Non-parametric Methods

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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.
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 $R$ is given by

$$P = \int_{R} p(x') dx'. $$

The probability that $k$ of the $n$ will fall in $R$ 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 \( p(x) \) is continuous and \( \mathcal{R} \) is small enough so that \( p(x) \) does not vary significantly in it, we can get the approximation

\[
\int_{\mathcal{R}} p(x') \, dx' \approx p(x) V
\]

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

- Then, the density estimate becomes

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

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

\[ \lim_{n \to \infty} V_n = 0 \]
\[ \lim_{n \to \infty} k_n = \infty \]
\[ \lim_{n \to \infty} \frac{k_n}{n} = 0. \]
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.
Parzen Windows

- 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 $\varphi(u) = \mathcal{N}(0, I)$ 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 $\varphi(u) = N(0, 1)$ 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 $p(x)$ 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.