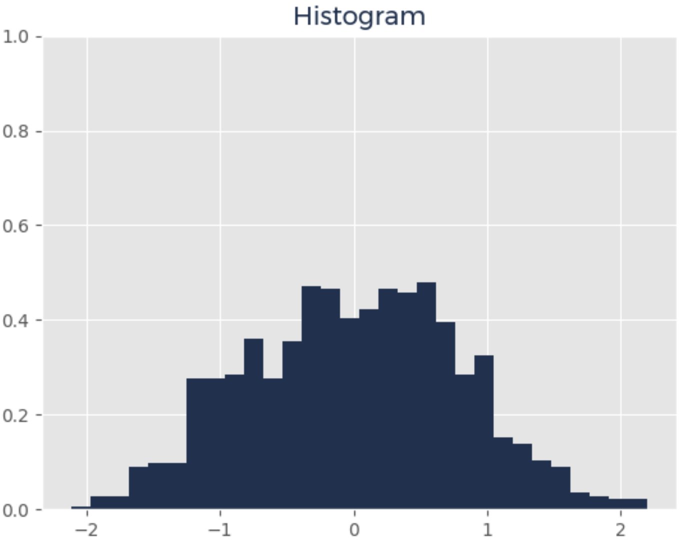
Unsupervised Learning - Density Estimation

Creating our own truth

Histograms



Histogram Bin Width

Scott's rule

$$w = 3.49\sigma n^{\frac{-1}{3}},$$

where σ is the standard deviation of the data and n is the number of samples.

Histogram Bin Width

Freedman and Diaconis' rule

$$w = 2dn^{\frac{-1}{3}},$$

where d is the interquartile range (difference between 75th percentile and 25th percentile), and n is the number of samples.

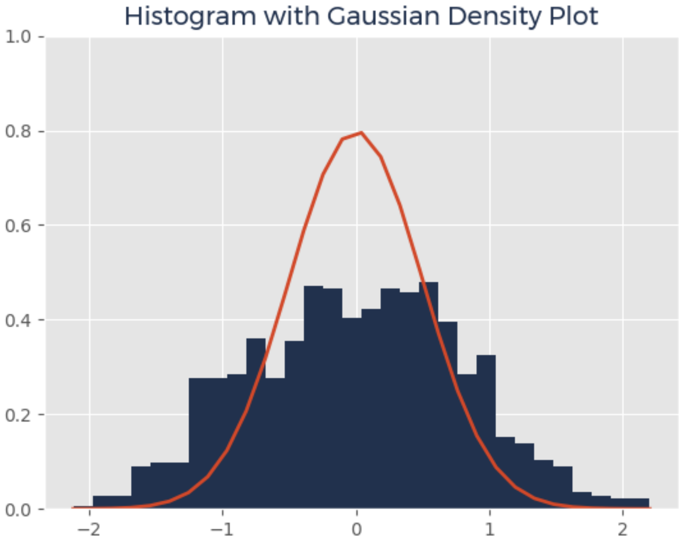
Histogram Bin Width

- Knuth's rule
- Bayesian block representations

Histogram Bin Width - Problems

Demo

Kernel Density Estimation



Kernel Density Estimation

The kernel density estimator of an unknown density f is,

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

where n is the number of samples, h is the bandwidth which is a smoothing parameter, and $K()$ is a kernel applied to the data.

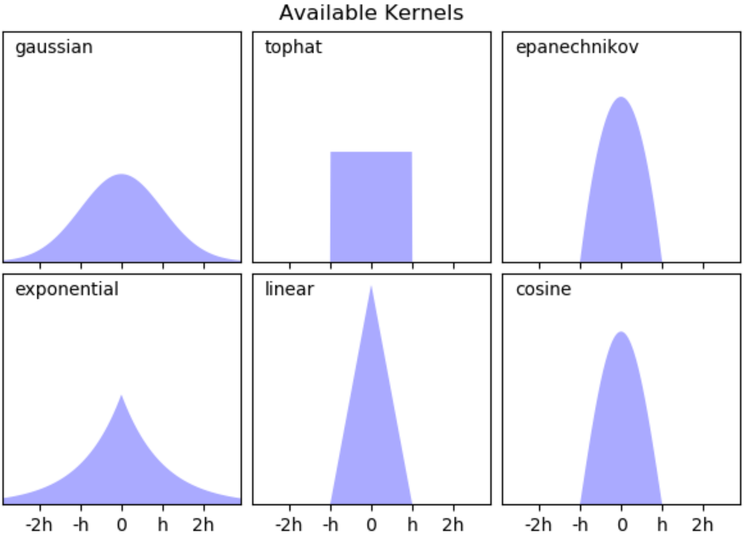
Scaled Kernel

$$K_h(x_i) = \frac{1}{h} K(\frac{x_i}{h}).$$

Kernels

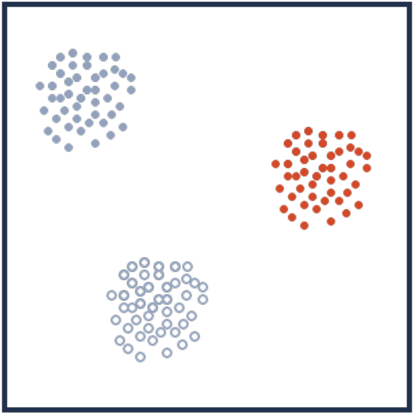
Gaussian	$K_h(x) \propto \exp \frac{-x^2}{2h^2},$
Uniform / Tophat	$K_h(x) \propto 1 \text{ if } x < h,$
Exponential	$K_h(x) \propto \exp \frac{-x}{h},$
Linear	$K_h(x) \propto 1 - \frac{x}{h},$
Epanechnikov	$K_h(x) \propto 1 - \frac{x^2}{h^2},$
Cosine	$K_h(x) \propto \cos \frac{\pi x}{2h}.$

Kernels



Available Kernels
gaussian
tophat
epanechnikov
exponential
linear
cosine
-2h
-h
0
h
2h

Demo



Clustering

Density-Based Clustering Methods

- Gaussian Mixture Models
- MeanShift
- DBSCAN

Gaussian Mixture Models

Clustering by assuming each cluster follows a Gaussian distribution.

MeanShift

$$\mathbf{x}_{i,t+1} = \mathbf{x}_{i,t} + \mathbf{m}_{i,t} \tag{1}$$

MeanShift

$$\mathbf{m}_i = \frac{\sum_{j \in N(\mathbf{x}_i)} K(\mathbf{x}_i - \mathbf{x}_j)\mathbf{x}_j}{\sum_{j \in N(\mathbf{x}_i)} K(\mathbf{x}_i - \mathbf{x}_j)} \tag{2}$$

where the set $N(\mathbf{x}_i)$ is the set of points within a specified distance of $\mathbf{x}_i$ called its *neighborhood*, and K is a kernel.

DBSCAN

Clustering by assigning points a status of core or border.

A core point is one that has a minimum number of points within a particular distance.

All other points are border points.

A cluster is defined as a set of connected core points.

Minimum number of points and the distance to check for in order to make a point a core point are hyperparameters.

Clusters do not have to form convex shapes.

Cluster number is **not** a hyperparameter.

Questions