A Simulation Study on Kernel Density Estimation

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Contents

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- This approach is **nonparametric density estimation.**
- The focus of discussion will be on this nonparametric approach.

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- We will see this fact verified shortly through our simulation.

Histograms by varying number of bins

- A sample $X_1, X_2, \ldots, X_n$ of size $n = 200$ from the density

$$f(x) = \phi(2(x-1)) + \frac{1}{2}\phi(x-5)$$

where $\phi(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$ is drawn.

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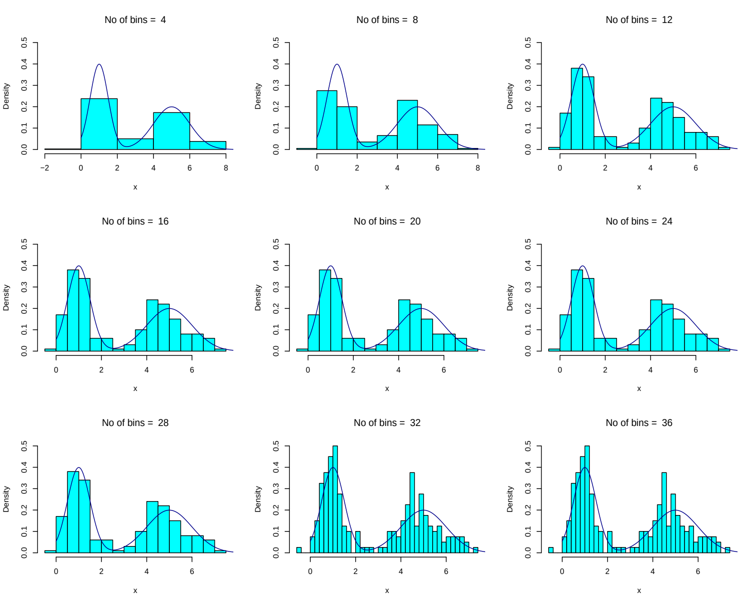
- See all the plots for varying *number of bins* or equivalently *varying binwidth* on the same panel to catch the difference:-

Histograms for varying number of bins



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- Thus,one of our main challenges is to find the **best choice of** h or **optimum binwidth** h_{opt} for our estimator.
- We will somehow try to achieve this goal through different approaches.

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- Derivatives of density function cannot be estimated.
- Difficult to extend this idea to high dimensions.

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- Due to some drawbacks hence we try to generalize this concept.

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- All other drawbacks remain as they are.

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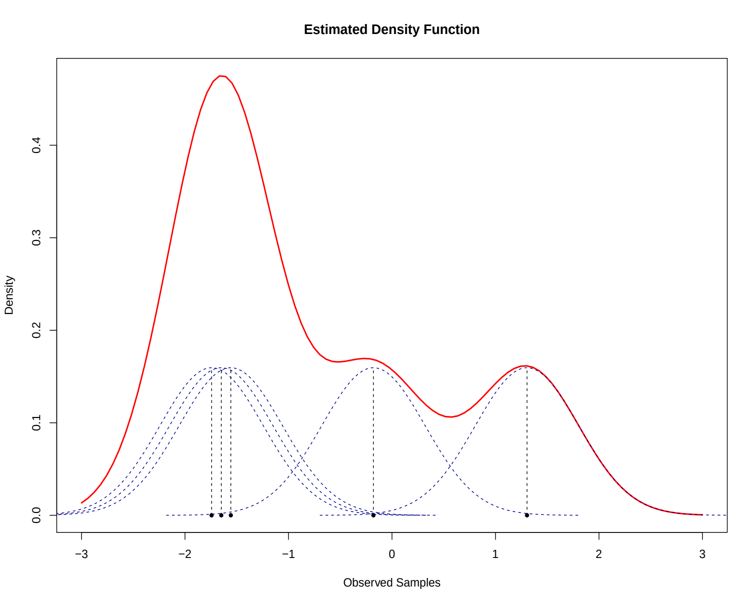
- The *Kernel Type Estimator* is thus given by :

