EE5907/EE5027 Week 5: Non-Parametric Techniques

BT Thomas Yeo

ECE, CIRC, Sinapse, Duke-NUS, HMS

Last Week Recap

- Discriminative Classifier p(y | x, w): Logistic Regression
- Numerical optimization
  - Gradient descent
  - Newton's method
  - Hessian positive definite everywhere => cost function convex => unique global minimum and every local minimum is global minimum
- Logistic regression
  - NLL is convex – optimize with Newton's method
  - Bias term
  - Regularization

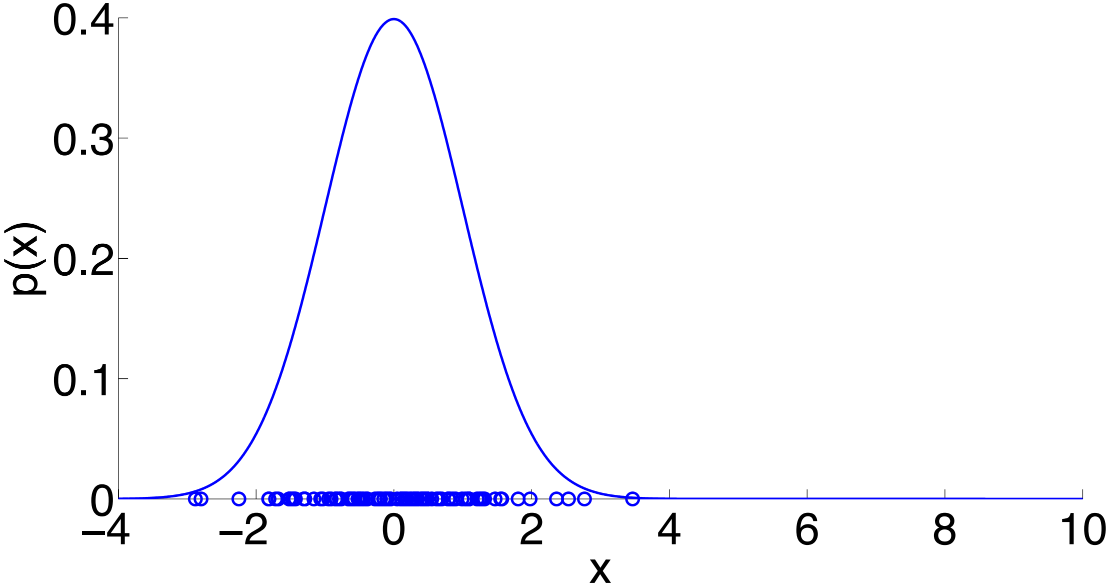
This week

- Non-parametric approaches
  - Parzen’s Window
  - K-nearest neighbors

Non-parametric Approaches

Motivation

- Problem 1: density estimation
  - Given data samples $x_1, \cdots, x_N$, estimate $p(x)$
  - Suppose we assume $p(x)$ is Gaussian with variance 1, then from previous class, ML estimate of mean $\mu_{ML} = \frac{1}{N}\sum_n x_n$, and so estimate of $p(x)$ is $\mathcal{N}(\mu_{ML}, 1)$



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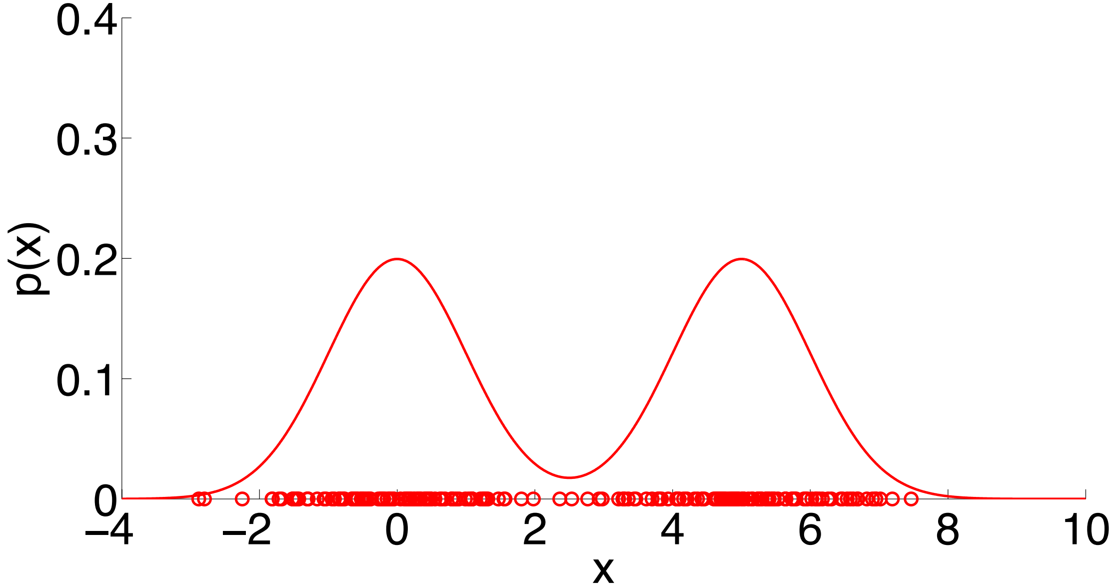
  - What if we do not know what kind of distribution p is?



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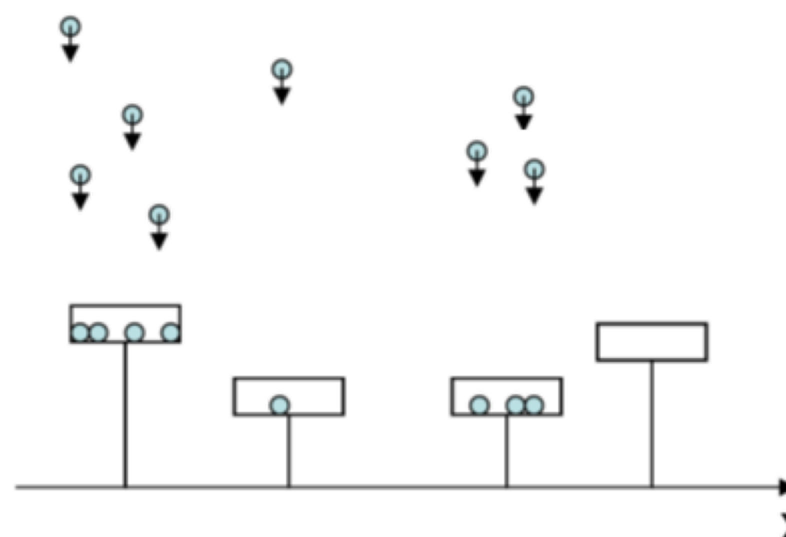
  - What if we do not know what kind of distribution p is?
- Problem 2: classification
  - Given input-output pairs $D = \{x_n, y_n\}_{n=1:N}$, learn mapping $y = f(x)$
  - What if we do not know what kind of function f is?
- Today: Non-parametric approach

