Lecture: Kernel Density Estimator

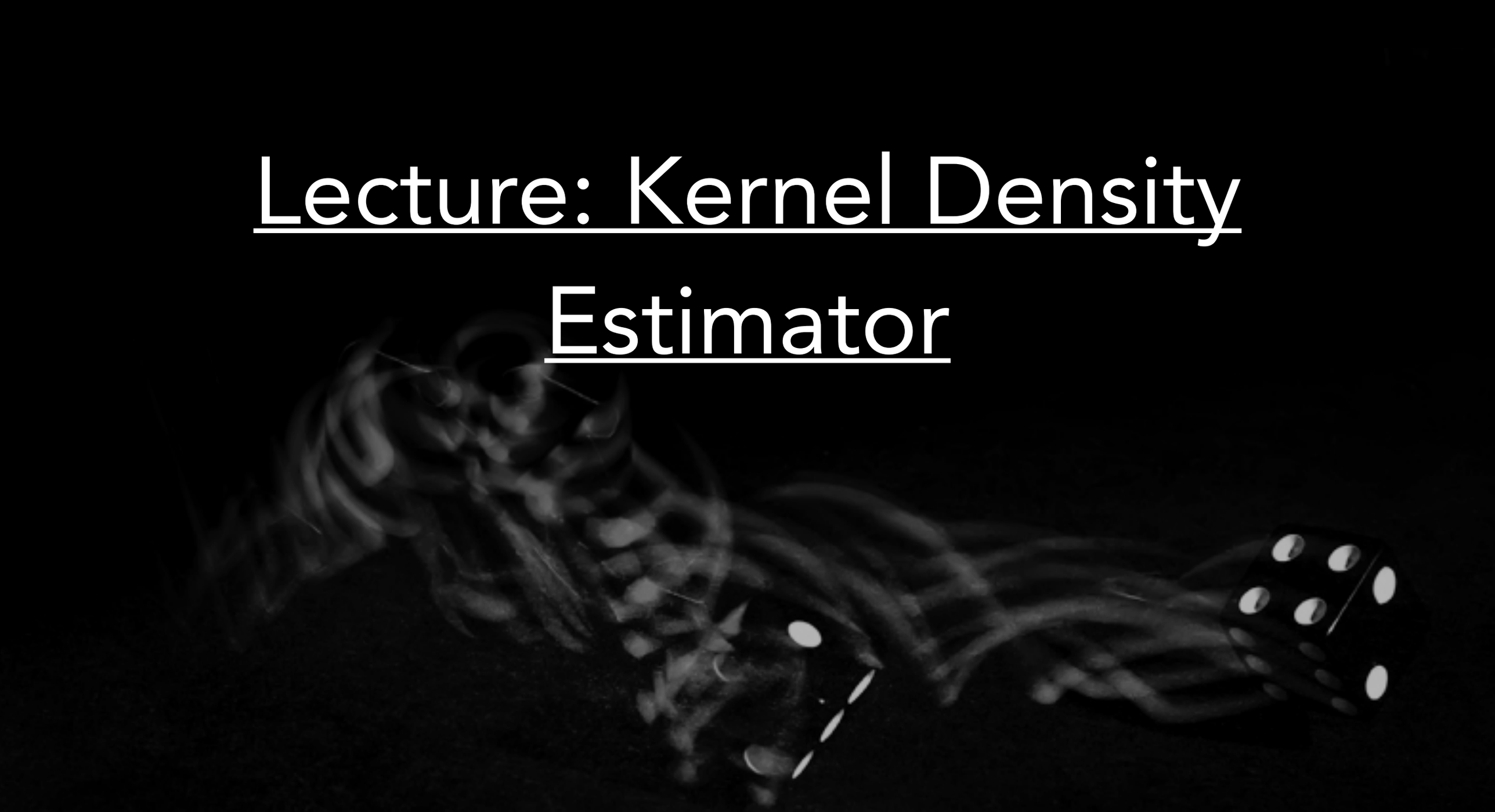

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Photo by Howard Jackman

Overview

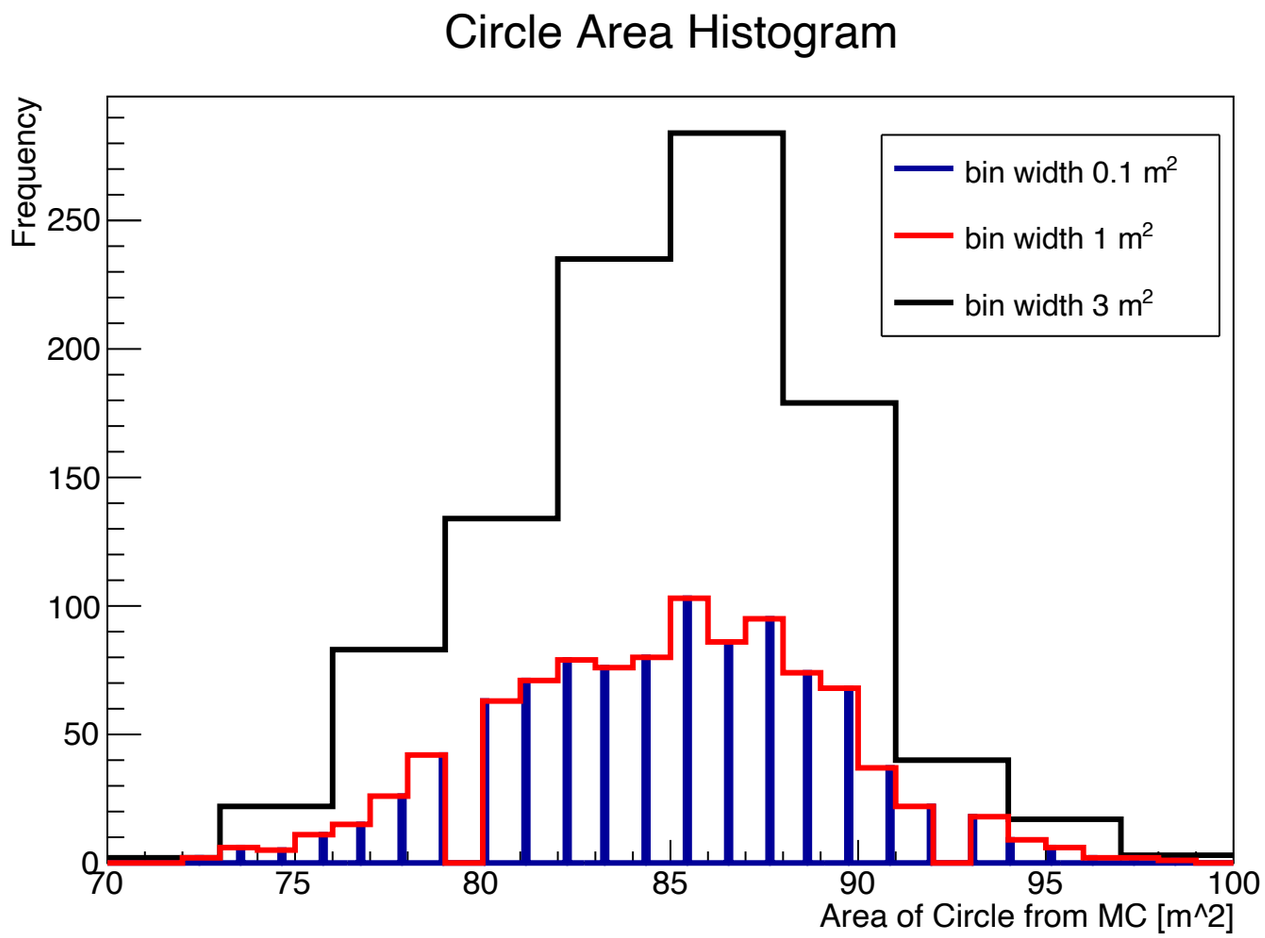
- Much of what we have covered has been parameter estimation — best-fit values and uncertainties — using analytic or defined density expressions
- Today we cover density estimates derived from the data or Monte Carlo itself

