

Knowledge Discovery & Data Mining

***k*-Nearest Neighbor Algorithm**

Khasha Dehnad

Supervised vs. Unsupervised Methods

- Data mining methods are categorized as either Unsupervised or Supervised
- **Unsupervised Methods**
 - A target variable is not specified
 - Instead, the algorithm searches for patterns and structure among the variables
 - Clustering is the most common unsupervised method
 - For example, political consultants analyze voter clusters in congressional districts that may be responsive to their particular candidate
 - Important variables such as gender, age, income, and race are input to the clustering algorithm
 - Voter profiles for fund-raising and advertising are created

Supervised vs. Unsupervised Methods (*cont'd*)

- **Supervised Methods**
 - A target variable is specified
 - The algorithm “learns” from the examples by determining which values of the predictor variables are associated with different values of the target variable
 - For example, the regression methods discussed in Chapter 4 are supervised. The observed values of the response (target) variable are read by the least-squares algorithm, while it attempts to minimize the prediction error
 - All classification methods in Chapters 5 – 7 are supervised methods including: Decision Trees, Neural Networks, and k-Nearest Neighbors

Methodology for Supervised Modeling

- Supervised data mining methods use Training, Test, and Validation data sets as part of the model building and evaluation process
- **Training**
 - The Training Set includes records with predictor variables and pre-classified values for the target variable
 - This is the initial stage where a provisional data mining model is built using the training set
 - The model “learns” from the examples in the training set
 - What happens if the model blindly applies all patterns learned from the training set to future data?

Methodology for Supervised Modeling (*cont'd*)

- For example, suppose every customer in a training set named “David” happens to be in the high-income bracket
- A data mining model that “memorizes” this idiosyncrasy in the training set is actually overfitting the data
- Most likely we would not want our model to apply this rule to future or unseen data
- Therefore, the next step in the process is to examine the performance of the provisional data model using a different set of data

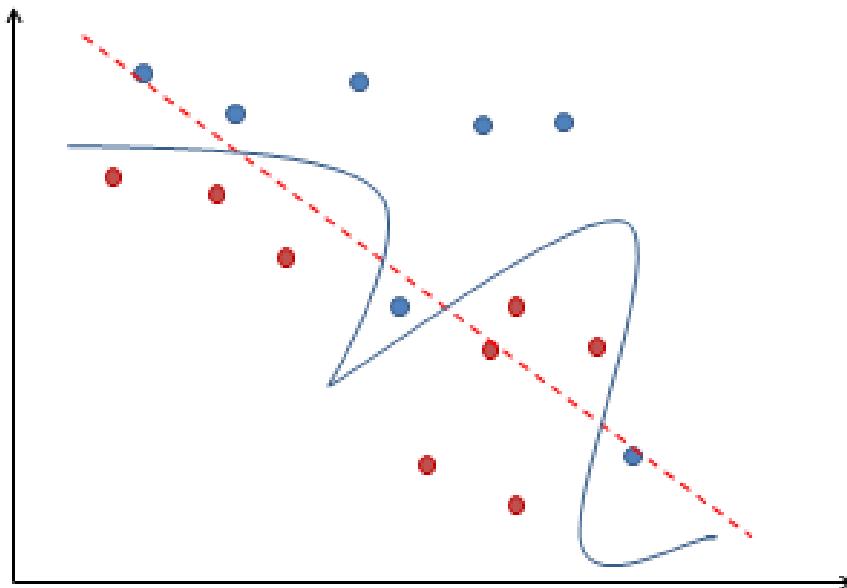
Methodology for Supervised Modeling (*cont'd*)