$$f_n(x) = \frac{1}{nh_n} \sum_{i=1}^{n} K(\frac{x - X_i}{h_n})$$

$h_n \to 0$ as $n \to \infty$

Demonstrating how KDE Works

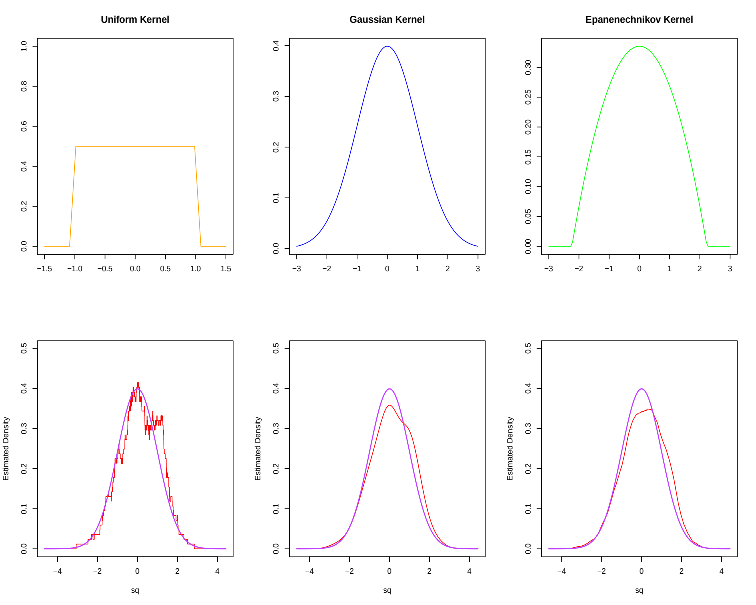


Some examples of Kernel Functions

Kernel Names	Functional Form $(K(x))$	Efficiency relative to Epanechnikov Kernel
Uniform	$\frac{1}{2}\boldsymbol{I}_{\lvert x\rvert\leq 1}$	92.9%
Triangular	$(1-\lvert x\rvert)\,\boldsymbol{I}_{\lvert x\rvert\leq 1}$	98.5%
Epanechnikov	$\frac{3}{4\sqrt{5}}\left(1-\frac{t^2}{5}\right)\boldsymbol{I}_{\lvert x\rvert\leq\sqrt{5}}$	1
Gaussian	$\frac{1}{\sqrt{2\pi}}e^{-\frac{t^2}{2}}\boldsymbol{I}_{x\in\mathbb{R}}$	95.1%
Cosine	$\frac{\pi}{4}\cos\left(\frac{\pi}{2}x\right)\boldsymbol{I}_{\lvert x\rvert\leq 1}$	99.9%

Here,we have done a comparative study between these kernels to show our results.To compare how different choices of kernels influence the estimated density, we make the KDE plots for the same observed data and different kernels.

Comparison between different kernels



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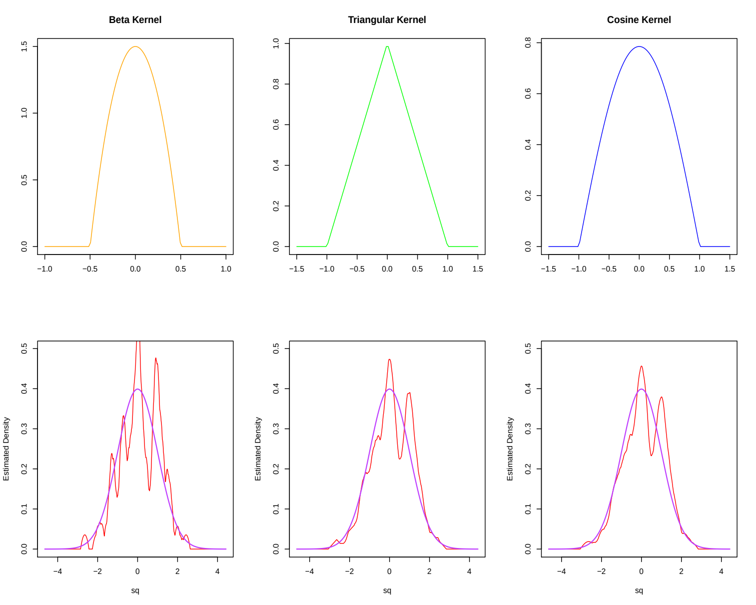

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- Let's take a look at the plot of the estimated density.

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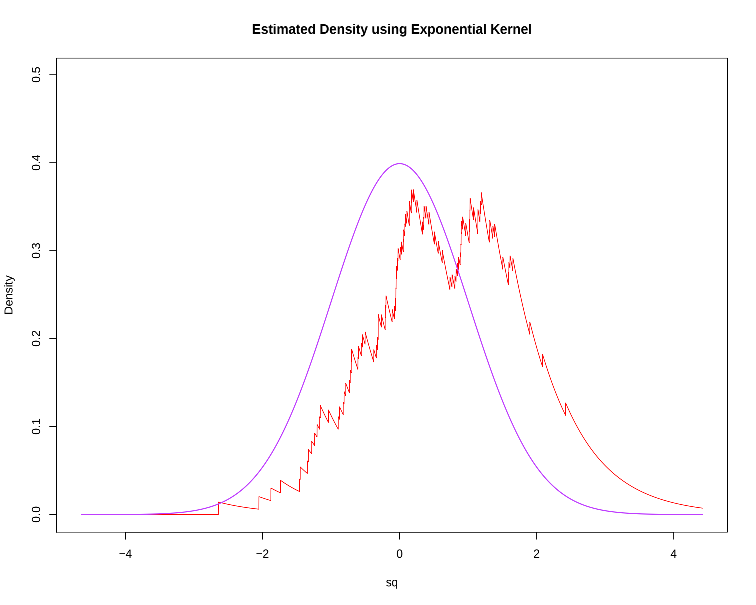

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- Why does this happen?

Observation

- The reason behind this is the form of the kernel density estimate at any point x is defined as

$$\begin{aligned}
\widehat{f}_n(x) &= \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x-X_i}{h}\right) \\
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- On the left portion, lesser number of points contribute which results in such a type of estimated density.

