Nonparametric Methods
Lecture 5

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Nonparametric Methods Lecture 5 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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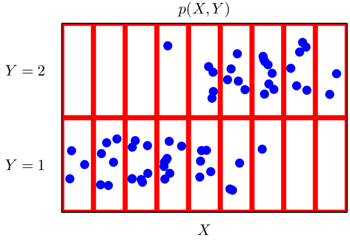
- **But, what if this is not the case?**
- Indeed, for most real-world pattern recognition scenarios this assumption is suspect.
- For example, most real-world entities have multimodal distributions whereas all classical parametric densities are unimodal.
- We will examine **nonparametric** procedures 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

Histograms



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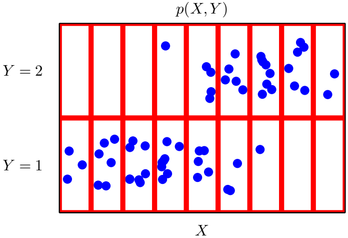

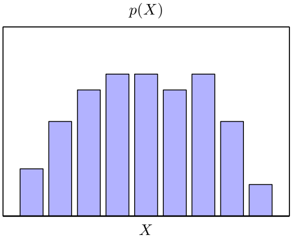

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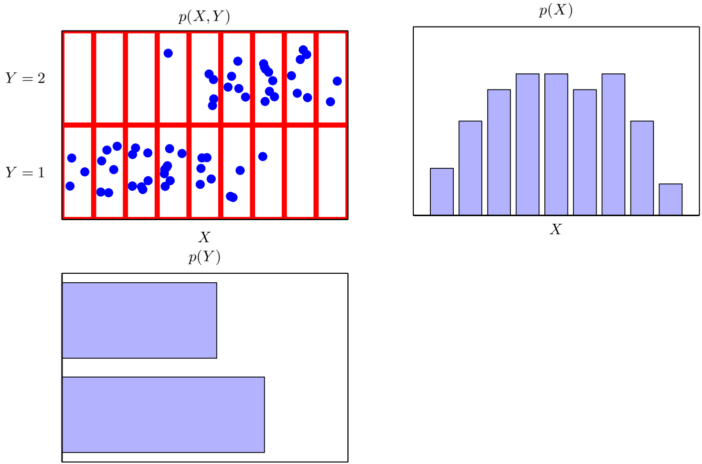

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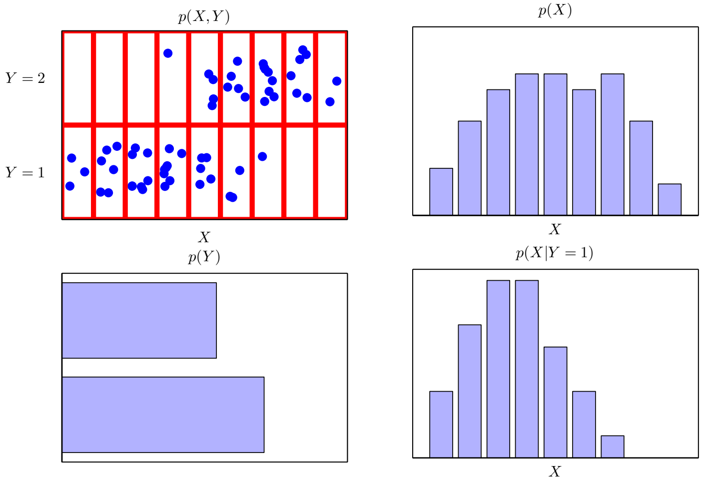

