Nonparametric Methods

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CS182: Introduction to Machine Learning (Fall 2021)
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Outline

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Introduction

Nonparametric Density Estimation

Generalization to Multivariate Case

Nonparametric Classification

Nonparametric Regression

Parametric, Semiparametric, and Nonparametric Methods

- Parametric:
  - $p(\mathbf{x} \mid C_i)$ is represented by a single global parametric model.
  - Topic 3 (Parameter Estimation for Generative Models)
- Semiparametric:
  - $p(\mathbf{x} \mid C_i)$ is represented by a small number of local parametric models.
  - Topic 10 (Clustering and Mixture Models)
- Nonparametric:
  - $p(\mathbf{x} \mid C_i)$ cannot be represented by a single parametric model or a mixture model; the data speaks for itself.
  - Assumption: similar inputs have similar outputs, i.e., smooth functions (e.g., probability density functions, discriminant functions, regression functions).
  - Given a test instance, find a small number of nearest (or most similar) training instances and interpolate from them.
  - A.k.a. instance-based, memory-based, case-based or lazy learning algorithms.

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Nonparametric Density Estimation: Univariate Case

- Sample $\mathcal{X} = \{x^{(\ell)}\}_{\ell=1}^{N}$, drawn i.i.d. from some unknown probability density $p(x)$, with cumulative distribution function $F(x)$.
- Estimator $\hat{F}(x)$ for $F(x)$:

$$\hat{F}(x) = \frac{\#\{x^{(\ell)} \leq x\}}{N}$$

- Estimator $\hat{p}(x)$ for $p(x)$:

$$\hat{p}(x) = \frac{1}{h}\left[\frac{\#\{x^{(\ell)} \leq x + h\} - \#\{x^{(\ell)} \leq x\}}{N}\right]$$

where h is the length of the interval and instances $x^{(\ell)}$ that fall in this interval are assumed to be "close enough".

Histogram Estimator

- The input space is divided into equal-sized intervals called bins:

$$\left[x_0 + mh, x_0 + (m+1)h\right)$$

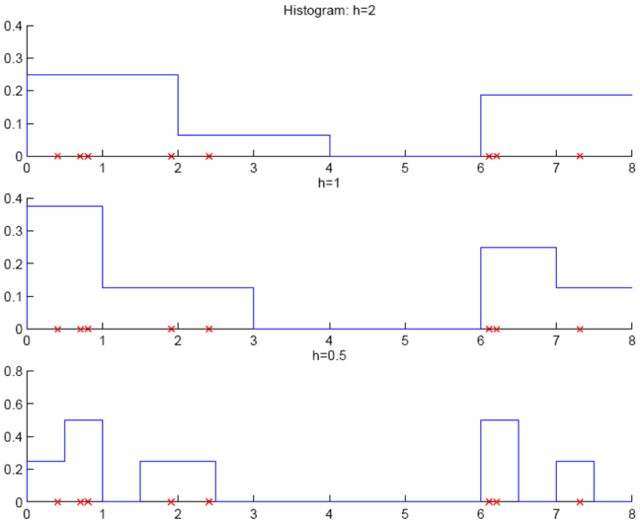
  where x_0 is the origin, h is the bin width, and m is an integer.

- Histogram estimator:

$$\hat{p}(x) = \frac{\#\{x^{(\ell)} \text{ in the same bin as } x\}}{Nh}$$

- Once the bin estimates are calculated and stored, we do not need to retain the training set.

Histogram Estimator with Different Bin Sizes



Naive Estimator

- Unlike the histogram estimator, this estimator frees us from setting an origin.
- Naive estimator:

$$\hat{p}(x) = \frac{\#\{x - h/2 < x^{(\ell)} \le x + h/2\}}{Nh}$$

- The bin is of size h and x is always at its center.
- Alternative form of estimator:

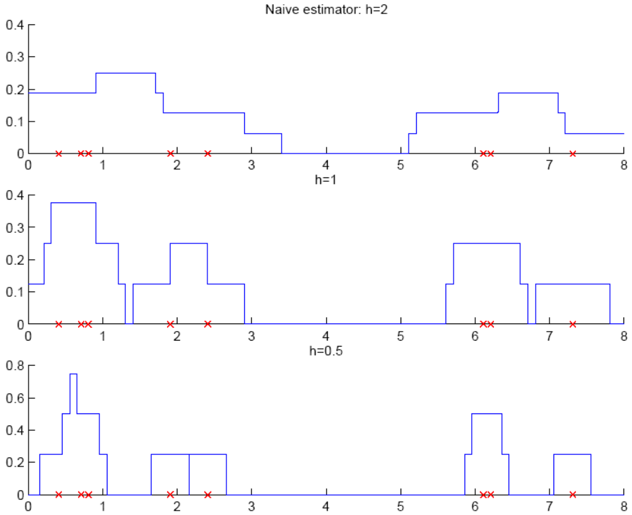
$$\hat{p}(x) = \frac{1}{Nh} \sum_{\ell=1}^{N} w\left(\frac{x - x^{(\ell)}}{h}\right)$$

  with weight function:

$$w(u) = \begin{cases} 1 & \text{if } |u| < 1/2 \\ 0 & \text{otherwise} \end{cases}$$

- Each $x^{(\ell)}$ has a symmetric region of influence of size h around it and contributes 1 for an x falling in its region. The nonparametric estimate is the sum of influences of $x^{(\ell)}$ whose regions include x, i.e., sum of "boxes."

Naive Estimator with Dieffrent Bin Sizes



Kernel Estimator

- Histogram estimator and naive estimator are not smooth at bin boundaries.
- To get a smooth estimator, a smooth weight function called kernel function is used, e.g., Gaussian kernel:

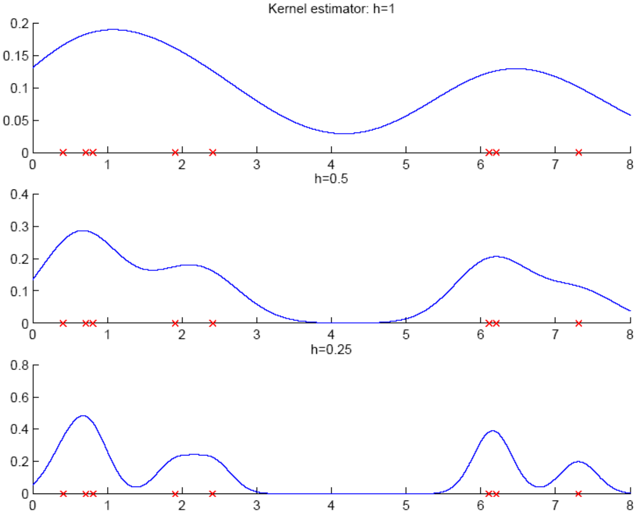
$$K(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$$

- Kernel estimator (a.k.a. Parzen windows):

$$\hat{p}(x) = \frac{1}{Nh} \sum_{\ell=1}^{N} K\left(\frac{x - x^{(\ell)}}{h}\right)$$

  where $K(\cdot)$ determines the shape of the influences and h determines the width. $K(\cdot)$ should be everywhere nonnegative and integrates to 1.
- It is a sum of N smooth local functions.

Kernel Estimator with Different Window Widths



Properties of Kernel Estimator

- All the $x^{(\ell)}$ have an effect on the estimate at x and this effect decreases smoothly as $|x - x^{(\ell)}|$ increases.
- When h is small, each training instance has a large effect in a small region.
- When h is large, there is more overlap of the kernels and the estimator is smoother.
- One problem with this estimator is that the window width h is fixed across the entire input space.

k-Nearest Neighbor Estimator I

- While kernel estimator uses the same window width everywhere, the nearest neighbor class of estimators adapts the amount of smoothing to the local density of data.
- The degree of smoothing is controlled by $k(\ll N)$, the number of neighbors taken into account.
- k-nearest neighbor (k-NN) estimator:

$$\hat{p}(x) = \frac{k}{2Nd_k(x)}$$

  where $d_k(x)$ is the distance from x to the kth nearest instance.
- This is like a naive estimator with $h = 2d_k(x)$, the difference being that instead of fixing h and checking how many samples fall in the bin, we fix k, the number of observations to fall in the bin, and compute the bin size.
- When the data density is high, the bins are small; when it is low, the bins are larger.

