colon \mathbb{R} \to \mathbb{R}$, where $\hat{f}_h(x)$ is given by (1) for every $x \in \mathbb{R}$.

2.2 The Bias of the Estimate

As ususal, the **bias** of our estimate is the difference between what the estimator gives on average and the truth. For our estimation problem we get

$$\operatorname{bias}(\hat{f}_h(x)) = \mathbb{E}(\hat{f}_h(x)) - f(x).$$

The expectation on the right-hand side averages over the randomness in the data, by using $X_1, \dots, X_n$ from the model in place of the data.

Substituting in the definition of $\hat{f}_h(x)$ from equation (1) we find

$$\begin{aligned}\mathbb{E}(\hat{f}_h(x)) &= \mathbb{E}\Big(\frac{1}{n}\sum_{i=1}^{n} K_h(x - X_i)\Big) \\ &= \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}(K_h(x - X_i))\end{aligned}$$

and since the X_i are identically distributed, we can replace all X_i with X_1 (or any other of them) to get

$$\begin{aligned}\mathbb{E}(\hat{f}_h(x)) &= \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}(K_h(x - X_1)) \\ &= \frac{1}{n} n\, \mathbb{E}(K_h(x - X_1)) \\ &= \mathbb{E}(K_h(x - X_1)).\end{aligned}$$

Since the model assumes X_1 (and all the other X_i) to have density f, we can write this expectation as an integral to get

$$\begin{aligned}\mathbb{E}(\hat{f}_h(x)) &= \int_{-\infty}^{\infty} K_h(x-y)\, f(y)\, dy \\ &= \int_{-\infty}^{\infty} f(y)\, K_h(y-x)\, dy \\ &= \int_{-\infty}^{\infty} f(z+x)\, K_h(z)\, dz\end{aligned}$$

where we used the symmetry of K_h and the substitution $z = y - x$.

2.3 Moments of Kernels

To understand how the bias changes as h varies, we will need to consider properties of K and K_h in more detail.

Definition 2.1. The kth **moment** of a kernel K, for $k \in \mathbb{N}_0 = \{0, 1, 2, ...\}$, is given by

$$\mu_k(K) = \int_{-\infty}^{\infty} x^k K(x)\, dx.$$

The second moment μ_2 is sometimes also called the *variance* of the kernel K.

Using the properties of K, we find the following results:

- Since $x^0 = 1$ for all $x \in \mathbb{R}$, the 0th moment is $\mu_0(K) = \int_{-\infty}^{\infty} K(x)\, dx = 1$ for every kernel K.
- Since K is symmetric, the function $x \mapsto xK(x)$ is antisymmetric and we have

  $$\mu_1(K) = \int_{-\infty}^{\infty} xK(x)\, dx = 0$$

  for every kernel K.

The moments of the rescaled kernel K_h, given by

$$K_h(x-y) = \frac{1}{h} K\Big(\frac{x-y}{h}\Big),$$

can be computed from the moments of K.

Lemma 2.1. *Let K be a kernel, $k \in \mathbb{N}_0$ and $h > 0$. Then*

$$\mu_k(K_h) = h^k \mu_k(K).$$

Proof. We have

$$\begin{aligned}\mu_k(K_h) &= \int_{-\infty}^{\infty} x^k K_h(x)\, dx \\ &= \int_{-\infty}^{\infty} x^k \frac{1}{h} K\Big(\frac{x}{h}\Big)\, dx.\end{aligned}$$

Using the substitution $y = x/h$ we find

$$\begin{aligned}\mu_k(K_h) &= \int_{-\infty}^{\infty} (hy)^k \frac{1}{h} K(y)\, h\, dy \\ &= h^k \int_{-\infty}^{\infty} y^k K(y)\, dy \\ &= h^k \mu_k(K).\end{aligned}$$

This completes the proof. □

It is easy to check that if K is a kernel, then K_h is also a kernel which implies that K_h is a probability density. If Y is a random variable with density K_h, written as $Y \sim K_h$ in short, then we find

$$\mathbb{E}(Y) = \int y K_h(y)\, dy = \mu_1(K_h) = 0$$

and

$$\mathrm{Var}(Y) = \mathbb{E}(Y^2) = \int y^2 K_h(y)\, dy = \mu_2(K_h) = h^2\, \mu_2(K). \tag{3}$$

Thus, Y is centred and the variance of Y is proportional to h^2.

