Nonparametric Methods

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Nonparametric Methods Overview

- Previously, we've assumed that the forms of the underlying densities were of some particular known parametric form.
- But, what if this is not the case?
- Indeed, for most real-world pattern recognition scenarios this assumption is suspect.
- For example, most real-world entities have multimodal distributions whereas all classical parametric densities are unimodal.



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- Previously, we've assumed that the forms of the underlying densities were of some particular known parametric form.
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- Indeed, for most real-world pattern recognition scenarios this assumption is suspect.
- For example, most real-world entities have multimodal distributions whereas all classical parametric densities are unimodal.
- We will examine nonparametric procedures that can be used with arbitrary distributions and without the assumption that the underlying form of the densities are known.

Histograms.

Kernel Density Estimation / Parzen Windows.

- k-Nearest Neighbor Density Estimation.
- Real Example in Figure-Ground Segmentation

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Histograms



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Histograms



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Histogram Density Representation

• Consider a single continuous variable x and let's say we have a set \mathcal{D} of N of them $\{x_1, \ldots, x_N\}$. Our goal is to model p(x) from \mathcal{D} .

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- Standard histograms simply partition x into distinct bins of width Δ_i and then count the number n_i of observations x falling into bin i.
- To turn this count into a normalized probability density, we simply divide by the total number of observations N and by the width Δ_i of the bins.
- This gives us:

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



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- To turn this count into a normalized probability density, we simply divide by the total number of observations N and by the width Δ_i of the bins.
- This gives us:

$$p_i = \frac{n_i}{N\Delta_i} \tag{1}$$

• Hence the model for the density p(x) is constant over the width of each bin. (And often the bins are chosen to have the same width $\Delta_i = \Delta$.)



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Histogram Density as a Function of Bin Width



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Histogram Density as a Function of Bin Width

 The green curve is the underlying true density from which the samples were drawn. It is a mixture of two Gaussians.



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- When Δ is very small (top), the resulting density is quite spiky and hallucinates a lot of structure not present in p(x).



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- When Δ is very big (bottom), the resulting density is quite smooth and consequently fails to capture the bimodality of p(x).
- It appears that the *best results* are obtained for some intermediate value of Δ , which is given in the middle figure.
- In principle, a histogram density model is also dependent on the choice of the edge location of each bin.

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Analyzing the Histogram Density

• What are the advantages and disadvantages of the histogram density estimator?

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- Advantages:
 - Simple to evaluate and simple to use.
 - One can throw away $\mathcal D$ once the histogram is computed.
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- Advantages:
 - Simple to evaluate and simple to use.
 - $\bullet\,$ One can throw away ${\cal D}$ once the histogram is computed.
 - Can be computed sequentially if data continues to come in.
- Disadvantages:
 - The estimated density has discontinuities due to the bin edges rather than any property of the underlying density.
 - Scales poorly (curse of dimensionality): we would have M^D bins if we divided each variable in a D-dimensional space into M bins.

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What can we learn from Histogram Density Estimation?

- Lesson 1: To estimate the probability density at a particular location, we should consider the data points that lie within some local neighborhood of that point.
 - This requires we define some distance measure.
 - There is a natural smoothness parameter describing the spatial extent of the regions (this was the bin width for the histograms).

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- Lesson 2: The value of the smoothing parameter should neither be too large or too small in order to obtain good results.

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 - There is a natural smoothness parameter describing the spatial extent of the regions (this was the bin width for the histograms).
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- With these two lessons in mind, we proceed to kernel density estimation and nearest neighbor density estimation, two closely related methods for density estimation.

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- Consider again samples \mathbf{x} from underlying density $p(\mathbf{x})$.
- Let \mathcal{R} denote a small region containing \mathbf{x} .



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- \bullet The probability mass associated with ${\cal R}$ is given by

$$P = \int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}'$$
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- Suppose we have n samples x ∈ D. The probability of each sample falling into R is P.
- How will the total number of k points falling into $\mathcal R$ be distributed?

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- Suppose we have a more amples $\mathbf{x} \in \mathcal{D}$. The probability of each sample falling into \mathcal{R} (2.1)
- How will the total number of k points falling into \mathcal{R} be distributed?
- This will be a **binomial distribution**:

$$P_k = \binom{n}{k} P^k (1-P)^{n-k} \tag{3}$$

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• The expected value for k is thus

$$\mathcal{E}[k] = nP \tag{4}$$

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The binomial for k peaks very sharply about the mean. So, we expect k/n to be a very good estimate for the probability P (and thus for the space-averaged density).

