Instance-based Learning

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Outline

- Non-parametric approach
 - Unsupervised: Non-parametric density estimation
 - Parzen Windows
 - Kn-Nearest Neighbor Density Estimation
 - Supervised: Instance-based learners
 - Classification
 - □ kNN classification
 - □ Weighted (or kernel) kNN
 - Regression
 - □ kNN regression
 - Locally linear weighted regression

Introduction

Estimation of arbitrary density functions

- Parametric density functions cannot usually fit the densities we encounter in practical problems.
 - e.g., parametric densities are unimodal.
- Non-parametric methods don't assume that the model (from) of underlying densities is known in advance
- Non-parametric methods (for classification) can be categorized into
 - Generative
 - Estimate $p(\mathbf{x}|C_i)$ from \mathcal{D}_i using non-parametric density estimation
 - Discriminative
 - Estimate $p(C_i | \mathbf{x})$ from \mathcal{D}

Parametric vs. nonparametric methods

- Parametric methods need to find parameters from data and then use the inferred parameters to decide on new data points
 - Learning: finding parameters from data
- Nonparametric methods
 - Training examples are explicitly used
 - Training phase is not required
- Both supervised and unsupervised learning methods can be categorized into parametric and non-parametric methods.

Histogram approximation idea

Histogram approximation of an unknown pdf

$$P(b_l) \approx k_n(b_l)/n \quad l = 1, \dots, L$$

• $k_n(b_l)$: number of samples (among n ones) lied in the bin b_l



The corresponding estimated pdf:

$$\hat{p}(x) = \frac{P(b_l)}{h} \qquad \left| x - \bar{x}_{b_l} \right| \le \frac{h}{2}$$

Mid-point of the bin b_l

Non-parametric density estimation

• Probability of falling in a region \mathcal{R} :

•
$$P = \int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}'$$
 (smoothed version of $p(\mathbf{x})$)

•
$$\mathcal{D} = \{x^{(i)}\}_{i=1}^{n}$$
: a set of samples drawn i.i.d. according to $p(x)$

• The probability that k of the n samples fall in \mathcal{R} :

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

•
$$E[k] = nP$$

This binomial distribution peaks sharply about the mean:

•
$$k \approx nP \Rightarrow \frac{k}{n}$$
 as an estimate for *P*
• More accurate for larger *n*

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Non-parametric density estimation

- We can estimate smoothed p(x) by estimating P:
- Assumptions: p(x) is continuous and the region \mathcal{R} enclosing x is so small that p is near constant in it:

$$P = \int_{\mathcal{R}} p(\mathbf{x}')d\mathbf{x}' = p(\mathbf{x}) \times V$$
$$V = Vol(\mathcal{R})$$
$$\mathbf{x} \in \mathcal{R} \Rightarrow p(\mathbf{x}) = \frac{P}{V} \approx \frac{k/n}{V}$$

• Let V approach zero if we want to find p(x) instead of the averaged version.

Necessary conditions for converge

- $p_n(x)$ is the estimate of p(x) using n samples:
 - V_n : the volume of region around x
 - k_n : the number of samples falling in the region

$$p_n(\boldsymbol{x}) = \frac{k_n/n}{V_n}$$

- Necessary conditions for converge of $p_n(x)$ to p(x):
 - $\lim_{n\to\infty}V_n=0$
 - $\lim_{n \to \infty} k_n = \infty$
 - $\lim_{n \to \infty} k_n / n = 0$

Non-parametric density estimation: Main approaches

- Two approaches of satisfying conditions:
 - k-nearest neighbor density estimator: fix K and determine the value of V from the data
 - Volume grows until it contains K neighbors of x
 - Kernel density estimator (Parzen window): fix V and determine
 K from the data
 - Number of points falling inside the volume can vary from point to point

