Master Program in *Data Science and Business Informatics*

# Statistics for Data Science

## Lesson 15 - Graphical summaries

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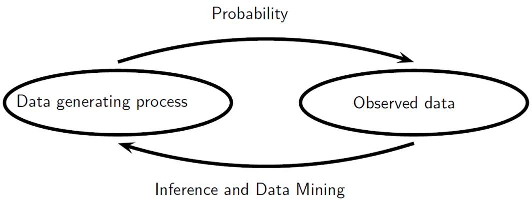
# Condensed observations




- 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-parameteric (general) methods
- Record observations $x_1, \ldots, x_n$ (a dataset)
- $n$ can be large: need to condense for easy visual comprehension
- Graphical summaries:
  - Univariate: empirical distribution functions, histograms, kernel density estimates
  - Multi-variate: kernel density estimates, scatter plots

# The empirical CDF

- A r.v. $X$ is completely characterized by its CDF $F$
- Record observations $x_1, \ldots, x_n$ (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): $\bar{F}_n(x) = 1 - F_n(x)$
- Estimating $F$ through $F_n$ [**Glivenko-Cantelli Thm**]

$$P(\lim_{n \to \infty} \sup_x |F(x) - F_n(x)| = 0) = 1$$

allow for estimating other quantities by plugging $F_n$ in the place of $F$, e.g., $E[X]$ as

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

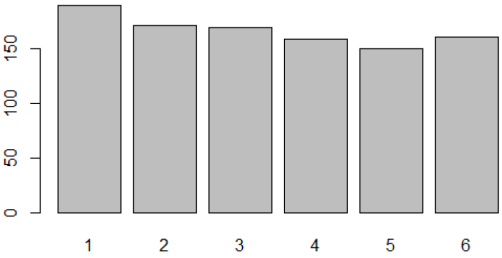
- What about p.m.f. and d.f.?

**See R script**

# p.m.f.: Barplots

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

$$P(X = a) \approx \frac{|\{i \mid x_i = a\}|}{n}$$




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

**See R script**

# d.f.: Histograms

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

$$B_1, \ldots, B_m$$

  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 $A_i$

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

**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

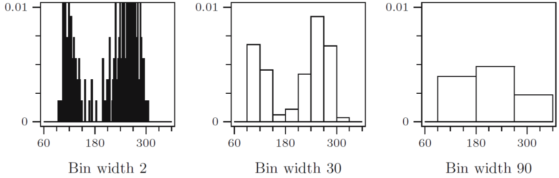



**Fig. 15.2.** Histograms of the Old Faithful data with different bin widths.

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

$$MISE = E\left[\int (\hat{f}(u) - f(u))^2 du\right] = \int \int (\hat{f}(u) - f(u))^2 f(x_1) \dots f(x_n) du dx_1 \dots dx_n$$

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

$b = 3.49 \cdot s \cdot n^{-1/3}$, 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 $x_1, \ldots, x_n$
  - $Q_1$ is 25% percentile of $x_1, \ldots, x_n$
- 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: $0, 1, \ldots, m-1$
    - 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**

# d.f.: Kernels

- 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 $-\infty < u < \infty$

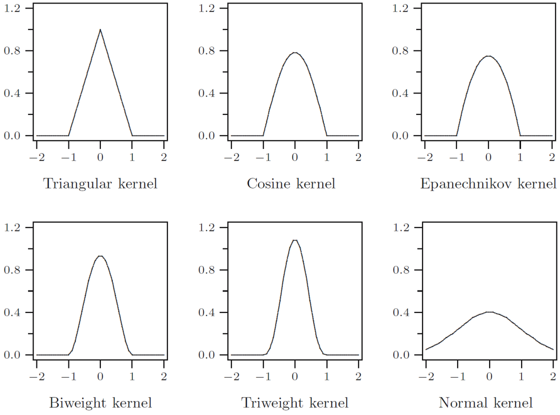



**Fig. 15.4.** Examples of well-known kernels $K$.

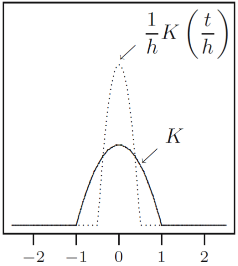
# Kernel density estimation (KDE)

