Non-parametric density estimation

Probability distributions

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Non-parametric density estimation

So far, probability distributions with specific functional forms governed by a number of parameters, whose values are to be computed from data

- This is called the **parametric** approach to density modelling

Limitation: The chosen density might be a poor model of the distro that generates the data, which can result in poor predictive performance

- if the data generating process is multimodal, then this aspect of the distribution can never be captured by the (unimodal) Gaussian

We consider some **non-parametric** approaches to density estimation that make very few assumptions about the form of the distribution

- Focus mainly on simple frequentist methods

Outline

1. Histograms

2. Kernel density estimators

3. Nearest-neighbour methods
   - Classification with k-NN

Histograms

Non-parametric density estimation

Histograms

Let us start with the classic **histogram methods** for density estimation

- Already seen in the context of marginal/conditional distributions
- We explore the properties of histogram density models
- Focus on a single continuous variable x

Standard histograms simply partition x into distinct bins of width Δ_i

- then count the number n_i of observations of x falling in bin i

To turn this count into a normalised probability density, we divide n_i by the total number N of observations and by the width Δ_i of the bins

- We get probabilities values for each bin

$$p_i = \frac{n_i}{N\Delta_i}, \qquad \text{such that} \int p(x)dx = 1 \tag{1}$$

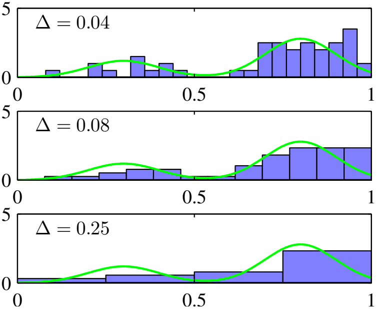
This gives a model for density $p(x)$ that is constant over the bin

- The bins are often chosen to have the same width $\Delta_i = \Delta$

Histograms (cont.)

Data (50 observations) is drawn from the distribution, corresponding to the green curve, which is formed from a mixture of two Gaussians

Three density estimates with three different choices of bin width Δ



- Small Δ, spiky density with structure not in the distribution
- Large Δ, smooth density model without underlying bi-modality
- Best from an intermediate Δ

Useful technique for getting a quick visualisation of the data in 1 or 2D

- Discontinuities, D variables divided in M bins each means M^D bins

Histograms (cont.)

Hardly useful in density estimation applications, but teaches lessons

- To estimate a probability density at a particular location, we should consider points that lie within a local neighbourhood of that point

The **notion of locality** needs some form of **distance measure**

- For histograms, locality was defined by the bins' width
- Locality should be neither too large nor too small

Kernel density estimation

Non-parametric density estimation

Kernel density estimators

Suppose our observations have been drawn from some unknown probability density $p(\mathbf{x})$ in some D-dimensional space, which we consider Euclidean

- We wish to estimate the value of $p(\mathbf{x})$

Let us consider some small region $\mathcal{R}$ containing $\mathbf{x}$

- The probability mass associated with this region is

$$P = \int_{\mathcal{R}} p(\mathbf{x}) d\mathbf{x} \tag{2}$$

Suppose that we have collected a set with N observations from $p(\mathbf{x})$

- Each point has a probability P of falling within $\mathcal{R}$

The number of points K in $\mathcal{R}$ is distributed with a binomial distro

$$\text{Bin}(K|N, P) = \frac{N!}{K!(N-K)!} P^K (1-P)^{1-K} \tag{3}$$

Kernel density estimators (cont.)

Using results for binomial distribution

- the mean fraction of points in the region is $\mathbb{E}[K/N] = P$
- the variance around this mean is $\text{var}[K/N] = P(1-P)/N$

For large N, the distribution will be sharply peaked around its mean

$$K \simeq NP \tag{4}$$

If we assume that the region $\mathcal{R}$ is sufficiently small (of volume V) that the probability density is roughly constant over the region, then we have

$$P \simeq p(\mathbf{x})V \tag{5}$$

Combining the results, we obtain our density estimate in the form

$$p(\mathbf{x}) = \frac{K}{NV} \tag{6}$$

Kernel density estimators (cont.)

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

Either

- We can fix K and determine the value of V from the data
- We get the **K-nearest-neighbour estimators**

or

- We can fix V and determine the value if K from the data
- We get a class of **kernel-based estimators**

For $N \to \infty$, both techniques converge to the true probability density

- Provided that V shrinks suitably with N and that K grows with N

Kernel density estimators (cont.)

