Kernel Density Estimation

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Suppose we have n independent, identically distributed random variables $X_1, X_2, \ldots, X_n$ (known as samples) from a distribution whose density function, $f_X(x)$ is not known but is assumed to exist. Then Kernel Density Estimation (also known as Parzen Windows or the empirical probability density function) provides an easy, if computationally intensive [Dekking et al., 2005], way of estimating the density function and as shown in [Parzen, 1962], will converge to the true distribution as the number of samples $n \to \infty$.

Historical context

Kernel Density Estimation (KDE) was only seriously considered in research beginning in the late 1950's. At its core, KDE seeks to infer the nature of the probability density function (pdf) of a random variable given a number of samples from that random variable. Prior to the development of KDE by [Rosenblatt, 1956] & [Parzen, 1962] in the mid 20th century, inference of pdfs from data was limited to histograms. Histograms are of limited usefulness because they very discrete and a small change in bin width or shift in bin location may result in a plot of a very different nature. [Dekking et al., 2005] The lack of research was in spite of the admission by [Parzen, 1962] of "the obvious importance of these [estimation] problems."

The Method

Intuitively, one expects areas with a high density of samples to have a higher density function, and those areas which are more sparse to have a lesser density function.

To that end, a kernel function $K(y)$ is introduced which in general is a probability density, is radially symmetric and unimodal. [Dekking et al., 2005] The kernel functions are evaluated at each data point and then summed together, with an appropriate normalisation constant (namely n^{-1} where n is the number of samples) to give the empirical probability density function. That is to say, given each sample $(X_i)_{i=1}^n$ and assuming a bandwidth h, the empirical probability density function, $\hat{f}(x)$ is [Sheather and Jones, 1991]

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

Choices and parameters

Fundamentally, there are two key choices to be made when implementing KDE, viz. the choice of kernel function and the choice of bandwidth. We consider both in turn.

Choice of Kernel Function

The two most common choices of kernel function are the rectangular and the Gaussian, although others exist such as Epanechnikov [Epanechnikov, 1969] and the triangular kernel.

The simplest choice of kernel function is the rectangular (or window) function which has the formula:

$$K_r(x) = \begin{cases} \frac{1}{h} & \text{if } |x - X_i| \leq \frac{h}{2}, \\ 0 & \text{otherwise} \end{cases}$$

and can be seen in Figure 1 on the left. This kernel function has the disadvantage of weighing all points within a certain distance (the bandwidth) of the data point equally. It would be natural to assume that we should weigh points closest to the data point the heaviest.

The Gaussian kernel function is precisely that, it fits a Gaussian (or normal) function about each data point and then sums these together to give the empirical density function. The formula for this type of density

function is given (in 1-dimension) by

$$K_G(x) = \frac{1}{h\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x - X_i}{h}\right)^2\right).$$

The shape of this kernel function is the familiar bell-curve as can be seen on the right hand side of Figure 1.

```
plot(density.default(10, bw=2, kernel = "rectangular"))
plot(density.default(10, bw=2, kernel = "gaussian"))
```

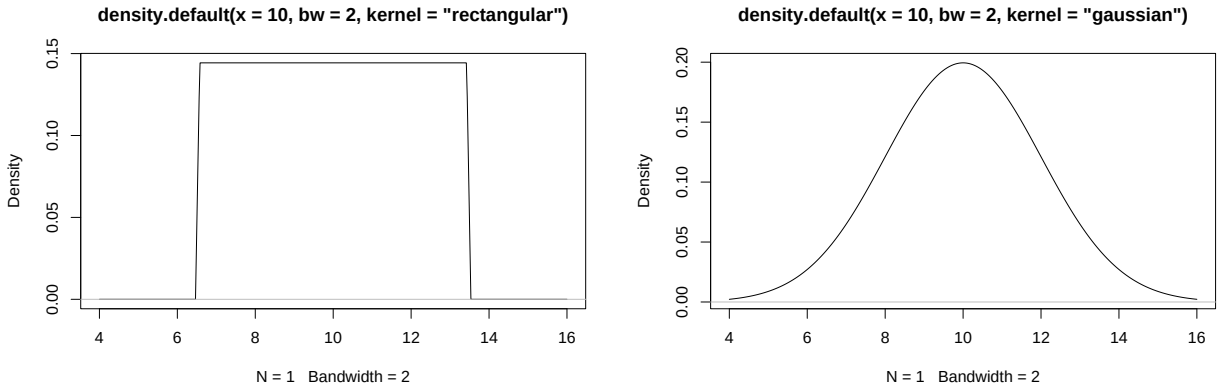


Figure 1: The window and Gaussian Kernel Functions, both centred at 10 with bandwidth $h = 2$.