2.4 The Bias for Small Bandwidth

Considering again the formula

$$\mathbb{E}(\hat{f}_h(x)) = \int_{-\infty}^{\infty} f(x+y)\, K_h(y)\, dy,$$

we see that we can interpret this integral as an expectation with respect to a random variable $Y \sim K_h$:

$$\mathbb{E}(\hat{f}_h(x)) = \mathbb{E}(f(x+Y)). \tag{4}$$

Equation (3) shows that for $h \downarrow 0$ the random variable concentrates more and more around 0 and thus $x+Y$ concentrates more and more around x. For this reason we expect $\mathbb{E}(\hat{f}_h(x)) \approx f(x)$ for small h.

To get a more qualitative version of this argument, we consider the Taylor approximation of f around the point x:

$$f(x+y) \approx f(x) + y f'(x) + \frac{y^2}{2} f''(x).$$

Substituting this into equation (4) we find

$$\begin{aligned}
\mathbb{E}(\hat{f}_h(x)) &\approx \mathbb{E}\Big(f(x) + Y f'(x) + \frac{Y^2}{2} f''(x)\Big) \\
&= f(x) + \mathbb{E}(Y) f'(x) + \frac{1}{2}\mathbb{E}(Y^2) f''(x) \\
&= f(x) + \frac{1}{2} h^2 \mu_2(K) f''(x)
\end{aligned}$$

for small h. Considering the bias again, this gives

$$\mathrm{bias}(\hat{f}_h(x)) = \mathbb{E}(\hat{f}_h(x)) - f(x) \approx \frac{\mu_2(K) f''(x)}{2} h^2 \tag{5}$$

which shows that the bias of the estimator descreases quadratically as h gets smaller.

In contrast, we will see in the next section that the variance of the estimator *increases* as $h \downarrow 0$. We will need to balance these two effects to find the optimal value of h.

Summary

- We have introduced a statistical model for density estimation.
- The bias for kernel density estimation can be written as an integral.
- We learned how the moments of a kernel are defined.
- The bias for small bandwidth depends on the second moment of the kernel and the second derivative of the density.

3 The Variance of Kernel Density Estimates

In the previous section we considered the bias of the estimator

$$\hat{f}_h(x) = \frac{1}{n}\sum_{i=1}^{n} K_h(x - x_i).$$

We found

$$\mathbb{E}(\hat{f}_h(x)) = \mathbb{E}(K_h(x - X_i)) \tag{6}$$

for all $i \in \{1, \dots, n\}$ (we used $i = 1$), and we used this relation to compute the bias. In this section, we will use similar arguments to compute the variance and the mean squared error of the estimator.

3.1 Variance

We use the formula

$$\mathrm{Var}(\hat{f}_h(x)) = \mathbb{E}(\hat{f}_h(x)^2) - \mathbb{E}(\hat{f}_h(x))^2$$

and consider the two terms separately.