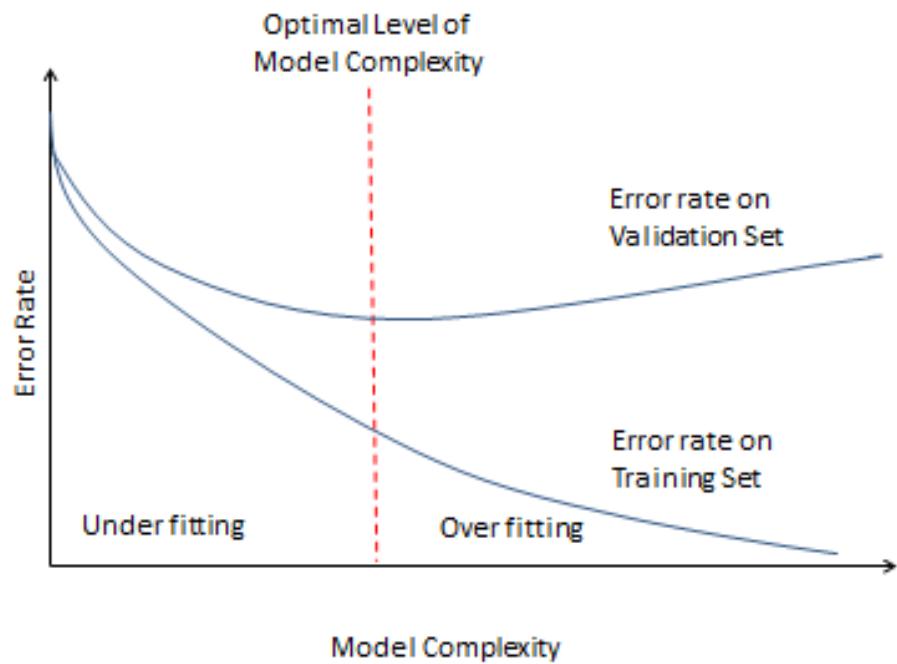
- **Testing**
 - The Test Set is a “holdout” set of data independent from the training set that was used to build the provisional data model
 - The true values of the target variable in the test set are hidden temporarily from the provisional data model
 - The provisional data model simply classifies the records in the test set according to the rules and patterns it learned from the records in the training set
 - The performance of the provisional data model is evaluated by comparing its classifications against the actual values of the target variable
 - The provisional data model is then adjusted in an effort to minimize the error rate on the test set

Methodology for Supervised Modeling (*cont'd*)