Kernel-Smoothed Cumulative Distribution Function

Since, we define the kernel density estimator as :-

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

where $K(.)$ is the kernel function, an obvious extension of this idea is to make smoothed estimators of CDF as :-

$$\begin{aligned}
\widehat{F}_n(x) &= \int_{-\infty}^{x} \widehat{f}_n(t)\, dt \\
&= \int_{-\infty}^{x} \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{t - X_i}{h}\right) dt \\
&= \frac{1}{n}\sum_{i=1}^{n}\int_{-\infty}^{x} \frac{1}{h} K\left(\frac{t - X_i}{h}\right) dt \\
&= \frac{1}{n}\sum_{i=1}^{n} \widetilde{K}\left(\frac{x - X_i}{h}\right) dt
\end{aligned}$$

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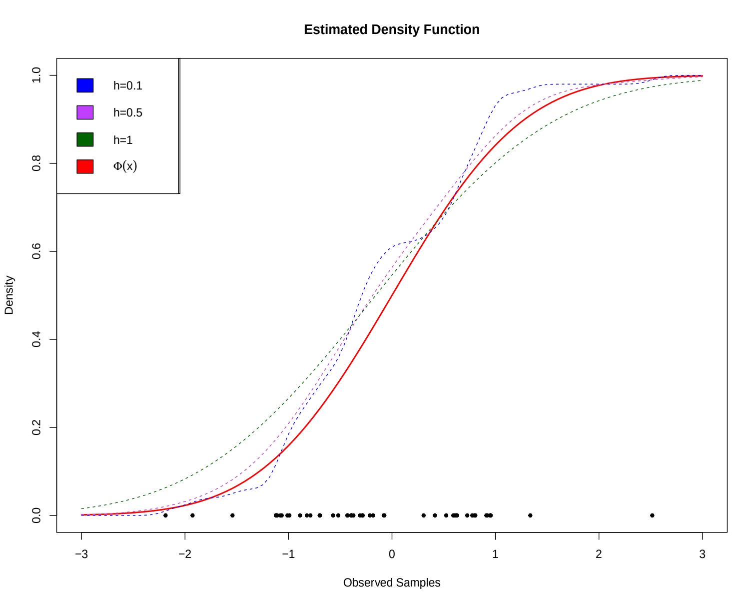
- Let's take a look at the plot for different choices of bandwidths.

Kernel Smoothed CDF Estimators



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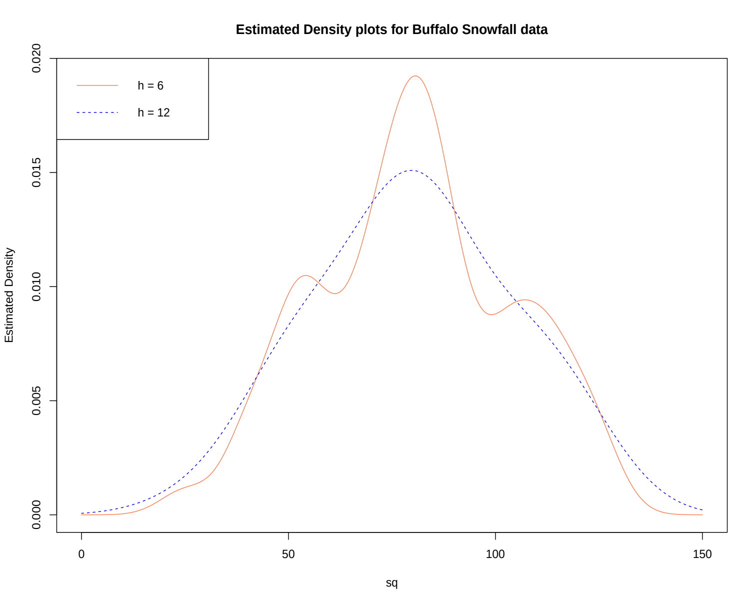
- For many applications this approach will be perfectly satisfactory. Indeed, the process of examining several plots of the data, all smoothed by different amounts, may well give more insight into the data than merely considering a single automatically produced curve.
- Consider, as an example, the estimate given in following plot, the data underlying these estimates are the amounts of winter snowfall (in inches) at Buffalo, New York, for each of the 63 winters from 1910/11 to 1972/73.

Kernel estimates for annual snowfall data



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- For many purposes, particularly for model and hypothesis generation, it is by no means unhelpful for the statistician to supply the scientist with a range of possible presentations of the data. A choice between the two alternative models suggested by our figures is a very useful step forward from the enormous number of possible explanations that could conceivably be considered.