Non-parametric Density Estimation: Parzen Window

Overview

- Previously assume parametric probability distributions (e.g. Gaussians), but now assume non-parametric
  - Does not mean no parameter!
  - Number and nature of parameters change with data
  - Less assumptions, but need much more data to work well
- Idea: Given $x_1, \cdots, x_N$ i.i.d. sampled from unknown $p(x)$
  - For particular x, count number of samples k falling in window of volume V centered at x
  - $p(x) \approx \frac{k/N}{V}$
- Two approaches
  - Parzen windows: fix V, estimate k
  - KNN: fix k, determine V

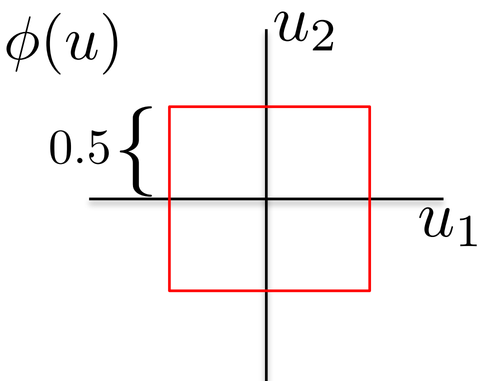


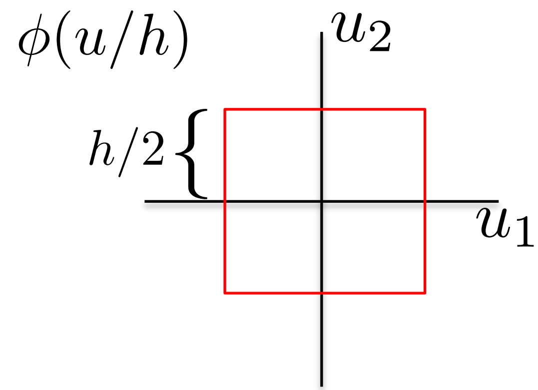
More samples in window => larger p(x)

Parzen Window

j indexes dimensionality of data

- Square cube: $\phi(u) = \begin{cases} 1 & |u_j| \leq 0.5, j = 1, \cdots, d \\ 0 & \text{otherwise} \end{cases}$





- $\phi(\frac{x - x_i}{h}) = \begin{cases} 1 & x_i \text{ inside hypercube of width } h \text{ centered at x} \\ 0 & \text{otherwise} \end{cases}$

- $k(x) = \sum_i \phi(\frac{x - x_i}{h}) = \#$ samples in hypercube centered at x

x_i = i-th data point
x_i = vector of length d

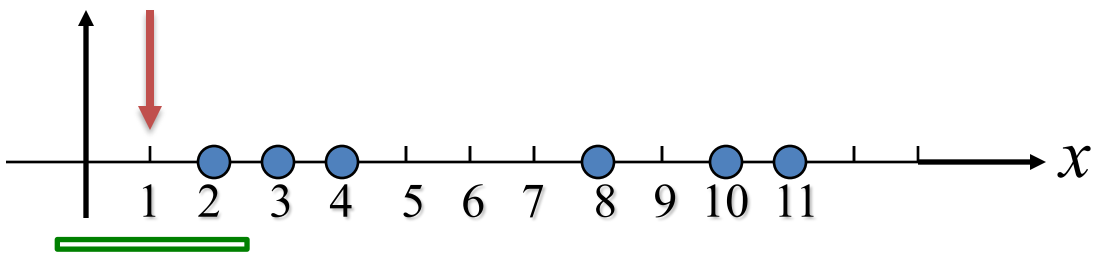
- Parzen window estimation:

$$p(x) = \frac{k(x)/N}{V} = \frac{\sum_i \phi(\frac{x - x_i}{h})/N}{h^d} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h^d} \phi\left(\frac{x - x_i}{h}\right)$$

Parzen Window as Histogramming

Parzen window estimate: $p(x) = \frac{1}{N}\sum_{i=1}^{N} \frac{1}{h^d}\phi\left(\frac{x-x_i}{h}\right)$

- Interpretation 1: At x, count fraction of samples in hypercube centered at x
- Example:
  - 6 samples at $2, 3, 4, 8, 10, 11$



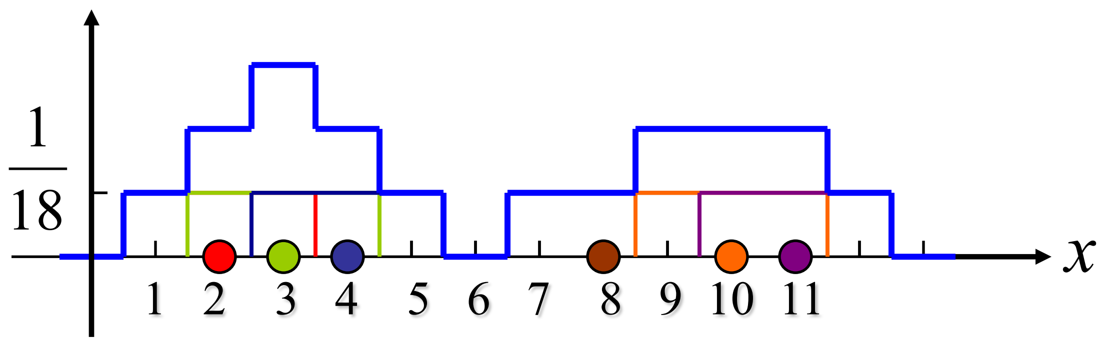
  - $d = 1, h = 3, x = 1$:

$$p(1) = \frac{1}{6}\sum_{i=1}^{6}\frac{1}{3}\phi\left(\frac{1-x_i}{3}\right) = \frac{1}{18}[1+0+0+0+0+0] = \frac{1}{18}$$

Parzen Window as Interpolation

Parzen window estimate: $p(x) = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h^d} \phi\left(\frac{x - x_i}{h}\right)$