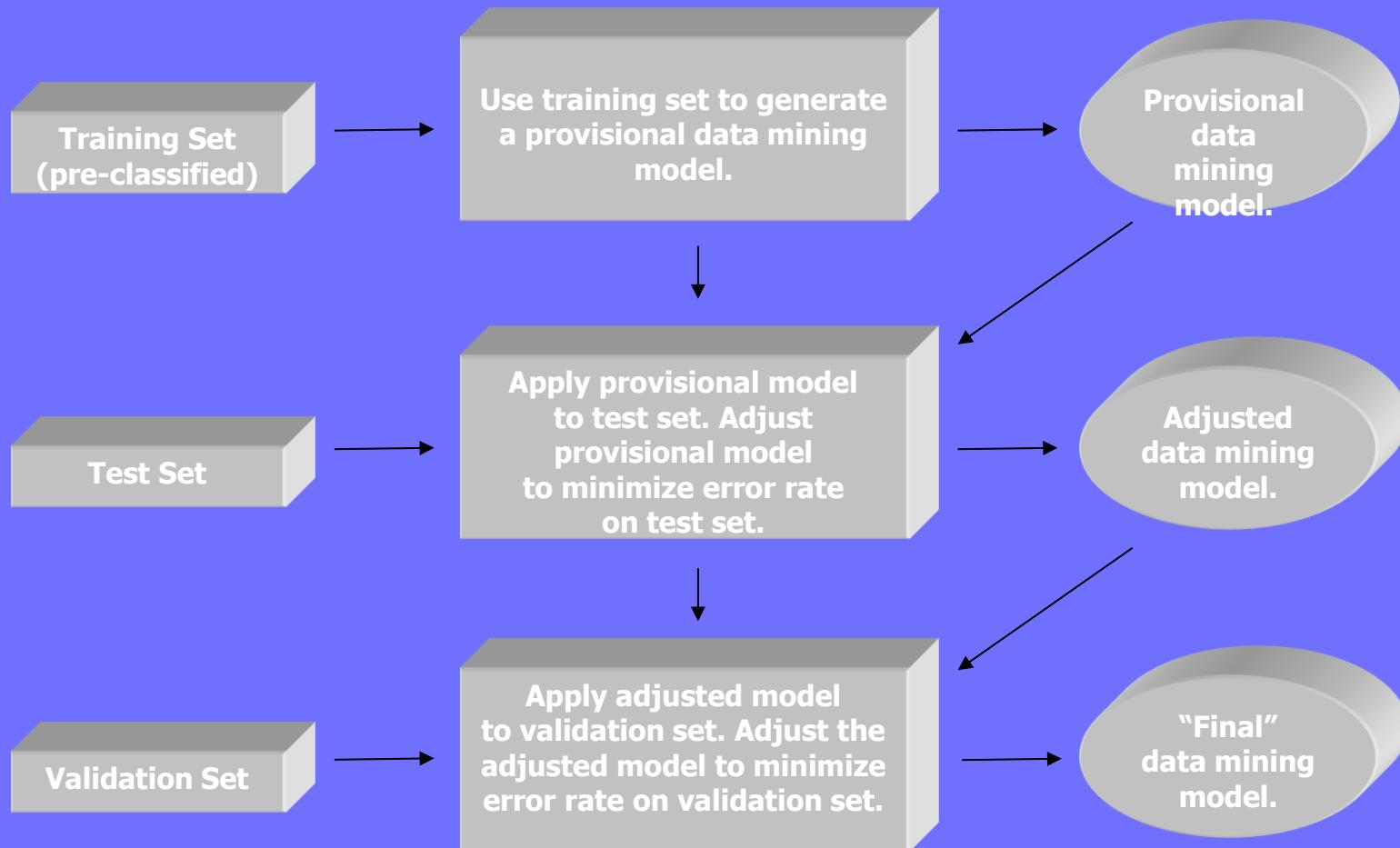
- **Validation**
 - Next, the adjusted data model is applied to another set of data called the Validation Set
 - The validation set is another “holdout” set of data independent of the training and test sets
 - The performance of the adjusted data model is evaluated against the validation set
 - If required, the adjusted data model is modified to minimize the error rate on the validation set
 - Estimates of data model performance for future, unseen data are computed using evaluative measures applied to results obtained when classifying the validation set

BIAS-Variance Trade off





Methodology for Supervised Modeling (*cont'd*)



Data Mining View

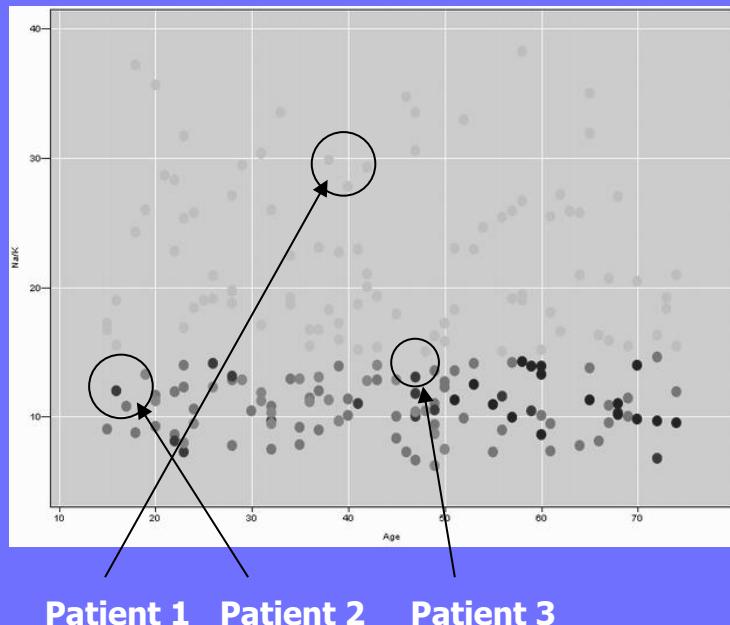
- Traditional Analytics:
 - Have techniques that can be applied to different problems
- Data mining view
 - Needing a solution for a given problem no matter where it comes from
 - Example: How to treat a patient