Choice of Bandwidth

The bandwidth (h in expressions above) is the breadth of influence each data point has. Its selection is always a trade off between being overly specific (with a narrow bandwidth) and hiding the underlying nature of the data (with too wide a bandwidth). R, by default, will use the method described in [Sheather and Jones, 1991] that seeks to "[choose] the bandwidth to (approximately) minimize good quality estimates of the mean integrated squared error". All three cases are demonstrated below.

Examples of KDE in Practice

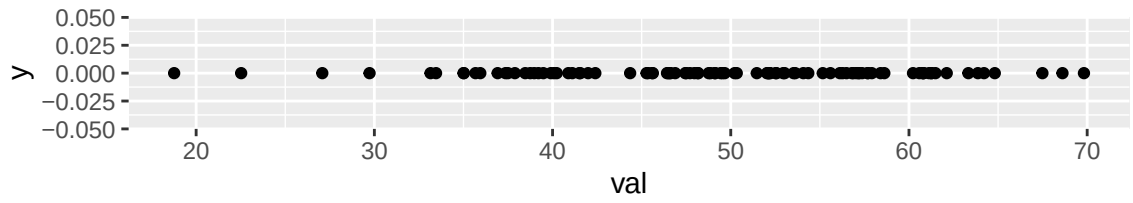
For reproducibility, we set the seed and include some R libraries as follows.

```
set.seed(184); library(tidyverse); library(bbmle)
```

A Limited Number of Samples from a (Unimodal) Normal Distribution

We first demonstrate KDE in practice and the importance of the choice of kernel function by considering a random variable $X \sim N(50, 10)$ of which we take 100 i.i.d. samples, namely $X_1, X_2, \ldots, X_{100}$ and plot.

```
normSample <- rnorm(100,50,10); normSampDF <- tibble(val = normSample)
ggplot(data = normSampDF) + geom_point(aes(val, 0))
```



The data points are more concentrated towards the mean as expected. We now plot the kernel density estimate using both the window and Gaussian kernel functions, and include the true density function (dashed line) since $X \sim N(50, 10)$.

```
ggplot(data = normSampDF) +
  xlim(10,90) + geom_point(aes(val, 0)) + geom_density(aes(val), kernel = "rectangular") +
  geom_function(fun = dnorm, args = list(mean = 50, sd = 10), linetype = "dashed")
ggplot(data = normSampDF) +
  xlim(10,90) + geom_point(aes(val, 0)) + geom_density(aes(val)) +
  geom_function(fun = dnorm, args = list(mean = 50, sd = 10), linetype = "dashed")
```

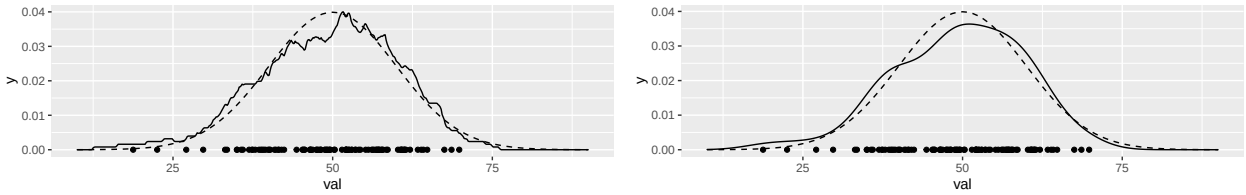


Figure 2: Evaluating the emprirical probability density using the window (left) and Gaussian (right) functions.

Clearly, the Gaussian kernel gives a much smoother empirical pdf and in this case is more appropriate, however it is more computationally expensive and has an unlimited support.

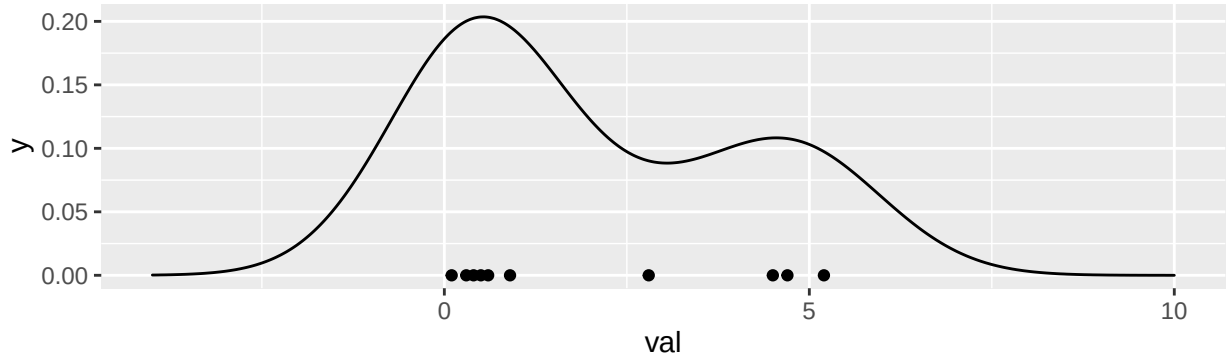
Bandwidth Selection

Now suppose we have the data set `(0.1,0.3,0.4,0.5,0.6,0.9,2.8,4.5,4.7,5.2)` which we plot:

```
interest<- c(0.1,0.3,0.4,0.5,0.6,0.9,2.8,4.5,4.7,5.2)
interestingDF <- tibble(val = interest)
ggplot(data = interestingDF) + geom_point(aes(val, 0))
```

