THE UNIVERSITY OF
SYDNEY

Lecture 3:
Density estimation

STAT5003

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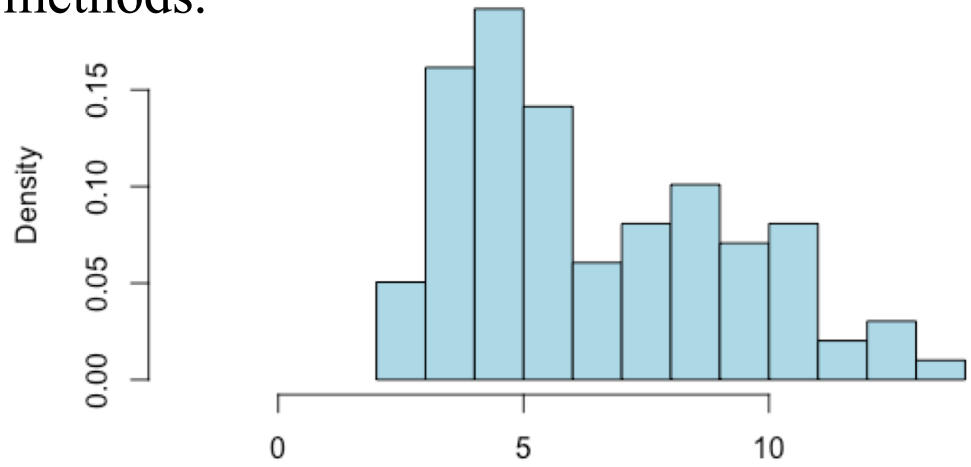
Readings

- An Introduction to Statistical Learning with Applications in R
  - Chapter 7 : Moving Beyond Linearity. Sections 7.1 to 7.5

Density estimation

- In this section of the unit we will introduce density estimation and smoothing methods.



- There are two types of methods classified as *parametric* and *nonparametric*. Compared to *parametric* methods *nonparametric* methods lack of a formal statistical model.
- The methods are generally intended for *description* rather than formal *inference*.
- We learn methods to describe the probability distribution of univariate random variable and multivariate random variables.

Usage of estimating a density function

- In exploratory data analysis, an estimate of the density function can be used
  - to assess multimodality, skew, tail behaviour, etc.
  - in decision making, classification, and summarizing Bayesian posteriors
  - as a useful visualisation tool (a simple summary of a distribution)

- This week our concern is the estimation of a *density function f* using observations of random variables $x_1, \ldots, x_n$ sampled independently from f.

Parametric density estimation

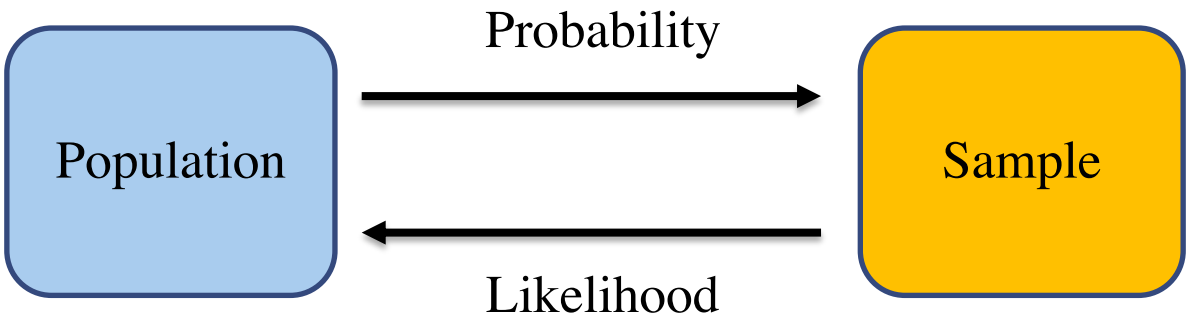
- The *parametric* approach to a density estimation assumes a *parametric* model, $x_1, \ldots, x_n \sim$ i.i.d. $f_{\boldsymbol{\theta}}$, (where $\boldsymbol{\theta}$ is a low-dimensional parameter vector).

  For example, assume $x_i \sim N(m, s)$

- We typically estimate parameters $\widehat{\boldsymbol{\theta}}$ using maximum likelihood.

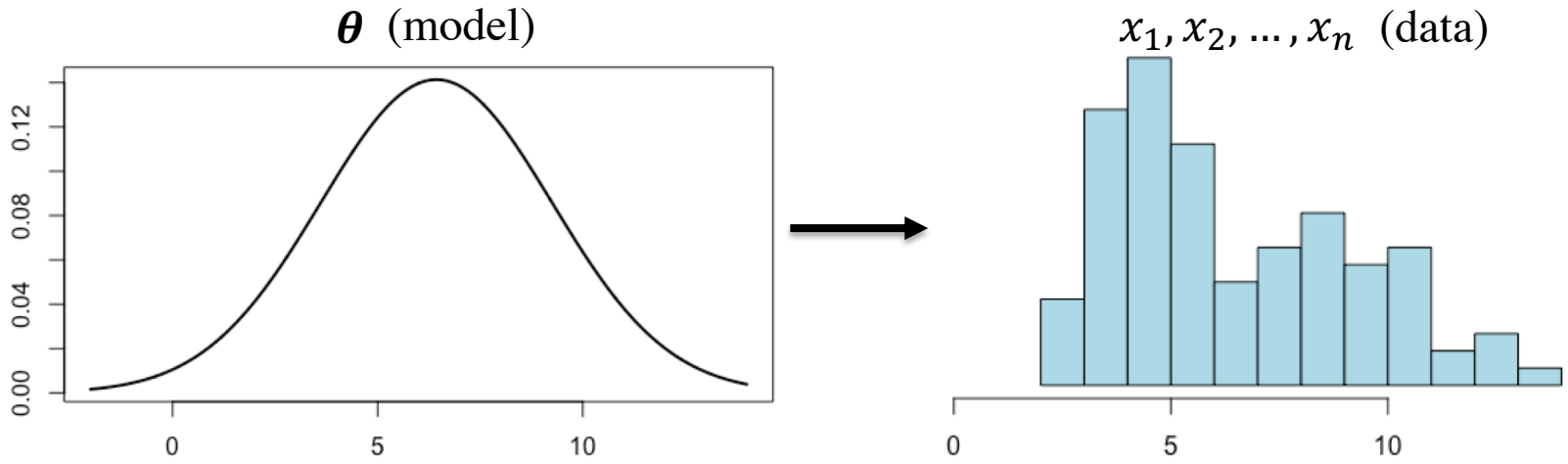
  density at x can be estimated as $f(x|\widehat{\boldsymbol{\theta}})$

- What is likelihood?