k-Nearest Neighbor Algorithm

- The *k*-Nearest Neighbor algorithm is an example of instance-based learning where training set records are first stored
 - Next, the classification of a new unclassified record is performed by comparing it to records in the training set it is most similar to
 - *k*-Nearest Neighbor is used most often for classification, although it is also applicable to estimation and prediction tasks
- **Example: Patient 1**
 - Recall from Chapter 1 that we were interested in classifying the type of drug a patient should be prescribed
 - The training set consists of 200 patients with Na/K ratio, age, and drug attributes
 - Our task is to classify the type of drug new a patient should be prescribed that is 40-years-old and has a Na/K ratio of 29

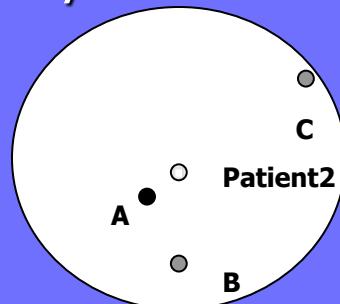
k -Nearest Neighbor Algorithm (*cont'd*)

- This scatter plot of Na/K against Age shows the records in the training set that patients 1, 2, and 3 are most similar to
- A “drug” overlay is shown where Light points = drug Y, Medium points = drug A or X, and Dark points = drug B or C



k-Nearest Neighbor Algorithm (*cont'd*)

- Which drug should Patient 1 be prescribed?
 - Since Patient 1's profile places them in the scatter plot near patients prescribed drug Y, we classify Patient 1 as drug Y
 - All points near Patient 1 are prescribed drug Y, making this a straightforward classification
- **Example: Patient 2**
 - Next we classify a new patient who is 17-years-old with a Na/K ratio = 12.5. A close-up shows the neighborhood of training points in close proximity to Patient 2

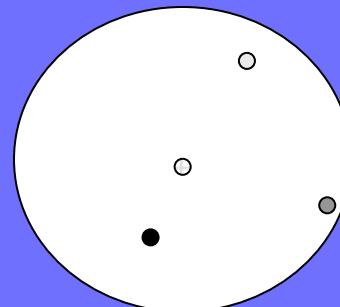


k -Nearest Neighbor Algorithm (*cont'd*)

- Suppose we let $k = 1$ for our k -Nearest Neighbor algorithm
- This means we classify Patient 2 according to whichever single point in the training set it is closest to
- In this case, Patient 2 is closest to the Dark point, and therefore we classify them as drug B or C
- Suppose we let $k = 2$ and reclassify Patient 2 using k -Nearest Neighbor
- Now, Patient 2 is closest to a Dark point and Medium point
- How does the algorithm decide which drug to prescribe?
- A simple voting scheme does not help

k -Nearest Neighbor Algorithm (*cont'd*)

- However, with $k = 3$, voting determines that two of the three closest points to Patient 2 are Medium
 - Therefore, Patient 2 is classified as drug A or X
 - Note that the classification of Patient 2 differed based on the value chosen for k
- Example: Patient 3
 - Patient 3 is 47-years-old and has a Na/K ratio of 13.5. A close-up shows Patient 3 in the center, with the closest 3 training data points



k-Nearest Neighbor Algorithm (*cont'd*)

- With $k = 1$, Patient 3 is closest to the Dark point, based on a distance measure
 - Therefore, Patient 3 is classified as drug B or C
 - Using $k = 2$ or $k = 3$, voting does not help since each of the three nearest training points have different target values
- Considerations when using *k*-Nearest Neighbor
 - How many neighbors should be used? $k = ?$
 - How is the distance between points measured?
 - How is the information from two or more neighbors combined when making a classification decision?
 - Should all points be weighted equally, or should some points have more influence?