- Interpretation 2: At x, sum of N hypercubes centered at x_i



- Instead of hypercube, can use other windows (e.g., Gaussians):

$$\phi(u) \geq 0 \text{ and } \int \phi(u) du = 1,$$

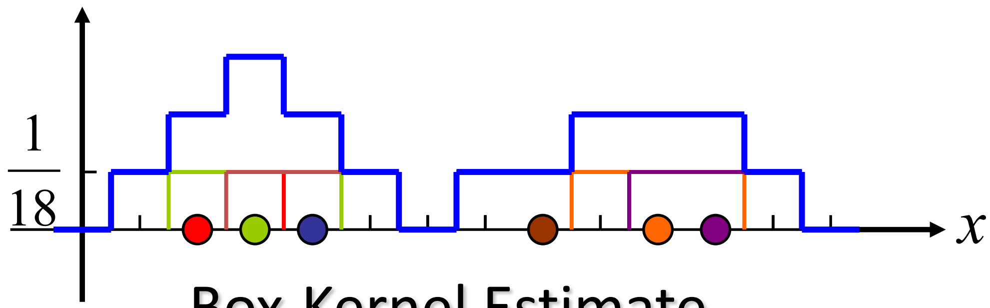
guaranteeing $p(x) \geq 0$ and integrates to 1 because $\frac{1}{h^d} \int \phi\left(\frac{x - x_i}{h}\right) dx = 1$

- Window function used for interpolation: $p(x)$ is weighted average of samples

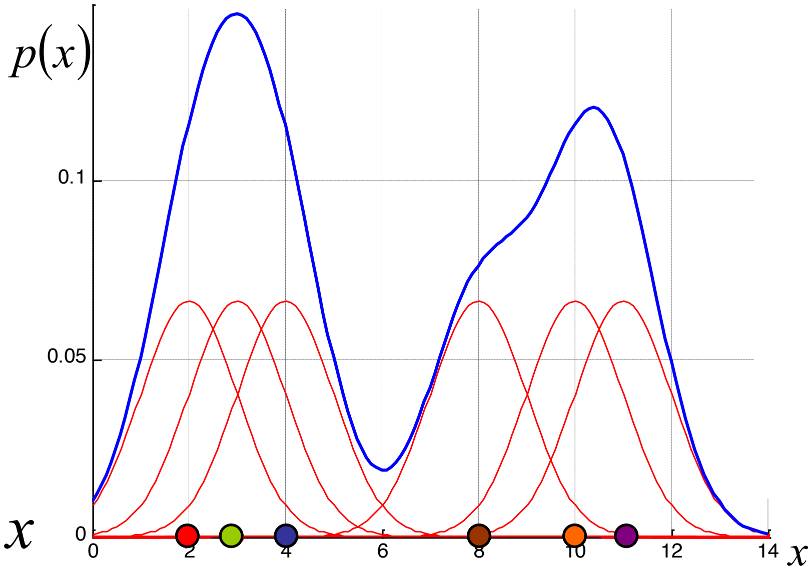
Smooth Windows

Parzen window estimate: $p(x) = \frac{1}{N}\sum_{i=1}^{N} \frac{1}{h^d}\phi\left(\frac{x-x_i}{h}\right)$

- With smooth windows (e.g., Gaussians), resulting $p(x)$ is smooth



Box-Kernel Estimate



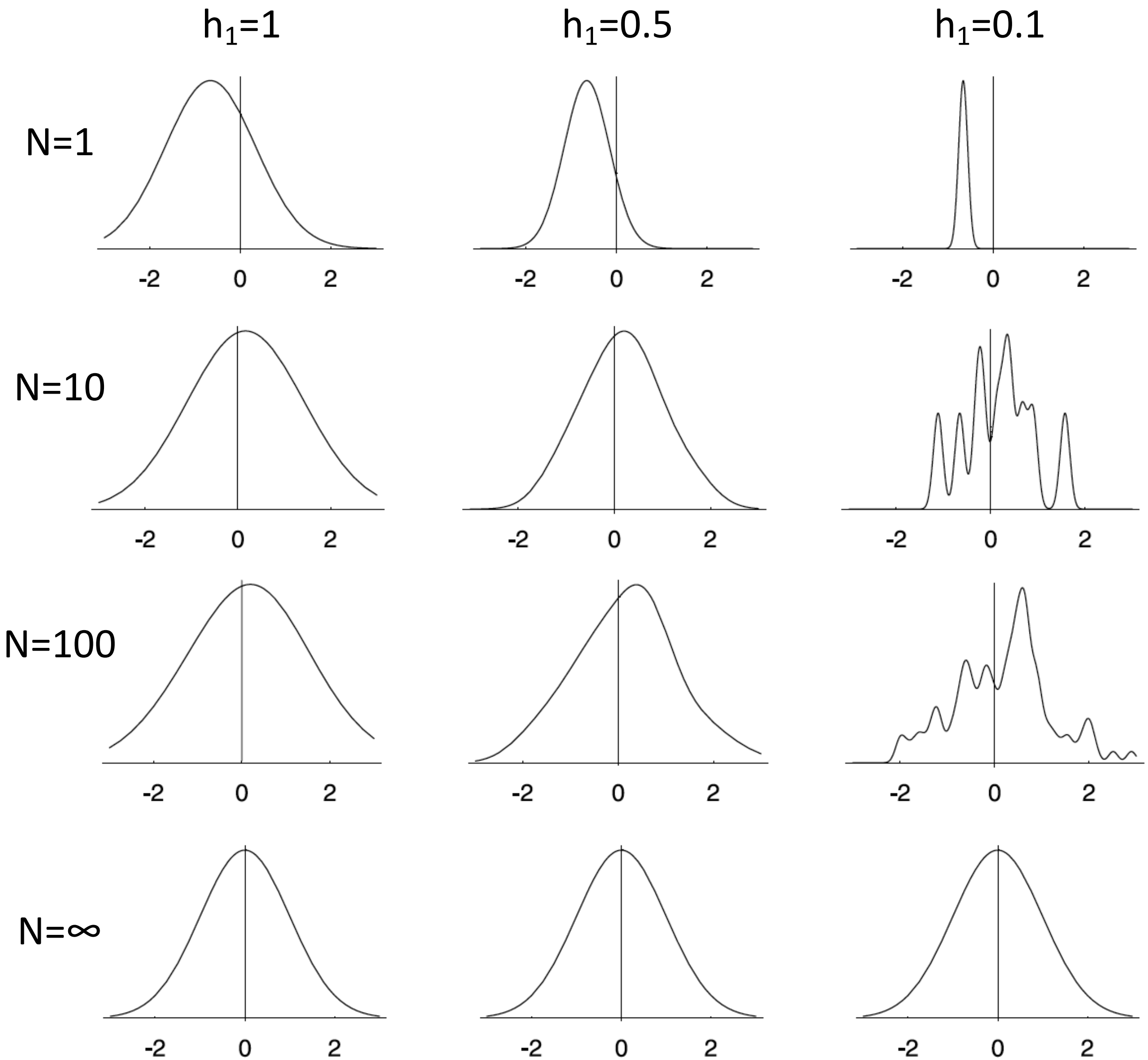
Gaussian-Kernel Estimate

Convergence Conditions

Parzen window estimate: $p_N(x) = \frac{k_N(x)/N}{V_N} = \frac{1}{N}\sum_{i=1}^{N} \frac{1}{h_N^d}\phi\left(\frac{x-x_i}{h_N}\right)$

