Non-parametric Methods

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Introduction

- Density estimation with parametric models assumes that the forms of the underlying density functions are known.
- However, common parametric forms do not always fit the densities actually encountered in practice.
- In addition, most of the classical parametric densities are unimodal, whereas many practical problems involve multimodal densities.
- Non-parametric methods can be used with arbitrary distributions and without the assumption that the forms of the underlying densities are known.

Non-parametric Density Estimation

- Suppose that n samples $\mathbf{x_1}, \ldots, \mathbf{x_n}$ are drawn i.i.d. according to the distribution $p(\mathbf{x})$.
- The probability P that a vector $\mathbf{x}$ will fall in a region $\mathcal{R}$ is given by

$$P = \int_{\mathcal{R}} p(\mathbf{x'}) d\mathbf{x'}.$$

- The probability that k of the n will fall in $\mathcal{R}$ is given by the binomial law

$$P_k = \binom{n}{k} P^k (1 - P)^{n-k}.$$

- The expected value of k is $E[k] = nP$ and the MLE for P is $\hat{P} = \frac{k}{n}$.

Non-parametric Density Estimation

- If we assume that $p(\mathbf{x})$ is continuous and $\mathcal{R}$ is small enough so that $p(\mathbf{x})$ does not vary significantly in it, we can get the approximation

$$\int_{\mathcal{R}} p(\mathbf{x'}) d\mathbf{x'} \simeq p(\mathbf{x}) V$$

  where $\mathbf{x}$ is a point in $\mathcal{R}$ and V is the volume of $\mathcal{R}$.
- Then, the density estimate becomes

$$p(\mathbf{x}) \simeq \frac{k/n}{V}.$$

Non-parametric Density Estimation

- Let n be the number of samples used, $\mathcal{R}_n$ be the region used with n samples, V_n be the volume of $\mathcal{R}_n$, k_n be the number of samples falling in $\mathcal{R}_n$, and $p_n(\mathbf{x}) = \frac{k_n/n}{V_n}$ be the estimate for $p(\mathbf{x})$.
- If $p_n(\mathbf{x})$ is to converge to $p(\mathbf{x})$, three conditions are required:

$$\lim_{n\to\infty} V_n = 0$$
$$\lim_{n\to\infty} k_n = \infty$$
$$\lim_{n\to\infty} \frac{k_n}{n} = 0.$$

Histogram Method

- A very simple method is to partition the space into a number of equally-sized cells (*bins*) and compute a *histogram*.

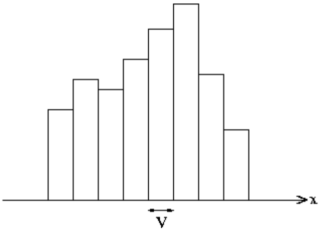


Figure 1: Histogram in one dimension.

- The estimate of the density at a point $\mathbf{x}$ becomes

$$p(\mathbf{x}) = \frac{k}{nV}$$

where n is the total number of samples, k is the number of samples in the cell that includes $\mathbf{x}$, and V is the volume of that cell.

Histogram Method

- Although the histogram method is very easy to implement, it is usually not practical in high-dimensional spaces due to the number of cells.
- Many observations are required to prevent the estimate being zero over a large region.
- Modifications for overcoming these difficulties:
  - Data-adaptive histograms,
  - Independence assumption (naive Bayes),
  - Dependence trees.

Non-parametric Density Estimation

- Other methods for obtaining the regions for estimation:
  - Shrink regions as some function of n, such as $V_n = 1/\sqrt{n}$. This is the *Parzen window* estimation.
  - Specify k_n as some function of n, such as $k_n = \sqrt{n}$. This is the *k-nearest neighbor* estimation.

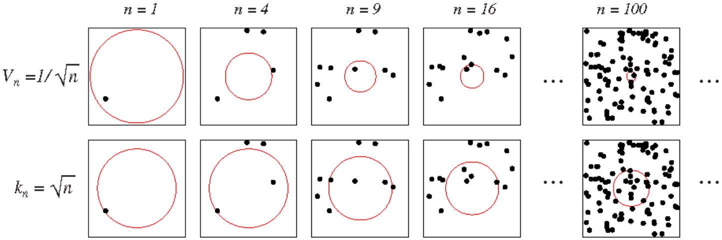


Figure 2: Methods for estimating the density at a point, here at the center of each square.