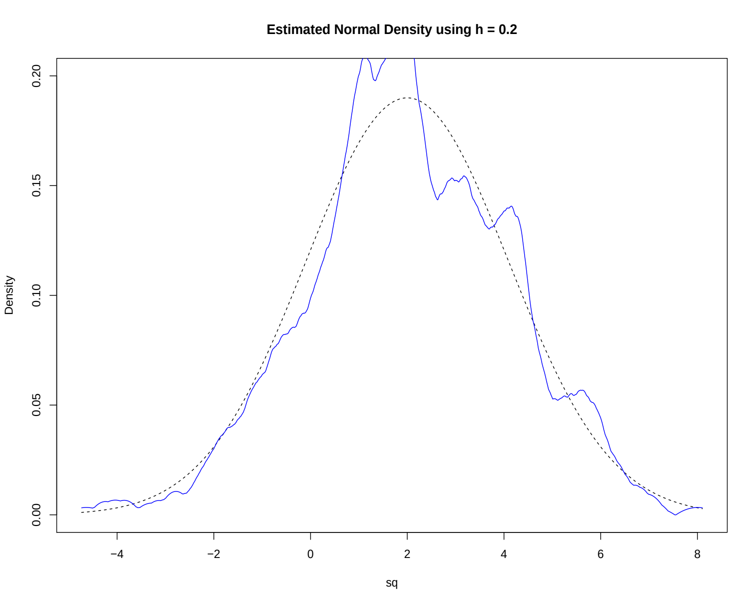
Reference to a standard distribution

If we assume a standard family of distributions while estimating the density, then we can obtain an exact expression of the optimal bin width h_{opt}. For example if we assume the density to be normally distributed with variance σ^2, and if we use gaussian kernel for estimation (i.e. $K(x) = \phi(x)$), then we get :-

$$
\begin{aligned}
h_{\text{opt}} &= (4\pi)^{-1/10} \left(\frac{3}{8} \pi^{-1/2} \right)^{-1/5} \sigma n^{-1/5} \\
&= \left(\frac{4}{3} \right)^{1/5} \sigma n^{-1/5} = 1.06 \sigma n^{-1/5}
\end{aligned}
$$

We draw a sample of size $n = 500$ from a $N\left(0, \sigma^2 = 4.41\right)$ distribution which gives $h_{\text{opt}} \approx 0.628$.

Effect of Undersmoothing



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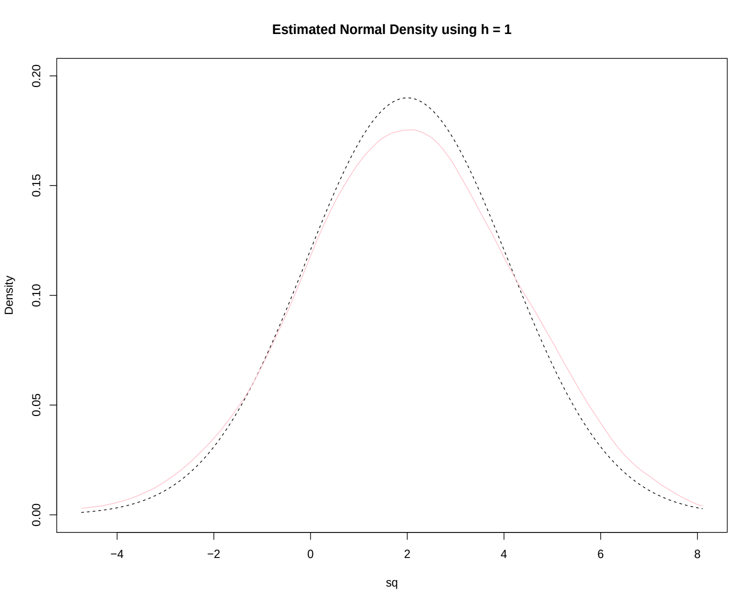
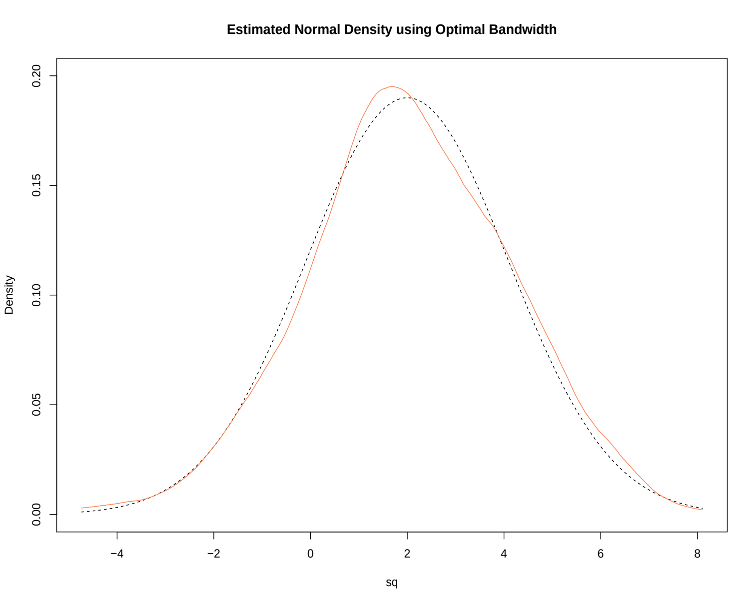


Using optimal bandwidth



Least Squares cross validation

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- The basic principle of least square cross validation is to construct a estimator of $R(\hat{f})$ and minimise the estimator with respect to h.

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- We will find our optimum value of h by minimising this quantity.

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- Without loss of generality, we transform this observations linearly so that they lie in the range $[0, 1]$ by doing the transformation $y_i = \frac{x_i - \min\limits_{1 \le j \le n}(x_j)}{\max\limits_{1 \le j \le n}(x_j) - \min\limits_{1 \le j \le n}(x_j)}$.

