

Master Program in *Data Science and Business Informatics*

Statistics for Data Science

Lesson 15 - Graphical summaries

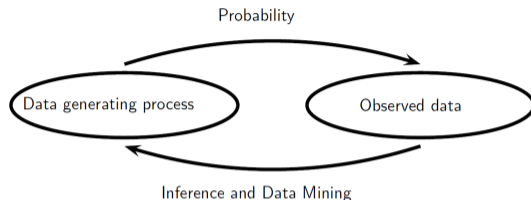
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Condensed observations



- Probability models governs some random phenomena
- Confronted with a new phenomenon, we want to learn about the randomness associated with it
 - ▶ Parametric (efficient) vs non-parametric (general) methods
- Record observations x_1, \dots, x_n (a dataset)
- n can be large: need to condense for easy visual comprehension
- Graphical summaries:
 - ▶ Univariate: histograms, kernel density estimates, empirical distribution functions
 - ▶ Multi-variate: scatter plots

The empirical CDF

- Record observations x_1, \dots, x_n (a dataset)
- Empirical cumulative distribution function (CDF):

$$F_n(x) = \frac{|\{i \in [1, n] \mid x_i \leq x\}|}{n}$$

- Empirical complementary cumulative distribution function (CCDF):

$$\bar{F}_n(x) = 1 - F_n(x)$$

- A r.v. X is completely characterized by its CDF F_X
- Estimating F_X through F_n allow for estimating other quantities by plugging F_n in the place of F_X , e.g., $E[X]$ as

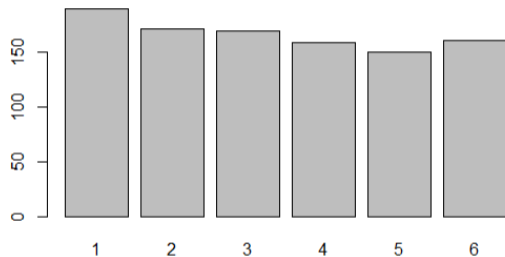
$$E[X] = \sum_a a \cdot P(X = a) = \sum_a a \cdot \frac{|\{i \mid x_i = a\}|}{n} = \frac{1}{n} \sum_i x_i$$

- What about p.m.f. and d.f.?

See R script

Barplots

- For discrete data, barplots provide frequency counts for values
 - ▶ approximate the p.m.f. due to the law of large numbers



- For continuous data, frequency counting of distinct values do not work. Why?

See R script

Histograms

- Histograms provide frequency counts for ranges of values:
 - ▶ Split the support to intervals, called *bins*:

$$B_1, \dots, B_m$$

where the length $|B_i|$ is called the *bin width*

- ▶ Count observations in each bin and normalize them:

$$A_i = \frac{|\{j \in [1, n] \mid x_j \in B_i\}|}{n} \approx P(X \in B_i)$$

- ▶ Plot bars whose **area** is proportional to A_i

$$A_i = |B_i| \cdot H_i \quad H_i = \frac{|\{j \in [1, n] \mid x_j \in B_i\}|}{n|B_i|}$$

See R script

Choice of the bin width

- Bins of equal width:

$$B_i = (r + (i - 1)b, r + ib] \quad \text{for } i \in [1, m]$$

where $r \leq$ minimum point and b is the bin width

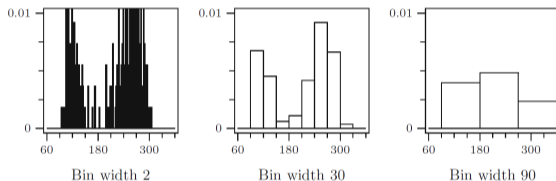


Fig. 15.2. Histograms of the Old Faithful data with different bin widths.