Parametric approach – maximum likelihood

$f\ (x_1, x_2, \ldots, x_n|\boldsymbol{\theta})$ Probability of observing $x_1, x_2, \ldots, x_n$ given parameter(s) $\boldsymbol{\theta}$



$$f\ (x_1, x_2, \ldots, x_n|\boldsymbol{\theta}) = f(x_1|\boldsymbol{\theta}) \cdot f(x_2|\boldsymbol{\theta}) \cdot \cdots \cdot f(x_n|\boldsymbol{\theta}) = \prod_{i=1}^{n} f(x_i|\boldsymbol{\theta})$$

Likelihood function is defined as $L(\boldsymbol{\theta}|x_i) = \prod_{i=1}^{n} f(x_i|\boldsymbol{\theta})$

Because maximise log-likelihood is often easier so we commonly maximise the following:

$$L(\boldsymbol{\theta}|x_i) = \prod_{i=1}^{n} f(x_i|\boldsymbol{\theta}) \text{ -> } \ln L(\boldsymbol{\theta}|x_i) = \sum_{i=1}^{n} \ln f(x_i|\boldsymbol{\theta})$$

Non-parametric density estimation

- *Danger with parametric approach*:

  When the assumed model f_θ is incorrect this approach can lead to serious inferential errors.

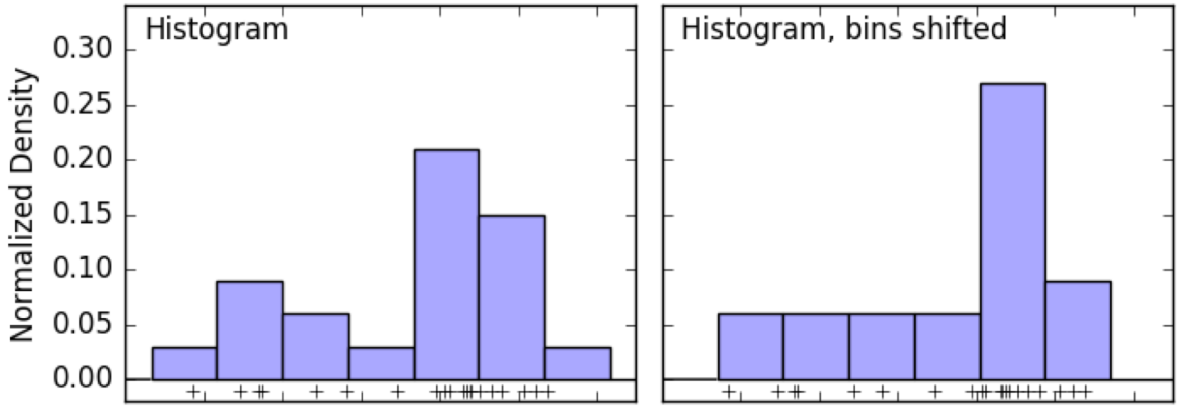
- *Nonparametric* approaches to density estimation
  - ✓ assume very little about the form of f .
  - ✓ use *local information* to estimate f at a point x.

- *Histograms are*
  - ✓ one type of nonparametric density estimators
  - ✓ *piecewise* constant density estimators
  - ✓ produced automatically by most software packages

Histograms

- A histogram can be used as a simple visualization of data;
- In a histogram bins are first defined and then the number of data points within each bin is used to determine the height of the bar plot.

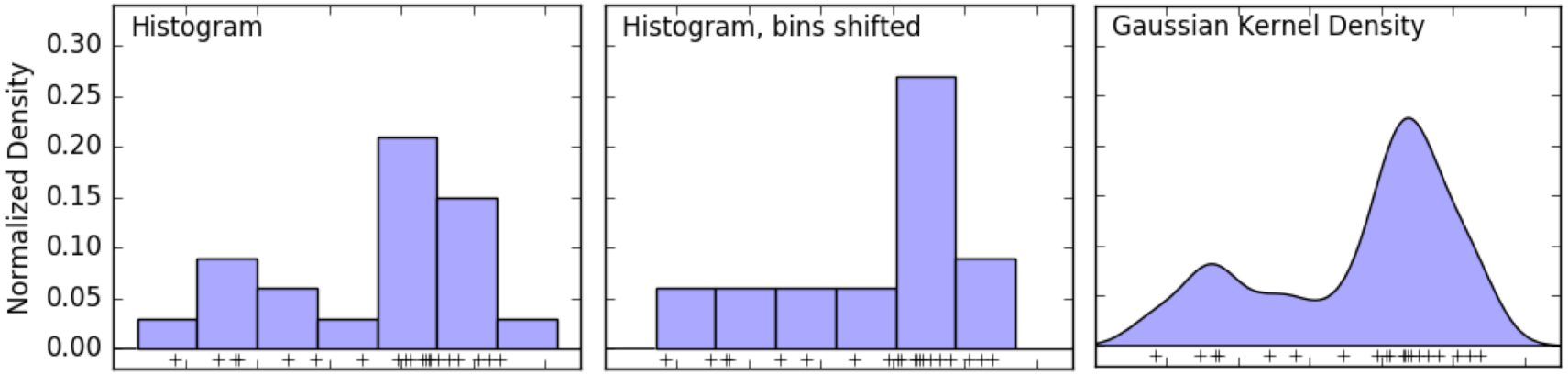
- Two histograms of the same data are shown below (how would you interpret the data according to each of these two histograms?):



- The number of bins are slightly different (7 vs 6)
- Different interpretations of the data.