Histogram Density Representation

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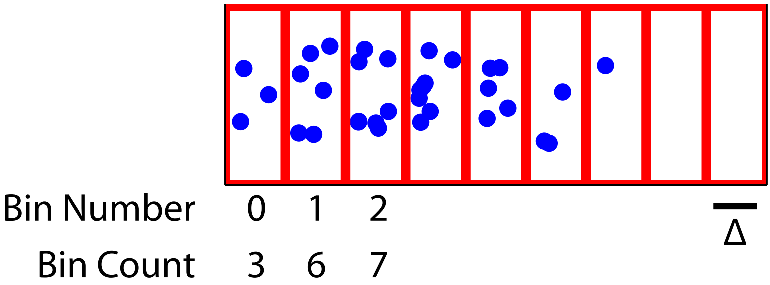
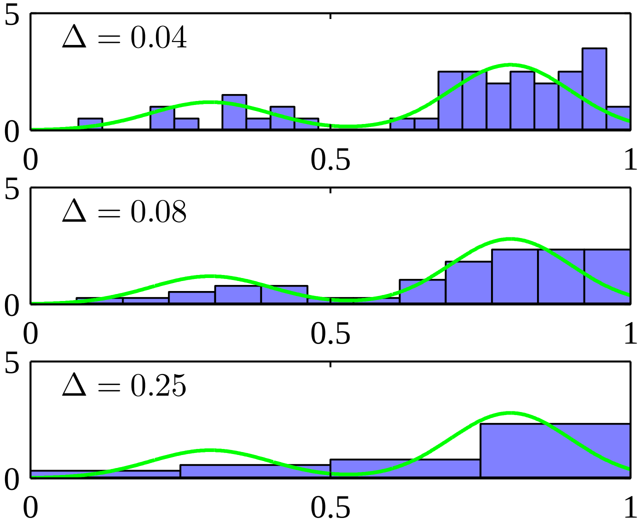
- Hence the model for the density $p(x)$ is constant over the width of each bin. (And often the bins are chosen to have the same width $\Delta_i = \Delta$.)


Bin Number
0
1
2
Bin Count
3
6
7
Δ

Histogram Density as a Function of Bin Width



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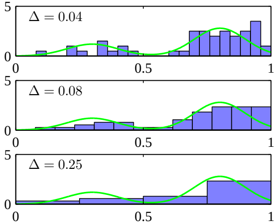

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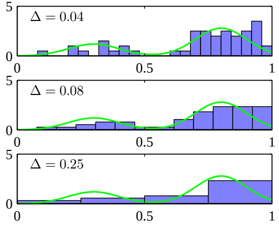

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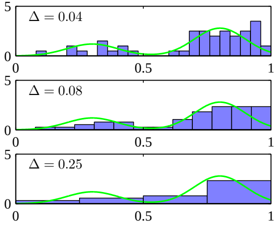

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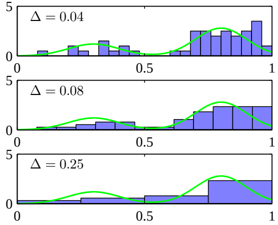

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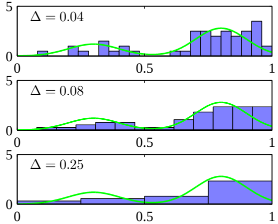

- When Δ is very big (bottom), the resulting density is quite smooth and consequently fails to capture the bimodality of $p(x)$.
- It appears that the *best results* are obtained for some intermediate value of Δ, which is given in the middle figure.
- In principle, a histogram density model is also dependent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

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  - One can throw away $\mathcal{D}$ 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.

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.
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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.
- 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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- This will be a **binomial distribution**:

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

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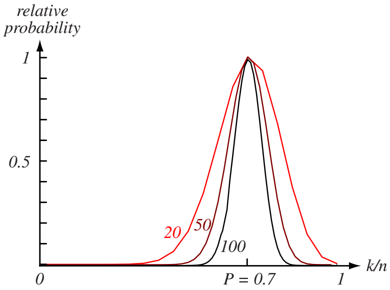
- This estimate is increasingly accurate as n increases.



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

$$\int_{\mathcal{R}} p(\mathbf{x}')d\mathbf{x}' \simeq p(\mathbf{x})V \tag{5}$$

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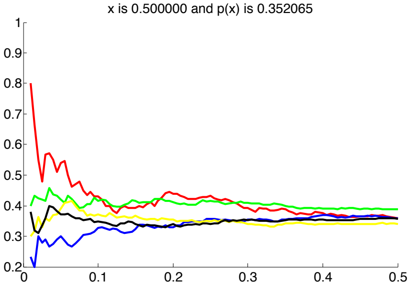
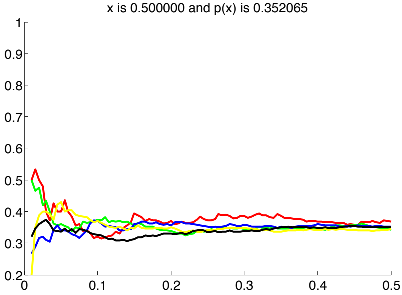
- After some rearranging, we get the following estimate for $p(\mathbf{x})$

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

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.
- Red=1000, Green=2000, Blue=3000, Yellow=4000, Black=5000.