To start with we take the region $\mathcal{R}$ to be a small hypercube centred on the point $\mathbf{x}$ at which we wish to determine the probability density

To count the number K of points falling within $\mathcal{R}$, define the function

$$k(\mathbf{u}) = \begin{cases} 1, & \text{if } |u_i| \leq 1/2 \quad \text{with } i = 1, \dots, D \\ 0, & \text{otherwise} \end{cases} \tag{7}$$

It represents a unit cube centred on the origin

- Function $k(\mathbf{u})$ is an example of a **kernel function**
- In this context it is also called a **Parzen window**

If a data point x_n lies inside a cube of side h centred on $\mathbf{x}$, then the quantity $\dfrac{k(\mathbf{x} - \mathbf{x}_n)}{h}$ will be one and zero otherwise

- The total number of points lying inside this cube will be

$$K = \sum_{n=1}^{N} k\Big(\frac{\mathbf{x} - \mathbf{x}_n}{h}\Big) \tag{8}$$

Kernel density estimators (cont.)

Substitute $K = \sum_{n=1}^{N} k\Big(\dfrac{\mathbf{x} - \mathbf{x}_n}{h}\Big)$ in $p(\mathbf{x}) = \dfrac{K}{NV}$, the density at $\mathbf{x}$ is

$$p(\mathbf{x}) = \frac{1}{N}\sum_{n=1}^{N} \frac{1}{h^D} k\Big(\frac{\mathbf{x} - \mathbf{x}_n}{h}\Big) \qquad (9)$$

$h^D = V$ is the volume of the hypercube of side h in D dimensions

We can interpret this equation, not a single cube centred on $\mathbf{x}$,
but as the sum over N cubes centred on the N data points $\mathbf{x}_n$

Kernel density estimators (cont.)

Remark

This density estimator shares some of the problems of the histograms

- Discontinuities, at the boundaries of the cubes

A smoother model is obtained by choosing a smoother kernel function

Kernel density estimators (cont.)

Usual choice: The kernel function of the estimator is the Gaussian

$$p(\mathbf{x}) = \frac{1}{N}\sum_{n=1}^{n} \frac{1}{(2\pi h^2)^{D/2}} \exp\Big(-\frac{||\mathbf{x}-\mathbf{x}_n||^2}{2h^2}\Big) \qquad (10)$$

h now denotes the standard deviation of Gaussian components

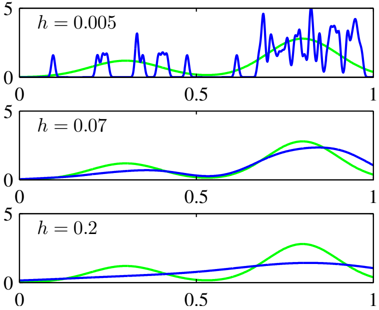
This density model is obtained by placing a Gaussian over each data point, and then adding up the contributions over the whole dataset

- Divide by N to correctly normalise the density

Kernel density estimators (cont.)

Kernel density model applied to the same data set used with histograms

Three density estimates with three different choices of h



- Small h, noisy density with structure not in the distribution
- Large h, smooth density model without underlying bi-modality
- Best, from an intermediate h

Parameter h plays the role of a smoothing term, and there is a trade-off between sensitivity to noise at small h and over-smoothing at large h

Kernel density estimators (cont.)

We can choose any other kernel function $k(\mathbf{u})$ subject to the conditions

$$\begin{aligned} k(\mathbf{u}) &\geq 0 \qquad (11) \\ \int k(\mathbf{u}) d\mathbf{u} &= 1 \qquad (12) \end{aligned}$$

They ensure that the resulting probability distribution is nonnegative everywhere and that integrates to one

Nearest-neighbour methods

Non-parametric density estimation

Nearest-neighbour methods

One of the difficulties with the kernel approach to density estimation is that the parameter h governing the kernel width is fixed for all kernels

- In regions of high density, a large h may lead to over-smoothing
- Reducing h, may lead to noisy estimates where density is low

An optimal choice of h may be dependent on location within the space

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

Instead of fixing V and determining K from data, we consider a fixed value of K and use the data to find an appropriate value for V

Nearest-neighbour methods (cont.)