Distance Function

- How is similarity defined between an unclassified record and its neighbors?
- A distance metric is a real-valued function d used to measure the similarity between coordinates x , y , and z with properties:

1. $d(x, y) \geq 0$, and $d(x, y) = 0$ if and only if $x = y$
2. $d(x, y) = d(y, x)$
3. $d(x, z) \leq d(x, y) + d(y, z)$

- Property 1: Distance is always non-negative
- Property 2: Commutative, distance from “A to B” is distance from “B to A”
- Property 3: Triangle inequality holds, distance from “A to C” must be less than or equal to distance from “A to B to C”

Distance Function (*cont'd*)

- The Euclidean Distance function is commonly-used to measure distance

$$d_{\text{Euclidean}}(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_i (x_i - y_i)^2}$$

where $\mathbf{x} = x_1, x_2, \dots, x_m$, and $\mathbf{y} = y_1, y_2, \dots, y_m$
represent the m attributes

● Example

- Suppose Patient A is 20-years-old and has a Na/K ratio = 12, and Patient B is 30-years-old and has a Na/K ratio = 8
- What is the Euclidean distance between these instances?

$$d_{\text{Euclidean}}(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_i (x_i - y_i)^2} = \sqrt{(20-30)^2 + (12-8)^2} = 10.77$$

Distance Function (*cont'd*)

- The Minkowski Distance function is commonly-used to measure distance

$$d_{\text{Minkowski}}(\mathbf{x}, \mathbf{y}) = \left(\sum_i (x_i - y_i)^p \right)^{1/p}$$

where $\mathbf{x} = x_1, x_2, \dots, x_m$, and $\mathbf{y} = y_1, y_2, \dots, y_m$
represent the m attributes

Distance Function (*cont'd*)

- Example 1: What is the distance between customer A and B?
 - Customer A age= 20-years-old Income= 10,000
 - Customer B age= 30-years-old Income= 20,000
- Example 2: What is the distance between customer A and B?
 - Customer A age= 20-years-old Income= 10K
 - Customer B age= 30-years-old Income= 20K

Distance Function (*cont'd*)

	Age	Income		Age	Income
A	20	10,000		A	20
B	30	20,000		B	30

$$\sqrt{(10,000^2) + (10^2)} = 10,000$$

$$\sqrt{(10^2) + (10^2)} = 14.14$$

Distance Function (*cont'd*)

- Example 3: What is the distance between customer A and B?
 - Customer A income=\$100k Assets= \$1 Million
 - Customer B income=\$110k Assets= \$.7 Million
- Example 4: What is the distance between customer A and c?
 - Customer A income=\$100k Assets= \$1 Million
 - Customer C income=\$70k Assets= \$1.1 Million

Remember to Normalize the data!!!

Distance Function (*cont'd*)

- When measuring distance, one or more attributes can have very large values, relative to the other attributes
 - For example, *income* may be scaled 30,000-100,000, whereas *years_of_service* takes on values 0-10
 - In this case, the values of *income* will overwhelm the contribution of *years_of_service*
 - To avoid this situation we use normalization
- **Normalization**
 - Continuous data values should be normalized using Min-Max Normalization or Z-Score Standardization

$$\text{Min - Max Normalization} = \frac{X - \min(X)}{\max(X) - \min(X)}$$

$$\text{Z - Score Standardization} = \frac{X - \text{mean}(X)}{\text{standard deviation}(X)}$$

Distance Function (*cont'd*)

- For categorical attributes, the Euclidean Distance function is not appropriate
- Instead, we define a function called “different”

$$\text{different}(x_i, y_i) = \begin{cases} 0 & \text{if } x_i = y_i \\ 1 & \text{otherwise} \end{cases}$$

- We substitute $\text{different}(x, y)$ for each categorical attribute in the Euclidean Distance function
- **Example**
- Which patient is more similar to a 50-year-old male: a 20-year-old male or a 50-year-old female?