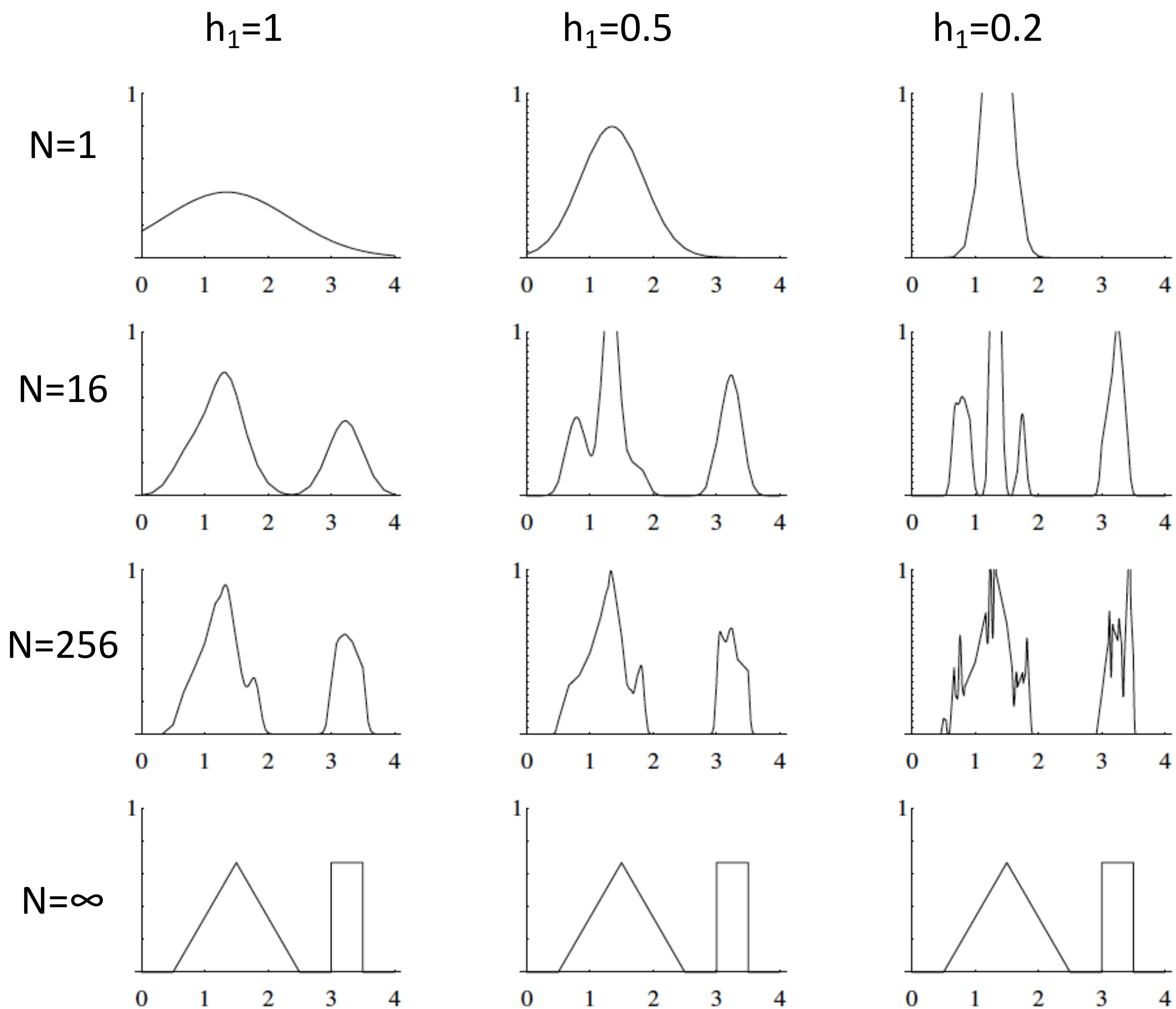
- As $N \to \infty$, want $p_N(x) \to$ true $p(x)$
- 4 sufficient conditions
  - $\sup_u \phi(u) < \infty$
  - $\lim_{||u|| \to \infty} \phi(u) \prod_{i=1}^{d} u_i = 0$
  - $\lim_{N \to \infty} V_N = 0$
  - $\lim_{N \to \infty} N V_N = \infty$
- First two conditions easy to satisfy
- Last two conditions $\implies$ volume around data sample must fall to 0, but at a rate slower than $1/N$

N(0, 1) Window to Estimate N(0, 1)



$$h_N = h_1/\sqrt{N}$$

N(0, 1) Window to Estimate Bimodal Distribution



$$h_N = h_1/\sqrt{N}$$

Setting Window Size h

Parzen window estimate: $p(x) = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{h^d}\phi\big(\frac{x-x_i}{h}\big)$

- In practice, N fixed, need to set h
- Can use cross-validation
  - Divide training data into training and validation set
  - For different h, compute estimate $p_h(x)$ from training set
  - "Test" on validation set: $\sum_i \log p_h(x_i)$, where $x_i \in$ validation set
  - Pick h with highest log probability on validation set
  - Notice we never touch test set!