- The methods are regularly employed on finite data samples that may benefit from smoothing, or require non-parametric methods to get a probability distribution (function)

- Last few slides of this lecture contain extended literature for further reading

Histogram

- The histogram is one of the most simple forms of a non-parametric data-driven density estimator
- But, the only two histogram parameters (bin width and bin position(s)) are arbitrary



*From Lecture 1

Histograms

- The histogram is one of the most simple forms of a non-parametric data-driven density estimator
- But, the only two histogram parameters (bin width and bin position(s)) are **arbitrary**
  - Histograms are not smooth, but if the underlying true PDF *is smooth* then it would be good that our density estimator/function is smooth
  - More dimensions requires more data in order to have a multi-dimensional histogram which can match the true PDF
- We can avoid some of these issues with density estimates by using something more sensible than a histogram

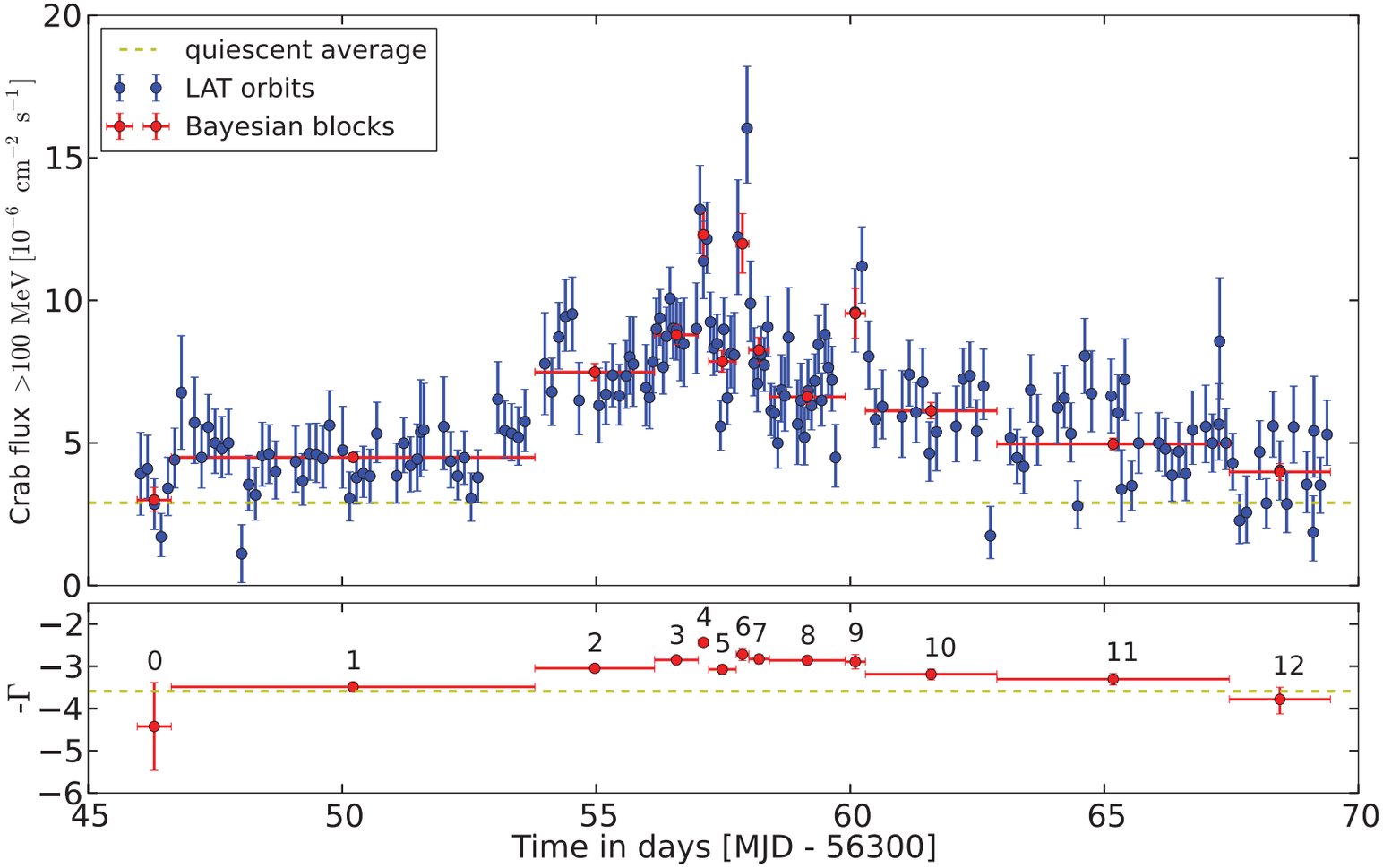
Wish List

- For density estimates what do we want?
  - Non-parametric, i.e. no explicit requirement for the form of the PDF
  - (Easily) extendable to higher dimensions
  - Use data to get local point-wise density estimates which can be combined to get an overall density estimate
    - Smooth
      - At least smoother than a ‘jagged’ histogram
  - Preserves real probabilities, i.e. any transformation has to give PDFs which integrate to 1 and don’t ever go negative
- The answer… Kernel Density Estimation (KDE)
  - Sometimes it is “Estimator” too for KDE

