Non-parametric Methods

Selim Aksoy

Department of Computer Engineering
Bilkent University
saksoy@cs.bilkent.edu.tr

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

\[
P = \int_{\mathcal{R}} p(x') \, dx'.
\]

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

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

where $x$ is a point in $\mathcal{R}$ and $V$ is the volume of $\mathcal{R}$.

Then, the density estimate becomes

$$p(x) \simeq \frac{k/n}{V}.$$
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 $p_n(x) = \frac{k_n}{V_n}$ be the estimate for $p(x)$.

If $p_n(x)$ is to converge to $p(x)$, three conditions are required:

\[
\lim_{n \to \infty} V_n = 0 \quad \lim_{n \to \infty} k_n = \infty \quad \lim_{n \to \infty} \frac{k_n}{n} = 0.
\]
A very simple method is to partition the space into a number of equally-sized cells (bins) and compute a histogram.

The estimate of the density at a point $x$ becomes

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

where $n$ is the total number of samples, $k$ is the number of samples in the cell that includes $x$, and $V$ is the volume of that cell.
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.](image)
Suppose that \( \varphi \) is a \( d \)-dimensional window function that satisfies the properties of a density function, i.e.,

\[
\varphi(u) \geq 0 \quad \text{and} \quad \int \varphi(u) \, du = 1.
\]

A density estimate can be obtained as

\[
p_n(x) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{V_n} \varphi \left( \frac{x - x_i}{h_n} \right)
\]

where \( h_n \) is the window width and \( V_n = h_n^d \).
The density estimate can also be written as

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

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 \( \delta_n(x) \).
Parzen Windows

- If $h_n$ is very large, $p_n(x)$ is the superposition of $n$ broad functions, and is a smooth “out-of-focus” estimate of $p(x)$.

- If $h_n$ is very small, $p_n(x)$ is the superposition of $n$ sharp pulses centered at the samples, and is a “noisy” estimate of $p(x)$.

- As $h_n$ approaches zero, $\delta_n(x - x_i)$ approaches a Dirac delta function centered at $x_i$, and $p_n(x)$ 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 $\varphi(u) = N(0, I)$ 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 $\phi(u) = N(0, 1)$ 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.
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 $p(x)$ from $n$ samples, we can center a volume about $x$ 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 $x$.

If the density is high near $x$, 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.
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 $x$ includes $k$ samples, $k_i$ of which are labeled as belonging to class $w_i$.

As estimate for the joint probability $p(x, w_i)$ becomes

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

and gives an estimate for the posterior probability

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

Continuous $x$

- Use as is
- Quantize

$\hat{p}(x) = \frac{k/n}{V}$

- Fixed window, variable $k$
  (Parzen windows)
- Variable window, fixed $k$
  ($k$-nearest neighbors)

$\hat{p}(x) = \text{pmf using relative frequencies (histogram method)}$
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 ($\Delta$).
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.