- Mean Integrated Square Error (MISE), for $\hat{f}(\cdot)$ density estimation of $f(\cdot)$:

$$MISE = E\left[\int (\hat{f}(u) - f(u))^2 du\right] = \int \int (\hat{f}(u) - f(u))^2 (f(x))^n du dx$$

- Scott's normal reference rule (minimize MISE for Normal density):

$$b = 3.49 \cdot s \cdot n^{-1/3}, \quad \text{where } s = \hat{\sigma} = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2}$$
 is the sample standard deviation

Choice of the bin width

- $b = 2 \cdot IQR \cdot n^{-1/3}$, where $IQR = Q_3 - Q_1$ *[Freedman–Diaconis' choice]*
 - ▶ It replaces $3.49 \cdot s$ in the Scott's rule by $2 \cdot IQR$ (more robust to outlier)
 - ▶ Q_3 is 75% percentile of x_1, \dots, x_n
 - ▶ Q_1 is 25% percentile of x_1, \dots, x_n
- Variable bin width
 - ▶ Logarithmic binning in power laws
- Alternative: number of bins given equal bin width b :
 - ▶ $m = \lceil \frac{\max x_i - \min x_i}{b} \rceil$
 - ▶ $m = \lceil \sqrt{n} \rceil$
 - ▶ $m = \lceil \log_2 n \rceil + 1$ *[Sturges' formula]*
 - ▶ Sturges's formula:
 - assume m bins: $0, 1, \dots, m - 1$
 - assume normal distribution of true density
 - approximate normal density as $Bin(n, 0.5)$, hence absolute frequency of i^{th} bin is $\binom{m-1}{i}$
 - total frequency is $n = \sum_{i=0}^{m-1} \binom{m-1}{i} = 2^{m-1}$, hence $m = \lceil \log_2 n \rceil + 1$

N.B. R's `hist` method take bin width as a suggestion, then it rounds bins differently

See R script

Density estimation

- Problem with histograms: as m increases, histogram becomes unusable
- Idea: estimate density function by putting a **pile (of sand)** around each observation
- Kernels state the shape of the pile
 - ▶ Epanechnikov $\frac{3}{4}(1 - u^2)$ for $-1 \leq u \leq 1$
 - ▶ Triweight $\frac{35}{32}(1 - u^2)^3$ for $-1 \leq u \leq 1$
 - ▶ Normal $\frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}u^2}$ for $-\infty < u < \infty$

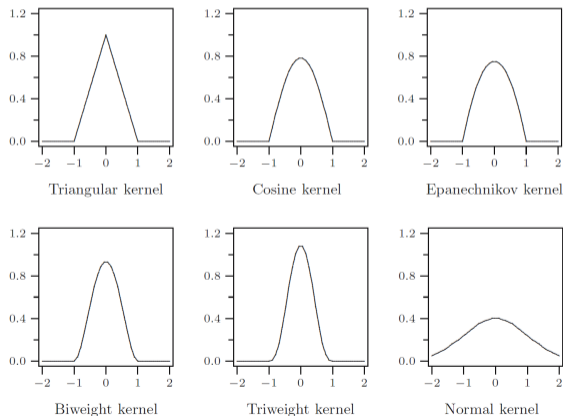


Fig. 15.4. Examples of well-known kernels K .

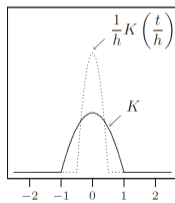
Kernel density estimation (KDE)

A Kernel is a function $K : \mathbb{R} \rightarrow \mathbb{R}$ such that

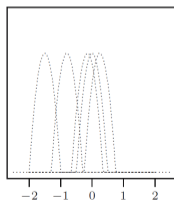
- K is a probability density, i.e., $K(u) \geq 0$ and $\int_{-\infty}^{\infty} K(u)du = 1$
- K is symmetric, i.e., $K(-u) = K(u)$
- [sometime, it is required that] $K(u) = 0$ for $|u| > 1$

A bandwidth h is a scaling factor over the support of K (from $[-1, 1]$ to $[-h, h]$)