Parzen window

- Extension of histogram idea:
 - Hyper-cubes with length of side h (i.e., volume h^d) are located on the samples
- Hypercube as a simple window function:

$$\varphi(\boldsymbol{u}) = \begin{cases} 1 & (|u_1| \le \frac{1}{2} \land \dots \land |u_d| \le \frac{1}{2}) \\ 0 & o.w. \end{cases}$$

$$p_n(\mathbf{x}) = \frac{k_n}{nV_n} = \frac{1}{nV_n} \sum_{i=1}^n \varphi\left(\frac{\mathbf{x} - \mathbf{x}^{(i)}}{h_n}\right)$$

$$k_n = \sum_{i=1}^n \varphi\left(\frac{\mathbf{x} - \mathbf{x}^{(i)}}{h_n}\right) \longrightarrow \text{number}$$

$$V_n = (h_n)^d$$

number of samples in the hypercube around x





Window function

- Necessary conditions for window function to find legitimate density function:
 - $\varphi(\mathbf{x}) \ge 0$
 - $\int \varphi(\mathbf{x}) d\mathbf{x} = 1$
- Windows are also called **kernels** or potential functions.

Density estimation: non-parametric

$$\hat{p}_n(x) = \frac{1}{n} \sum_{i=1}^n \frac{N(x|x^{(i)}, h^2)}{\sqrt{2\pi}h} \xrightarrow{1} \frac{1}{\sqrt{2\pi}h} e^{-\frac{(x-x^{(i)})^2}{2h^2}}$$

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Density estimation: non-parametric



Window (or kernel) function: Width parameter

$$p_n(x) = \frac{1}{n} \times \frac{1}{h_n^d} \sum_{i=1}^n \varphi\left(\frac{x - x^{(i)}}{h_n}\right)$$

- Choosing h_n :
 - Too large: low resolution
 - Too small: much variability
 [Duda, Hurt, and Stork]
- For unlimited n, by letting V_n slowly approach zero as n increases $p_n(x)$ converges to p(x)

Width parameter

- For fixed n, a smaller h results in higher variance while a larger h leads to higher bias.
- For a fixed h, the variance decreases as the number of sample points n tends to infinity
 - for a large enough number of samples, the smaller h the better the accuracy of the resulting estimate
- In practice, where only a finite number of samples is possible, a compromise between h and n must be made.
 - h can be set using techniques like cross-validation where the density estimation used for learning tasks such as classification

Practical issues: Curse of dimensionality

- Large n is necessary to find an acceptable density estimation in high dimensional feature spaces
 - n must grow exponentially with the dimensionality d.
 - If n equidistant points are required to densely fill a one-dim interval, n^d points are needed to fill the corresponding d-dim hypercube.
 - We need an exponentially large quantity of training data to ensure that the cells are not empty



k_n -nearest neighbor estimation

Cell volume is a function of the point location

- To estimate p(x), let the cell around x grow until it captures k_n samples called k_n nearest neighbors of x.
 - k_n is a function of n
- Two possibilities can occur:
 - high density near $x \Rightarrow$ cell will be small which provides a good resolution
 - Iow density near x ⇒ cell will grow large and stop until higher density regions are reached

k_n -nearest neighbor estimation

Necessary and sufficient conditions of convergence:

- $\lim_{n \to \infty} k_n \to \infty$
- $\lim_{n \to \infty} k_n / n \to 0$
- A family of estimates by setting $k_n = k_1 \sqrt{n}$ and choosing different values for k_1 :

$$p_n(\mathbf{x}) = \frac{k_n/n}{V_n} \Rightarrow V_n \approx \frac{1/p(\mathbf{x})}{\sqrt{n}} \qquad k_1 = 1$$

$$V_n \text{ is a function of } \mathbf{x}$$

 k_n -Nearest Neighbor Estimation: Example

Discontinuities in the slopes



Non-parametric density estimation: Summary

- Generality of distributions
 - With enough samples, convergence to an arbitrarily complicated target density can be obtained.
- The number of required samples must be very large to assure convergence
 - grows exponentially with the dimensionality of the feature space
- These methods are very sensitive to the choice of window width or number of nearest neighbors
- There may be severe requirements for computation time and storage (needed to save all training samples).
 - 'training' phase simply requires storage of the training set.
 - computational cost of evaluating p(x) grows linearly with the size of the data set.