Non-parametric Density Estimation: KNN

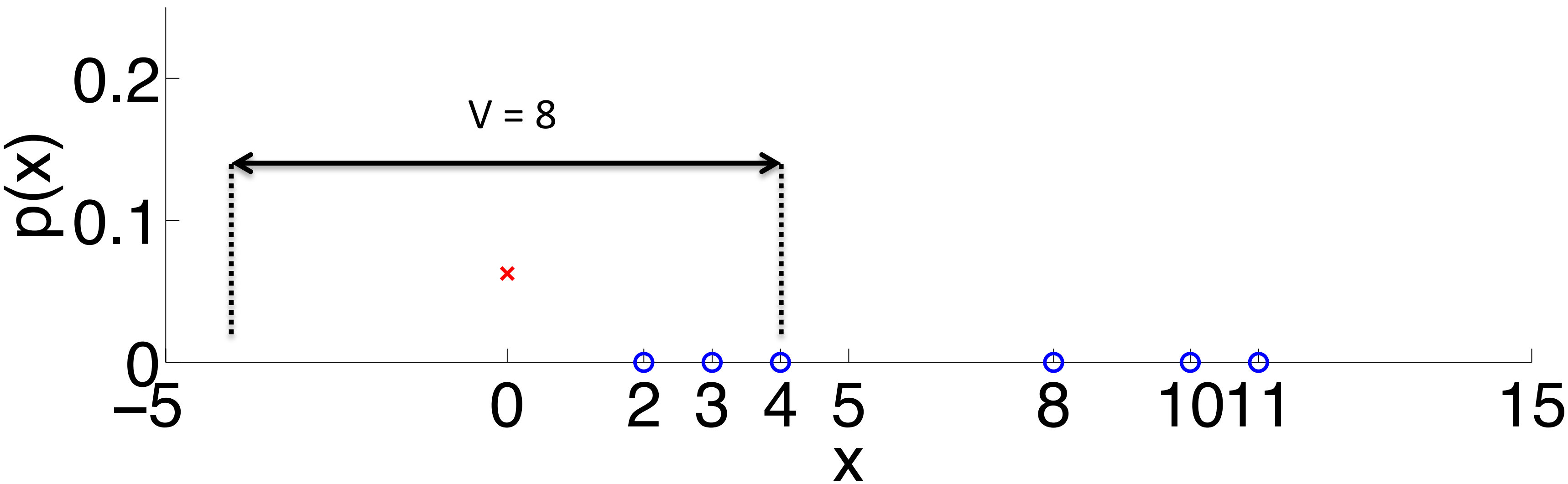
K-Nearest Neighbors (KNN) Density Estimation

KNN estimate: $p_N(x) = \frac{k_N(x)/N}{V_N}$

- Rather than fix window size, grows volume around x until $k_N(x)$ samples
- If $p(x)$ high, then volume will be small; if $p(x)$ low, then volume will be big
- Convergence: $p_N(x) \to p(x) \iff \begin{cases} \lim_{N\to\infty} k_N = \infty \\ \lim_{N\to\infty} k_N/N = 0 \end{cases}$

KNN Example

- $\{x_n\}_{n=1:6} = \{2, 3, 4, 8, 10, 11\}$, $K = 3$
- At $x = 0$, $V = 8$, so $p(x) = (K/N)/V = (3/6)/8 = 1/16$



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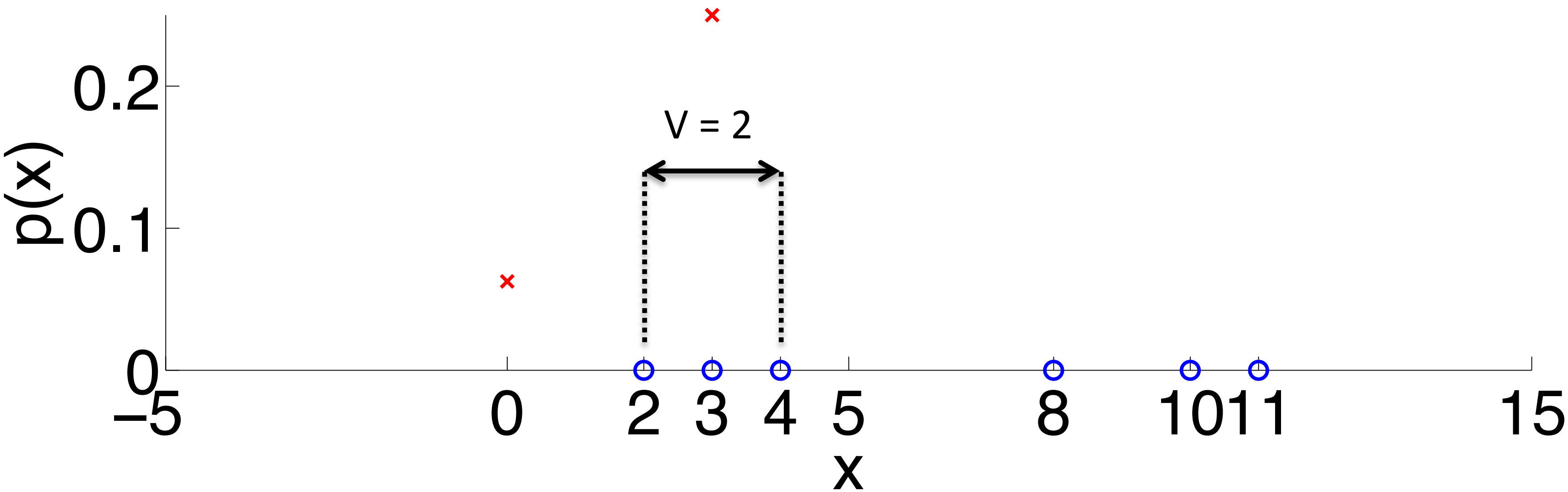

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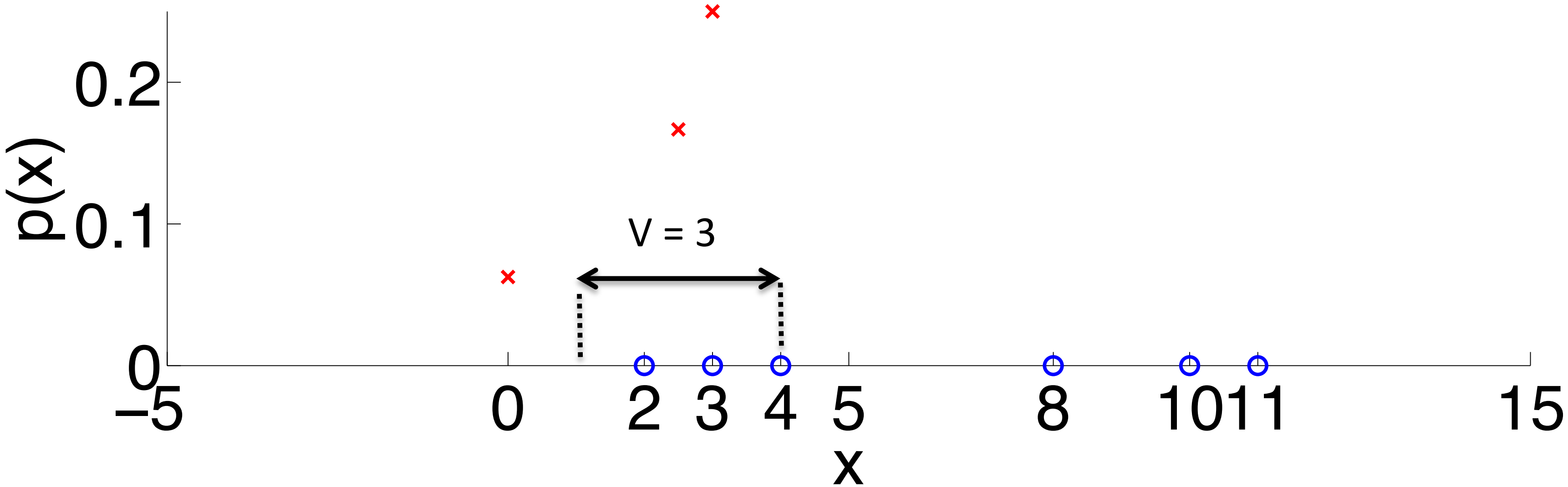
- At $x = 2.5$, $V = 3$, so $p(x) = (K/N)/V = (3/6)/3 = 1/6$