Clearly, this data set is bimodal. We perform KDE to illustrate the importance of bandwidth selection using the Gaussian kernel. First using the default from [Sheather and Jones, 1991],

```
ggplot(data = interestingDF) +
  xlim(-4,10) + geom_point(aes(val, 0)) + geom_density(aes(val))
```



In this case, R estimates the best bandwidth to be 1.1805817 which can be seen to show the underlying sturcture of the data; maintaining two peaks whilst not overfitting.

Let us now consider two extremes, a very narrow bandwidth ($h = 0.05$) and a very wide bandwidth ($h = 3$).

```
ggplot(data = interestingDF) +
  xlim(-1,7) + geom_point(aes(val,0)) + geom_density(aes(val), bw = 0.05)
ggplot(data = interestingDF) +
  xlim(-5,15) + geom_point(aes(val,0)) + geom_density(aes(val), bw = 3)
```

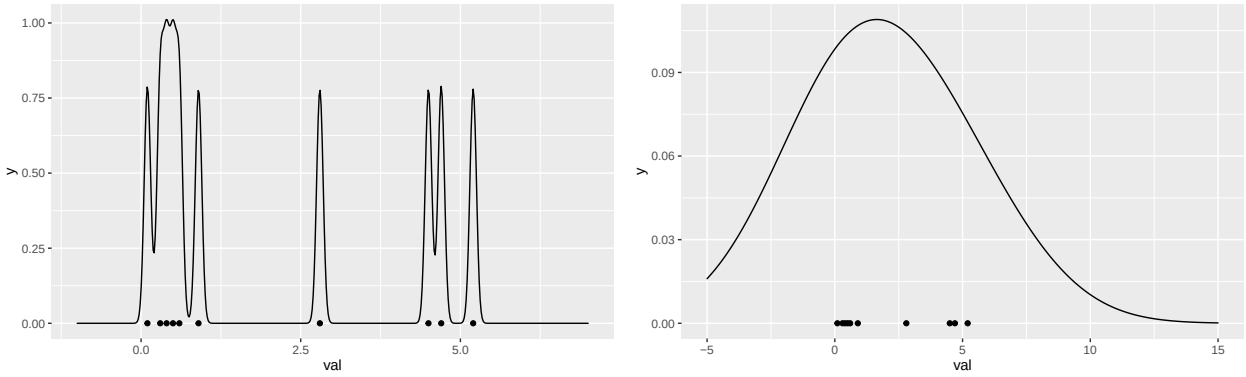


Figure 3: Evaluating the emprirical probability density using a bandwidth of 0.05 (left) and 3 (right).

Both bandwidths in Figure 3 are totally inappropriate. In the first case with a narrow bandwidth, the density is totally concentrated about the data points. This suggests overfitting so this estimate is unlikely to generalise to other examples from the same distribution. On the other hand, using a very wide bandwidth of 3 totally masks the underlying structure of the data; the two peaks are completely washed away and so we lose the characteristic of this dataset.

References

[Dekking et al., 2005] Dekking, F. M., Kraaikamp, C., Lopuhaä, H. P., and Meester, L. E. (2005). *A Modern Introduction to Probability and Statistics : Understanding Why and How*. Springer Texts in Statistics. Springer-Verlag London Limited, London.

[Epanechnikov, 1969] Epanechnikov, V. A. (1969). Non-parametric estimation of a multivariate probability density. *Theory of Probability & Its Applications*, 14(1):153–158.

[Parzen, 1962] Parzen, E. (1962). On estimation of a probability density function and mode. *The Annals of Mathematical Statistics*, 33(3):1065–1076.

[Rosenblatt, 1956] Rosenblatt, M. (1956). Remarks on some nonparametric estimates of a density function. *The Annals of Mathematical Statistics*, 27(3):832–837.

[Sheather and Jones, 1991] Sheather, S. J. and Jones, M. C. (1991). A reliable data-based bandwidth selection method for kernel density estimation. *Journal of the Royal Statistical Society. Series B, Methodological*, 53(3):683–690.

[Whittle, 1958] Whittle, P. (1958). On the smoothing of probability density functions. *Journal of the Royal Statistical Society. Series B, Methodological*, 20(2):334–343.