Nonparametric learners

Memory-based or instance-based learners

- Iazy learning: (almost) all the work is done at the test time.
- Generic description:
 - Memorize training $(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})$.
 - Given test x predict: $\hat{y} = f(x; x^{(1)}, y^{(1)}, \dots, x^{(n)}, y^{(n)})$.
- f is typically expressed in terms of the similarity of the test sample x to the training samples $x^{(1)}, \ldots, x^{(n)}$

Parzen window & generative classification

$$\mathsf{If} \frac{\frac{1}{n_1} \times \frac{1}{h^d} \sum_{x^{(i)} \in \mathcal{D}_1} \varphi\left(\frac{x - x^{(i)}}{h}\right)}{\frac{1}{n_2} \times \frac{1}{h^d} \sum_{x^{(i)} \in \mathcal{D}_2} \varphi\left(\frac{x - x^{(i)}}{h}\right)} > \frac{P(\mathcal{C}_2)}{P(\mathcal{C}_1)} \text{ decide } \mathcal{C}_1$$

otherwise decide C_2

- *n_j* = |D_j| (*j* = 1,2): number of training samples in class C_j
 D_j: set of training samples labels as C_j
- For large n, it needs both high time and memory requirements

Parzen window & generative classification: Example



[Duda, Hurt, and Stork]

k_n -nearest neighbor estimation & generative classification

If
$$\frac{kn_2V_2}{kn_1V_1} > \frac{P(\mathcal{C}_2)}{P(\mathcal{C}_1)}$$
 decide \mathcal{C}_1

otherwise decide \mathcal{C}_2

- ▶ $n_j = |D_j|$ (j = 1,2): number of training samples in class C_j
 - \mathcal{D}_j : set of training samples labels as \mathcal{C}_j
- \triangleright V_i shows the hypersphere volumes
 - r_j: the radius of the hypersphere centered at x containing k samples of the class C_j (j = 1,2)
- \triangleright k may not necessarily be the same for all classes

k-Nearest-Neighbor (kNN) rule

• k-NN classifier: k > 1 nearest neighbors

Label for x predicted by majority voting among its k-NN.



 $x = [x_1, x_2]$

What is the effect of k?

kNN classifier

Given

- Fraining data $\{(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})\}$ are simply stored.
- Test sample: x
- To classify *x*:
 - Find k nearest training samples to \boldsymbol{x}
 - Out of these k samples, identify the number of samples k_j belonging to class C_j (j = 1, ..., C).
 - Assign x to the class C_{j^*} where $j^* = \underset{j=1,...,c}{\operatorname{argmax}} k_j$
- It can be considered as a discriminative method.

Probabilistic perspective of kNN

kNN as a discriminative nonparametric classifier

- Non-parametric density estimation for $P(C_j|x)$
 - $P(C_j | \mathbf{x}) \approx \frac{k_j}{k}$ where k_j shows the number of training samples among k nearest neighbors of \mathbf{x} that are labeled C_j
- Bayes decision rule for assigning labels

Nearest-neighbor classifier: Example

- Voronoi tessellation:
 - Each cell consists of all points closer to a given training point than to any other training points
 - All points in a cell are labeled by the category of the corresponding training point.