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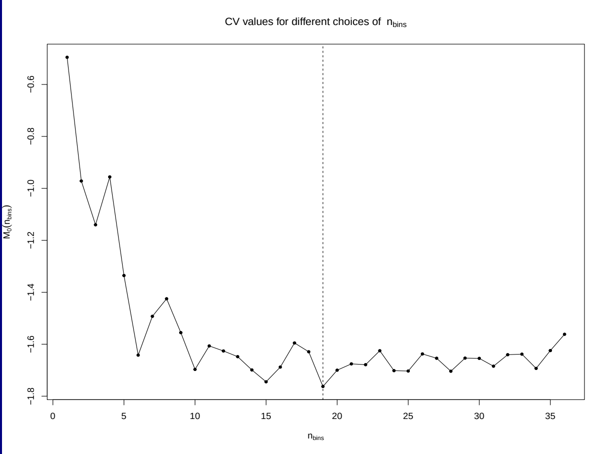
- We take a range of values of n_{bins} as $\{1,\ldots,40\}$ and then, for each of the choices we calculate $M_0(h)$ where $h = \frac{1}{n_{bins}}$ is the binwidth since we have normalized the range to $[0,1]$. (Hence, $n_{bins}h = 1$.)

Least Squares cross validation

- After calculating the risk estimates, we plot them and the plot looks like this :-



Least Squares cross validation

- So from the plot we can see that the estimated risk is minimum when $n_{bins} = 19 \implies h \approx 0.0526$ and indeed it is quite similar to the heuristic observations, we made earlier.

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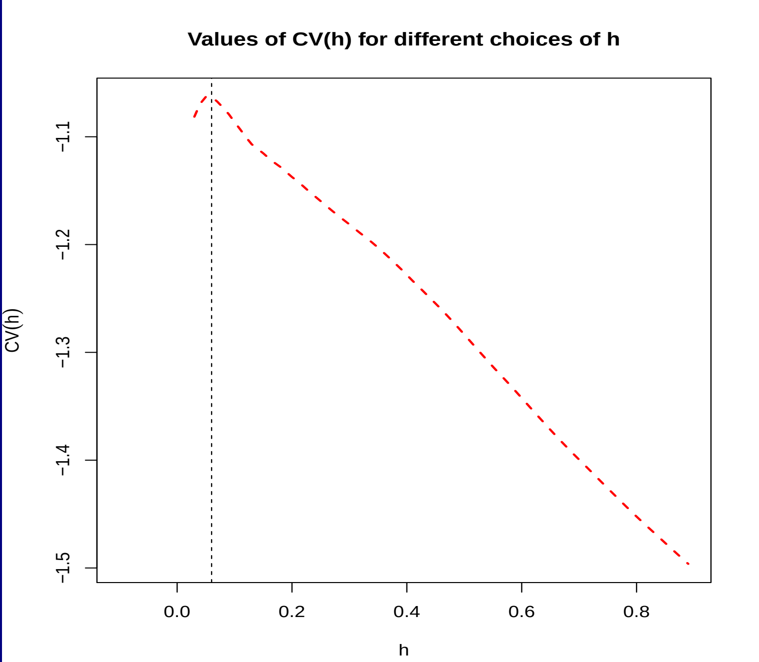

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- Let us have a look at them.

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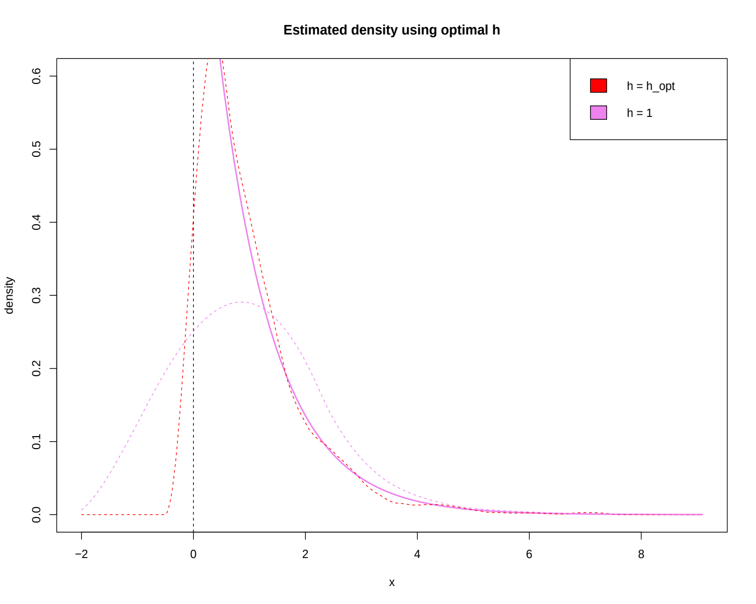

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- Another important drawback to mention here is that the estimated density is non-zero for negative values of x as well which is occuring due to positive weight that is being assigned due to observations whose values are near zero.