Demonstrate histogram and parametric method

Refining histogram



- Right plot uses a smoother kernel
  Gaussian kernel density estimate
- each point contributes to a Gaussian curve to the total

→ a smooth density estimate derived from the data,

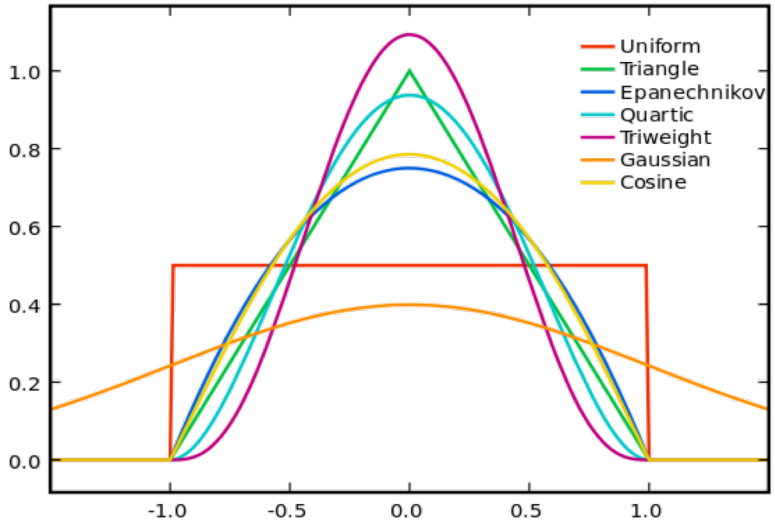
→ a powerful non-parametric model of the distribution of points.

Kernel

- A kernel is a special type of probability density function (PDF) which is *symmetric*.
- A kernel is a function and has the following properties
  - ✓ non-negative
  - ✓ real-valued
  - ✓ symmetric
  - ✓ its definite integral over its support set must equal to 1

- Some common PDFs are kernels:

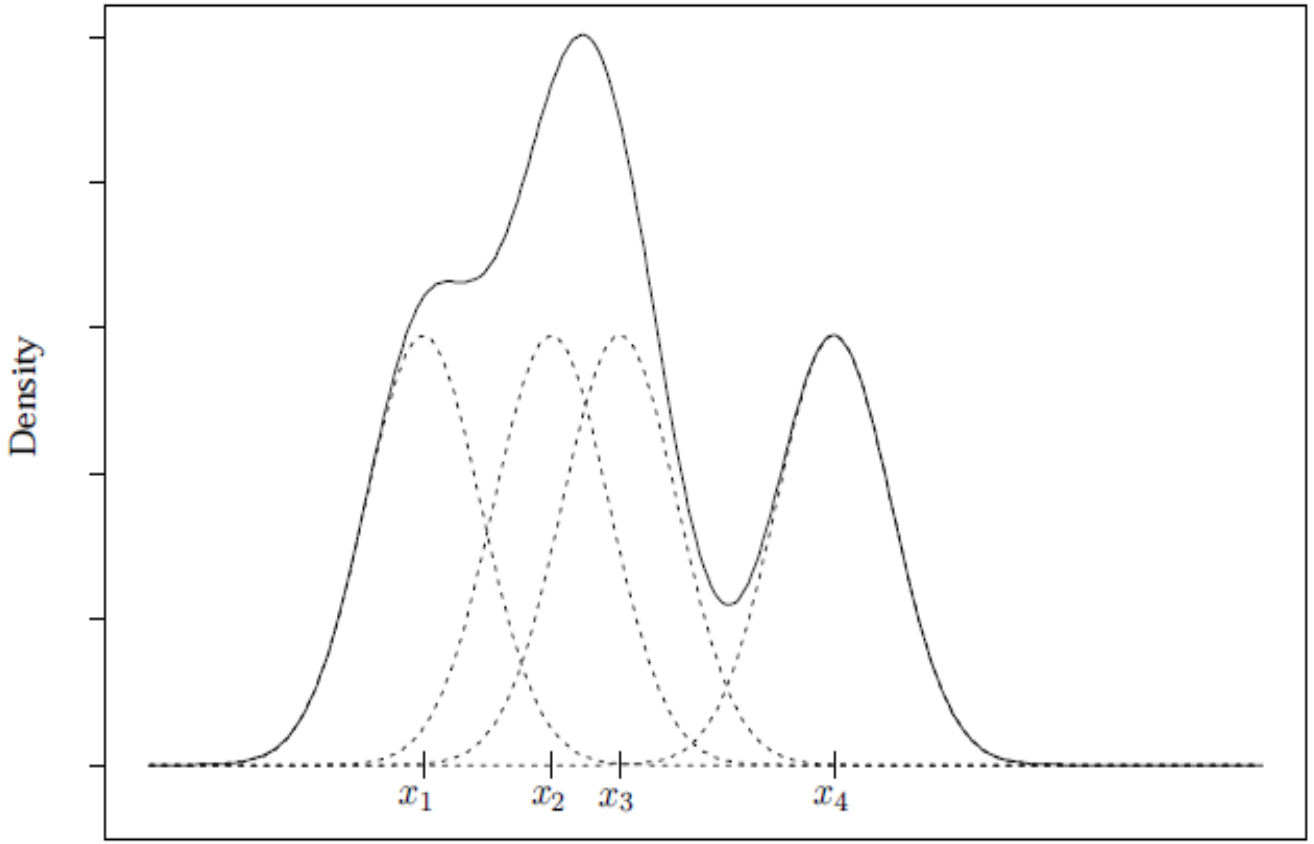
  e.g. Uniform(-1,1) and standard normal distributions.