Distance Function (*cont'd*)

- Let Patient A = 50-year-old male, Patient B = 20-year-old male, and Patient C = 50-year-old female
- Suppose that the *Age* variable has a range = 50, minimum = 10, mean = 45, and standard deviation = 15
- The table contains original, Min-Max Normalized, and Z-Score Standardized values for *Age*

Patient	Age	Age_{MMN}	$\text{Age}_{\text{Zscore}}$	Gender
A	50	$\frac{50-10}{50} = 0.8$	$\frac{50-45}{15} = 0.33$	Male
B	20	$\frac{20-10}{50} = 0.2$	$\frac{20-45}{15} = -1.67$	Male
C	50	$\frac{50-10}{50} = 0.8$	$\frac{50-45}{15} = 0.33$	Female

Distance Function (*cont'd*)

- **Age not normalized**

- Assume we do not normalize *Age* and calculate the distance between Patient A and Patient B, and Patient A and Patient C

$$d(A, B) = \sqrt{(50 - 20)^2 + 0^2} = 30$$
$$d(A, C) = \sqrt{(50 - 50)^2 + 1^2} = 1$$

- We determine, although perhaps incorrectly, that Patient C is nearest Patient A
 - Is Patient B really 30 times more distant than Patient C is to Patient A?
 - Perhaps neglecting to normalize the values of *Age* is creating this discrepancy?

Distance Function (*cont'd*)

- Age Normalized using Min-Max
 - Age is normalized using Min-Max Normalization. Values lie in the range [0, 1]
 - Again, we calculate the distance between Patient A and Patient B, and Patient A and Patient C

$$d_{MMN}(A, B) = \sqrt{(0.8 - 0.2)^2 + 0^2} = 0.6$$

$$d_{MMN}(A, C) = \sqrt{(0.8 - 0.8)^2 + 1^2} = 1.0$$

- In this case, Patient B is now closer to Patient A
- Age Standardized using Z-Score
 - This time, Age is standardized using Z-Score Standardization

Distance Function (*cont'd*)

$$d_{Zscore}(A, B) = \sqrt{(0.33 - (-1.67))^2 + 0^2} = 2.0$$

$$d_{Zscore}(A, C) = \sqrt{(0.33 - 0.33)^2 + 1^2} = 1.0$$

- Using Z-Score Standardization, most values are typically contained in the range [-3, 3]
 - Now, Patient C is nearest Patient A. This is different from the results obtained using Min-Max Normalization
- Conclusion
 - The use of different normalization techniques resulted in Patient A being nearest to different patients in the training set
 - This underscores the importance of understanding which technique is being used

Distance Function (*cont'd*)

- Note that the $distance(x,y)$ and Min-Max Normalization functions produce values in the range [0, 1]
- Perhaps, when calculating the distance between records containing both numeric and categorical attributes, the use of Min-Max Normalization is preferred

Combination Function

- The Euclidean Distance function determines the similarity of a new unclassified record to those in the training set
 - How should the most similar (k) records combine to provide a classification?
- **Simple Unweighted Voting**
 - This is the most simple combination function
 - Decide on the value for k to determine the number of similar records that “vote”
 - Compare each unclassified record to its k nearest (most similar) neighbors according to the Euclidean Distance function
 - Each of the k similar records vote

Combination Function (*cont'd*)

- Recall that we classified a new patient 17-years-old with a Na/K ratio = 12.5, using $k = 3$
- Simple unweighted voting determined that two of the three closet points to Patient 2 are Medium
- Therefore, Patient 2 is classified as drug A or X with a confidence of $2/3 = 66.67\%$
- We also classified a new patient 47-years-old that has a Na/K ratio of 13.5, using $k = 3$
- However, simple unweighted voting did not help and resulted in a tie
- Perhaps weighted voting should be considered?