A Kernel is a function $K : \mathbb{R} \to \mathbb{R}$ 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 $|u| > 1$, i.e., support is $[-1, 1]$

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

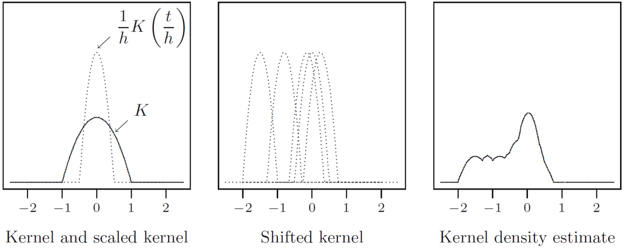
- $h$ controls for how the probability density extends around 0
- if $X \sim K$, then $hX \sim \frac{1}{h} K(\frac{u}{h})$ *[Change-of-units transformation, see Lesson 09]*




CHANGE-OF-UNITS TRANSFORMATION. Let $X$ be a continuous random variable with distribution function $F_X$ and probability density function $f_X$. If we change units to $Y = rX + s$ for real numbers $r > 0$ and $s$, then

$$F_Y(y) = F_X\left(\frac{y-s}{r}\right) \quad \text{and} \quad f_Y(y) = \frac{1}{r} f_X\left(\frac{y-s}{r}\right).$$

# Kernel density estimation (KDE)




Let $x_1, \ldots, x_n$ be the observations

- if $X \sim K$, then $hX + x_i \sim \frac{1}{h}K(\frac{u-x_i}{h})$ *[Change-of-units transformation, see Lesson 09]*
- *$K$ scaled and shifted* at $x_i$, with support $[x_i - h, x_i + h]$

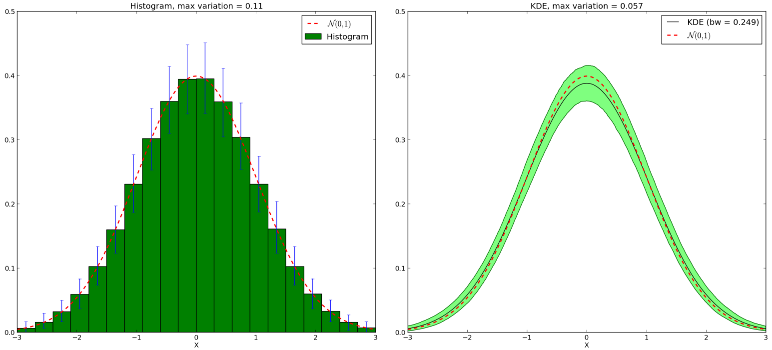
The *kernel density estimate* is defined as the mixture of scaled and shifted kernel densities:

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

- It is a probability density function! **[Prove it!]**

**See R script**

# Histograms vs KDE




- 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 bandwith $h$ is critical (and it may depend on the kernel)
- Mean Integrated Squared Error (MISE) is

$$E[\int_{-\infty}^{\infty}(f_{n,h}(u) - f(u))^2 du] = \int \int_{-\infty}^{\infty}(f_{n,h}(u) - f(u))^2 f(x_1) \dots f(x_n) du dx_1 \dots dx_n$$

  where $f(x)$ is the true density function and observations are independent
- For $f(x)$ being the Normal density, the MISE is minimized for

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

**See R script**

# Kernel density estimation (KDE)

- **A problem.** The choice of the bandwith $h$ is critical (and it may depend on the kernel)
- Automatic selection of $h$
  - Plug-in selectors (iterative bandwith 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.*