3.1.1 Second Moment

For the second moment term in the definition of the variance we get

$$\begin{aligned}
\mathbb{E}(\hat{f}_h(x)^2) &= \mathbb{E}\Big(\frac{1}{n}\sum_{i=1}^{n} K_h(x - X_i)\frac{1}{n}\sum_{j=1}^{n} K_h(x - X_j)\Big) \\
&= \frac{1}{n^2}\mathbb{E}\Big(\sum_{i,j=1}^{n} K_h(x - X_i)K_h(x - X_j)\Big) \\
&= \frac{1}{n^2}\sum_{i,j=1}^{n} \mathbb{E}\Big(K_h(x - X_i)K_h(x - X_j)\Big)
\end{aligned}$$

Since the X_i are independent, the values of i and j in this sum do not matter. For the n terms where $i = j$ we can assume that both indices equal 1, and for the $n(n-1)$ terms where $i \neq j$ we can assume $i = 1$ and $j = 2$, without changing the value of the expectation. So we get

$$\begin{aligned}
\mathbb{E}(\hat{f}_h(x)^2) &= \frac{1}{n^2}\Big(n\mathbb{E}(K_h(x - X_1)^2) + n(n-1)\mathbb{E}(K_h(x - X_1)K_h(x - X_2))\Big) \\
&= \frac{1}{n^2}\Big(n\mathbb{E}(K_h(x - X_1)^2) + n(n-1)\mathbb{E}(K_h(x - X_1))\mathbb{E}(K_h(x - X_2))\Big) \\
&= \frac{1}{n^2}\Big(n\mathbb{E}(K_h(x - X_1)^2) + n(n-1)\mathbb{E}(K_h(x - X_1))^2\Big) \\
&= \frac{1}{n}\mathbb{E}\Big(K_h(x - X_1)^2\Big) + \frac{n-1}{n}\mathbb{E}(\hat{f}_h(x))^2,
\end{aligned}$$

where we used equation (6) for the last term. Using this equation, we can write the expectation as

$$\begin{aligned}
\mathrm{Var}(\hat{f}_h(x)) &= \mathbb{E}(\hat{f}_h(x)^2) - \mathbb{E}(\hat{f}_h(x))^2 \\
&= \frac{1}{n}\mathbb{E}(K_h(x - X_1)^2) + \Big(\frac{n-1}{n} - 1\Big)\mathbb{E}(\hat{f}_h(x))^2.
\end{aligned}$$

Since $(n-1)/n - 1 = -1/n$ we get

$$\mathrm{Var}(\hat{f}_h(x)) = \frac{1}{n}\Big(\mathbb{E}(K_h(x - X_1)^2) - \mathbb{E}(\hat{f}_h(x))^2\Big). \tag{7}$$

3.1.2 The Roughness of a Kernel

Similar to what we did in the last section, we will use Taylor expansion of f around the point x to understand the behaviour of the variance for small h. Some more care is needed here, because this time

the result also depends on the sample size n and we will consider the joint limit of $n \to \infty$ and $h \to 0$. For the first term in equation (7) we find

$$\begin{aligned}\mathbb{E}(K_h(x - X_1)^2) &= \int K_h(x-y)^2 f(y)\, dy \\ &= \int K_h(y-x)^2 f(y)\, dy \\ &= \int \frac{1}{h^2} K\Big(\frac{y-x}{h}\Big)^2 f(y)\, dy.\end{aligned}$$

Now we use the substitution $z = (y - x)/h$. This gives

$$\mathbb{E}(K_h(x - X_1)^2) = \int \frac{1}{h^2} K(z)^2 f(x + hz)\, h\, dz$$

Finally, we use Taylor approximation to get

$$\begin{aligned}\mathbb{E}(K_h(x - X_1)^2) &\approx \int \frac{1}{h} K(z)^2 \Big(f(x) + hz\, f'(x) + \frac{1}{2}h^2 z^2\, f''(x)\Big)\, dz \\ &= \frac{1}{h} f(x) \int K(z)^2\, dz + f'(x) \int zK(z)^2\, dz + \frac{1}{2} h f''(x) \int z^2 K(z)^2\, dz \\ &= \frac{1}{h} f(x) \int K(z)^2\, dz + \frac{1}{2} h f''(x) \int z^2 K(z)^2\, dz\end{aligned}$$

where the first-order term disappears since $z \mapsto zK(z)^2$ is an asymmetric function. As a shorthand we use the following definition.