Parzen Windows

- Suppose that φ is a d-dimensional window function that satisfies the properties of a density function, i.e.,

$$\varphi(\mathbf{u}) \geq 0 \quad \text{and} \quad \int \varphi(\mathbf{u}) d\mathbf{u} = 1.$$

- A density estimate can be obtained as

$$p_n(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{V_n} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right)$$

where h_n is the window width and $V_n = h_n^d$.

Parzen Windows

- The density estimate can also be written as

$$p_n(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} \delta_n(\mathbf{x} - \mathbf{x}_i) \quad \text{where} \quad \delta_n(\mathbf{x}) = \frac{1}{V_n} \varphi\left(\frac{\mathbf{x}}{h_n}\right).$$

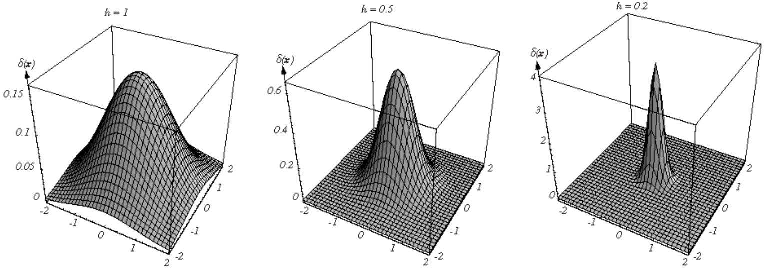


Figure 3: Examples of two-dimensional circularly symmetric Parzen windows functions for three different values of h_n. The value of h_n affects both the amplitude and the width of $\delta_n(\mathbf{x})$.

Parzen Windows

- If h_n is very large, $p_n(\mathbf{x})$ is the superposition of n broad functions, and is a smooth "out-of-focus" estimate of $p(\mathbf{x})$.
- If h_n is very small, $p_n(\mathbf{x})$ is the superposition of n sharp pulses centered at the samples, and is a "noisy" estimate of $p(\mathbf{x})$.
- As h_n approaches zero, $\delta_n(\mathbf{x} - \mathbf{x}_{\boldsymbol{i}})$ approaches a Dirac delta function centered at $\mathbf{x}_{\boldsymbol{i}}$, and $p_n(\mathbf{x})$ is a superposition of delta functions.

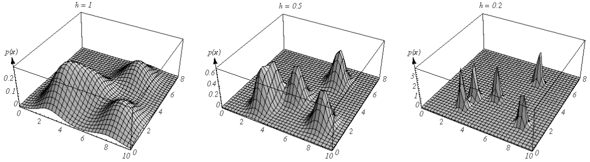


Figure 4: Parzen window density estimates based on the same set of five samples using the window functions in the previous figure.

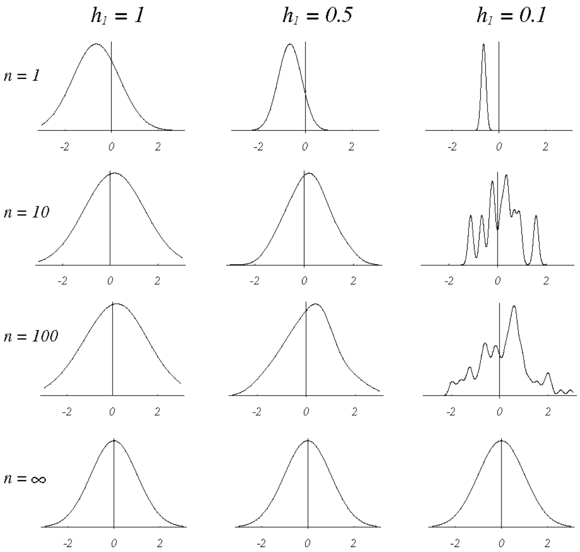


Figure 5: Parzen window estimates of a univariate Gaussian density using different window widths and numbers of samples where $\varphi(u) = N(0, 1)$ and $h_n = h_1/\sqrt{n}$.