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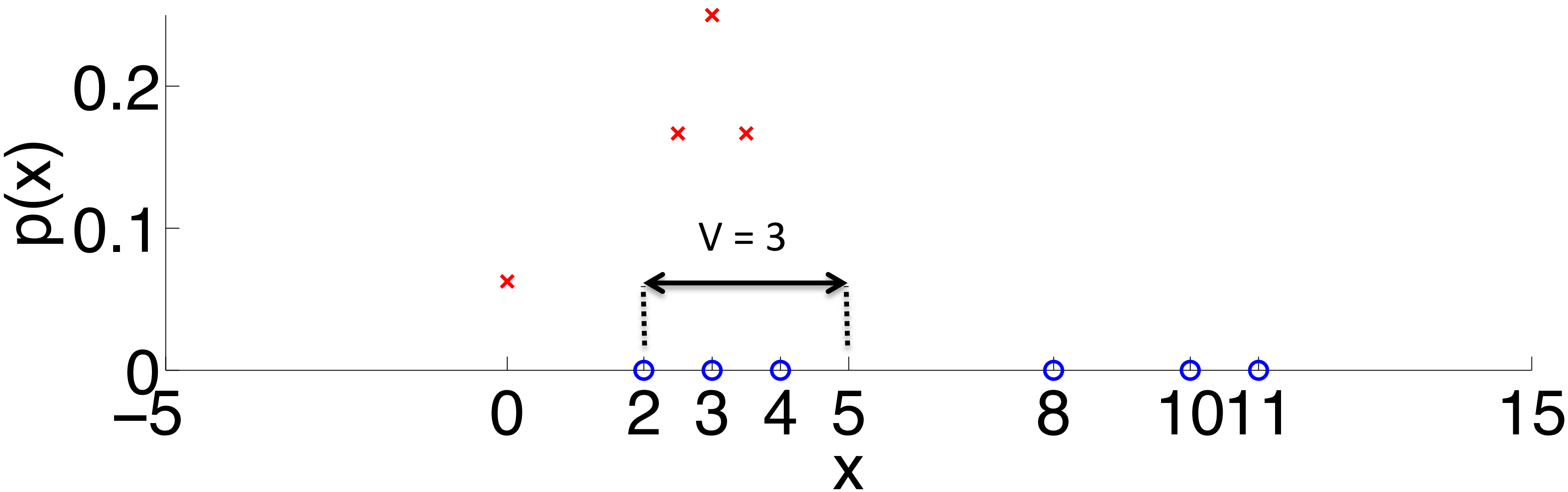