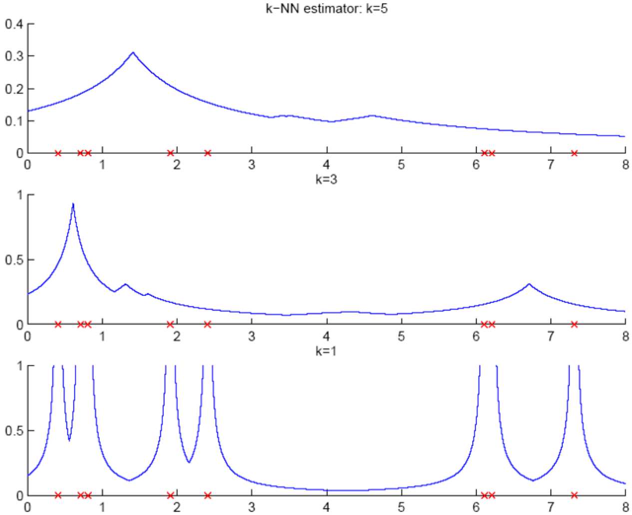
k-Nearest Neighbor Estimator II

- The k-NN estimator is not continuous and hence is not a probability density function since it integrates to ∞, not 1.
- k-nearest neighbor (k-NN) estimator with a kernel function:

$$\hat{p}(x) = \frac{1}{N d_k(x)} \sum_{\ell=1}^{N} K\left(\frac{x - x^{(\ell)}}{d_k(x)}\right)$$

  where $K(\cdot)$ is typically chosen to be the Gaussian kernel.
- This estimator is like a kernel estimator with adaptive smoothing parameter $h = d_k(x)$.

k-Nearest Neighbor Estimator with Different k Values



Outline

Generalization to Multivariate Case I

- A sample of *d*-dimensional observations $\mathcal{X} = \{\mathbf{x}^{(\ell)}\}_{\ell=1}^{N}$
- Multivariate kernel density estimator:

$$\hat{p}(x) = \frac{1}{Nh^d} \sum_{\ell=1}^{N} K\Big(\frac{\mathbf{x} - \mathbf{x}^{(\ell)}}{h}\Big)$$

  with the requirement that

$$\int_{\mathbb{R}^d} K(\mathbf{x}) d\mathbf{x} = 1$$

- Multivariate Gaussian kernel:

$$K(\mathbf{u}) = \Big(\frac{1}{\sqrt{2\pi}}\Big)^d \exp\Big(-\frac{\|\mathbf{u}\|^2}{2}\Big)$$

Generalization to Multivariate Case II

- Instead of using a single smoothing parameter h for all dimensions which corresponds to using the Euclidean distance, generalization to Mahalanobis distance gives the multivariate ellipsoidal Gaussian kernel:

$$K(\mathbf{u}) = \frac{1}{(2\pi)^{d/2}|\mathbf{S}|^{1/2}} \exp\left(-\frac{1}{2}\mathbf{u}^T\mathbf{S}^{-1}\mathbf{u}\right)$$

  where $\mathbf{S}$ is the (general) sample covariance matrix.
- Curse of dimensionality: nonparametric estimation in high-dimensional spaces may require many bins, most of which end up being empty.

Outline

Nonparametric Classification I

- Classification based on density estimation:
  - **Step 1**: estimate the class-conditional densities $p(\mathbf{x} \mid C_i)$ (parametric or nonparametric approach).
  - **Step 2**: use Bayes' rule to compute the posterior class probabilities and make optimal decision.
- Kernel estimator of class-conditional densities:

$$\hat{p}(\mathbf{x} \mid C_i) = \frac{1}{N_i h^d} \sum_{\ell=1}^{N} K\left(\frac{x - x^{(\ell)}}{h}\right) r_i^{(\ell)}$$

where

$$r_i^{(\ell)} = \begin{cases} 1 & \text{if } \mathbf{x}^{(\ell)} \text{ is in } C_i \\ 0 & \text{otherwise} \end{cases}$$

and $N_i = \sum_\ell r_i^{(\ell)}$.