[Bishop]

Nearest neighbor classifier: error bound

• Nearest-Neighbor: kNN with k = 1

• Decision rule: $\hat{y} = y^{NN(x)}$ where $NN(x) = \underset{i=1,...,N}{\operatorname{argmin}} \|x - x^{(i)}\|$

Cover & Hart 67: asymptotic risk of NN classifier satisfies:

$$R^* \le R_{\infty}^{NN} \le 2R^*(1-R^*) \le 2R^*$$

 R_n : expected risk of NN classifier with n training examples drawn from p(x, y)

$$R_{\infty}^{NN} = \lim_{n \to \infty} R_n^{NN}$$

 R^* : the optimal Bayes risk

k-NN classifier: error bound

• Devr 96: the asymptotic risk of the kNN classifier $R_{\infty} = \lim_{n \to \infty} R_n$ satisfies

$$R^* \le R_{\infty}^{kNN} \le R^* + \sqrt{\frac{2R_{\infty}^{NN}}{k}}$$

where R^* is the optimal Bayes risk.

Instance-based learner

- Main things to construct an instance-based learner:
 - A distance metric
 - Number of nearest neighbors of the test data that we look at
 - A weighting function (optional)
 - How to find the output based on neighbors?

Distance measures

Euclidean distance

$$d(\mathbf{x}, \mathbf{x}') = \sqrt{\|\mathbf{x} - \mathbf{x}'\|_2^2} = \sqrt{(x_1 - x_1')^2 + \dots + (x_d - x_d')^2}$$

Sensitive to irrelevant features

- Distance learning methods for this purpose
 - Weighted Euclidean distance

•
$$d_{w}(x, x') = \sqrt{w_1(x_1 - x_1')^2 + \dots + w_d(x_d - x_d')^2}$$

Mahalanobis distance

$$d_A(x, x') = \sqrt{(x_1 - x_1')^T A(x_1 - x_1')}$$

Other distances:

Hamming, angle, ...

•
$$L_p(\mathbf{x}, \mathbf{x}') = \sqrt[p]{\sum_{i=1}^d (x_i - x_i')^p}$$

Distance measure: example



0.5

0.6

0.7

0.8

0.9

Weighted kNN classification

Weight nearer neighbors more heavily:

$$\hat{y} = f(\boldsymbol{x}) = \underset{c=1,\dots,C}{\operatorname{argmax}} \sum_{j \in N_k(\boldsymbol{x})} w_j(\boldsymbol{x}) \times I(c = y^{(j)})$$

 $w_j(\mathbf{x}) = \frac{1}{\|\mathbf{x} - \mathbf{x}^{(j)}\|^2}$ An example of weighting function

In the weighted kNN, we can use all training examples instead of just k (Stepard's method):

$$\hat{y} = f(\boldsymbol{x}) = \underset{c=1,\dots,C}{\operatorname{argmax}} \sum_{j=1}^{n} w_j(\boldsymbol{x}) \times I(c = y^{(j)})$$

• Weights can be found using a kernel function $w_j(x) = K(x, x^{(j)})$:

• e.g.,
$$K(x, x^{(j)}) = e^{-\frac{d(x, x^{(j)})}{\sigma^2}}$$

Weighting functions

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[Fig. has been adopted from Andrew Moore's tutorial on "Instance-based learning"]

kNN regression

Simplest k-NN regression:

• Let $x'^{(1)}, \dots, x'^{(k)}$ be the k nearest neighbors of x and $y'^{(1)}, \dots, y'^{(k)}$ be their labels.

$$\hat{y} = \frac{1}{k} \sum_{j=1}^{k} y^{\prime(j)}$$

- Problems of kNN regression for fitting functions:
 - Problem I: Discontinuities in the estimated function
 - Solution:Weighted (or kernel) regression
 - INN: noise-fitting problem
 - kNN (k > 1) smoothes away noise, but there are other deficiencies.
 - flats the ends

kNN regression: examples

Dataset I





Dataset 3









[Figs. have been adopted from Andrew Moore's tutorial on "Instance-based learning"]

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k = 1

Weighted (or kernel) kNN regression

Higher weights to nearer neighbors:

$$\hat{y} = f(\boldsymbol{x}) = \frac{\sum_{j \in N_k(x)} w_j(x) \times y^{(j)}}{\sum_{j \in N_k(x)} w_j(x)}$$

In the weighted kNN regression, we can use all training examples instead of just k in the weighted form:

$$\hat{y} = f(\boldsymbol{x}) = \frac{\sum_{j=1}^{n} w_j(\boldsymbol{x}) \times y^{(j)}}{\sum_{j=1}^{n} w_j(\boldsymbol{x})}$$

Kernel kNN regression



Choosing a good parameter (kernel width) is important.