Bayesian Blocks

- An alternative to constant bins for histograms is to use Bayesian Blocks developed by J.D. Scargle*
  - Bayesian Blocks are very useful for determining time varying changes
  - Covers many, but not all, wish list items

$$\text{Crab Flux} = \frac{dN}{dE} \propto E^{-\Gamma}$$



*arXiv:1308.6698

Basics of Data Driven Estimation

- Localized regions in parameter space are expected to have approximately equal probabilities
  - The smaller the region(s) the more supported our assumption that probability is constant
  - The more data in each region the more accurate the density estimate

- We will keep the region fixed and find some compromise; large enough to collect some data, but small enough that our probability assumption is reasonable
  - For more thorough treatment of the original idea see the articles by Parzen and Rosenblatt in the last slides of this lecture

Example in 1 dimension

- Start with a uniform probability 'box' around data points:

$$K(u) = \begin{cases} 0.5, & \text{for } |u| \leq 1 \\ 0, & \text{for } |u| > 1 \end{cases}$$

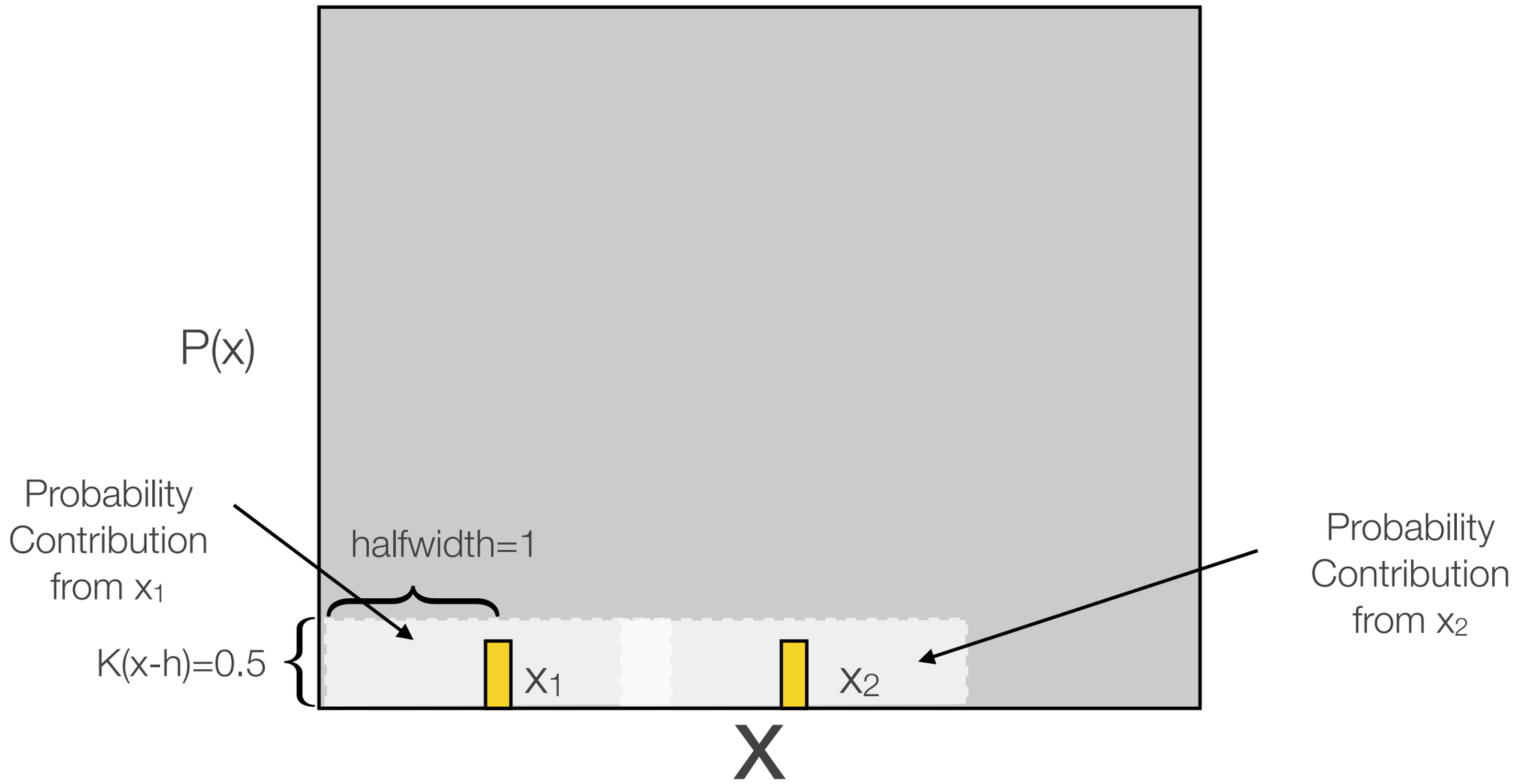
- Notice that this kernel K(u) is normalized. The **kernel is always normalized!!** The total width is 2*1, so the 'height' (h) must be

$$h = \frac{1}{2 * 1}$$

- For a 1D set of data ($\vec{x}$), then $u = (x - x_n)/L$, where L is a distance near a data point that has a non-zero probability
  - The value of h or L is set by the analyzer
  - Here, the L=1
  - x_n are all the individual data points in the total data set ($\vec{x}$)
  - Similar to a function, e.g. f(x), 'x' represents all possible values of x.