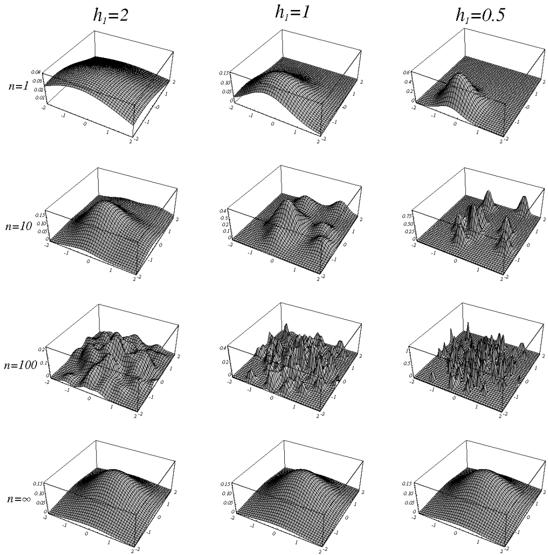


Figure 6: Parzen window estimates of a bivariate Gaussian density using different window widths and numbers of samples where $\varphi(\mathbf{u}) = N(\mathbf{0}, \mathbf{I})$ and $h_n = h_1/\sqrt{n}$.

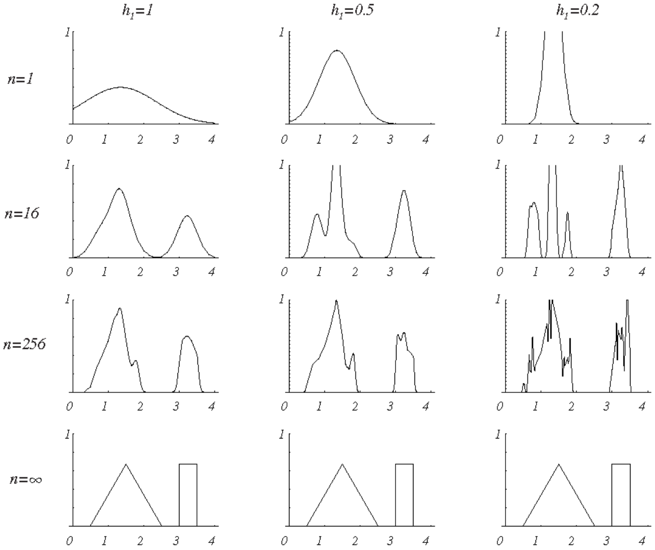


Figure 7: Estimates of a mixture of a uniform and a triangle density using different window widths and numbers of samples where $\varphi(u) = N(0,1)$ and $h_n = h_1/\sqrt{n}$.

Parzen Windows

- Densities estimated using Parzen windows can be used with the Bayesian decision rule for classification.
- The training error can be made arbitrarily low by making the window width sufficiently small.
- However, the goal is to classify novel patterns so the window width cannot be made too small.

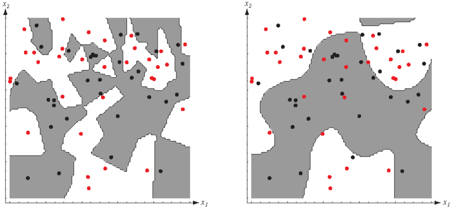


Figure 8: Decision boundaries in 2-D. The left figure uses a small window width and the right figure uses a larger window width.

k-Nearest Neighbors

- A potential remedy for the problem of the unknown "best" window function is to let the estimation volume be a function of the training data, rather than some arbitrary function of the overall number of samples.
- To estimate $p(\mathbf{x})$ from n samples, we can center a volume about $\mathbf{x}$ and let it grow until it captures k_n samples, where k_n is some function of n.
- These samples are called the k-nearest neighbors of $\mathbf{x}$.
- If the density is high near $\mathbf{x}$, the volume will be relatively small. If the density is low, the volume will grow large.

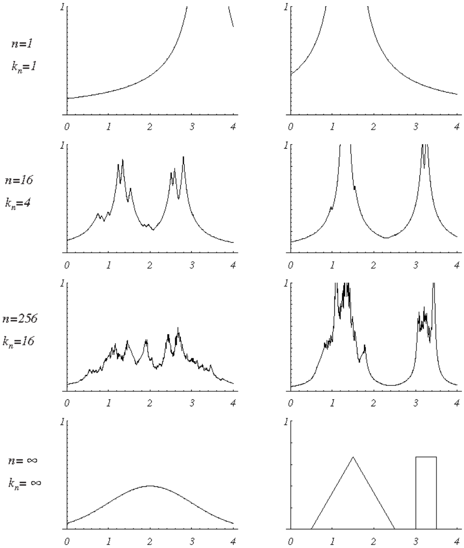


Figure 9: k-nearest neighbor estimates of two 1-D densities: a Gaussian and a bimodal distribution.