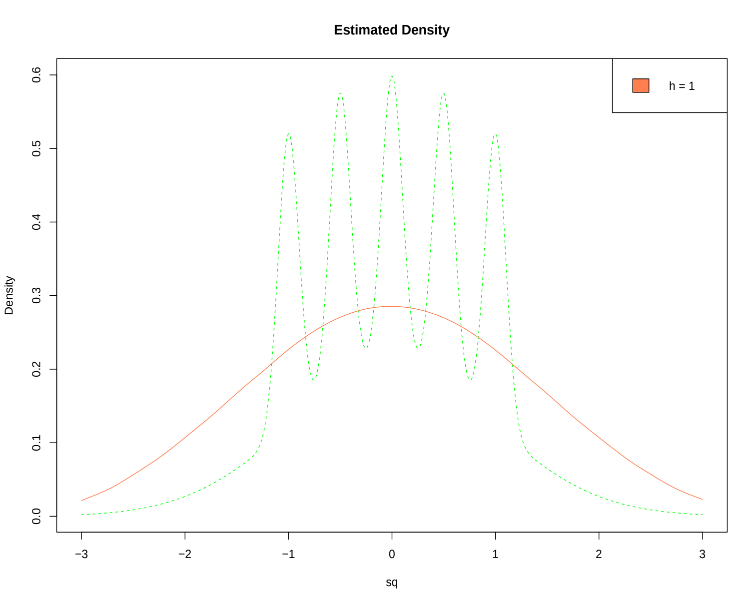
Demonstrating importance of choosing h optimally

Suppose we generate a random sample of size 1000 from a density $f(x)$ of the form :-

$$f(x) = \frac{1}{2}\phi(x;0,1) + \sum_{i=1}^{4} \phi\left(x;\left(\frac{i}{2}-1\right),\frac{1}{10}\right)$$

We have estimated this "claw shaped" density known as "Bart Simpson" density using **epanechnikov** kernel based on the sample observations.

Demonstrating importance of choosing h optimally



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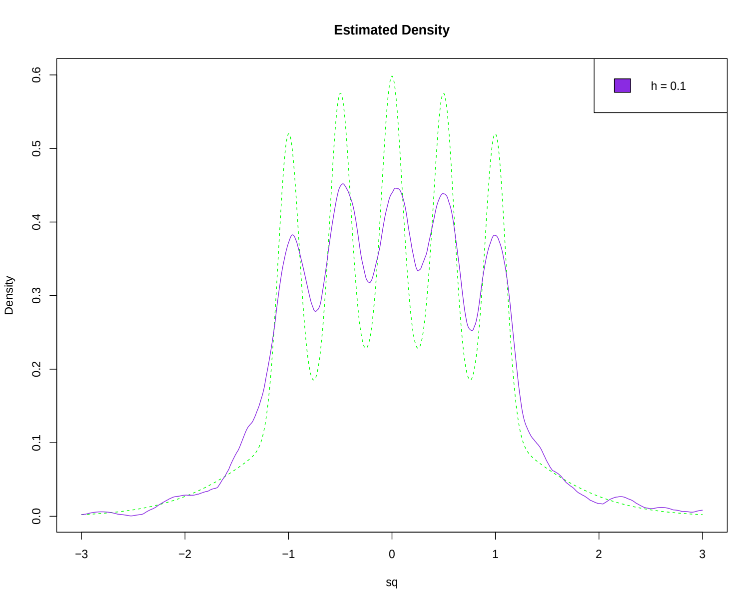

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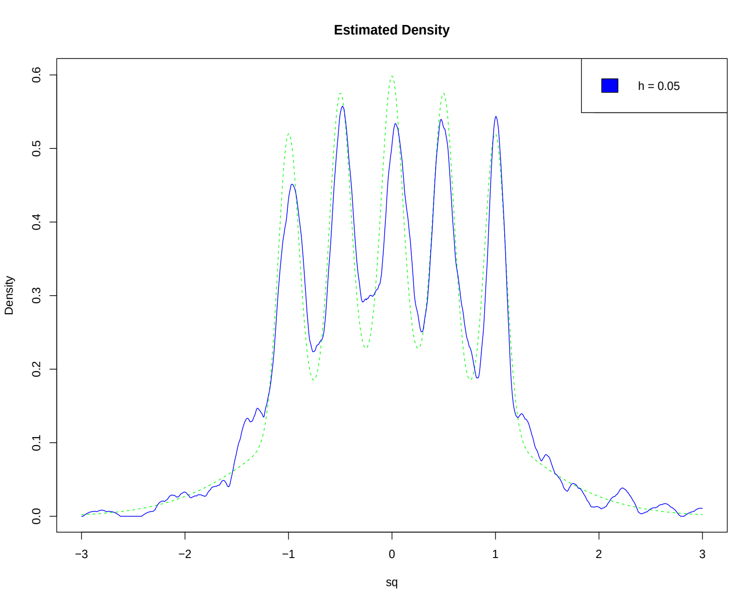

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- For a particular value of bin width the kernel density estimates the true density precisely.
- For small bin width, the estimated kernel density is over smoothed and it doesn't capture the true nature of the density.
- So, it is very crucial to find the optimal bin width for estimating the density using kernel estimation.