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- The validity of our estimate depends on two contradictory assumptions:
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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: $p(\mathbf{x}) \simeq 0$.
- Note that in practice, we cannot let V to become arbitrarily small because the number of samples is always limited.

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

- To estimate the density at $\mathbf{x}$, form a sequence of regions $\mathcal{R}_1, \mathcal{R}_2, \ldots$ containing $\mathbf{x}$ with the $\mathcal{R}_1$ having 1 sample, $\mathcal{R}_2$ having 2 samples and so on.

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- 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 nth estimate for $p(\mathbf{x})$:

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- If $p_n(\mathbf{x})$ 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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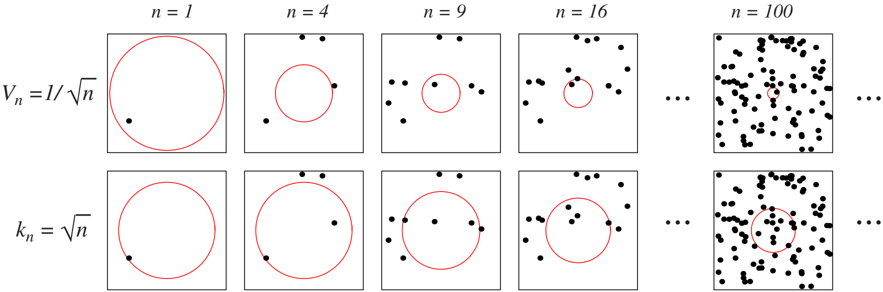
Both of these methods converge...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...

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- We can derive an analytic expression for k_n:
  - Define a **windowing function**:

$$\varphi(\mathbf{u}) = \begin{cases} 1 & |u_j| \leq 1/2 \qquad j = 1, \dots, d \\ 0 & \text{otherwise} \end{cases} \tag{12}$$

  - This windowing function φ defines a unit hypercube centered at the origin.
  - Hence, $\varphi((\mathbf{x} - \mathbf{x}_i)/h_n)$ is equal to unity if $\mathbf{x}_i$ falls within the hypercube of volume V_n centered at $\mathbf{x}$, and is zero otherwise.

- The number of samples in this hypercube is therefore given by

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$$p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{V_n}\varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right) \quad . \tag{14}$$

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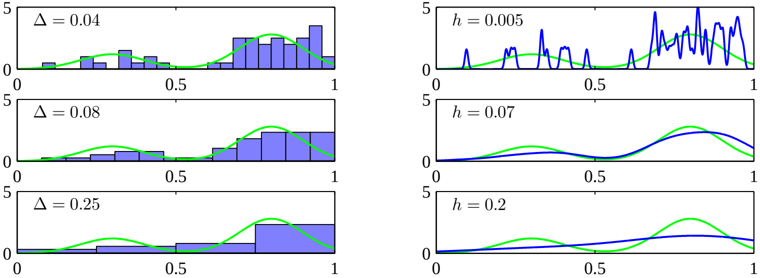
- Hence, the windowing function φ, in this context called a **Parzen window**, tells us how to **weight** all of the samples in $\mathcal{D}$ to determine $p(\mathbf{x})$ at a particular $\mathbf{x}$.

Example



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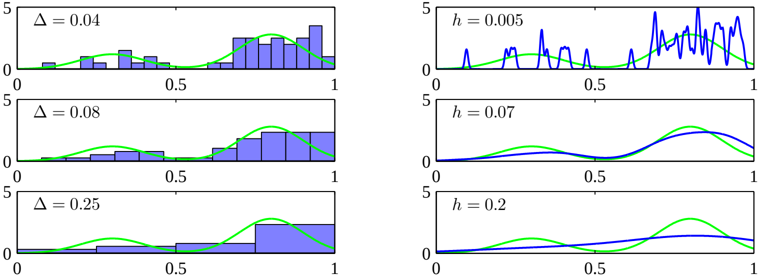

- But, what undesirable trait from histograms are inherited by Parzen window density estimates of the form we've just defined?