KNN Example

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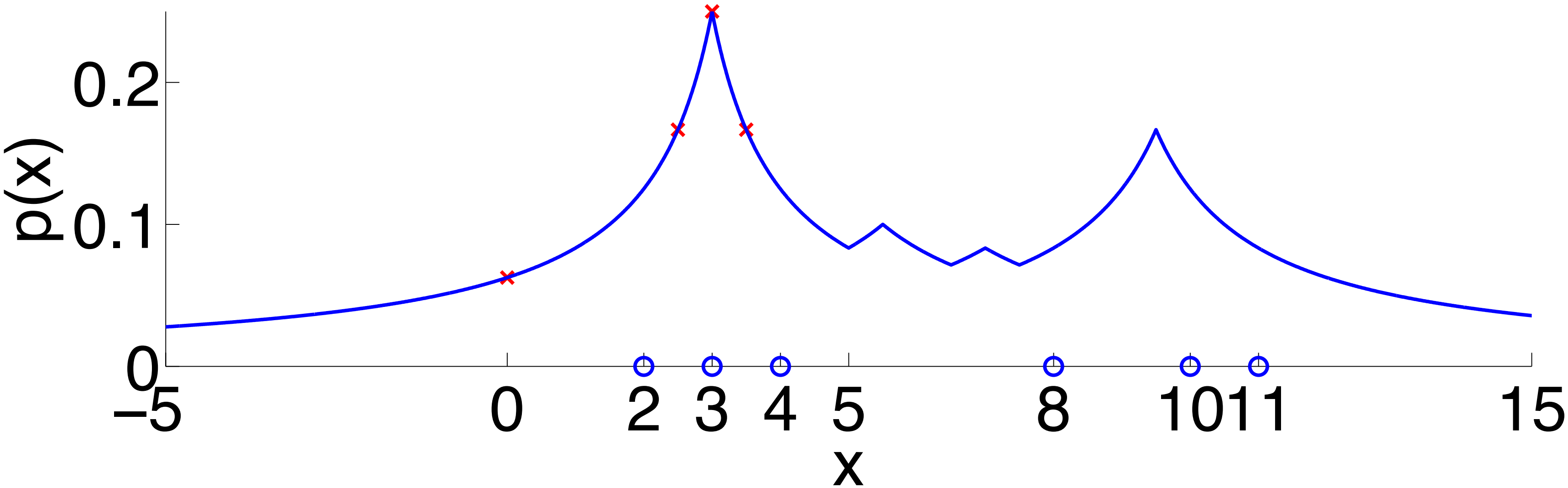
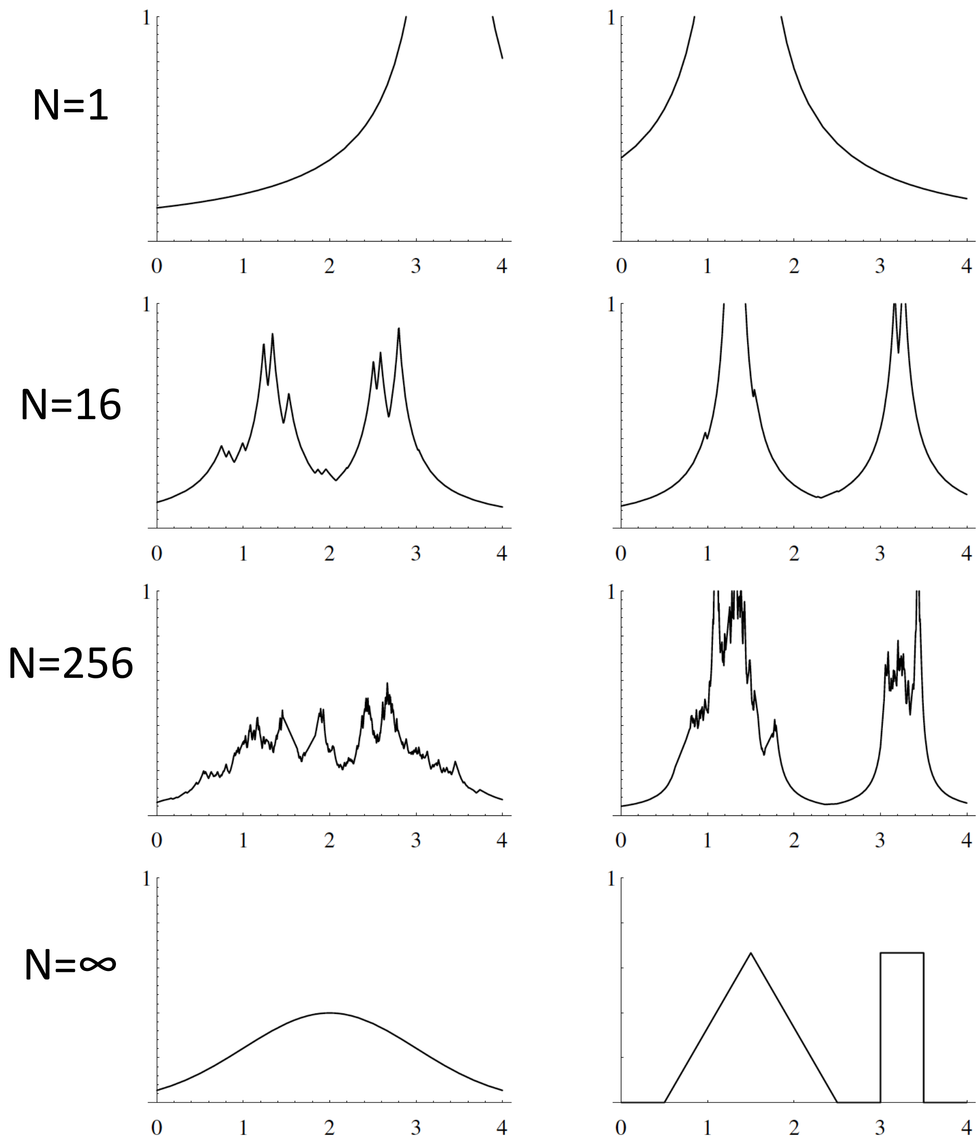
- At $x = 3.5$, $V = 3$, so $p(x) = (K/N)/V = (3/6)/3 = 1/6$
- In general, $p(x)$ continuous but not differentiable
- In general, $p(x)$ may not be proper distribution ($\int p(x)dx = \infty$)



Estimating N(0, 1) and Bi-modal Distribution



$$k_N = k_1\sqrt{N}$$

$$k_1 = 1$$

Results do not look very impressive. For density estimation, most people use Parzen's approach. But KNN used for classification instead (see later slides)

Setting # Neighbors K

KNN estimate: $p(x) = \frac{k(x)/N}{V}$

- In practice, N fixed, need to set K
- Can use cross-validation
  - Divide training data into training and validation set
  - For different K, compute estimate $p_K(x)$ from training set
  - "Test" on validation set: $\sum_i \log p_K(x_i)$, where $x_i \in$ validation set
  - Pick K with highest log probability on validation set
  - Notice we never touch test set!

Non-parametric Classification

Classification

- Given features x, want to estimate label y
- Estimate joint density $p(x, y)$ non-parametrically
- Suppose volume V around x capture K samples, k_c were from class $y = c$
  - Joint probability $p(x, y = c) = \frac{k_c/N}{V}$
  - Posterior $p(y = c|x) = \frac{p(x,y=c)}{\sum_{c'=1}^{C} p(x,y=c')} = \frac{(k_c/N)/V}{\sum_{c'=1}^{C}(k_{c'}/N)/V} = \frac{k_c}{\sum_{c'=1}^{C} k_{c'}} = \frac{k_c}{K}$
- Therefore posterior probability of class c is simply fraction of neighbors with class label c
  - MAP estimation: output class c with highest posterior probability
  - Parzen's window approach of fixing volume V obtained by cross-validation procedure
  - KNN approach of fixing K obtained by cross-validation procedure (more common, see programming assignment)