Definition 3.1. The **roughness** of a kernel K is given by

$$R(K) := \int_{-\infty}^{\infty} K(x)^2\, dx.$$

This gives the result

$$\mathbb{E}(K_h(x - X_1)^2) \approx \frac{1}{h} f(x) R(K) + \frac{1}{2} h f''(x) \int z^2 K(z)^2\, dz \tag{8}$$

for small h.

3.1.3 The Variance for Small Bandwidth

Here we consider the term $\mathbb{E}(\hat{f}_h(x))^2$ in the formula for the variance. From the previous section we know

$$\mathbb{E}(\hat{f}_h(x)) \approx f(x) + \frac{1}{2} h^2 \mu_2(K) f''(x)$$

and thus we get

$$\mathbb{E}(\hat{f}_h(x))^2 \approx f(x)^2 + h^2 \mu_2(K) f(x) f''(x) + \frac{1}{4} h^4 \mu_2(K)^2 f''(x)^2 \tag{9}$$

for small h.

Substituting (8) and (9) into equation (7) we finally find

$$\mathrm{Var}(\hat{f}_h(x)) = \frac{1}{n}\Big(\frac{1}{h} f(x) R(K) - f(x)^2 + \cdots\Big),$$

where all the omitted terms go to zero as $h \downarrow 0$. Omitting one more term and keeping only the leading term we find

$$\mathrm{Var}(\hat{f}_h(x)) \approx \frac{1}{nh} f(x) R(K) \tag{10}$$

as $h \downarrow 0$.

3.2 Mean Squared Error

The Mean Squared Error of the estimator $\hat{f}_h(x)$ for $f(x)$ is given by

$$\mathrm{MSE}(\hat{f}_h(x)) = \mathbb{E}\Big((\hat{f}_h(x) - f(x))^2\Big).$$

It is an easy exercise to show that this can equivalently be written as

$$\mathrm{MSE}(\hat{f}_h(x)) = \mathrm{Var}(\hat{f}_h(x)) + \mathrm{bias}(\hat{f}_h(x))^2.$$

Substituing equations (5) and (10) into the formula for the MSE, we get

$$\mathrm{MSE}(\hat{f}_h(x)) \approx \frac{1}{nh} f(x)R(K) + \frac{1}{4}\mu_2(K)^2 f''(x)^2 h^4. \tag{11}$$

Some care is needed to make sure that the omitted terms from the Taylor approximations really don't make a significant contribution in this formula for the MSE: The additional contributions from the variance have the form $e_1(h)/n$, where the error term e_1 does not depend on n and is negligible compared to $f(x)R(K)/h$ as $h \downarrow 0$. Using little-o notation, This is sometimes denoted by $e_1(h) = o(1/h)$, which indicates that $e_1(h)/(1/h) \to 0$ as $h \downarrow 0$. The additional terms from the squared bias, say $e_2(h)$, do not depend on n and are negligible compared to $\mu_2(K)^2 f''(x)^2 h^4$. We can write $e_2(h) = o(h^4)$ as $n \downarrow 0$, to reflect this fact. We can summarise these results as

$$\mathrm{MSE}(\hat{f}_h(x)) = \frac{1}{nh} f(x)R(K) + \frac{1}{4}\mu_2(K)^2 f''(x)^2 h^4 + o(1/nh) + o(h^4)$$

as $h \downarrow 0$, with the understanding that the constants in the definition of $o(h^4)$ do not depend on n and that $o(1/nh)$ really means "$o(1/h)$, where the constants are proportional to $1/n$."