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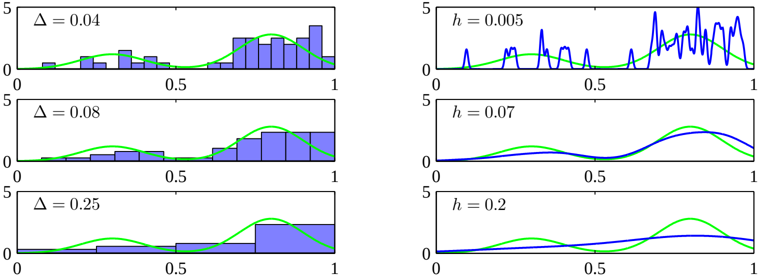

- But, what undesirable trait from histograms are inherited by Parzen window density estimates of the form we've just defined?
- Discontinuities...

Generalizing the Kernel Function

- What if we allow a more general class of windowing functions rather than the hypercube?
- If we think of the windowing function as an interpolator, rather than considering the window function about $\mathbf{x}$ only, we can visualize it as a kernel sitting on each data sample $\mathbf{x}_i$ in $\mathcal{D}$.

Generalizing the Kernel Function

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- If we think of the windowing function as an interpolator, rather than considering the window function about $\mathbf{x}$ only, we can visualize it as a kernel sitting on each data sample $\mathbf{x}_i$ in $\mathcal{D}$.
- And, if we require the following two conditions on the kernel function φ, then we can be assured that the resulting density $p_n(\mathbf{x})$ will be proper: non-negative and integrate to 1.

$$\varphi(\mathbf{x}) \geq 0 \tag{15}$$

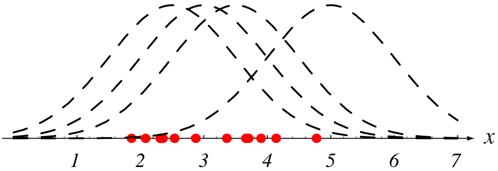
$$\int \varphi(\mathbf{u}) d\mathbf{u} = 1 \tag{16}$$

- For our previous case of $V_n = h_n^d$, then it follows $p_n(\mathbf{x})$ will also satisfy these conditions.

Example: A Univariate Guassian Kernel

- A popular choice of the kernel is the Gaussian kernel:

$$\varphi_h(u) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}u^2\right] \tag{17}$$



- The resulting density is given by:

$$p(x) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h_n\sqrt{2\pi}} \exp\left[-\frac{1}{2h_n^2}(\mathbf{x}-\mathbf{x}_i)^2\right] \tag{18}$$

- It will give us smoother estimates without the discontinuites from the hypercube kernel.

Effect of the Window Width
Slide I

- An important question is what effect does the window width h_n have on $p_n(\mathbf{x})$?
- Define $\delta_n(\mathbf{x})$ as

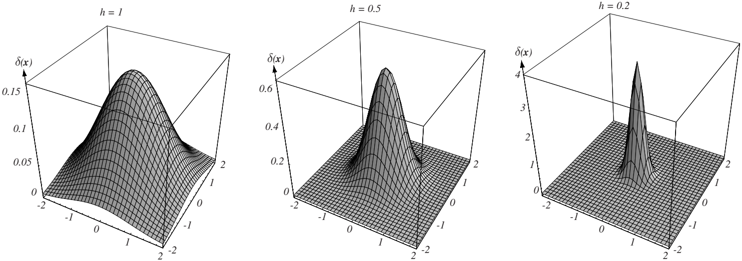
$$\delta_n(\mathbf{x}) = \frac{1}{V_n}\varphi\left(\frac{\mathbf{x}}{h_n}\right) \tag{19}$$

and rewrite $p_n(\mathbf{x})$ as the average

$$p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\delta_n(\mathbf{x}-\mathbf{x}_i) \tag{20}$$

Effect of the Window Width
Slide II

- h_n clearly affects both the amplitude and the width of $\delta_n(\mathbf{x})$.