k-Nearest Neighbors

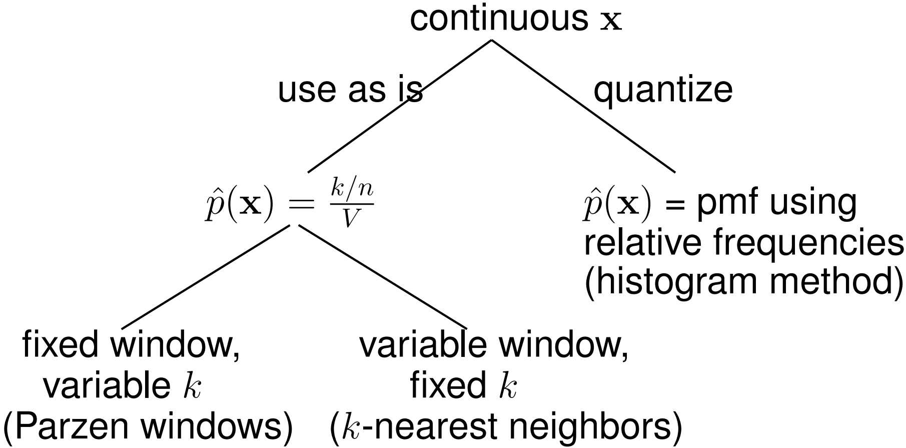
- Posterior probabilities can be estimated from a set of n labeled samples and can be used with the Bayesian decision rule for classification.
- Suppose that a volume V around $\mathbf{x}$ includes k samples, k_i of which are labeled as belonging to class w_i.
- As estimate for the joint probability $p(\mathbf{x}, w_i)$ becomes

$$p_n(\mathbf{x}, w_i) = \frac{k_i/n}{V}$$

and gives an estimate for the posterior probability

$$P_n(w_i|\mathbf{x}) = \frac{p_n(\mathbf{x}, w_i)}{\sum_{j=1}^{c} p_n(\mathbf{x}, w_j)} = \frac{k_i}{k}.$$

Non-parametric Methods



Non-parametric Methods

- Advantages:
  - No assumptions are needed about the distributions ahead of time (generality).
  - With enough samples, convergence to an arbitrarily complicated target density can be obtained.
- Disadvantages:
  - The number of samples needed may be very large (number grows exponentially with the dimensionality of the feature space).
  - There may be severe requirements for computation time and storage.

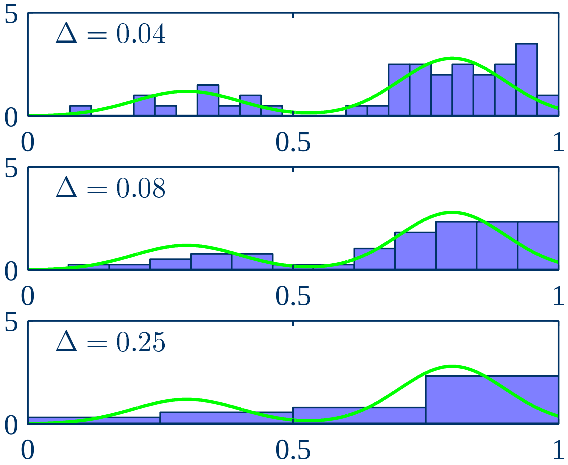


Figure 10: An illustration of the histogram approach to density estimation, in which a data set of 50 points is generated from the distribution shown by the green curve. Histogram density estimates are shown for various values of the cell volume (Δ).

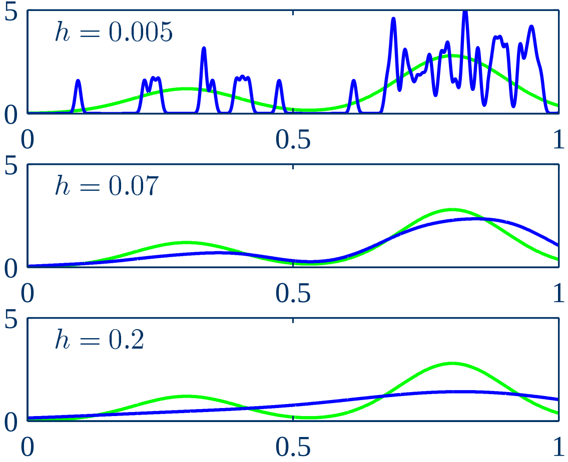


Figure 11: Illustration of the Parzen density model. The window width (h) acts as a smoothing parameter. If it is set too small (top), the result is a very noisy density model. If it is set too large (bottom), the bimodal nature of the underlying distribution is washed out. An intermediate value (middle) gives a good estimate.