Kernel density estimation

- Kernel density estimation is a non-parametric approach for estimating the probability density function (*pdf*) of a continuous random variable.
- It is non-parametric because it does not assume any underlying distribution for the *variable* (a.k.a. X does not need to be assumed to follow any specific distribution).
- Essentially, at every data point, a kernel function is created with the point at its centre.
- → the kernel is symmetric around the point.
- The *pdf is estimated* by adding all of these kernel functions and dividing by the number of data to ensure that it satisfies
  - ✓ every possible value of the *pdf* is non-negative.
  - ✓ the definite integral of the *pdf* over its support set equals 1.

Normal kernel density estimate



Normal kernel density estimate (solid) and kernel contributions (dotted) for the sample $x_1, \ldots, x_4$. The kernel density estimate at any x is the sum of the kernel contributions centered at each x_i.

Kernel density estimator

- The simple density estimator that weights all points within h of x equally.

$$\hat{f}(x) = \frac{1}{2hn} \sum_{i=1}^{n} 1_{\{|x - Xi| < h\}},$$

- A univariate *kernel density estimator* allows a more flexible weighting scheme, fitting

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

where

K is a *kernel function* and

h is a fixed number, called the *bandwidth*, *window width*, or *smoothing parameter*.

Constructing a kernel density estimator

1. Choose a kernel; the common ones are normal (Gaussian), uniform (rectangular) and triangular (*kernel functions are positive everywhere and symmetric at zero*).
2. At each point, X_i, build the scaled kernel function

where $$\frac{1}{h} K\left[\frac{(x-X_i)}{h}\right]$$

K[] is the chosen kernel function,
the parameter *h* is the *bandwidth*, window width or ***smoothing parameter***.

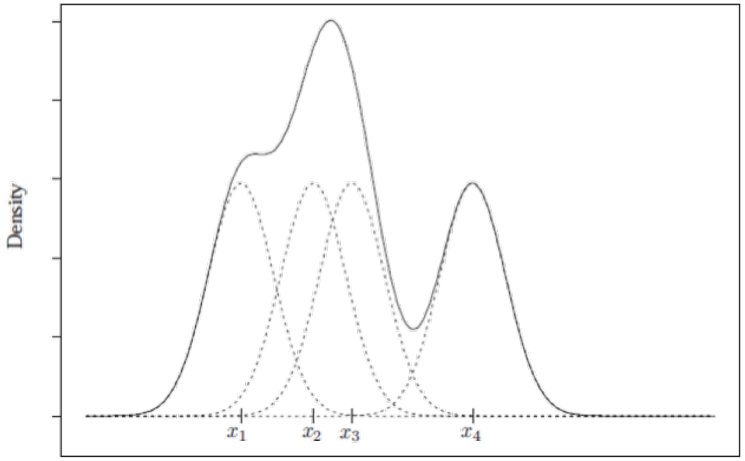
3. Add the individual scaled kernel functions and divide by *n*;

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

- ✓ this places a probability of $^1/_n$ to each x_i
- ✓ it also ensures that the kernel density estimate integrates to 1

Constructing kernel density estimate

- Figure on the right illustrates how a kernel density estimate is constructed from a sample of four univariate observations, $x_1, \ldots, x_4$.



- Centred at each observed data point is a scaled kernel: in this case, *a normal density function divided by 4*. (These contributions are shown with the dotted lines).
- Summing the contributions yields the estimate $\hat{f}$ (solid line).

A sum of "bumps"

- **Intuitively, a kernel density estimate is a sum of "bumps"**.
- A "bump" is assigned to every point, and the size of the "bump" represents the probability assigned at the *neighbourhood of values* around that point;
- thus, if the data set contains
  - 2 data points at $x = 1.5$
  - 1 data point at $x = 0.5$
- then the "bump" at x=1.5 is twice as big as the "bump" at x=0.5.

- Each "bump" is centred at the point, and spreads out symmetrically to cover the neighbouring values around the point.

Choice of kernels

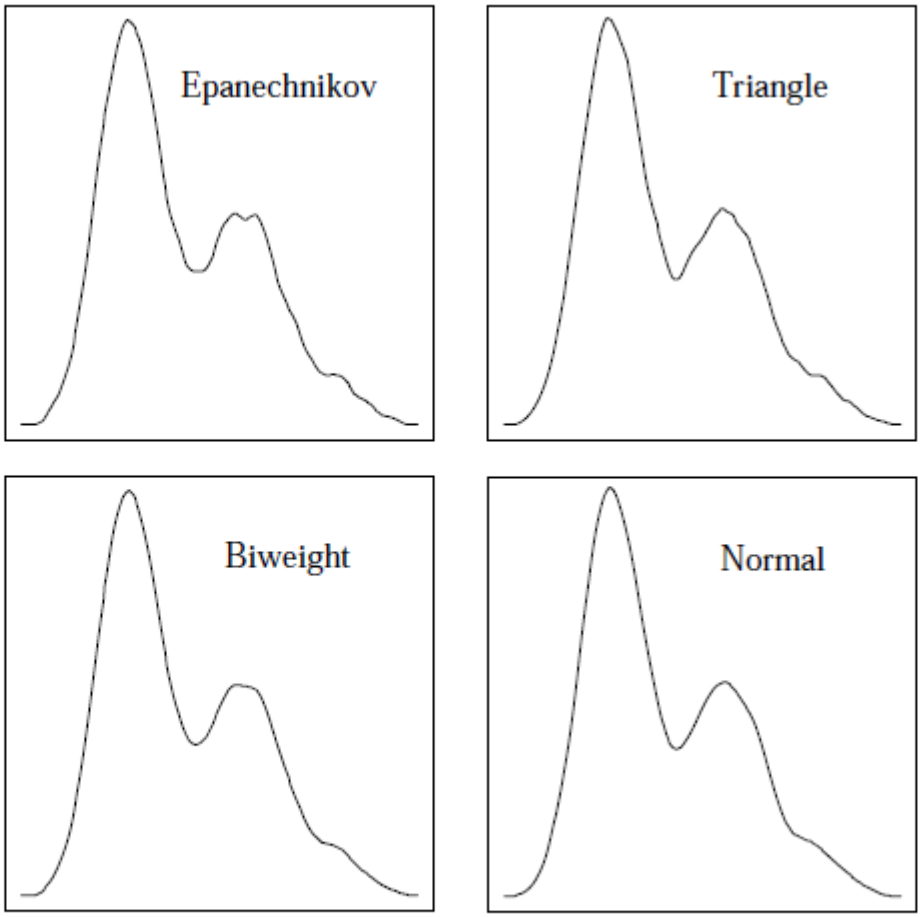
- Kernel density estimation requires specification of two components: the kernel and the bandwidth.