3.3 Optimal Bandwidth

The two terms on the right-hand side of (11) are balanced in that the first term decreases for large h while the second term decreases for small h. By taking derivatives with respect to h, we can find the optimal value of h. Ignoring the higher order terms, we get

$$\frac{\partial}{\partial h}\mathrm{MSE}(\hat{f}_h(x)) = -\frac{1}{nh^2} f(x)R(K) + \mu_2(K)^2 f''(x)^2 h^3$$

and thus the derivative equals zero, if

$$\frac{1}{nh^2} f(x)R(K) = \mu_2(K)^2 f''(x)^2 h^3$$

or, equivalently,

$$h = h_{\mathrm{opt}} := \Big(\frac{f(x)R(K)}{n\mu_2(K)^2 f''(x)^2}\Big)^{1/5}.$$

It is easy to check that this h corresponds to the minimum of the MSE. This shows how the optimal bandwidth depends both on the kernel and on the target density f. In practice, this formula is hard to use, since f'' is unknown. (We don't even know f!)

Substituting the optimal value of h back into equation (11), we get

$$\begin{aligned}\mathrm{MSE}_{\mathrm{opt}} &= \frac{1}{n} f(x)R(K)\Big(\frac{n\mu_2(K)^2 f''(x)^2}{f(x)R(K)}\Big)^{1/5} + \frac{1}{4}\mu_2(K)^2 f''(x)^2\Big(\frac{f(x)R(K)}{n\mu_2(K)^2 f''(x)^2}\Big)^{4/5} \\ &= \frac{5}{4}\,\frac{1}{n^{4/5}}\,\Big(R(K)^2\mu_2(K)\Big)^{2/5}\,\Big(f(x)^2|f''(x)|\Big)^{2/5}.\end{aligned}$$

This expression clearly shows the contribution of n, K and f:

- If the bandwidth is chosen optimally, as n increases the bandwidth h decreases proportionally to $1/n^{1/5}$ and the MSE decreases proportionally to $1/n^{4/5}$. For comparison, in a Monte Carlo estimate for an expectation, the MSE decreases proportionally to $1/n$. The error in kernel density estimation decreases slightly slower than for Monte Carlo estimates.

- The error is proportional to $\left(R(K)^2\mu_2(K)\right)^{2/5}$. Thus we should use kernels where the value $R(K)^2\mu_2(K)$ is small.
- The error is proportional to $f(x)^2|f''(x)|$. We cannot influence this term, but we can see that x where f is large or has high curvature have higher estimation error.

Summary

- We found the variance of the kernel density estimate.
- We studied the mean squared error for small h.
- We derived a formula for the optimal value of the bandwidth h.

4 Kernel Density Estimation in Practice

In this section we conclude our discussion of kernel density estimation by considering different aspects which are important when using the method in practice.

4.1 Integrated Error

From equation (11) we know

$$\mathrm{MSE}(\hat{f}_h(x)) \approx \frac{1}{nh} f(x) R(K) + \frac{1}{4}\mu_2(K)^2 f''(x)^2 h^4.$$

This gives the mean squared error when trying to estimate the density $f(x)$ at a fixed point x. Usually we are interested in estimating the function f rather than individual points $f(x)$. In this case, we consider the **integrated mean squared error (IMSE)**:

$$\mathrm{IMSE}(\hat{f}_h) := \int_{-\infty}^{\infty} \mathrm{MSE}(\hat{f}_h(x))\, dx.$$

Using our result from above we find

$$\begin{aligned}
\mathrm{IMSE}(\hat{f}_h) &\approx \int \Big(\frac{1}{nh} f(x) R(K) + \frac{1}{4}\mu_2(K)^2 f''(x)^2 h^4 \Big)\, dx \\
&= \frac{1}{nh} R(K) \int f(x)\, dx + \frac{h^4}{4}\mu_2(K)^2 \int f''(x)^2\, dx \\
&= \frac{1}{nh} R(K) + \frac{1}{4}\mu_2(K)^2 R(f'') h^4,
\end{aligned}$$

where we (mis-)use the definition of roughness as an abbreviation to express the integral over f''.