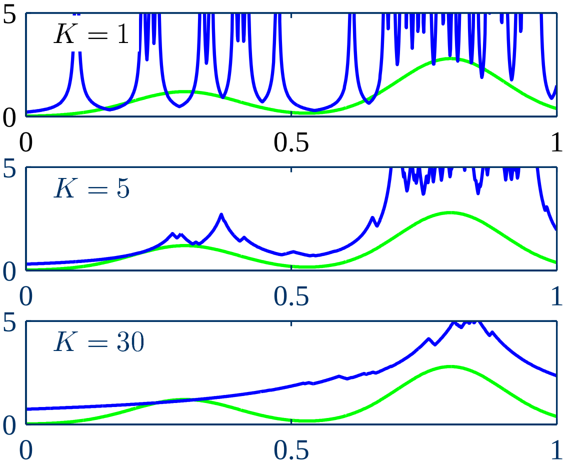


Figure 12: Illustration of the k-nearest neighbor density model. The parameter k governs the degree of smoothing. A small value of k (top) leads to a very noisy density model. A large value (bottom) smoothes out the bimodal nature of the true distribution.

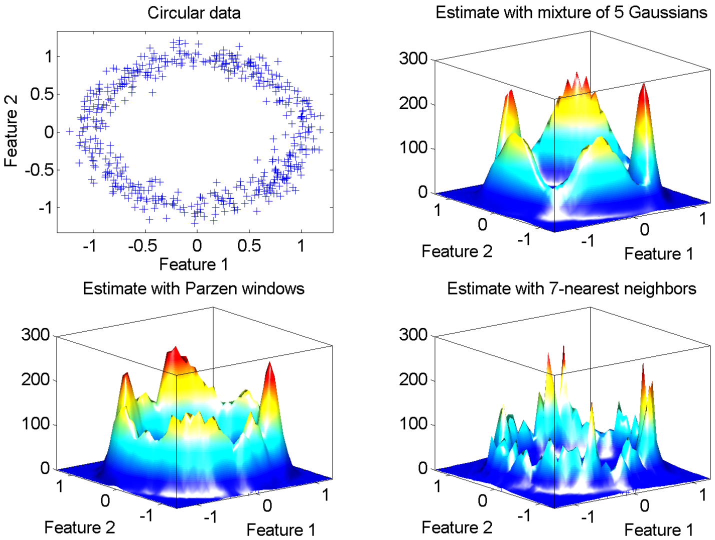


Figure 13: Density estimation examples for 2-D circular data.

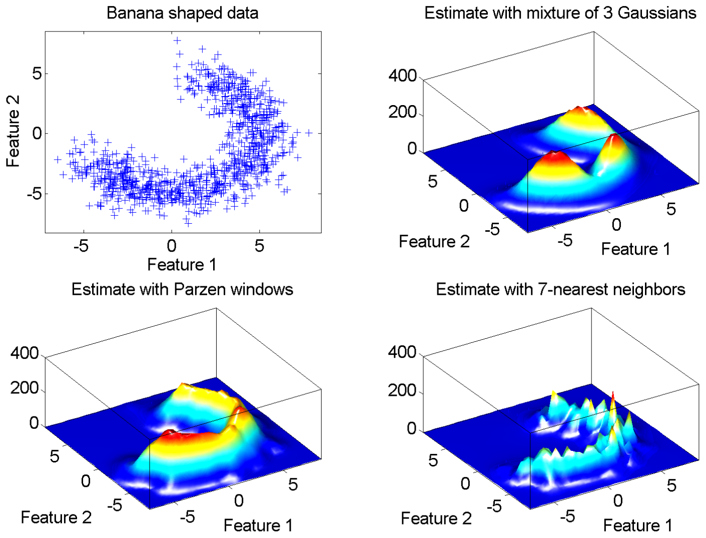


Figure 14: Density estimation examples for 2-D banana shaped data.