CS 1675 Introduction to Machine Learning
Lecture 8

Non-parametric density estimation

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Nonparametric Density Estimation

- **Parametric distribution models** are:
  - restricted to specific functional forms, which may not always be suitable;
  - **Example:** modelling a multimodal distribution with a single, unimodal model.

- **Nonparametric approaches:**
  - Do not make any strong assumptions about the overall shape of the distribution being modelled.

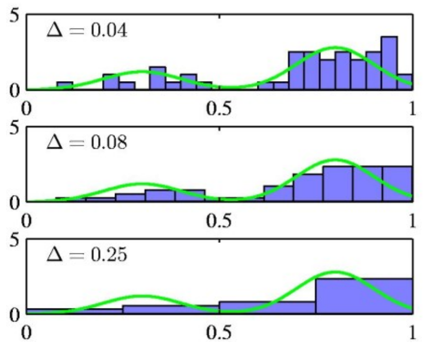
Nonparametric Methods

Histogram methods:

partition the data space into distinct bins with widths Δ_i and count the number of observations, n_i, in each bin.

$$p_i = \frac{n_i}{N\Delta_i}$$

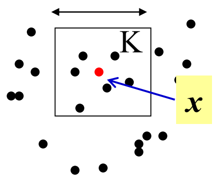
- Often, the same width is used for all bins, $\Delta_i = \Delta$.
- Δ acts as a smoothing parameter.



- Binning does not work well in the in a d-dimensional space,

Nonparametric Methods

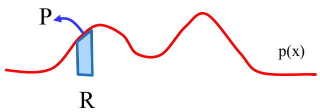
- Binning does not work well in the in a d-dimensional space,
  - M bins in each dimension will require M^d bins!
- **Solution:**
  - Build the estimates of p(**x**) by considering the data points in D and how similar (or close) they are to **x**
  - **Example: Parzen window**
    - As if we build a bin dynamically for **x** for which we need p(**x**)



Nonparametric Methods

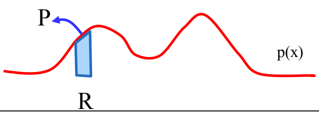
- Assume observations drawn from a density p(x) and consider a small region R containing x such that

$$P = \int_R p(x)dx$$



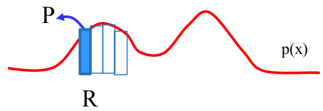
- The probability that K out of N observations lie inside R is *Bin(K,N,P)* and if N is large

$$K \cong NP$$



If the volume of R, V, is sufficiently small, p(x) is approximately constant over R and

$$P \cong p(x)V$$



Thus
$$p(x) = \frac{P}{V}$$

Putting things together we get:

$$p(x) = \frac{K}{NV}$$

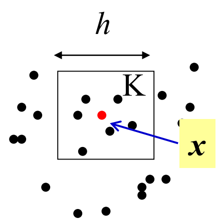
Nonparametric methods: kernel methods

Solution 1: Estimate the probability for **x** based on the fixed volume **V** built around **x**

$$p(x) = \frac{K}{NV}$$

- **Fix V, estimate K from the data**

Example: Parzen window



Nonparametric methods: kernel methods

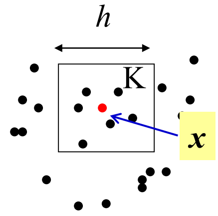
Kernel Density Estimation:

- **Parzen window:** Let R be a hypercube centred on **x** that defines the **kernel function:**

$$k\left(\frac{x-x_n}{h}\right)=\begin{cases}1 & |(x_i-x_{ni})|/h\le 1/2 \qquad i=1,\dots D\\ 0 & otherwise\end{cases}$$

- **It follows that**

$$K=\sum_{n=1}^{N}k\left(\frac{x-x_n}{h}\right)$$



- **and hence**

$$p(x)=\frac{K}{NV}=\frac{1}{Nh^D}\sum_{n=1}^{N}k\left(\frac{x-x_n}{h}\right)$$

Nonparametric Methods: smooth kernels

To avoid discontinuities in p(x) because of sharp boundaries we can use a **smooth kernel**, e.g. a Gaussian

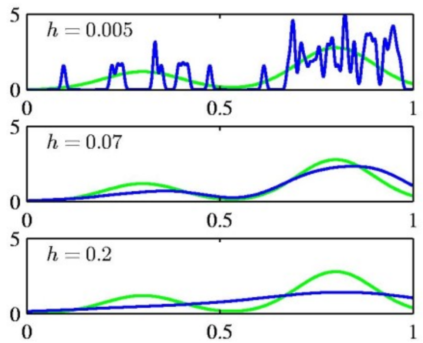
$$p(\mathbf{x})=\frac{1}{N}\sum_{n=1}^{N}\frac{1}{\left(2\pi h^2\right)^{D/2}}\exp\left[-\frac{\|\mathbf{x}-\mathbf{x}_n\|}{2h^2}\right]$$

- Any kernel such that

$$k(\mathbf{u})\ge 0$$

$$\int k(\mathbf{u})d\mathbf{u}=1$$

- will work.



h acts as a smoother.

Nonparametric Methods: kNN estimation

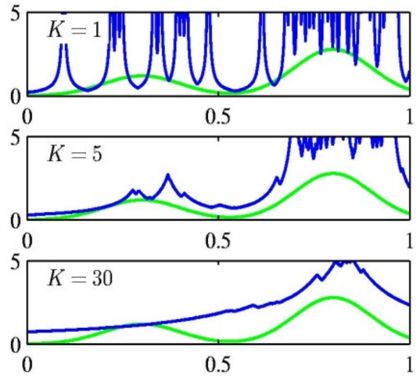
Solution 2: Estimate the probability for **x** based on a fixed count **K** for a variable volume **V** built around **x**

fix K, estimate V from the data

Nearest Neighbour Density Estimation:

Consider a hyper-sphere centred on x and let it grow to a volume, V*, that includes K of the given N data points. Then

$$p(\mathbf{x}) \simeq \frac{K}{NV^{\star}}.$$



K acts as a smoother

Nonparametric vs Parametric Methods

Nonparametric models:

- More flexibility – no density model is needed
- But require storing the entire dataset
- and the computation is performed with all data examples.

Parametric models:

- Once fitted, only parameters need to be stored
- They are much more efficient in terms of computation
- But the model needs to be picked in advance