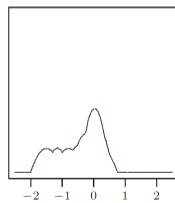
- if $X \sim K$, then $\frac{X}{h} \sim \frac{1}{h}K\left(\frac{u}{h}\right)$ *[Change-of-Unit rule]*



Kernel and scaled kernel

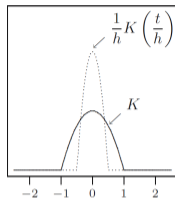


Shifted kernel

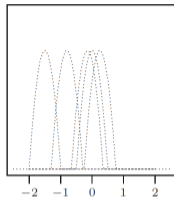


Kernel density estimate

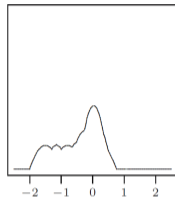
Kernel density estimation (KDE)



Kernel and scaled kernel



Shifted kernel



Kernel density estimate

Let x_1, \dots, x_n be the observations

- K scaled and shifted at x_i is $\frac{1}{h}K\left(\frac{u-x_i}{h}\right)$, with support $[x_i - h, x_i + h]$

The *kernel density estimate* is defined as:

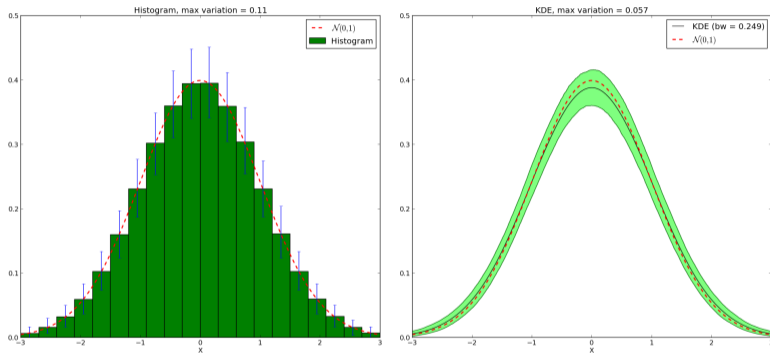
$$f_{n,h}(u) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{u-x_i}{h}\right)$$

- It is a probability density!

[Prove it]

See R script

KDE vs histograms



- KDE has less variability!

Choice of the bandwidth

- **Note.** The choice of the kernel is not critical: different kernels give similar results
- **A problem.** The choice of the bandwidth h is critical (and it may depend on the kernel)
- Mean Integrated Squared Error (MISE) is

$$E\left[\int_{-\infty}^{\infty} (f_{n,h}(u) - f(u))^2 du\right] = \int \int_{-\infty}^{\infty} (f_{n,h,x}(u) - f(u))^2 (f(x))^n du dx$$

where $f(x)$ is the true density function and observations are independent

- For $f(x)$ being the Normal density, the MISE is minimized for

$$h = \left(\frac{4}{3}\right)^{\frac{1}{5}} \cdot s \cdot n^{-\frac{1}{5}} \quad [\textit{Normal reference method}]$$

See R script

Kernel density estimation (KDE)

- **A problem.** The choice of the bandwidth h is critical (and it may depend on the kernel)
- Automatic selection of h
 - ▶ Plug-in selectors (iterative bandwidth selection)
 - ▶ Cross-validation selectors (part of data for estimation and part for evaluation)
- **Another problem.** When the support is finite, symmetric kernels give meaningless results
- Boundary kernels
 - ▶ Kernel (truncation) and renormalization
 - ▶ Linear (combination) kernel
 - ▶ Beta boundary kernels
 - ▶ Reflective kernels (density=0 at boundaries)
- See [[Scott, 2015](#)] for a complete book on KDE

See R script

Optional reference



David W. Scott (2015)

Multivariate density estimation: Theory, practice, and visualization.

John Wiley & Sons, Inc.