Limiting Distribution of V_n

- If $K(.)$ is a kernel function of bounded variation and the series $\sum_{n=1}^{\infty} e^{-\gamma n h_n^2}$ converges $\forall\ \gamma > 0$ where h_n denotes the bandwidth. Then

$$V_n = \sup_x \left| \widehat{f}_n(x) - f(x) \right| \to 0 \text{ w.p. } 1$$

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$$\int_{-\infty}^{\infty} uK(u)\, du = 0, \int_{-\infty}^{\infty} u^2 K(u)\, du < \infty$$

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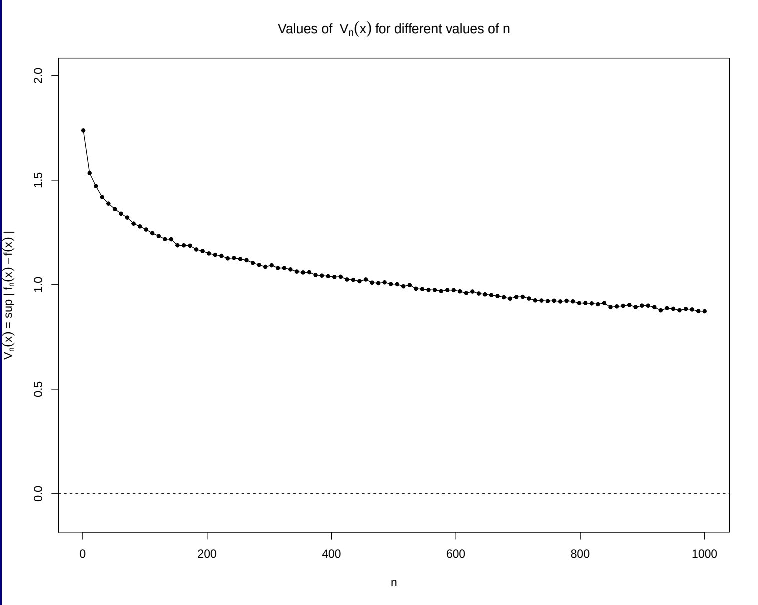
- which indicates that the rate at which $\sup_x \left|\widehat{f}_n(x) - f(x)\right|$ goes to 0 is very slow which can also be verified from the plots we made using simulation

Asymptotic distribution of V_n



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- is that, for every $\varepsilon > 0$.

$$nP[|Z_{n1} - E(Z_{n1})|\{var(Z_{n1})\}^{-\frac{1}{2}} \geq \varepsilon n^{1/2}] \longrightarrow 0 \quad as \text{ n} \longrightarrow \infty$$

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- A sufficient condition for

$$\frac{\hat{f}_n(x) - E(\hat{f}_n(x))}{\sqrt{var(\hat{f}_n(x))}} \xrightarrow{\mathcal{L}} N(0,1)$$

is that, for some $\delta > 0$

$$\frac{E|Z_{n1} - E(Z_{n1})|^{2+\delta}}{n^{\delta/2}[var(Z_{n1})]^{1+\delta/2}} \longrightarrow 0 \;\; as \text{ n} \to \infty$$

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- Now, we use simulation to verify the result stated above.
- Suppose, we have drawn a samples from standard normal distribution.Then $f(x) = \phi(x)$ which is a continuous function.
- We have estimated the true density using the **epanechnikov kernel** with a fixed bandwidth.

Asymptotic normality of kernel density estimator

- We plot the asymptotic distribution of

$$\frac{\hat{f}_n(x) - E(\hat{f}_n(x))}{\sqrt{var(\hat{f}_n(x))}}$$

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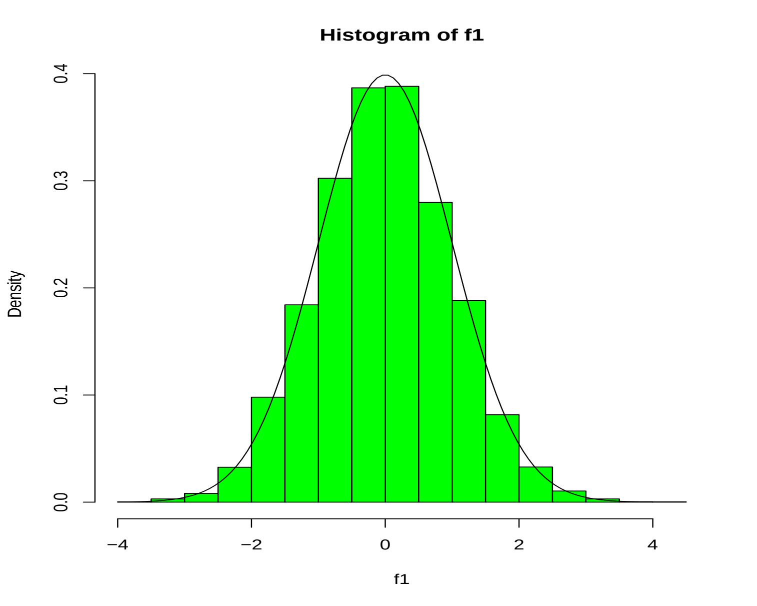
- We can clearly see that the histogram closely resembles that of a standard normal density as expected.