As before, we can use differentiation to find the optimal value of h. Here we get

$$h_{\mathrm{opt}} = \Big(\frac{R(K)}{n\mu_2(K)^2 R(f'')} \Big)^{1/5}.$$

and the corresponding error is

$$\mathrm{IMSE}_{\mathrm{opt}} = \frac{5}{4} \frac{1}{n^{4/5}} \Big(R(K)^2 \mu_2(K) \Big)^{2/5} R(f'')^{1/5}. \tag{12}$$

Thus, in order to minimise the error we still need to choose $h \propto n^{-1/5}$ and we should choose a kernel K which minimises the value $R(K)^2\mu_2(K)$.

4.2 Choice of Kernel

The integrated error in equation (12) is proportional to $\big(R(K)^2\mu_2(K)\big)^{2/5}$, and none of the remaining terms in the equation depends on the choice of the kernel. Thus, we can minimise the error by choosing a kernel which has minimal $R(K)^2\mu_2(K)$. For a given kernel, it is easy to work out the value of $R(K)^2\mu_2(K)$.

Example 4.1. For the uniform kernel we have

$$K(x) = \begin{cases} 1/2 & \text{if } -1 \le x \le 1 \\ 0 & \text{otherwise.} \end{cases}$$

From this we find

$$R(K) = \int_{-\infty}^{\infty} K(x)^2\, dx = \int_{-1}^{1} \frac{1}{4}\, dx = \frac{1}{2}$$

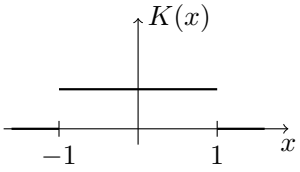
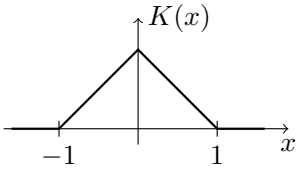
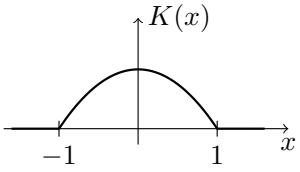
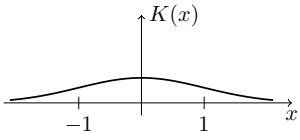
and

$$\mu_2(K) = \int_{-\infty}^{\infty} x^2 K(x)\, dx = \int_{-1}^{1} \frac{1}{2} x^2\, dx = \frac{1}{6} x^3 \Big|_{x=-1}^{1} = \frac{1}{6}(1 - (-1)) = \frac{1}{3}.$$

Thus, for the triangular kernel we have

$$R(K)^2\mu_2(K) = \Big(\frac{1}{2}\Big)^2 \frac{1}{3} = \frac{1}{12} \approx 0.083333.$$

Calculations similar to the ones in the example give the following values:

kernel		$\mu_2(K)$	$R(K)$	$R(K)^2\mu_2(K)$
Uniform		$\frac{1}{3}$	$\frac{1}{2}$	0.08333
Triangular		$\frac{1}{6}$	$\frac{2}{3}$	0.07407
Epanechnikov		$\frac{1}{5}$	$\frac{3}{5}$	0.07200
Gaussian		1	$\frac{1}{2\sqrt{\pi}}$	0.07958

The best value in the table is obtained for the Epanechnikov kernel, with $R(K)^2\mu_2(K) = 9/125 = 0.072$. One can show that this value is indeed optimal amongst all kernels. Since the difference in error for the kernels listed abive is only a few percent, any of these kernels would be a reasonable choice.

4.3 Bandwidth Selection

Our formulas for the optimal bandwidth contain the terms $f(x)^2|f''(x)|$ for fixed x and $R(f'')$ for the integrated error. Since f is unknown, neither of these quantities are available and instead different rules of thumb are used in the literature. Here we present one possible choice of bandwidth estimator.