Kernel kNN regression





In these datasets, some regions are without samples Best kernel widths have been used

Disadvantages:

- not capturing the simple structure of the data
- failure to extrapolate at edges

Locally weighted linear regression

- For each test sample, it produces linear approximation to the target function in a local region
- Instead of finding the output using weighted averaging (as in the kernel regression), we fit a parametric function locally:

$$\hat{y} = f(\mathbf{x}, \mathbf{x}^{(1)}, y^{(1)}, \dots, \mathbf{x}^{(n)}, y^{(n)})$$
$$\hat{y} = f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \dots + w_d x_d$$

$$J(\boldsymbol{w}) = \sum_{i \in N_k(\boldsymbol{x})} (y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)})^2$$

Unweighted linear

w is found for each test sample

Locally weighted linear regression

$$\hat{y} = f(\mathbf{x}, \mathbf{x}^{(1)}, y^{(1)}, \dots, \mathbf{x}^{(n)}, y^{(n)})$$

$$J(\boldsymbol{w}(\boldsymbol{x})) = \sum_{i \in N_k(\boldsymbol{x})} (y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)})^2 \qquad \text{unweighted} \\ \text{e.g. } K(\boldsymbol{x}, \boldsymbol{x}^{(i)}) = e^{-\frac{\left\|\boldsymbol{x} - \boldsymbol{x}^{(i)}\right\|^2}{2\sigma^2}} \\ J(\boldsymbol{w}(\boldsymbol{x})) = \sum_{i \in N_k(\boldsymbol{x})} K(\boldsymbol{x}, \boldsymbol{x}^{(i)}) (y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)})^2 \qquad \text{weighted} \end{cases}$$

$$J(\boldsymbol{w}(\boldsymbol{x})) = \sum_{i=1}^{n} K(\boldsymbol{x}, \boldsymbol{x}^{(i)}) (y^{(i)} - \boldsymbol{w}^{T} \boldsymbol{x}^{(i)})^{2}$$

$$\uparrow$$
Weighted on all training examples

Locally weighted linear regression: example



More proper result than weighted kNN regression

Locally weighted regression: summary

- Idea I: weighted kNN regression
 - using the weighted average on the output of x's neighbors (or on the outputs of all training data):

$$\hat{y} = \frac{\sum_{i=1}^{k} {y'}^{(i)} K(\boldsymbol{x}, \boldsymbol{x}'^{(i)})}{\sum_{j=1}^{k} K(\boldsymbol{x}, \boldsymbol{x}'^{(j)})}$$

- Idea 2: Locally weighted parametric regression
 - Fit a parametric model (e.g. linear function) to the neighbors of x (or on all training data).
 - Implicit assumption: the target function is reasonably smooth.

Parametric vs. nonparametric methods

Is SVM classifier parametric?

$$\hat{y} = \operatorname{sign}(w_0 + \sum_{\alpha_i > 0} \alpha_i y^{(i)} K(\boldsymbol{x}, \boldsymbol{x}^{(i)}))$$

- In general, we can not summarize it in a simple parametric form.
 - Need to keep around support vectors (possibly all of the training data).
- However, α_i are kind of parameters that are found in the training phase

Instance-based learning: summary

- Learning is just storing the training data
 - prediction on a new data based on the training data themselves
- An instance-based learner does not rely on assumption concerning the structure of the underlying density function.
- With large datasets, instance-based methods are slow for prediction on the test data
 - kd-tree, Locally Sensitive Hashing (LSH), and other kNN approximations can help.



T. Mitchell, "Machine Learning", 1998. [Chapter 8]