## Unit-III Classification and Prediction

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## Bayesian Classification



Thomas Bayes (1702-1761)

## Bayesian Classification: Why?

A statistical classifier: performs probabilistic prediction, i.e., predicts class membership probabilities, such as the probability that a given a tuple belong to a particular class.

- Foundation: Based on Bayes' Theorem.
- Performance: A simple Bayesian classifier, naïve Bayesian classifier, has comparable performance with decision tree and selected neural network classifiers.
- Incremental: Each training example can incrementally increase/decrease the probability that a hypothesis is correct - prior knowledge can be combined with observed data.
- Standard: Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured.


## Bayesian Classification: Why?

- Naïve Baysian classifiers assume that the effect of an attribute value on a given class is independent of the values of the other attributes.

This assumption is called class conditional independence.

## Bayesian Theorem: Basics

- Let $\mathbf{X}$ be a data tuple ("evidence"): class label is unknown
- Let H be a hypothesis that X belongs to class C .
- Classification is to determine $\mathrm{P}(\mathrm{H} \mid \mathbf{X})$, the probability that the hypothesis holds given the "evidence" or observed data tuple X.
- $\mathrm{P}(\mathrm{H})$ (prior probability), the initial probability
- E.g., $\mathbf{X}$ will buy computer, regardless of age, income, ...
- $P(\mathbf{X})$ : probability that tuple data is observed
- $\mathbf{P}(\mathbf{X} \mid H)$ (posteriori probability), the probability of observing the $\mathbf{X}$, given that the hypothesis holds
- E.g., Given that $\mathbf{X}$ will buy computer, the prob. that X is 31..40, medium income


## Bayesian Theorem: Basics

- $P(X)$ is the prior probability of $X$. An example is the probability that a person from our set of customers is 35 years old and earns \$40,000.


## Bayesian Theorem

- Given training data $\mathbf{X}$, posteriori probability of a hypothesis $\mathrm{H}, \mathrm{P}(\mathrm{H} \mid \mathbf{X})$, follows the Bayes theorem

$$
P(H \mid \mathbf{X})=\frac{P(\mathbf{X} \mid H) P(H)}{P(\mathbf{X})}
$$

- Informally, this can be written as posteriori $=$ likelihood $\times$ prior/evidence
- Predicts $\mathbf{X}$ belongs to $\mathrm{C}_{2}$ iff the probability $\mathrm{P}\left(\mathrm{C}_{\mathrm{i}} \mid \mathbf{X}\right)$ is the highest among all the $P\left(C_{k} \mid X\right)$ for all the $k$ classes
- Practical difficulty: require initial knowledge of many probabilities, significant computational cost


## Towards Naïve Bayesian Classifier

- Let D be a training set of tuples and their associated class labels, and each tuple is represented by an n-D attribute vector $\mathbf{X}=\left(x_{1}, x_{2}, \ldots, x_{n}\right)$
- Suppose there are $m$ classes $C_{1}, C_{2}, \ldots, C_{m}$.
- Classification is to derive the maximum posteriori, i.e., the maximal $\mathrm{P}\left(\mathrm{C}_{\mathrm{i}} \mid \mathbf{X}\right)$
- This can be derived from Bayes' theorem $P\left(C_{i} \mid \mathbf{X}\right)=\frac{P\left(\mathbf{X} \mid C_{i}\right) P\left(C_{i}\right)}{P(\mathbf{X})}$
- Since $\mathrm{P}(\mathrm{X})$ is constant for all classes, only $P\left(C_{i} \mid \mathbf{X}\right)=P\left(\mathbf{X} \mid C_{i}\right) P\left(C_{i}\right)$
needs to be maximized

Bayesian classifier predicts that tuple X belongs to the class Ci If and only if $\mathrm{P}(\mathrm{Ci} / \mathrm{X})>\mathrm{P}(\mathrm{Cj} / \mathrm{X})$ for $\mathrm{i}<=\mathrm{j}<=\mathrm{m}$, i not equal to j .