Let $\mathcal{B}(\mathbf{x})$ be a small sphere centred on point $\mathbf{x}$ at which we wish to estimate density $p(\mathbf{x})$ and let the sphere grow until it contains K points

The density estimate is

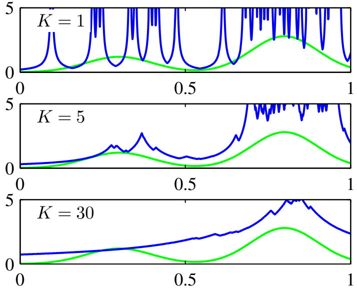
$$p(\mathbf{x}) = \frac{K}{NV}$$

with V set to the volume of the resulting sphere

This technique is known as **K-nearest neighbours**

The value of K now governs the degree of smoothing and there is an optimum choice for K that is neither too large nor too small

Nearest-neighbour methods (cont.)



The model produced by K-NN is not a true density model

- The integral over all space diverges ($\star$)

Classification with k-NN

The K-NN density estimator can be used for classification

1. We apply it to each class separately
2. We make use of the Bayes' theorem

We got data, N_k points in class C_k with N total points st $\sum_k N_k = N$

If we wish to classify a new point $\mathbf{x}$

Classification with k-NN (cont.)

Pseudocode

1. Draw a sphere centred in $\mathbf{x}$ with K points, whatever their class
2. Say, the volume of the sphere is V and contains K_k class-C_k points
3. Use $p(\mathbf{x}) = \dfrac{K}{NV}$ to estimate the density associated with each class

$$p(\mathbf{x}|c_k) = \frac{K_k}{N_k V} \tag{13}$$

4. The unconditional density and the class prior are given by

$$\begin{aligned} p(\mathbf{x}) &= \frac{K}{NV} && (14) \\ p(C_k) &= \frac{N_k}{N} && (15) \end{aligned}$$

5. Combine Equation 13, 14 and 15 using Bayes' theorem to get the posterior probability of the class membership

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})} = \frac{K_k}{K} \tag{16}$$

Classification with k-NN (cont.)

If we wish to minimise the probability of misclassification, we assign the test point $\mathbf{x}$ to the class having the largest posterior probability

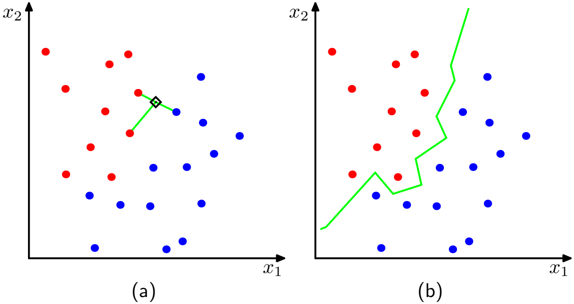
- The largest value of K_k/K

To classify $\mathbf{x}$, we identify the K nearest points from the training set and assign it to the class with largest number of representatives in this set

- Ties can be broken at random

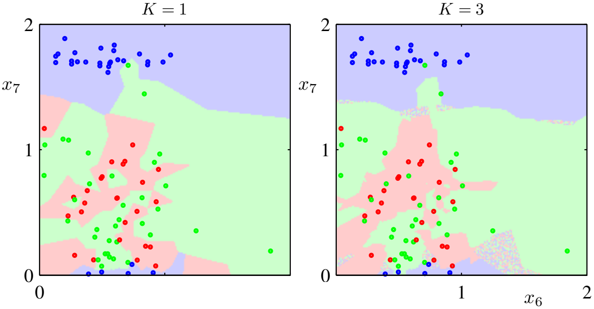
Classification with k-NN (cont.)

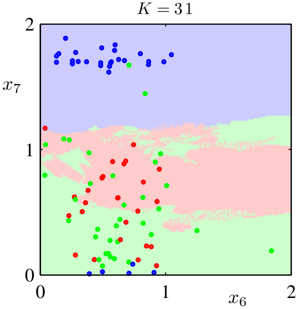
In the K-NN classifier, a new point (black), is classified according to the majority class membership of the K closest training points (here, $K = 3$)



(a) (b)

In the nearest-neighbour (K = 1) approach to classification, the decision boundary is composed of hyperplanes that form perpendicular bisectors of pairs of points from different classes


$K = 1$
$K = 3$
2
1
0
x_7
0
1
2
x_6


$K = 31$
2
1
0
x_7
0
1
2
x_6