Nonparametric Classification II

- MLE of prior probabilities:

$$\hat{p}(C_i) = \frac{N_i}{N}$$

- Discriminant functions:

$$g_i(\mathbf{x}) = \hat{p}(\mathbf{x} \mid C_i)\hat{P}(C_i) = \frac{1}{Nh^d}\sum_{\ell=1}^{N} K\Big(\frac{x - x^{(\ell)}}{h}\Big) r_i^{(\ell)}$$

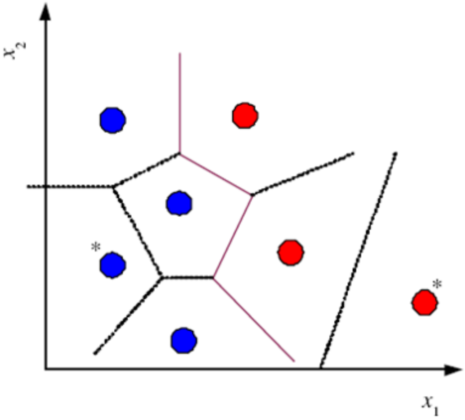
where the common factor $1/(Nh^d)$ can be ignored.

k-NN Classifier

- k-NN estimator:
$$\hat{p}(\mathbf{x} \mid C_i) = \frac{k_i}{N_i V^k(\mathbf{x})}$$
where k_i is the number of neighbors that belong to C_i and $V^k(\mathbf{x})$ is the volume of the d-dimensional hypersphere centered at $\mathbf{x}$ with radius $r = \|\mathbf{x} - \mathbf{x}_{(k)}\|$ where $\mathbf{x}_{(k)}$ is the k-th nearest observation to $\mathbf{x}$ (among all neighbors from all classes of $\mathbf{x}$).
- Posterior class probabilities:
$$\hat{P}(C_i \mid \mathbf{x}) = \frac{\hat{p}(\mathbf{x} \mid C_i)\hat{P}(C_i)}{\sum_j \hat{p}(\mathbf{x} \mid C_j)\hat{P}(C_j)} = \frac{k_i/NV^k(\mathbf{x})}{\sum_j k_j/NV^k(\mathbf{x})} = \frac{k_i}{k}$$
- k-NN classifier: assigns the input $\mathbf{x}$ to the class C_i having most examples among the k neighbors of $\mathbf{x}$, i.e.,
$$i = \arg\max_j \hat{P}(C_j \mid \mathbf{x}) = \arg\max_j k_j$$

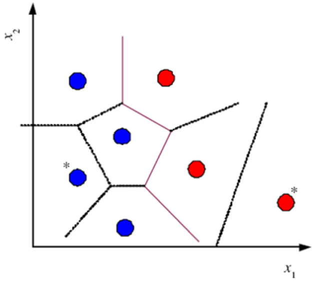
Nearest Neighbor Classifier

- Nearest neighbor classifier: special case of k-NN classier with $k = 1$.
- Voronoi tessellation formed in input space:



Condensed Nearest Neighbor

- Time/space complexity of nonparametric methods (e.g., k-NN): $O(N)$
- Condensing methods: find a small (hopefully smallest) subset $\mathcal{Z}$ of $\mathcal{X}$ such that the error does not increase when $\mathcal{Z}$ is used in place of $\mathcal{X}$.
- Condensed nearest neighbor classier: only the instances that define the discriminant need to be kept but those inside the class regions can be removed (cf. support vector machines).



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Nonparametric Regression

- Nonparametric regression is a.k.a. smoothing models.
- Regression problem:
$$y^{(\ell)} = g(\mathbf{x}^{(\ell)}) + \epsilon$$
where $y^{(\ell)} \in \mathbb{R}$.
- Nonparametric regression is needed when we cannot find an appropriate parametric model (e.g., polynomial) for $g(\cdot)$.
- Nonparametric regression estimators (a.k.a. smoothers):
  - Running mean smoother
  - Kernel smoother
  - Running line smoother
- Here we consider the univariate case, which can be extended easily to the multivariate case.

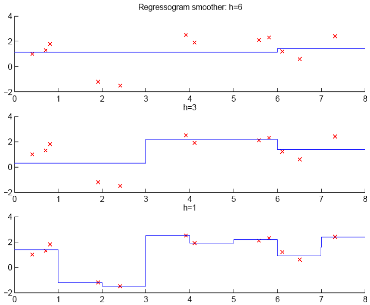
Running Mean Smoother I

- Regressogram:

$$\hat{g}(x) = \frac{\sum_{\ell=1}^{N} b(x, x^{(\ell)}) y^{(\ell)}}{\sum_{\ell=1}^{N} b(x, x^{(\ell)})}$$

where

$$b(x, x^{(\ell)}) = \begin{cases} 1 & \text{if } x^{(\ell)} \text{ is in the same bin with } x \\ 0 & \text{otherwise} \end{cases}$$