## Derivation of Naïve Bayes Classifier

- A simplified assumption: attributes are conditionally independent (i.e., no dependence relation between attributes):

$$
P\left(\mathbf{X} \mid C_{i}\right)=\prod_{k=1}^{n} P\left(x_{k} \mid C_{i}\right)=P\left(x_{1} \mid C_{i}\right) \times P\left(x_{2} \mid C_{i}\right) \times \ldots \times P\left(x_{n} \mid C_{i}\right)
$$

- This greatly reduces the computation cost: Only counts the class distribution
- If $A_{k}$ is categorical, $P\left(x_{k} \mid C_{i}\right)$ is the \# of tuples in $C_{i}$ having value $x_{k}$ for $A_{k}$ divided by $\left|C_{i, ~}\right|$, the no. of tuples of $C_{i}$ in $D$
- If $A_{k}$ is continous-valued, $P\left(x_{k} \mid C_{i}\right)$ is usually computed based on Gaussian distribution with a mean $\mu$ and standard deviation $\sigma$
defined as $g(x, \mu, \sigma)=\frac{1}{\sqrt{2 \pi} \sigma} e^{-\frac{(x-\mu)^{2}}{2 \sigma^{2}}}$
so that $P\left(\mathbf{X} \mid C_{i}\right)=g\left(x_{k}, \mu_{C_{i}}, \sigma_{C_{i}}\right)$


## Towards Naïve Bayesian Classifier

- In order to predict the class label of $\mathrm{X}, \mathrm{P}(\mathrm{X} / \mathrm{Ci})$ is evaluated for each class Ci.
- The classifier predicts that the class label of tuple $X$ is the class Ci if and only if
- $P(X \mid C i) P(C i)>P(X / C j) P(C j)$ for $i<=j<=m, j$ not equal to $i$.


## Naïve Bayesian Classifier: Training Dataset

| age | income | studen | tredit_ratin | com | Class: <br> C1:buys_computer = 'yes' <br> C2:buys_computer = 'no' <br> Data sample $X=\text { (age }<=30,$ <br> Income = medium, <br> Student $=$ yes <br> Credit_rating $=$ Fair) |
| :---: | :---: | :---: | :---: | :---: | :---: |
| <=30 | high | no | fair | no |  |
| $<=30$ | high | no | excellent | no |  |
| $31 . .40$ | high | no | fair | yes |  |
| >40 | medium | no | fair | yes |  |
| $>40$ | low | yes | fair | yes |  |
| $>40$ | low | yes | excellent | no |  |
| $31 . .40$ | low | yes | excellent | yes |  |
| $<=30$ | medium | no | fair | no |  |
| $<=30$ | low | yes | fair | yes |  |
| >40 | medium | yes | fair | yes |  |
| <=30 | medium | yes | excellent | yes |  |
| $31 . .40$ | medium | no | excellent | yes |  |
| $31 . .40$ | high | yes | fair | yes |  |
| $>40$ | medium | no | excellent | no |  |

## Naïve Bayesian Classifier: An Example

- We need to maximize $P\left(X / C_{i}\right) P\left(C_{i}\right)$ : The prior probability of each class

$$
\begin{aligned}
& \text { P(buys_computer }=\text { "yes") }=9 / 14=0.643 \\
& P(\text { buys_computer }=\text { "no") }=5 / 14=0.357
\end{aligned}
$$

- Compute $\mathrm{P}\left(\mathrm{X} \mid \mathrm{C}_{\mathrm{i}}\right)$ for each class
$P($ age $=$ " $<=30 " \mid$ buys_computer $=$ "yes") $=2 / 9=0.222$
$\mathrm{P}($ age $=$ " $<=30 " \mid$ buys_computer $=" n o ")=3 / 5=0.6$
$\mathrm{P}($ income $=$ "medium" $\mid$ buys_computer $=$ "yes") $=4 / 9=0.444$
$\mathrm{P}($ income $=$ "medium" $\mid$ buys_computer $=$ "no") $=2 / 5=0.4$
$\mathrm{P}($ student $=$ "yes" $\mid$ buys_computer $=" y e s)=6 / 9=0.667$
P (student = "yes" | buys_computer = "no") $=1 / 5=0.2$
P(credit_rating $=$ "fair" | buys_computer $=$ "yes") $=6 / 9=0.667$
$\mathrm{P}($ credit_rating $=$ "fair" $\mid$ buys_computer $=$ "no") $=2 / 5=0.4$
- $X=$ (age $<=\mathbf{3 0}$, income $=$ medium, student $=$ yes, credit_rating = fair)
$\mathbf{P}\left(\mathbf{X} \mid \mathbf{C}_{\mathbf{i}}\right): \mathbf{P ( X | b u y s}$ computer $=$ "yes") $=0.222 \times 0.444 \times 0.667 \times 0.667=0.044$
$\mathrm{P}(\mathrm{X} \mid$ buys_computer $=$ "no") $=0.6 \times 0.4 \times 0.2 \times 0.4=0.019$
$\mathbf{P}\left(\mathbf{X} \mid \mathbf{C}_{\mathbf{i}}\right) * \mathbf{P}\left(\mathbf{C}_{\mathbf{i}}\right): \mathbf{P}(\overline{\mathrm{X}} \mid$ buys_computer $=$ "yes") $* \mathrm{P}($ buys_computer $=$ "yes") $=0.028$ $P(X \mid$ buys_computer $=$ "no") * P(buys_computer = "no") $=0.007$