Asymptotic normality of kernel density estimator



Asymptotic Distribution

- Since, for large n ,

$$Z_n(x) = \frac{\widehat{f}_n(x) - E\widehat{f}_n(x)}{\sqrt{V\widehat{f}_n(x)}} \xrightarrow{\mathcal{L}} N(0,1)$$

where if we choose $K(u) = \phi(u)$, we get a closed form expression for the expectation term as,

$$E\widehat{f}_n(x) = \int_{-\infty}^{\infty} \frac{1}{h_n} K_n\left(\frac{x-u}{h_n}\right) f(u)\,du$$

$$= \frac{1}{2\pi h_n} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\left(\frac{x-u}{h_n}\right)^2} e^{-\frac{1}{2}u^2} du = (K_n * f)(x)$$

$$= \frac{1}{\sqrt{2\pi}\sqrt{h_n^2+1}} e^{-\frac{1}{2}\frac{x^2}{h_n^2+1}} = \frac{1}{\sqrt{h_n^2+1}} \phi\left(\frac{x}{\sqrt{h_n^2+1}}\right)$$

Asymptotic Distribution

- and,

$$
\begin{aligned}
\sigma_n^2(x) &= \frac{1}{n^2}\sum_{i=1}^{n} \operatorname{Var}\left(\frac{1}{h_n} K\left(\frac{x-X_i}{h_n}\right)\right) \\
&\approx \frac{f(x)}{nh_n} \int_{-\infty}^{\infty} K^2(u)\,du \\
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\end{aligned}
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$$= \frac{f(x)}{nh_n}\frac{1}{2\sqrt{\pi}}$$

- While doing simulation, here we know the actual pdf $f(x)$, hence we can use this property to visualize the CLT property of kernel density estimates by drawing upper and lower α points for each of the values of x that gives us two nice curves like :-

$$P\left(L_\alpha(x) \le \widehat{f}_n(x) \le U_\alpha(x)\right) \approx 1-\alpha$$

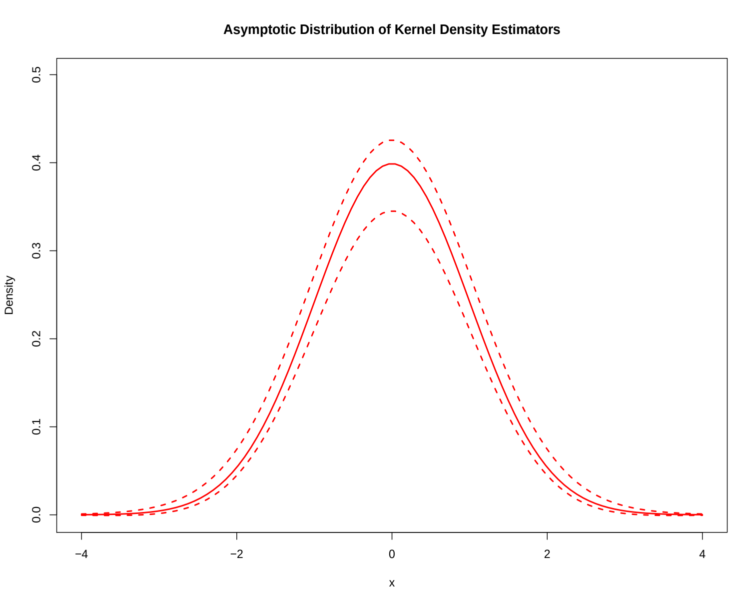
Asymptotic Distribution

- where ,

$$L_\alpha(x) = E\widehat{f_n}(x) - \tau_{\alpha/2}\sigma_n(x)$$
$$U_\alpha(x) = E\widehat{f_n}(x) + \tau_{\alpha/2}\sigma_n(x)$$

- if we draw these lines around the true density of the sample $(\phi(x))$, we get something like this :-

Asymptotic Distribution



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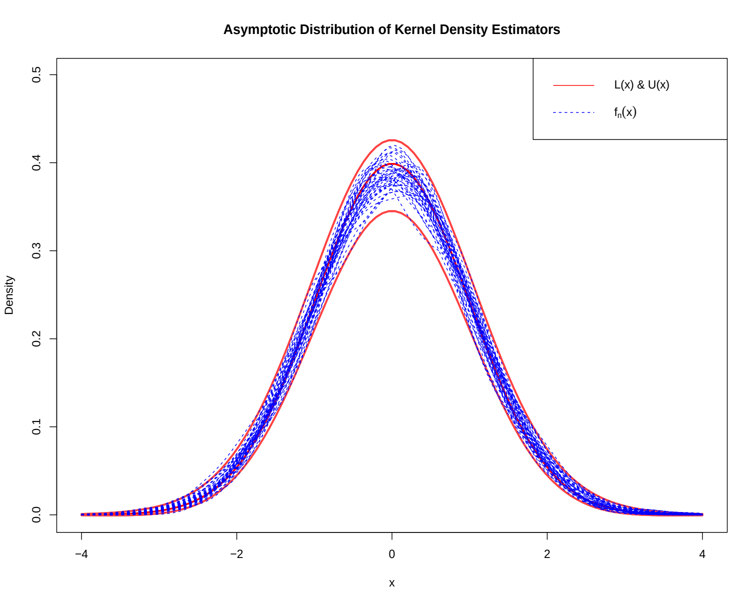

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Acknowledgements

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Acknowledgements

THANK YOU

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