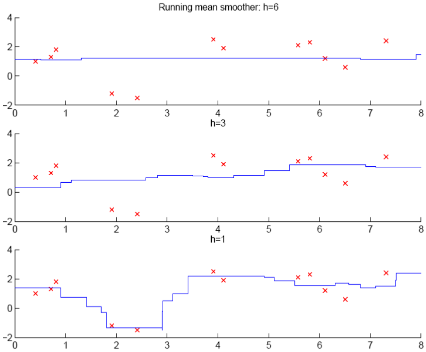
Running Mean Smoother II

- To avoid the need to fix an origin, the running mean smoother defines a bin symmetric around x:

$$\hat{g}(x) = \frac{\sum_{\ell=1}^{N} w\left(\frac{x - x^{(\ell)}}{h}\right) y^{(\ell)}}{\sum_{\ell=1}^{N} w\left(\frac{x - x^{(\ell)}}{h}\right)}$$

where

$$w(u) = \begin{cases} 1 & \text{if } |u| < 1 \\ 0 & \text{otherwise} \end{cases}$$



Kernel Smoother

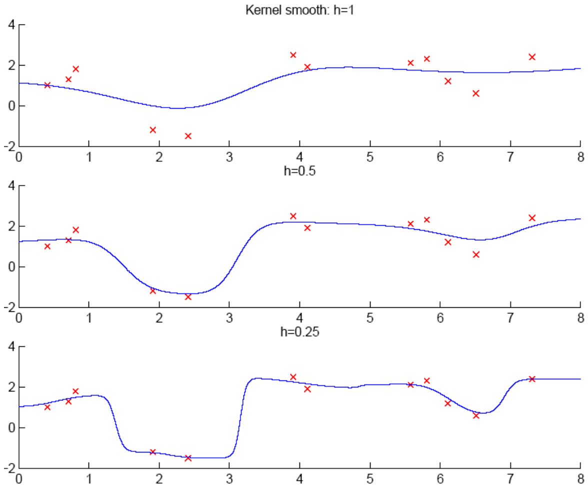
- Kernel smoother:

$$\hat{g}(x) = \frac{\sum_{\ell=1}^{N} K(\frac{x - x^{(\ell)}}{h}) y^{(\ell)}}{\sum_{\ell=1}^{N} K(\frac{x - x^{(\ell)}}{h})}$$

  where $K(\cdot)$ is a kernel, such as Gaussian kernel, that gives less weight to further points.

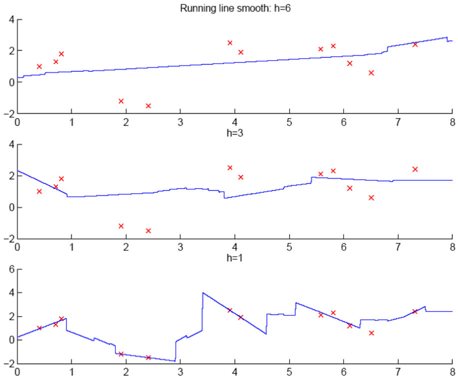
- k-NN smoother:
  Instead of fixing h, the number of neighbors k is fixed to adapt to the density around x.

Kernel Smoother with Different Bin Lengths



Running Line Smoother

- Unlike the running mean smoother which has discontinuities, the running line smoother uses continuous piecewise linear fit.



- Alternatively, kernel weighting may also be used to give the locally weighted running line smoother.

How to Choose h or k?

- Small h or k (undersmoothing): small bias but large variance.
- Large h or k (oversmoothing): large bias but small variance.
- Regularized cost function for smoothing splines:

$$\sum_{\ell} \left[y^{(\ell)} - \hat{g}(x^{(\ell)})\right]^2 + \lambda \int_a^b \left[\hat{g}''(x)\right]^2 dx$$

  - First term: error of fit
  - Second term: penalty for high variability, where $\hat{g}''(x)$ is the curvature of $\hat{g}(\cdot)$ and $[a, b]$ is the input range
  - λ: trades off error and variability and can also be determined by cross-validation.
- Cross-validation may be used to determine the best h or k.