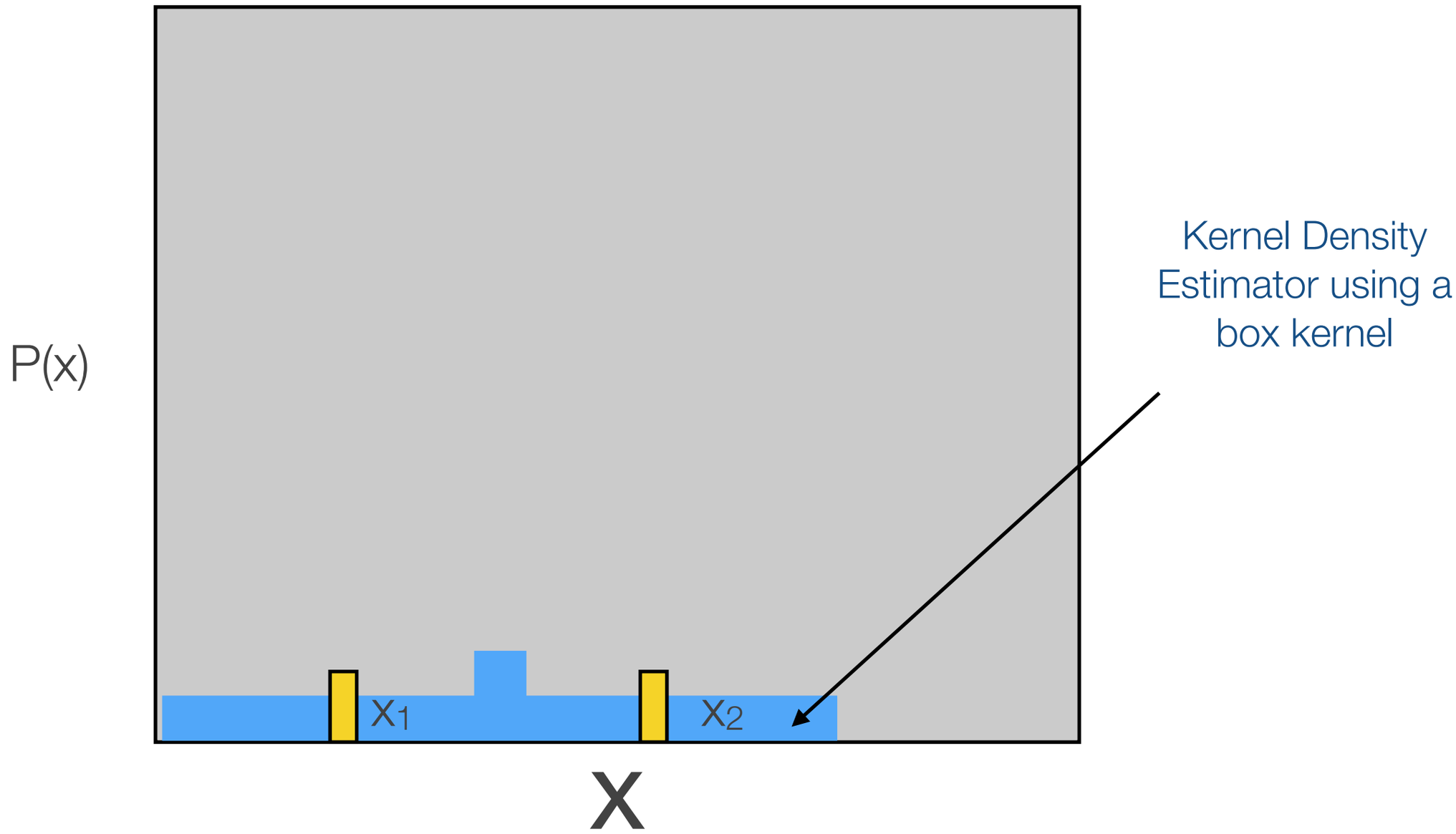
KDE by pieces

- For 2 data points (x_1 and x_2) we can produce a data driven probability density P(x) using a box of total width=2 and height=0.5 centered at each data point



Final KDE

- Combine the contributions, normalize the new function to 1, and we have generated a data driven PDF.



Hyper-Cube

- Our extended 'region' definition is a D-dimensional hyper-cube with lengths equal to $2h$ on each side
- We include all points within the hyper-cube volume via a weighting scheme. This is known as the kernel (K) which is for this KDE:

$$K(\vec{x}_i) = \begin{cases} 0.5, & \vec{x}_i \text{ in region } \mathfrak{R}_d \\ 0, & \vec{x}_i \text{ outside region } \mathfrak{R}_d \end{cases}$$

$$\text{for some } \mathfrak{R} \text{ centered at point } \vec{x}_d$$

- Sometimes you will see the kernel as K(u) where u is the 'distance' from x_i to x_d
- The above description is only for a box kernel, and will change depending on the kernel