Suppose that f is a normal density, with mean μ and variance σ^2. Then we have

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-(x-\mu)^2/2\sigma^2).$$

Taking derivatives we get

$$f'(x) = -\frac{1}{\sqrt{2\pi\sigma^2}} \frac{x-\mu}{\sigma^2} \exp(-(x-\mu)^2/2\sigma^2)$$

and

$$f''(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \Big(\frac{(x-\mu)^2}{\sigma^4} - \frac{1}{\sigma^2} \Big) \exp(-(x-\mu)^2/2\sigma^2)$$

Patiently integrating the square of this function gives

$$R(f'') = \int_{-\infty}^{\infty} f''(x)^2 \, dx = \cdots = \frac{3}{8\sigma^5\sqrt{\pi}}.$$

This can be used as a simple "plug-in rule" with σ estimated by the sample standard deviation.

We now demonstrate how this rule of thumb could be used in R to obtain a kernel density estimate for the snowfall data. We will use the Epanechnikov kernel. For compatibility with the kernels built into R, we rescale this kernel, so that $\mu_2(K) = 1$, i.e. we consider $K_{\sqrt{5}}$ in place of K. An easy calculation shows that the roughness is then $R(K) = 3/(5 * \sqrt(5))$.

```r
# downloaded from https://teaching.seehuhn.de/data/buffalo/
x <- read.csv("data/buffalo.csv")
snowfall <- x$snowfall
n <- length(snowfall)

# Roughness of the Epanechnikov kernel, after rescaling with h = sqrt(5)
# so that the second moment becomes mu_2 = 1:
R.K <- 3 / (5 * sqrt(5))

# Rule of thumb:
R.fpp <- 3 / (8 * sd(snowfall)^5 * sqrt(pi))

# formula for the optimal h
my.bw <- (R.K / (n * 1^2 * R.fpp))^0.2
my.bw
```

```
## [1] 11.58548
```

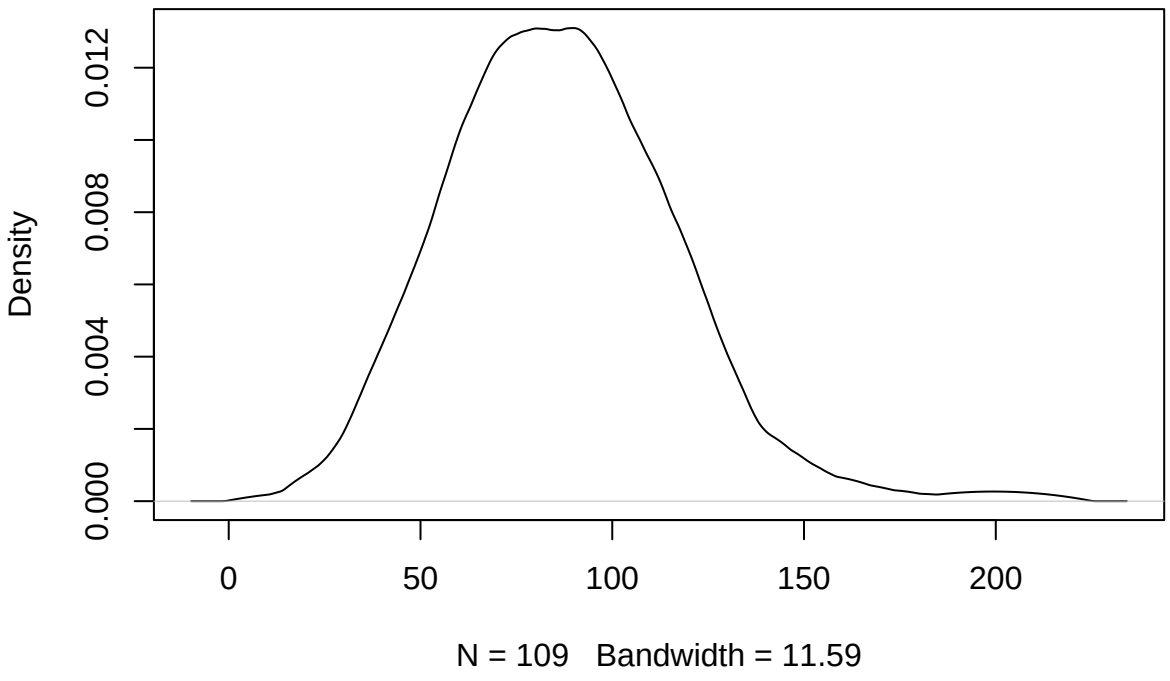
R has a variety of different builtin methods to estimate bandwidths. See stats/bandwidth for a description. For comparison to our result, we list here the bandwidths suggested by some of R's algorithms:

```r
data.frame(
  name = c("nrd0", "nrd", "SJ"),
  bw = c(bw.nrd0(snowfall), bw.nrd(snowfall), bw.SJ(snowfall)))
```

```
##   name       bw
## 1 nrd0  9.724206
## 2  nrd 11.452953
## 3   SJ 11.903840
```