- The shape of the kernel has much less influence on the results than does the bandwidth.
- Some choices for kernel functions are,

Kernel	**Equation**
Uniform	$k_0(u) = \frac{1}{2} 1\left(\lvert u\rvert \leq 1\right)$
Epanechnikov	$k_1(u) = \frac{3}{4}\left(1-u^2\right) 1\left(\lvert u\rvert \leq 1\right)$
Biweight	$k_2(u) = \frac{15}{16}\left(1-u^2\right)^2 1\left(\lvert u\rvert \leq 1\right)$
Triweight	$k_3(u) = \frac{35}{32}\left(1-u^2\right)^3 1\left(\lvert u\rvert \leq 1\right)$
Gaussian	$k_\phi(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$

- See also: https://en.wikipedia.org/wiki/Kernel_(statistics)#Kernel_functions_in_common_use

Different kernel estimates for “bimodal.dat”



Bimodal density, cont.

- Previous figure shows kernel density estimates for the data with equally weighted mixture of $N(4, 12)$ and $N(9, 22)$ densities.
- All the bandwidths were set at 0.69 for the canonical kernels of each shape.

➢ The results for all the kernels are qualitatively the same.

- Even quite different kernels can be scaled to produce such similar results that the choice of kernel is unimportant.

Kernel density estimation in R

- The density() function in R computes the values of the kernel density estimate.
- Applying the plot() function to an object created by density() will plot the estimate.
- Applying the summary() function to the object will reveal useful statistics about the estimate.

Demonstrate kernel density estimation

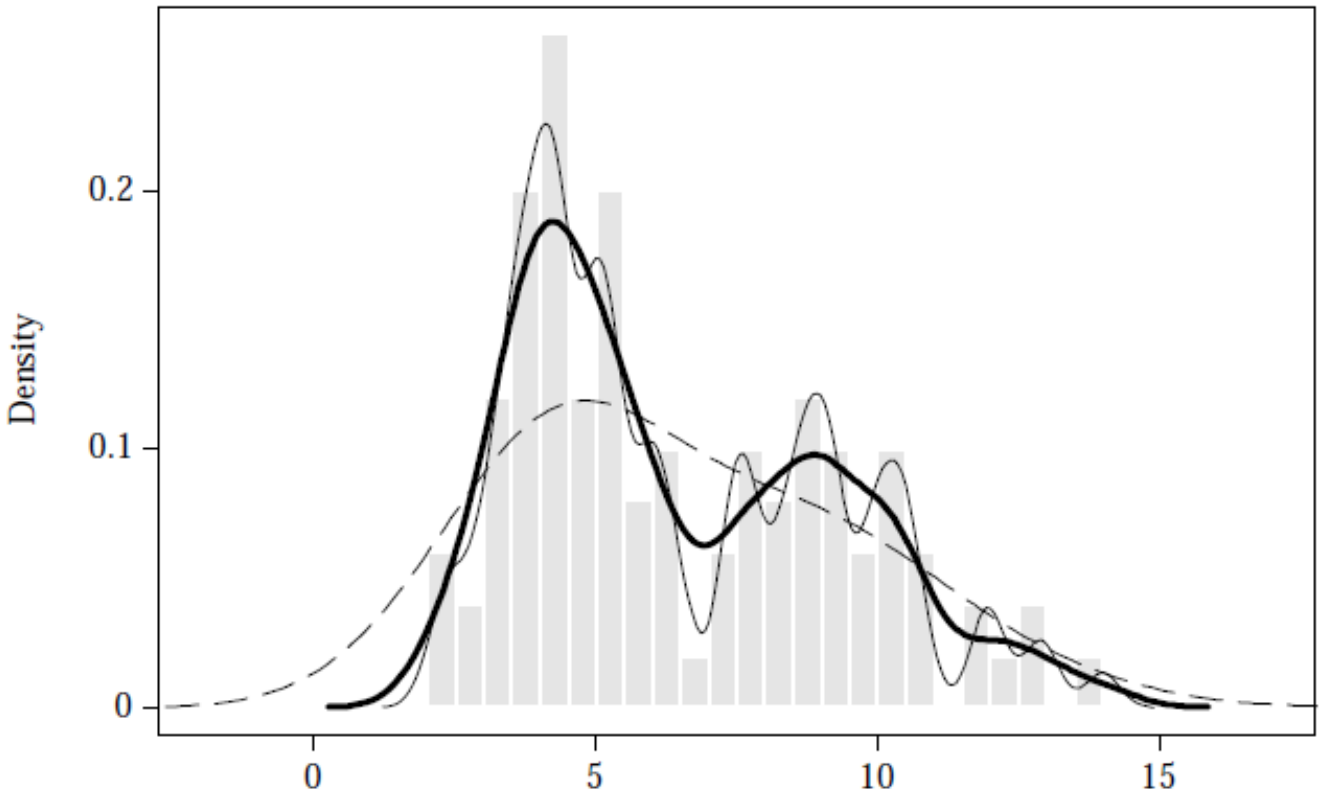
Value chosen for the bandwidth

- The density estimator

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

- is a *fixed-bandwidth kernel density estimator* since h is constant.
- The value chosen for the bandwidth exerts a strong influence on the estimator $\hat{f}$.
- If h is too small, the density estimator will tend to assign probability density too locally near observed data
  →a wiggly estimated density function with many false modes.
- If h is too large, the density estimator will spread probability density contributions too diffusely
  → smooths away important features of f.