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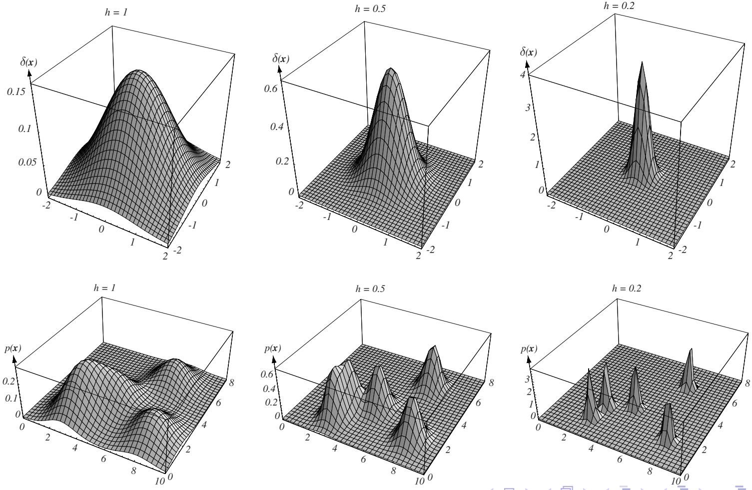

Effect of Window Width (And, hence, Volume V_n)

- But, for any value of h_n, the distribution is normalized:

$$\int \delta(\mathbf{x} - \mathbf{x}_i) d\mathbf{x} = \int \frac{1}{V_n} \varphi \left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n} \right) d\mathbf{x} = \int \varphi(\mathbf{u}) d\mathbf{u} = 1 \qquad (21)$$

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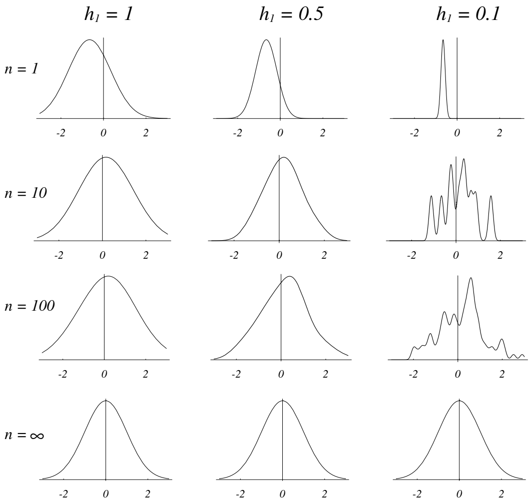
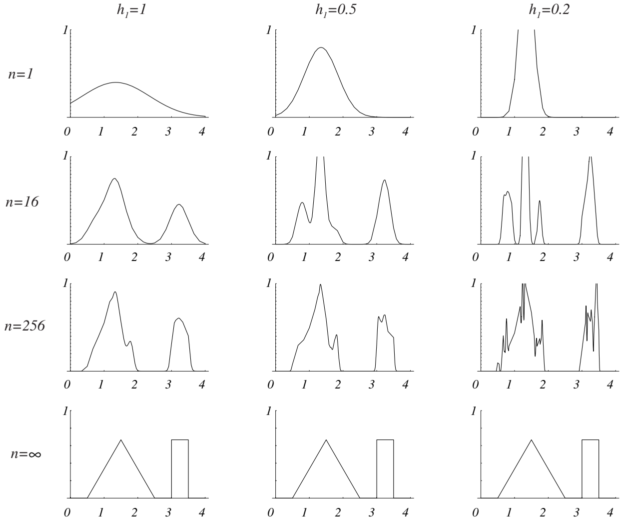
- If V_n is too large, the estimate will suffer from too little resolution.
- If V_n is too small, the estimte will suffer from too much variability.
- In theory (with an unlimited number of samples), we can let V_n slowly approach zero as n increases and then $p_n(\mathbf{x})$ will converge to the unknown $p(\mathbf{x})$. But, in practice, we can, at best, seek some compromise.

Example: Revisiting the Univariate Guassian Kernel



Example: A Bimodal Distribution



Parzen Window-Based Classifiers

- Estimate the densities for each category.
- Classify a query point by the label corresponding to the maximum posterior (i.e., one can include priors).