Kernel Characteristics

- The integrated kernel **always** equals 1, for any and every KDE

$$\int_{-\infty}^{+\infty} K(u)du = 1$$

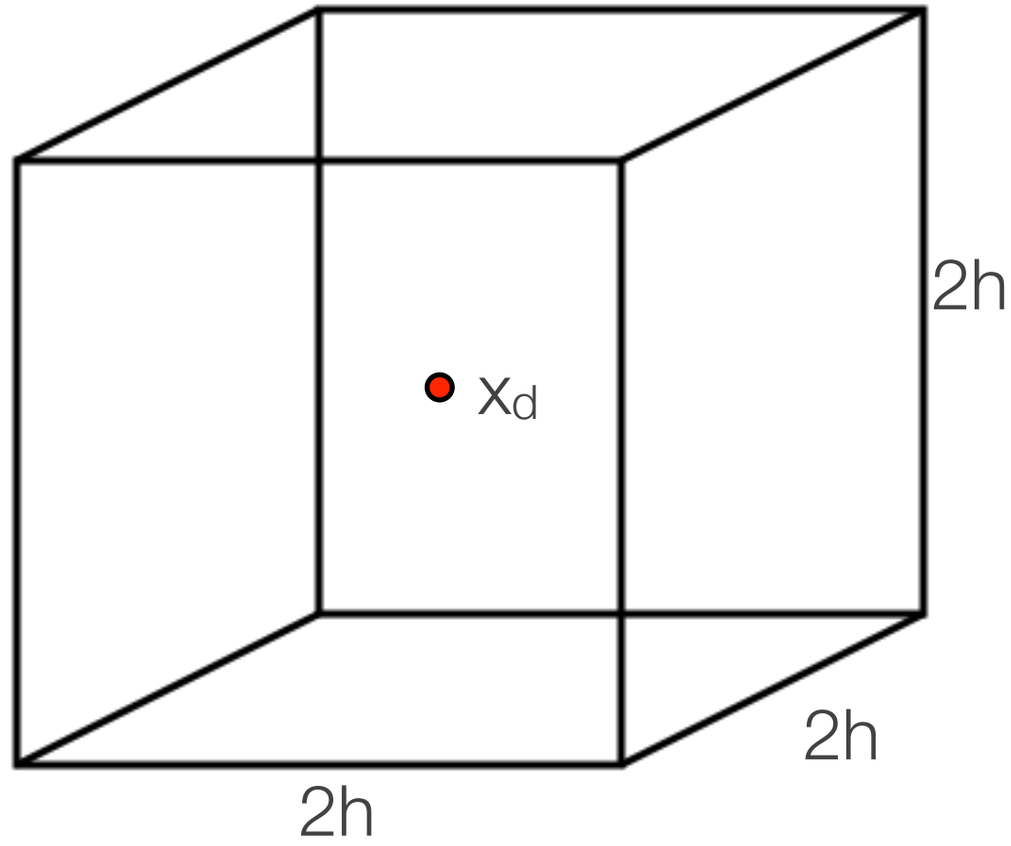
- If ‘u’ is multidimensional, then so is the integration. But, the integral is **always** 1.
- Even if the kernel is not transformed to be 1D, e.g. K(x,y,z) instead of K(u), the integral of the kernel is always 1.

$$\iiint K(x, y, z)\, dx\, dy\, dz = 1$$ 3D in cartesian coordinate x, y, and z

$$\int \cdots \int K(s_1, \ldots, s_k)\, ds_1 \ldots ds_k = 1$$ k-dimensions represented by $\vec{s}$

Visual Region

- Everything within the hyper-cube is included with an appropriate value (also known as a *weight*)
- For the density estimator we need:
  - To normalize by the total number of events in the sample (N)
  - The kernel is always normalized, i.e. integral or sum equals 1
- The PDF estimator (P_{KDE}) is now constructed from the individual data points
- The illustration is the estimation at a single point $x_d \in x$



$$P_{KDE}(\vec{x}) = \frac{1}{N}\sum_{n=1}^{N} K(\frac{\vec{x}-\vec{x}_n}{h})$$

Exercise 1

- Use a fixed length hyper-cube KDE in 1D

- Using the following data [1,2,5,6,12,15,16,16,22,22,22,23] for the finite data sample and h=1.5
  - Normalize the kernel!!!!!!!!
    - If the total width is 2h then kernel height is 1/(2h), i.e.K(u)=1/(2h) or K(u)=0
- Because the length is $2h$, to be in the hyper-cube each data point x_i only needs to be $\pm h$ in each dimension from x_d
- Calculate $P_{KDE}(x=6)$, $P_{KDE}(x=10.1)$, $P_{KDE}(x=20.499)$, and $P_{KDE}(x=20.501)$

Code this by-hand, i.e. no external packages

Exercise 1 Example

- Calculate the $P_{KDE}(x=6)$ by taking all 12 data points and seeing if they are within $\pm h$ of x=6, i.e. in the range 4.5 to 7.5.
- We include the data point at x=6 in the KDE

$$P_{KDE}(x=6) = \frac{1}{12}\sum_{n=1}^{N} K\left(\frac{6-\vec{x}_n}{1.5}\right)$$

$$= \frac{1}{12}\left[K\left(\frac{6-1}{1.5}\right) + K\left(\frac{6-2}{1.5}\right) + K\left(\frac{6-5}{1.5}\right) + K\left(\frac{6-6}{1.5}\right) + K\left(\frac{6-12}{1.5}\right) + ... + K\left(\frac{6-23}{1.5}\right)\right]$$

$$= \frac{1}{12}\left[0+0+\frac{1}{3}+\frac{1}{3}+0+0+0+0+0+0+0+0\right]$$

Exercise 1 (optional)

- Instead of examining KDEs in 1D, we can use the same kernel form, i.e. the top-hat, and extend it to 2D.
- We will use a 2D top-hat kernel with $h_x = 1.5$ and $h_y = 0.9$, and data as [(1,2), (2, 2.2), (5, 4.9), (6, 1.7), (12, 0.4), (15, 3.7), (16, 3.2), (16, 2.9), (22, 1.1), (22, 1.0), (22, 1.7), (23, 4.2)]
  - Remember that the kernels always integrate/sum to 1
- Calculate $P_{KDE}(6,\ 1.7)$, $P_{KDE}(10.2,\ 2.1)$, and $P_{KDE}(22.2,\ 2.1)$
- Make a colored 2D probability density plot from the $P_{KDE}(x, y)$

KDE Comments

- The function K() is known as the kernel, and *h* is the bandwidth
- Larger bandwidths mean more smoothing, but it can remove real features
- Smaller bandwidths will approach the true PDF better, but need lots of data points otherwise they are ‘bumpy’
- The fixed window KDE is similar to a histogram, but has better support for local densities
  - The bin ‘width’ is still arbitrary for this box/top-hat/Parzen-Rosenblatt kernel **and** a histogram, but unlike a histogram the bin ‘location’ is no longer arbitrary

Hyper-Cube

- We could use the hyper-cube kernel to construct a probability density, but there are a few drawbacks to a hyper-cube kernel
  - We have discrete jumps in density and limited smoothness
  - Nearby points in x have some sharp differences in probability density, e.g. $P_{KDE}(x=20.499)=0$ but $P_{KDE}(x=20.501)=0.08333$
  - All data have equal contribution to the estimated PDF density regardless of distance to the estimation point

- So let's switch to a different kernel with weights that decrease smoothly as a function of distance from the estimation point

Gaussian Kernel

- The generic KDE expression remains similar, e.g.

$$P_{KDE}(\vec{x}) = \frac{1}{N}\sum_{n=1}^{N} K(\frac{\vec{x} - \vec{x}_n}{h})$$

- The kernel is now (and there is no 'h' because we're switching to a gaussian kernel):