Value of bandwidth affects smoothness



- In above, the bandwidths are 0.3, 0.625, and 1.875
- Demonstrate the above effect in R.

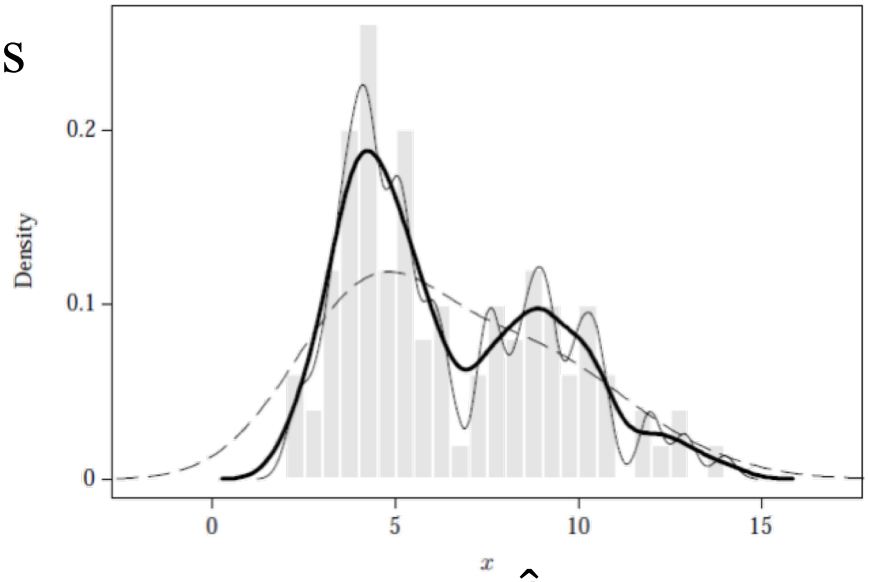
Bimodal density in the above example

- The effect of bandwidth is shown in previous slide.
- This histogram shows a sample of 100 points from an equally weighted mixture of $N(4,\ 12)$ and $N(9,\ 22)$ densities.
- Three density estimates that use a standard normal kernel are superimposed, with different bandwidths, h:

- $h = 1.875$ (*dashed*) is clearly *too large* → oversmooth density estimate that fails to reveal the bimodality of f.
- $h = 0.3$ (*solid*) is too small a bandwidth →undersmoothing, the density estimate is too wiggly with many false modes.
- $h = 0.625$ (*heavy*) is adequate → represents main features of f while suppressing most effects of sampling variability.

Choice of bandwidth

- The bandwidth parameter controls the smoothness of the density estimate.



- → the bandwidth determines the trade-off between the *bias* and *variance of estimator* $\hat{f}$.

✓ A small bandwidth produces a density estimator with wiggles indicative of *high variability* caused by under smoothing.

✓ A large bandwidth causes important features of *f* to be smoothed away, thereby causing *bias*.

- (the trade-off between the *bias* and the *variance of an estimator* is important in nearly all kinds of model selection, including density estimation, smoothing, regression, and classification)

Integrated squared error (ISE)

- To evaluate $\hat{f}$ as an estimator of f over the entire range of support, one could use the *integrated squared error* (ISE):

$$\mathrm{ISE}(h) = \int_{-\infty}^{\infty} \left[\hat{f}(x) - f(x)\right]^2 \, dx$$

the ISE(h) gives the square of the distances from $\hat{f}(x)$ to $f(x)$ for the *observed data*.

- To discuss the generic properties of an estimator, without reference to a particular observed sample, it is more sensible to average ISE(h) over *all* samples that might be observed.
- This gives the *mean integrated squared error* (MISE):

$$\mathrm{MISE}(h) = E\{\mathrm{ISE}(h)\}$$

See http://demonstrations.wolfram.com/VarianceBiasTradeoff/

Cross-validation

- Cross-validation, is a model validation technique for assessing how the results of a statistical analysis will generalize to an independent data set.
- It is mainly used when one wants to estimate how accurately a *predictive model* will perform in practice.
- In a prediction problem, a model is usually given

✓ a dataset of *known data* on which training is run (*training dataset*),

✓ and a dataset of *unknown data* (or *first seen* data) against which the model is tested (*testing dataset*).

Goal of cross-validation

- The goal of cross validation is to define a dataset to "test" the model in the training phase (i.e., the *validation dataset*), in order to
  - ➢ limit problems like overfitting,
  - ➢ give an insight on how the model will generalise to an independent dataset (i.e., an unknown dataset, for instance from a real problem), etc.
- One round of cross-validation involves