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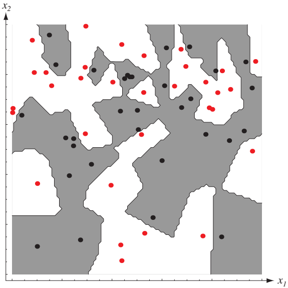
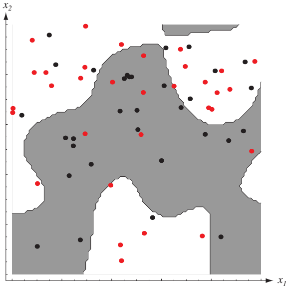
- As you guessed it, the **decision regions for a Parzen window-based classifier depend upon the kernel function**.





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- One possibility is to use cross-validation. Break up the data into a training set and a validation set. Then, perform training on the training set with varying bandwidths. Select the bandwidth that minimizes the error on the validation set.
- There is little theoretical justification for choosing one window width over another.

k_n Nearest Neighbor Methods

- Selecting the best window / bandwidth is a severe limiting factor for Parzen window estimators.
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- k_n-NN methods circumvent this problem by making the window size a function of the actual training data.
- The basic idea here is to center our window around $\mathbf{x}$ and let it grow until it capture k_n samples, where k_n is a function of n.
  - These samples are the k_n nearest neighbors of $\mathbf{x}$.
  - If the density is high near $\mathbf{x}$ then the window will be relatively small leading to good resolution.
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  - In either case, we estimate $p_n(\mathbf{x})$ according to

$$p_n(\mathbf{x}) = \frac{k_n}{nV_n} \tag{22}$$

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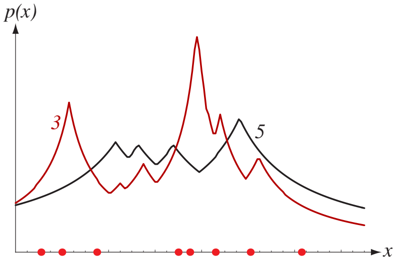
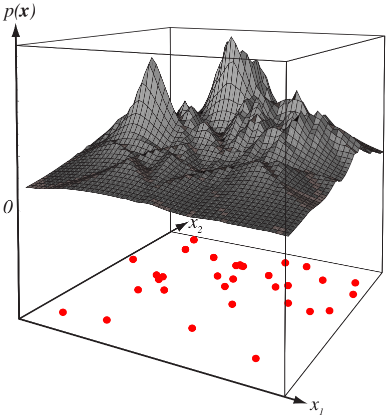
- Recall these conditions from the earlier discussion; these will ensure that $p_n(\mathbf{x})$ converges to $p(\mathbf{x})$ as n approaches infinity.

Examples of k_n-NN Estimation

- Notice the discontinuities in the slopes of the estimate.



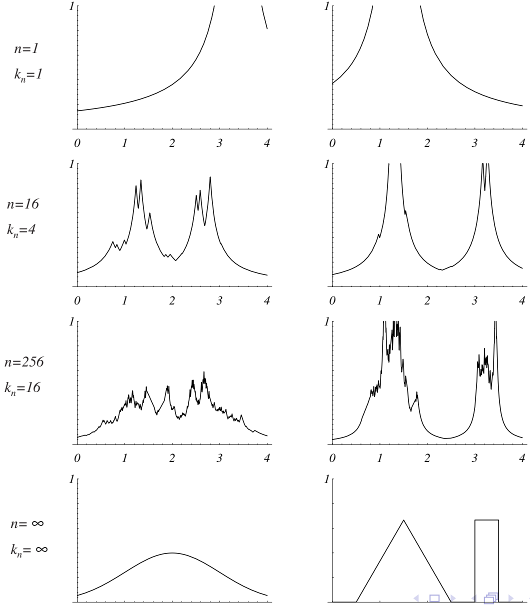


k-NN Estimation From 1 Sample

- We don't expect the density estimate from 1 sample to be very good, but in the case of k-NN it will diverge!
- With $n = 1$ and $k_n = \sqrt{n} = 1$, the estimate for $p_n(x)$ is

$$p_n(x) = \frac{1}{2|x - x_1|} \tag{23}$$

But, as we increase the number of samples, the estimate will improve.