KNN Example

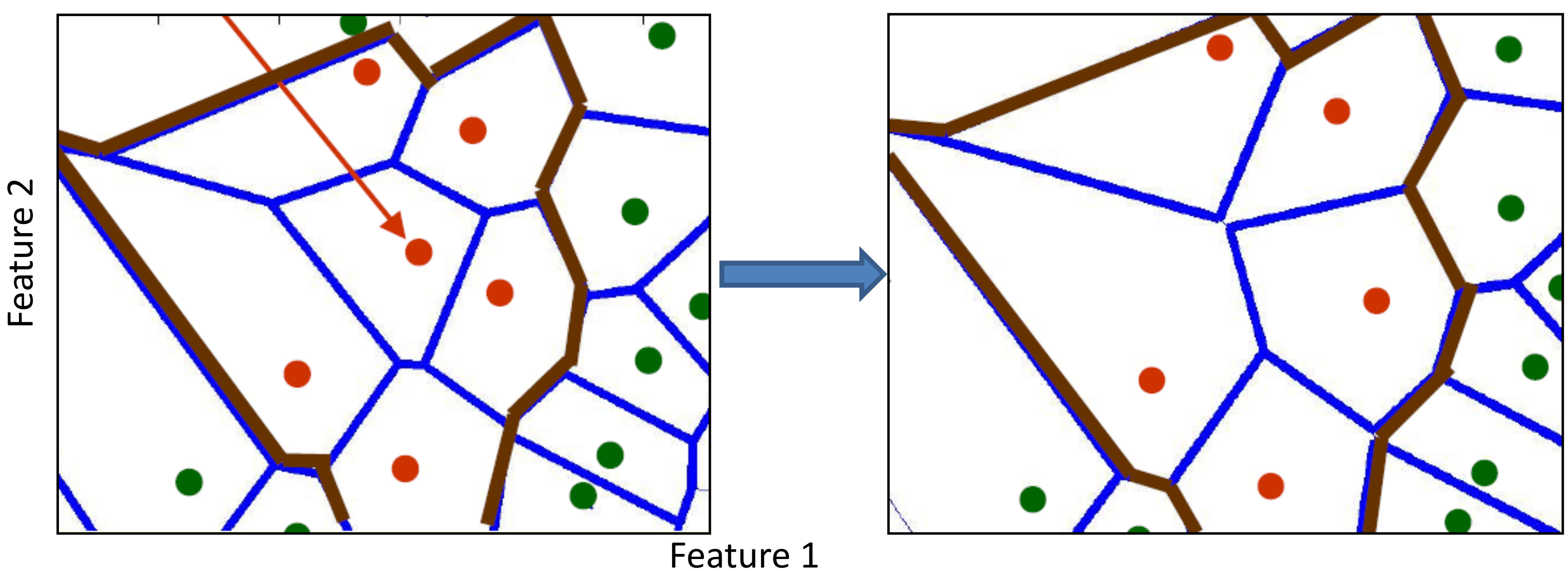
- Suppose we have training set consisting of N images & each image is labeled as a human, cat or dog
- Given a test image x, and suppose we set $K = 5$
  - Out of N training images, we find 5 images closest to the test image
  - Of these 5 images, let's say 3 images are humans (i.e., $k_{human} = 3$), 1 image is a cat (i.e., $k_{cat} = 1$) and 1 image is a dog (i.e., $k_{dog} = 1$).
  - Then $p(y = \text{human} \mid x) = k_{human}/K = 3/5$
  - $p(y = \text{cat} \mid x) = k_{cat}/K = 1/5$
  - $p(y = \text{dog} \mid x) = k_{dog}/K = 1/5$
  - So the MAP estimate of x is human

KNN Computational Complexity & Metrics

- Suppose features are D-dimensional => Compute distance between two samples require O(D) operations
- For test sample, to find closest neighbor among N training samples, need to compute distance between test sample and each training sample => N x O(D) = O(ND) operations
- To speed up:
  - Pruning/editing: for 1-NN, can remove data point surrounded by neighbors of the same class, resulting in subset of points (prototypes) used for classification

Red dots: class 1
Green dots: class 2

Blue lines: equidistant between 2 or more dots
Brown lines: 1-NN decision boundary



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  - Special data structure, e.g., https://en.wikipedia.org/wiki/K-d_tree
- Distance metrics
  - Minkowski $dist(a,b) = \left(\sum_{j=1}^{D} \left|a_j - b_j\right|^p\right)^{1/p}$, where j indexes feature dimension
  - Euclidean if $p = 2$, Manhattan if $p = 1$

Homework Assignment

- You don’t need to use any special tricks like pruning or kd-tree
- But if your code takes more than a few minutes, then your code is a bit inefficient, and you might want to speed things up
- You won’t be graded on how fast your code run, but if your code runs very slow, it will be difficult for you to debug

Summary

- Non-parametric approaches do not mean no parameters, but instead parameters grow with more data
  - Do not assume data is from specific distributions, such as Gaussian
  - Less assumptions imply non-parametric approaches need more data
- Two problems: density estimation and classification
- Two approaches
  - Parzen’s window: Count number of neighbors inside fixed window size
  - KNN: Expand window until K neighbors are captured

Optional Reading

- Notes based on
  - D&H Chapter 4.1-4.4, 4.5.5

- Some figures taken from Dr. Tam and Dr. Sun

Additional Material

Convergence Proof of Parzen Window

- Let's establish some notations and explain what we mean by convergence
- Let $\delta_n(x) = \frac{1}{h_n^d}\phi(\frac{x}{h_n})$, where $\phi(x) \geq 0$ and $\int \phi(x)dx = 1$
- Parzen window estimate: $p_n(x) = \frac{1}{n}\sum_{i=1}^{n} \delta_n(x - x_i)$
- $\lim_{h_n \to 0} \delta_n(x - x_i)$ is dirac delta function centered at x_i as $h_n \to 0$, i.e., $V_n \to 0$
- $p_n(x)$ depends on the samples $x_1, \cdots, x_n$, so $p_n(x)$ is also random with some mean $\bar{p}_n(x)$ and variance $\sigma_n^2(x)$.
- We say $p_n(x)$ converges to $p(x)$ in the mean square sense if $\lim_{n\to\infty} \bar{p}_n(x) = p(x)$ and $\lim_{n\to\infty} \sigma_n^2(x) = 0$

Convergence of Mean

- Let's consider convergence of the mean

$$\begin{aligned}\bar{p}_n(x) &= E[p_n(x)] \\ &= E[\frac{1}{n}\sum_{i=1}^{n}\delta_n(x-x_i)] \\ &= \frac{1}{n}\sum_{i=1}^{n}E[\delta_n(x-x_i)] \\ &= \int \delta_n(x-v)p(v)dv\end{aligned}$$

- From previous slide, $\lim_{n\to\infty}\delta_n(x-v)$ is a delta function centered at x if $\lim_{n\to\infty}V_n=0$

- Therefore $\lim_{n\to\infty}\bar{p}_n(x)=p(x)$ assuming $p(x)$ continuous at x

Convergence of Variance

- $\sigma_n^2(x)$ is sum of independent variables $\frac{1}{n}\delta_n(x - x_i)$, therefore $\sigma_n^2(x)$ is sum of the variance of the independent variables, so

$$\begin{aligned}
\sigma_n^2(x) &= \sum_{i=1}^{n} E\left[\left(\frac{1}{n}\delta_n(x-v) - \frac{1}{n}\bar{p}_n(x)\right)^2\right] \\
&= nE\left[\frac{1}{n^2}\delta_n^2(x-v)\right] - \frac{2}{n}\bar{p}_n^2(x) + \frac{1}{n}\bar{p}_n^2(x) \\
&= \int \frac{1}{n}\delta_n^2(x-v)p(v)dv - \frac{1}{n}\bar{p}_n^2(x) \\
&\leq \int \frac{1}{n}\left(\frac{1}{h_n^d}\phi\left(\frac{x-v}{h_n}\right)\right)\delta_n(x-v)p(v)dv \\
&\leq \frac{\sup(\phi(\cdot))}{nh_n^d}\int \delta_n(x-v)p(v)dv \\
&= \frac{\sup(\phi(\cdot))\bar{p}_n(x)}{nh_n^d} = C
\end{aligned}$$

- If $\sup_u \phi(u) < \infty$, and $\lim_{n\to\infty} V_n = \infty$, then $C \to 0$