All of these value seem close the value we obtained manually. Using our bandwidth estimate, we get the following estimated density.

```r
plot(density(snowfall, bw = my.bw, kernel = "epanechnikov"),
     main = NA)
```



In practice one would just use one of the built-in methods, for example using `bw="SJ"` instead of estimating the bandwidth manually.

4.4 Higher Dimensions

So far we have only considered the one-dimensional case, where the samples x_i are real numbers. In this subsection we will sketch how these methods will need to be adjusted for the multivariate case of $x_i = (x_{i,1}, \dots, x_{i,p}) \in \mathbb{R}^p$.

In this setup, a **kernel** is a function $K \colon \mathbb{R}^p \to \mathbb{R}$ such that

- $\int \cdots \int K(x)\, dx_p \cdots dx_1 = 1$,
- $K(x) = K(-x)$ and
- $K(x) \geq 0$ for all $x \in \mathbb{R}$,

where the integral in the first condition is now over all p coordinates.

Example 4.2. If $K_1, \dots, K_p$ are one-dimensional kernels, then the product

$$K(x_1, \dots, x_p) := K_1(x_1) \cdots K_p(x_p)$$

is a kernel in p dimensions. If we use the product of p Gaussian kernels, we get

$$\begin{aligned} K(x) &= \prod_{i=1}^{p} \frac{1}{\sqrt{2\pi}} \exp(-x_i^2/2) \\ &= \frac{1}{(2\pi)^{p/2}} \exp\Big(-\frac{1}{2}(x_1^2 + \cdots + x_p^2)\Big). \end{aligned}$$

There are different possibilities for rescaling these kernels:

- If all coordinates live on "comparable scales" (e.g., if they are measured in the same units), the formula
$$K_h(x) = \frac{1}{h^p} K(x/h)$$
for all $x \in \mathbb{R}^p$ can be used, where $h > 0$ is a bandwidth parameter as before. The scaling by $1/h^p$ is required to ensure that the integral of K_h equals 1, so that K_h is a kernel again.
- If different scaling is desirable for different components, the formula
$$K_h(x) = \frac{1}{h_1 \cdots h_p} K(x_1/h_1, \dots, x_p/h_p)$$
for all $x \in \mathbb{R}^p$ can be used, where $h = (h_1, \dots, h_p)$ is a vector of bandwidth parameters.
- A more general version would be to use a symmetric, positive definite bandwidth matrix $H \in \mathbb{R}^{p \times p}$. In this case the required scaling is
$$K_H(x) = \frac{1}{\det(H)} K(H^{-1}x)$$
for all $x \in \mathbb{R}^p$.

For all of these choices, the kernel density estimator is given by

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^{n} K_h(x - x_i)$$

(using K_H for the third option) for all $x \in \mathbb{R}^p$. Bandwidth selection in the multivariate case is a difficult problem and we will not discuss this here.