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- But, like the Parzen window size, one choice is as good as another absent any additional information.
- Similarly, in classification scenarios, we can base our judgement on classification error.

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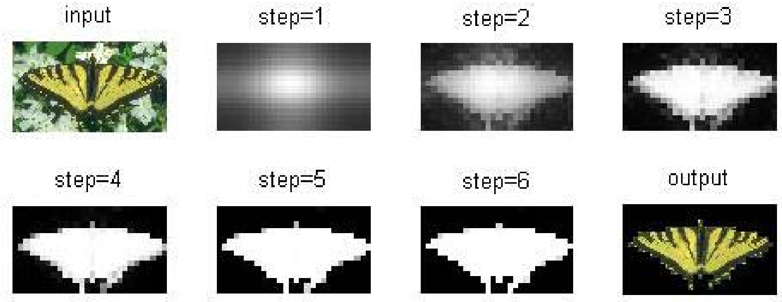
- Hence, the posterior probability for ω_i is simply the fraction of samples within the window that are labeled ω_i. This is a simple and intuitive result.

Example: Figure-Ground Discrimination

Source: Zhao and Davis. Iterative Figure-Ground Discrimination. ICPR 2004.

- Figure-ground discrimination is an important low-level vision task.
- Want to separate the pixels that contain some foreground object (specified in some meaningful way) from the background.



Example: Figure-Ground Discrimination

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- This paper presents a method for figure-ground discrimination based on non-parametric densities for the foreground and background.
- They use a subset of the pixels from each of the two regions.
- They propose an algorithm called **iterative sampling-expectation** for performing the actual segmentation.
- The required input is simply a region of interest (mostly) containing the object.

Example: Figure-Ground Discrimination

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- Given a set of n samples $S = \{\mathbf{x}_i\}$ where each $\mathbf{x}_i$ is a d-dimensional vector.
- We know the kernel density estimate is defined as

$$\hat{p}(\mathbf{y}) = \frac{1}{n\sigma_1 \ldots \sigma_d} \sum_{i=1}^{n} \prod_{j=1}^{d} \varphi\left(\frac{\mathbf{y}_j - \mathbf{x}_{ij}}{\sigma_j}\right) \tag{26}$$

where the same kernel φ with different bandwidth σ_j is used in each dimension.

The Representation

Source: Zhao and Davis. Iterative Figure-Ground Discrimination. ICPR 2004.

- The representation used here is a function of RGB:

$$r = R/(R+G+B) \tag{27}$$
$$g = G/(R+G+B) \tag{28}$$
$$s = (R+G+B)/3 \tag{29}$$

- Separating the chromaticity from the brightness allows them to us a wider bandwidth in the brightness dimension to account for variability due to shading effects.
- And, much narrower kernels can be used on the r and g chromaticity channels to enable better discrimination.

The Color Density

Source: Zhao and Davis. Iterative Figure-Ground Discrimination. ICPR 2004.

- Given a sample of pixels $S = \{\mathbf{x}_i = (r_i, g_i, s_i)\}$, the color density estimate is given by

$$\hat{P}(\mathbf{x} = (r, g, s)) = \frac{1}{n} \sum_{i=1}^{n} K_{\sigma_r}(r - r_i) K_{\sigma_g}(g - g_i) K_{\sigma_s}(s - s_i) \quad (30)$$

where we have simplified the kernel definition:

$$K_\sigma(t) = \frac{1}{\sigma} \varphi\left(\frac{t}{\sigma}\right) \quad (31)$$

- They use Gaussian kernels

$$K_\sigma(t) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{1}{2}\left(\frac{t}{\sigma}\right)^2\right] \quad (32)$$

with a different bandwidth in each dimension.

Data-Driven Bandwidth

Source: Zhao and Davis. Iterative Figure-Ground Discrimination. ICPR 2004.

- The bandwidth for each channel is calculated directly from the image based on sample statistics.

$$\sigma \approx 1.06\hat{\sigma}n^{-1/5} \tag{33}$$

where $\hat{\sigma}^2$ is the sample variance.