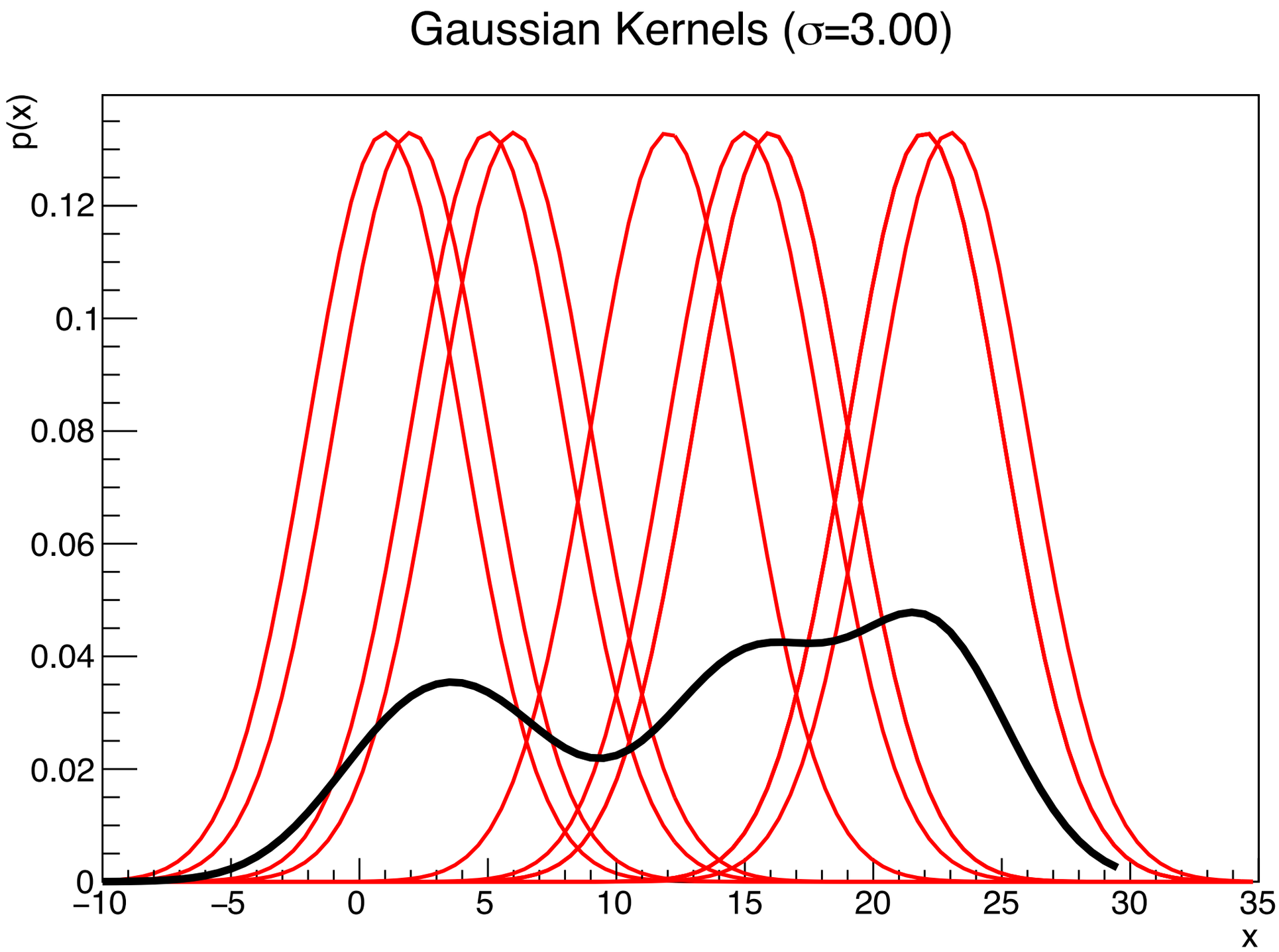
$$K(\vec{x}, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{|\vec{x}-\vec{x}_n|^2}{2\sigma^2}}$$

- The kernel at each data point now contributes a non-zero probability from [-∞,+∞] smoothly with decreasing contributions as a function of distance
  - Each data point and corresponding kernel integrate to 1 over the whole parameter space

Exercise 2

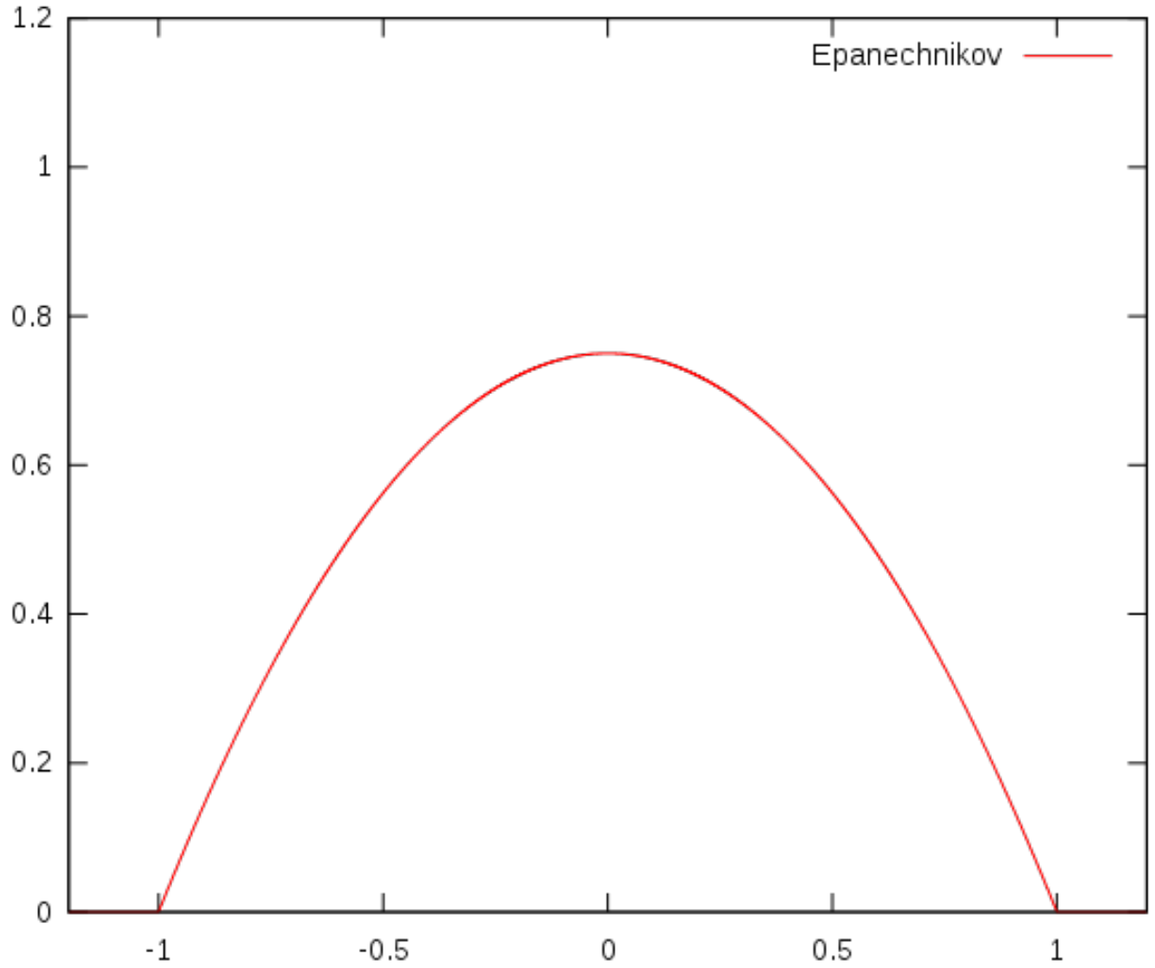
- Redo exercise 1 using the new Gaussian kernel
- For the gaussian width use $\sigma=3$
- Calculate the KDE two ways:
  - Writing software where you code the gaussian function
  - Using an external software package
- Plot the density estimate $P_{KDE}(x)$ over the following range of $-10 < x < 35$
- [Optional] If you have time, plot the individual kernel contributions too