Weighted Voting

- **Weighted Voting**
 - In this case, the closer the neighbor, the more influence it has in the classification decision
 - This method assumes a closer neighbor is more similar, and therefore its vote should be weighted more heavily, as compared that of more distant neighbors
 - The weight of particular record is inversely proportional to its distance to the unclassified record
 - A “tie” is unlikely to occur using this approach

Weighted Voting (*cont'd*)

- Example

Record	Age	Na/K	Age _{MMN}	Na/K _{MMN}
New Patient	17	12.5	0.05	0.25
A (Dark)	16.8	12.4	0.0467	0.2471
B (Med)	17.2	10.5	0.0533	0.1912
C (Med)	19.5	13.5	0.0917	0.2794

Weighted Voting (*cont'd*)

- **Example**

- Again, recall that we classified a new patient 17-years-old with a Na/K ratio = 12.5, using $k = 3$
- We determined, using unweighted voting, two of the closest points were Medium, and the third was Dark
- However, the Dark point is the most similar to the new patient
- Now, we reclassify the new patient using a weighted voting scheme using values from the table below

Record	Age	Na/K	Age _{MMN}	Na/K _{MMN}
New Patient	17	12.5	0.05	0.25
A (Dark)	16.8	12.4	0.0467	0.2471
B (Med)	17.2	10.5	0.0533	0.1912
C (Med)	19.5	13.5	0.0917	0.2794

Weighted Voting (*cont'd*)

- The distance of records A, B, and C to the new patient are:

$$d(new, A) = \sqrt{(.05 - .0467)^2 + (.25 - .2471)^2} = .004393$$

$$d(new, B) = \sqrt{(.05 - .0533)^2 + (.25 - .1912)^2} = .058893$$

$$d(new, C) = \sqrt{(.05 - .0917)^2 + (.25 - .2794)^2} = .051022$$

- Next, the votes of these records are weighted according to the inverse square of their distance to the new record
- Record A votes to classify the new patient as Dark (drug B or C)

$$Votes(Dark\ Gray) = \frac{1}{d(new, A)^2} = \frac{1}{.004393^2} \cong 51,818.$$

Weighted Voting (*cont'd*)

- Records B and C vote to classify the new patient as Medium (drug A or X)

$$Votes(Medium\ Gray) = \frac{1}{d(new, B)^2} + \frac{1}{d(new, C)^2} = \frac{1}{.058893^2} + \frac{1}{.051022^2} \cong 672.$$

- Convincingly (51,818 vs. 672) the weighted voting method classifies the new patient as Dark (drug B or C)
- Note that this procedure reverses our classification decision determined using unweighted voting, $k = 3$
- The inverse distance of 0 is undefined using weighted voting
- Theoretically, the value of k could be increased, such that all training records participate in voting; however, the computational complexity may result in poor performance

Quantifying Attribute Relevance: Stretching the Axes

- Not all attributes may be relevant to classification
- For example, Decision Trees only include attributes that contribute to improving classification accuracy
- In contrast, k -Nearest Neighbor's default behavior is to calculate distances using all attributes
- A relevant record may be proximate for important variables, while at the same time very distant for other, unimportant variables
- Taken together, the relevant record may now be moderately far away from the new record, such that it does not participate in the classification decision

Quantifying Attribute Relevance: Stretching the Axes (*cont'd*)

- Perhaps, we should consider restricting the algorithm to using the most important fields for classification
 - However, rather than making this determination *a priori*, we can make attributes either more, or less important
 - This is accomplished using cross-validation or applying domain knowledge expertise
- **Stretching the Axes**
 - Stretching the Axes finds the coefficient z_j by which to multiply the j^{th} axis. Larger values of z_j are associated with the more important variable axes
 - **Cross-validation**
 - Cross-validation selects a random subset of data from the training set and determines the set of z_1, z_2, \dots, z_m that minimize the classification error on the test set

Quantifying Attribute Relevance: Stretching the Axes (*cont'd*)

- Repeating the process leads to a more accurate set of values for z_1, z_2, \dots, z_m
- **Domain Expertise**
 - Alternately, we may call upon domain experts to recommend values for z_1, z_2, \dots, z_m
 - Using either approach the k -Nearest Neighbor algorithm may be made more precise
- **Example**
 - Suppose that the Na/K ratio was determined to be 3 times more important than the Age attribute, for performing drug classification

Quantifying Attribute Relevance: Stretching the Axes (*cont'd*)