✓ partitioning a sample of data into complementary subsets,

✓ performing the analysis on one subset (called the *training set*), and

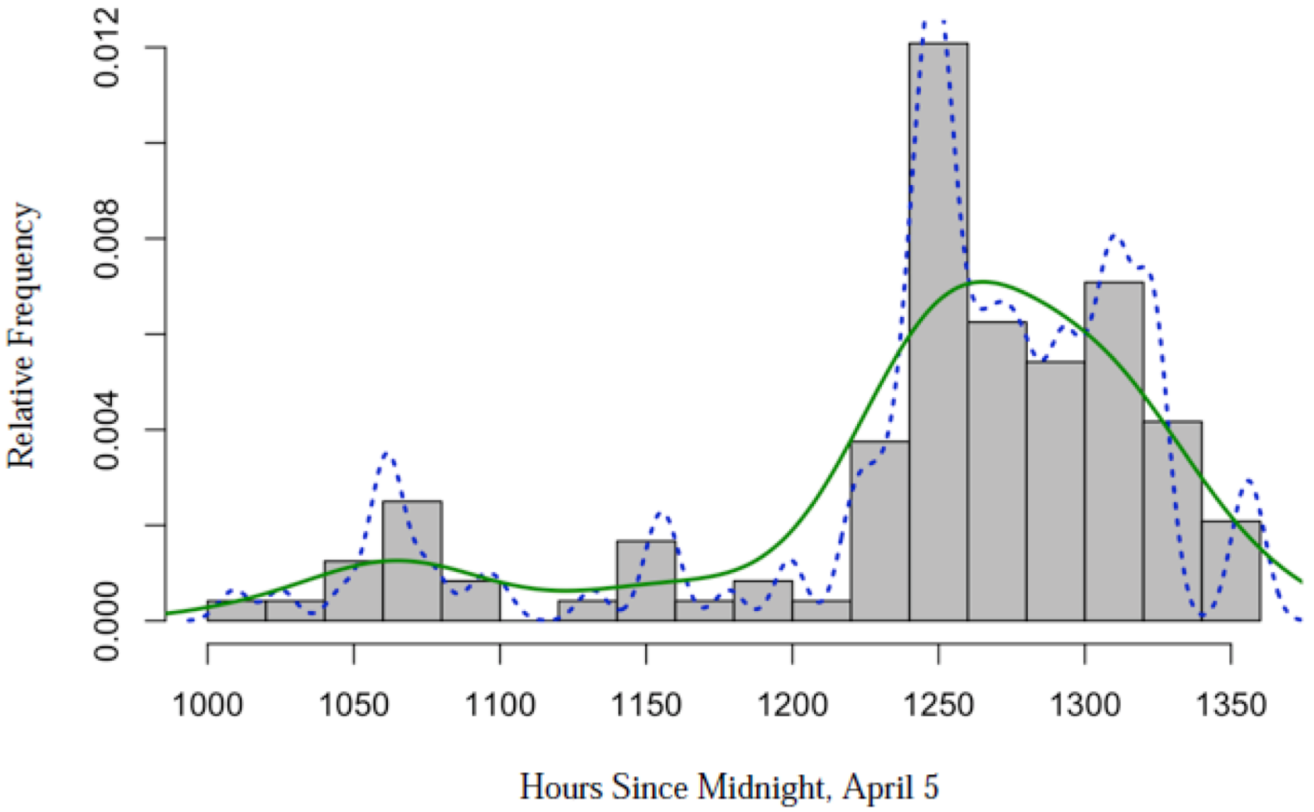
✓ validating the analysis on the other subset (called the *validation set* or *testing set*).

Why use cross-validation

- Many bandwidth selection strategies begin by relating h to some measure of the quality of $\hat{f}$ as an estimator of f.
- The quality is quantified by some $Q(h)$, whose estimate, $\widehat{Q}(h)$, is optimized to find h.
- If $\widehat{Q}(h)$ evaluates the quality of $\hat{f}$ based on how well it fits the observed data → observed data are being used twice:
  - ✓ once to calculate $\hat{f}$ from the data and a
  - ✓ second time to evaluate the quality of $\hat{f}$ as an estimator of f.
- Double use of the data provides an overoptimistic view of the quality of the estimator leading to overfitting.

- → Cross-validation provides a remedy to this problem.

Demonstration of CV for bandwidth selection



Using cross-validation criteria

- Previous figure shows the results of kernel density estimates for these data using the *normal kernel (see previous slide)*.

1. The result from using a $h = 5.18$ (dotted curve)
   → bad, the bandwidth is clearly too small.
2. Minimizing Biased CV(h) with respect to h yields $h = 26.43$ (solid line)
   → the better option in this case, emphasizes only the most prominent features of the data distribution.

- Biased CV [BCV(h)]: a type of CV that optimises asymptotic MISE (AMISE) instead of MISE. Lower variance but reasonable bias. (See additional reference)

- Perhaps a bandwidth around 26 would be preferable.