Exercise 2 KDE plot



Compact Kernel

- The gaussian kernel contributes across the whole space (infinite support), but sometimes we want compact support, i.e. probability of zero outside of a specific range
  - Maybe some parameters are constrained to be non-negative
  - Maybe, we know the physical system has either boundaries or effective cut-offs
- A common *compact support* kernel is the Epanechnikov kernel



$$K(u) = \begin{cases} \frac{3}{4}(1-u^2) & \text{for } |u| \leq 1 \\ 0 & \text{for } |u| > 1 \end{cases}$$

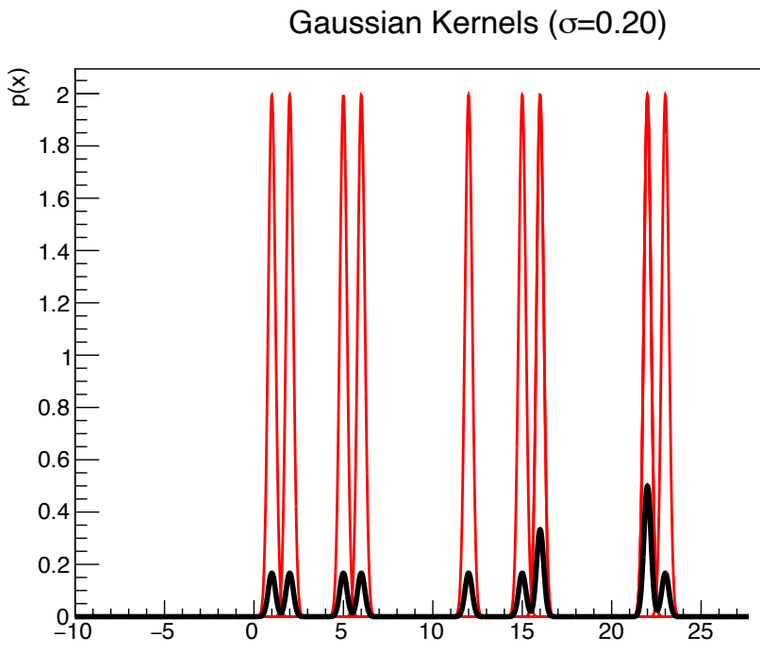
*https://en.wikipedia.org/wiki/Kernel_(statistics)