- The distance of the records A, B, and C to the new record are calculated as follows:

where $z_{Na/K} = 3$, $z_{Age} = 1$

$$d(new, A) = \sqrt{(.05 - .0467)^2 + ((3)(.25 - .2471))^2} = .009305$$

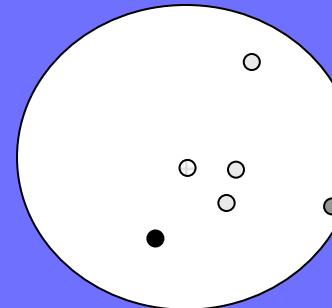
$$d(new, B) = \sqrt{(.05 - .0533)^2 + ((3)(.25 - .1912))^2} = .17643$$

$$d(new, C) = \sqrt{(.05 - .0917)^2 + ((3)(.25 - .2794))^2} = .097561$$

- The classification does not change by stretching the axes for Na/K ratio
- In many situations, stretching the axes leads to improved accuracy by quantifying the relevance of each variable used in the classification decision

Database Considerations

- Instance-based learning methods benefit from having access to learning examples composed of many attribute value combinations
- The data set should be balanced to include a sufficient number of records with common, as well as less-common, classifications
- One approach to balancing the data set is to reduce the proportion of records with more common classifications
- Restrictions on main memory space may limit the size of the training set used
- The training set may be reduced to include only those records that occur near a classification “boundary”



k -Nearest Neighbor Algorithm for Estimation and Prediction

- k -Nearest Neighbor may be used for estimation and prediction of continuous-valued target variables
 - A method used to accomplish this is Locally Weighted Averaging
- **Example**
 - We will estimate the systolic blood pressure for a 17-year-old patient with Na/K ratio equal to 12.5, using $k = 3$
 - The predictors are *Na/K* and *Age* and the target variable is *BP*
 - The three neighbors (A, B, and C) from the training set are shown below

Record	Age	Na/K	BP	Age _{MMN}	Na/K _{MMN}	Distance
New	17	12.5	?	0.05	0.25	--
A	16.8	12.4	120	0.0467	0.2471	0.009305
B	17.2	10.5	122	0.0533	0.1912	0.176430
C	19.5	13.5	130	0.0917	0.2794	0.097560

k -Nearest Neighbor Algorithm for Estimation and Prediction (*cont'd*)

- Assume BP has a range = 80, and minimum = 90
- We also stretch the axes for the Na/K ratio, to reflect its importance in estimating BP. In addition, we use the inverse square of the distances for the weights

$$\hat{y}_{new} = \frac{\sum_i w_i y_i}{\sum_i w_i}$$

where $w_i = \frac{1}{d(new, x_i)^2}$ for existing records x_1, x_2, \dots, x_k

- The estimated systolic blood pressure for the new record is:

$$\hat{y}_{new} = \frac{\sum_i w_i y_i}{\sum_i w_i} = \frac{\frac{120}{.009305^2} + \frac{122}{.17643^2} + \frac{130}{.09756^2}}{\frac{1}{.009305^2} + \frac{1}{.17643^2} + \frac{1}{.09756^2}} = 120.0954$$

- Since Record A is closest to the new record, its BP value of 120 makes a significant contribution to the estimated BP value

Choosing k

- What value of k is optimal?
 - There is not necessarily an obvious solution
- **Smaller k**
 - Choosing a small value for k may lead the algorithm to overfit the data
 - Noise or outliers may unduly affect classification
 - **Larger k**
 - Larger values will tend to smooth out idiosyncratic or obscure data values in the training set
 - If the values become too large, locally interesting values will be overlooked

Choosing k (*cont'd*)

- Choosing the appropriate value for k requires balancing these considerations
- Using cross-validation may help determine the value for k , by choosing a value that minimizes the classification error

Reading

- Text:
 - Chapter 3: Exploring Categorical Variables
 - Chapter 4: Statistical approaches to estimation and prediction -- confidence interval estimation
 - Chapter 5: Entire chapter
- SAS and R
- Next topic
 - K-means chapter 8