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- The binomial for k peaks very sharply about the mean. So, we expect k/n to be a very good estimate for the probability P (and thus for the space-averaged density).
- This estimate is increasingly accurate as n increases.



• Assuming continuous $p({\bf x})$ and that ${\cal R}$ is so small that $p({\bf x})$ does not appreciably vary within it, we can write:

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

where \mathbf{x} is a point within \mathcal{R} and V is the volume enclosed by \mathcal{R} .

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where x is a point within \mathcal{R} and V is the volume enclosed by \mathcal{R} .

• After some rearranging, we get the following estimate for $p(\mathbf{x})$

$$p(\mathbf{x}) \simeq \frac{k}{nV}$$
 (6)

Example

- Simulated an example of example the density at 0.5 for an underlying zero-mean, unit variance Gaussian.
- Varied the volume used to estimate the density.



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Practical Concerns

- The validity of our estimate depends on two contradictory assumptions:
 - ① The region \mathcal{R} must be sufficiently small the the density is approximately constant over the region.
 - 2 The region \mathcal{R} must be sufficiently large that the number k of points falling inside it is sufficient to yield a sharply peaked binomial.

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- Another way of looking it is to fix the volume V and increase the number of training samples. Then, the ratio k/n will converge as desired. But, this will only yield an estimate of the space-averaged density (P/V).

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- We want $p(\mathbf{x})$, so we need to let V approach 0. However, with a fixed n, \mathcal{R} will become so small, that no points will fall into it and our estimate would be useless: $p(\mathbf{x}) \simeq 0$.

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- Note that in practice, we cannot let V to become arbitrarily small because the number of samples is always limited.

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How can we skirt these limitations when an unlimited number of samples if available?

To estimate the density at x, form a sequence of regions R₁, R₂,... containing x with the R₁ having 1 sample, R₂ having 2 samples and so on.

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How can we skirt these limitations when an unlimited number of samples if available?

- To estimate the density at x, form a sequence of regions R₁, R₂,... containing x with the R₁ having 1 sample, R₂ having 2 samples and so on.
- Let V_n be the volume of \mathcal{R}_n , k_n be the number of samples falling in \mathcal{R}_n , and $p_n(\mathbf{x})$ be the *n*th estimate for $p(\mathbf{x})$:

$$p_n(\mathbf{x}) = \frac{k_n}{nV_n}$$

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• f $p_n(\mathbf{x})$ is to converge to $p(\mathbf{x})$ we need the following three conditions

$$\lim_{n \to \infty} V_n = 0 \tag{8}$$

$$\lim_{n \to \infty} k_n = \infty \tag{9}$$

$$\lim_{n \to \infty} k_n / n = 0 \tag{10}$$

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lim_{n→∞} V_n = 0 ensures that our space-averaged density will converge to p(x).

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- $\lim_{n\to\infty} k_n = \infty$ basically ensures that the frequency ratio will converge to the probability P (the binomial will be sufficiently peaked).

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- lim_{n→∞} k_n/n = 0 is required for p_n(x) to converge at all. It also says that although a huge number of samples will fall within the region R_n, they will form a negligibly small fraction of the total number of samples.

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- There are two common ways of obtaining regions that satisfy these conditions:
 - Shrink an initial region by specifying the volume V_n as some function of n such as $V_n = 1/\sqrt{n}$. Then, we need to show that $p_n(\mathbf{x})$ converges to $p(\mathbf{x})$. (This is like the Parzen window we'll talk about next.)

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- $\lim_{n\to\infty} V_n = 0$ ensures that our space-averaged density will converge to $p(\mathbf{x})$.
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 - ② Specify k_n as some function of n such as k_n = √n. Then, we grow the volume V_n until it encloses k_n neighbors of x. (This is the k-nearest-neighbor).

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 - 2 Specify k_n as some function of n such as $k_n = \sqrt{n}$. Then, we grow the volume V_n until it encloses k_n neighbors of \mathbf{x} . (This is the k-nearest-neighbor).

Both of these methods converge...

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