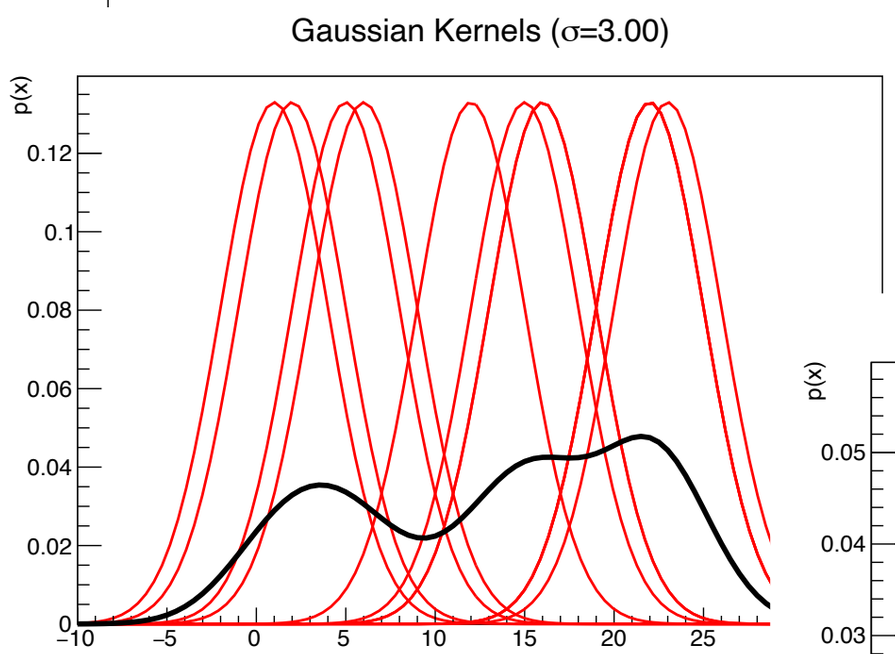
Exercise 3

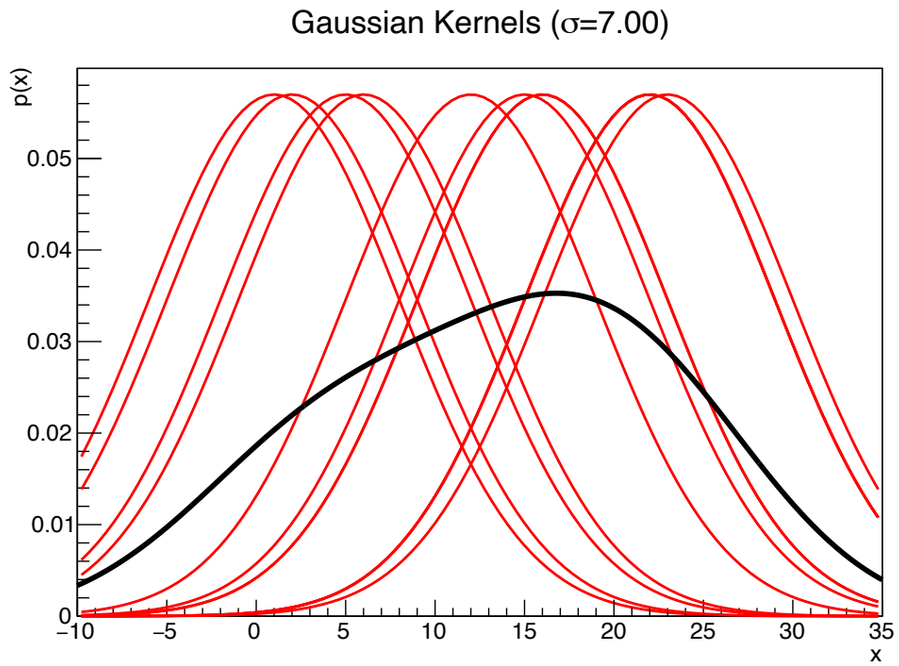
- Redo exercise 2 using the Epanechnikov kernel with a bandwidth that you choose
- In a nicely formatted table compare calculate $P_{KDE}(x=6)$, $P_{KDE}(x=10.1)$, $P_{KDE}(x=20.499)$, and $P_{KDE}(x=20.501)$ between the 3 different kernels; Parzen-Rosenblatt, gaussian, and Epanechnikov
- Use either your by-hand(s) version or external package

Kernel Bandwidth

- Every KDE is, unfortunately, strongly influenced by the kernel bandwidth, which is a user defined free parameter







Bandwidth Selection

- An analytic approach to bandwidth selection is to choose a bandwidth which minimizes the mean integrated square error (MISE)

$$MISE(h) = E\left[\int (P_{KDE}(\vec{x}) - P(\vec{x}))^2 dx\right]$$

- But analytically this requires some known form of the underlying distribution
- Assuming that the underlying distribution is gaussian, the optimal bandwidth is

$$h \approx 1.06\hat{\sigma}N^{-1/5}$$

$\hat{\sigma}$ standard deviation from data

N number of data points

Bandwidth Selection Non-parametric

- Instead of using a known function we can use subsets of the data as cross-validation of the kernel bandwidth with the integrated square error (ISE)

$$ISE(\hat{f}_h) = \int (\hat{f}_h(y) - f(y))^2 dy$$

$$= \int (\hat{f}_h(y))^2 dy - 2\int \hat{f}_h(y) f(y) dy + \int f(y)^2 dy$$

- This can be shown to converge to a least squares cross-validation (LSCV) expression as

$$LSCV(h) = \int (\hat{f}_h(y))^2 dy - \frac{2}{N}\sum_{i=1}^{n} \hat{f}_{-i}(y_i)$$

- The expression $\hat{f}_{-i}(y_i)$ is the kernel estimator from the data omitting the data point y_i which is also known as the "leave-one-out" density estimator

*https://projecteuclid.org/euclid.ss/1113832723

KDE in 2D, and more

- While the previous examples were for 1-dimension, the kernels work just fine in additional dimensions
  - No escaping the curse of dimensionality :-(
  - Similar to all other multi-dimensional problems, anything beyond 3D is difficult to visualize
- Kernel bandwidths do not have to be the same in each dimension
  - Either specify the bandwidth in each dimension, or
  - Transform the parameter space(s) to be uniform for a given bandwidth

Exercise 4

- There are many online tutorials covering different 2D density estimation problems in R, python, MatLab, etc.
  - Eruption of “Old Faithful” geyser
  - Rendering of text and numerals
  - Spread of diseases
  - Geographical population densities

Exercise 5

- Use the 500 pseudo-experiment bootstrap from Lecture "Parameter Estimation and Confidence Intervals" exercise 2b to produce a 2D KDE
  - Because the LLH method gives precise uncertainties, you can compare the contours from the KDE

The End

More KDE comments

- The kernel is symmetric about each data point
  - Makes sense, because the region near the data point should have a similar probability for a narrow (enough) bandwidth
  - Kernel symmetry is not technically a requirement, but in practice symmetry is often desirable because then the average (mean, median, and mode) of the kernel is centered on the data point
- The kernel density estimator PDF is often used for Monte Carlo sampling
  - E.g. N-body simulations (galaxy formation, astrophysical large scale structure, disease propagation in an ecosystem, etc.) can take months to generate 200 data points across 3 dimensions or parameters. Real data is much, much larger. In order to use our N-body PDF, we can sample from a smoothed PDF from a KDE.
- Because KDEs require ‘subjective’ input, clearly state the kernel, bandwidth, and any optimization from an analysis

Further Info

- Fixed kernel width window, Parzen-Rosenblatt window
  - Parzen (http://www.jstor.org/stable/2237880)
  - Rosenblatt (http://projecteuclid.org/euclid.aoms/1177728190)
- Nice list of various kernels at https://en.wikipedia.org/wiki/Kernel_(statistics)
- Very nice article on kernel bandwidth selection review https://projecteuclid.org/euclid.ss/1113832723
- Collection of other cross-validation techniques https://cran.r-project.org/web/packages/kedd/vignettes/kedd.pdf

Further Info (cont.)

- Variable bandwidth kernels
  - Z. I. Botev, et al., Kernel Density Estimation via Diffusion, Annals of Statistics, 38 5, 2916-2957 (2010).
  - I. S. Abramson, On bandwidth variation in kernel estimates—A square root law, Annals of Statistics, 10 4, 1217-1223 (1982).
- Any other suggestions?