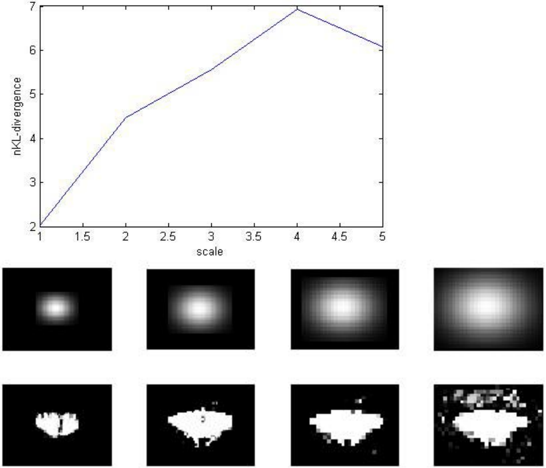
Initialization: Choosing the Initial Scale

Source: Zhao and Davis. Iterative Figure-Ground Discrimination. ICPR 2004.

- For initialization, they compute a distance between the foreground and background distribution by varying the scale of a single Gaussian kernel (on the foreground).
- To evaluate the "significance" of a particular scale, they compute the normalized KL-divergence:

$$\mathsf{nKL}(\hat{P}_{fg}||\hat{P}_{bg}) = \frac{-\sum_{i=1}^{n} \hat{P}_{fg}(\mathbf{x}_i) \log \frac{\hat{P}_{fg}(\mathbf{x}_i)}{\hat{P}_{bg}(\mathbf{x}_i)}}{\sum_{i=1}^{n} \hat{P}_{fg}(\mathbf{x}_i)} \tag{34}$$

where $\hat{P}_{fg}$ and $\hat{P}_{bg}$ are the density estimates for the foreground and background regions respectively. To compute each, they use about 6% of the pixels (using all of the pixels would lead to quite slow performance).


nKL-divergence
scale
7
6
5
4
3
2
1
1.5
2
2.5
3
3.5
4
4.5
5

Iterative Sampling-Expectation Algorithm

Source: Zhao and Davis. Iterative Figure-Ground Discrimination. ICPR 2004.

- Given the initial segmentation, they need to refine the models **and** labels to adapt better to the image.
- However, this is a chicken-and-egg problem. If we know the labels, we could compute the models, and if we knew the models, we could compute the best labels.

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- However, this is a chicken-and-egg problem. If we know the labels, we could compute the models, and if we knew the models, we could compute the best labels.
- They propose an EM algorithm for this. The basic idea is to alternate between estimating the probability that each pixel is of the two classes, and then given this probability to refine the underlying models.
- EM is guaranteed to converge (but only to a local minimum).

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- The overall probability of a pixel belonging to the foreground class

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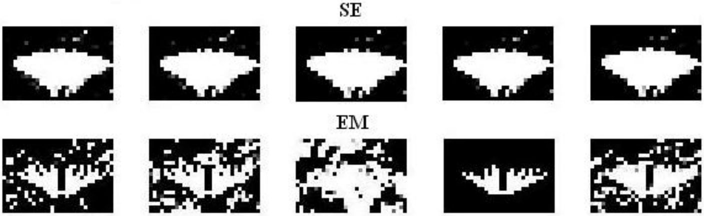
Results: Stability

Source: Zhao and Davis. Iterative Figure-Ground Discrimination. ICPR 2004.



Results

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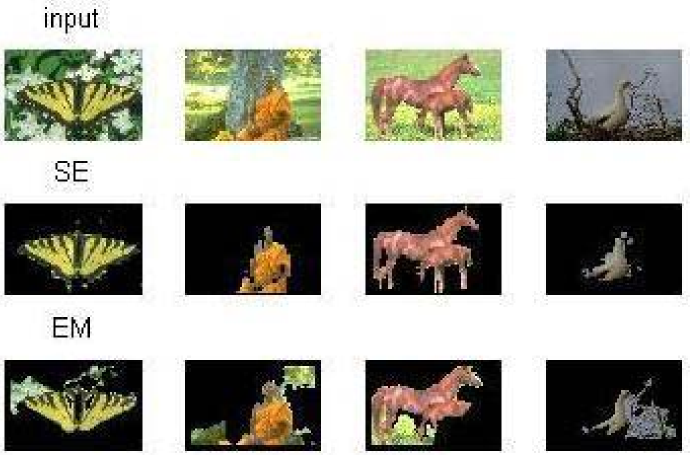

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