Spline methods

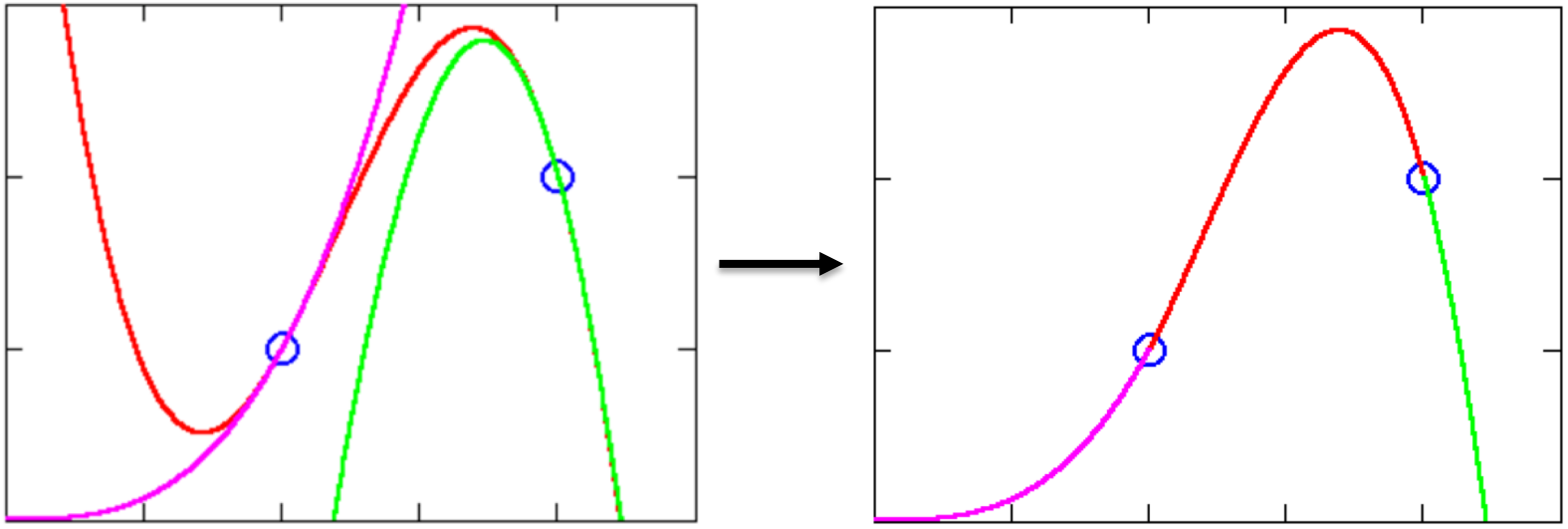
Cubic spline

- A *cubic spline* is a piecewise cubic function that is everywhere twice continuously differentiable but whose third derivative may be discontinuous at a finite number of pre-specified *knots*.

- A *cubic spline* is a function created from cubic polynomials on each *between-knot* interval by pasting them together twice continuously differentiable at the knots.

- https://www.youtube.com/watch?v=f4iNbNRKZKU
  http://wmueller.com/precalculus/families/splines.html

Visually, cubic spline “concatenate” cubic polynomial lines



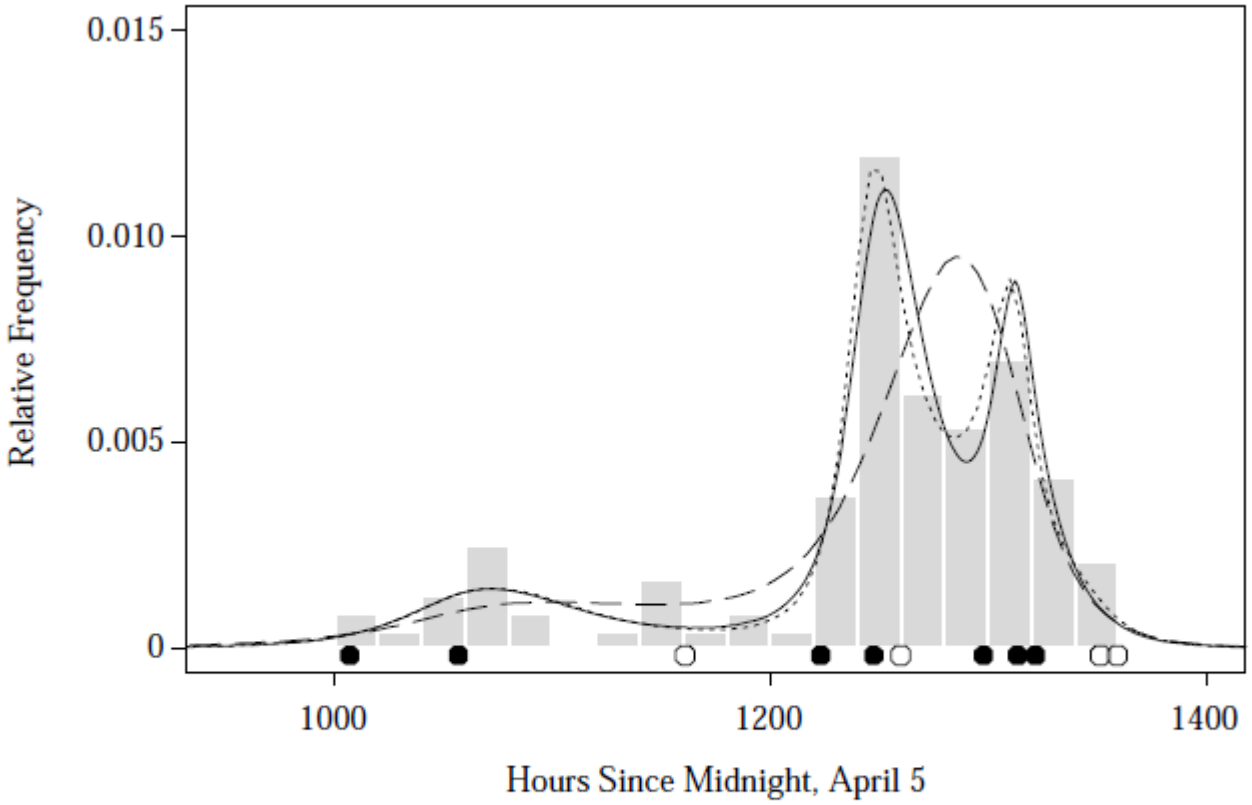
Cubic spline for density estimation

- Cubic spline can be used for estimating an unknown density function f based on sample data.
- One approach is to use maximum likelihood estimation to estimate $\log(f)$ by a cubic spline that have a finite number of pre-specified knots.
  - The knots are placed at selected order statistics of the sample data.
  - The number of knots can be determined either by a simple rule or by minimizing BIC (Bayes information criterion).

- The method works well both in obtaining smooth estimates and in picking up small details.

Logspline density estimate

Kooperberg and Stone's logspline density estimation approach estimates the log of f by a cubic spline



Whale migration example, continued

- Estimation of local modes can sometimes be a problem if there are too few knots or if they are poorly placed.
- The other lines in previous figure show the logspline density estimates with two other choices for the knots.
- The very poor estimate (dashed line) was obtained using 6 knots.
- The other estimate (dotted line) was obtained using all 11 knots shown in the figure with either hollow or solid dots.

Useful references and videos

- C. Kooperberg and C. J. Stone. Logspline density estimation for censored data. *Journal of Computational and Graphical Statistics*, 1:301–328, 1992
- https://cran.r-project.org/web/packages/HSAUR/vignettes/Ch_density_estimation.pdf

- https://www.youtube.com/watch?v=QSNN0no4dSI (first 53 mins)
- https://www.youtube.com/watch?v=WlK8PdHL_qc
- https://www.youtube.com/watch?v=f4iNbNRKZKU