Therefore, $\mathbf{X}$ belongs to class ("buys_computer = yes")

## Avoiding the 0-Probability Problem

- Naïve Bayesian prediction requires each conditional prob. be nonzero. Otherwise, the predicted prob. will be zero

$$
P\left(X \mid C_{i}\right)=\prod_{k=1}^{n} P\left(x_{k} \mid C_{i}\right)
$$

- Ex. Suppose a dataset with 1000 tuples, income=low (0) tuples, income $=$ medium (990) tuples, and income $=$ high (10) tuples,
- Use Laplacian correction (or Laplacian estimator)
- Adding 1 to each case

$$
\begin{aligned}
& \operatorname{Prob}(\text { income }=\text { low })=1 / 1003=0.001 \\
& \operatorname{Prob}(\text { income }=\text { medium })=991 / 1003=0.988 \\
& \operatorname{Prob}(\text { income }=\text { high })=11 / 1003=0.011
\end{aligned}
$$

- The "corrected" prob. estimates are close to their "uncorrected" counterparts


## Naïve Bayesian Classifier: Comments

- Advantages
- Easy to implement
- Good results obtained in most of the cases
- Disadvantages
- Assumption: class conditional independence, therefore loss of accuracy
- Practically, dependencies exist among variables
- E.g., hospitals: patients: Profile: age, family history, etc.

Symptoms: fever, cough etc., Disease: lung cancer, diabetes, etc.

- Dependencies among these cannot be modeled by Naïve Bayesian Classifier
- How to deal with these dependencies?
- Bayesian Belief Networks


## Bayesian Belief Networks

- Bayesian belief network allows a subset of the variables conditionally independent
- A graphical model of causal relationships
- Represents dependency among the variables
- Gives a specification of joint probability distribution

$\square$ Nodes: random variables
$\square$ Links: dependency
$\square X$ and $Y$ are the parents of $Z$, and $Y$ is the parent of $P$
$\square$ No dependency between $Z$ and $P$
$\square$ Has no loops or cycles


## Bayesian Belief Network: An Example



## Bayesian Belief Networks

The conditional probability table (CPT) for variable LungCancer:

| $(\mathrm{FH}, \mathrm{S})(\mathrm{FH}, \sim \mathrm{S})$ | $(\sim \mathrm{FH}, \mathrm{S})(\sim \mathrm{FH}, \sim \mathrm{S})$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| LC | 0.8 | 0.5 | 0.7 | 0.1 |
| $\sim \mathrm{LC}$ | 0.2 | 0.5 | 0.3 | 0.9 |

CPT shows the conditional probability for each possible combination of its parents

Derivation of the probability of a particular combination of values of $\mathbf{X}$, from CPT:

$$
P\left(x_{1}, \ldots, x_{n}\right)=\prod_{i=1}^{n} P\left(x_{i} \mid \text { Parents } \quad\left(Y_{i}\right)\right)
$$

## Training Bayesian Belief Networks

- Several scenarios:
- Given both the network structure and all variables observable: learn only the CPTs
- Network structure known, some hidden variables: gradient descent (greedy hill-climbing) method, analogous to neural network learning
- Network structure unknown, all variables observable: search through the model space to reconstruct network topology
- Unknown structure, all hidden variables: No good algorithms known for this purpose
- Ref. D. Heckerman: Bayesian networks for data mining


## Training Bayesian Belief Networks

- for data mining


## Rule Based Classification

## Using I F-THEN Rules for Classification

- Represent the knowledge in the form of IF-THEN rules

R: IF age = youth AND student = yes THEN buys_computer = yes

- Rule antecedent/precondition vs. rule consequent
- Assessment of a rule: coverage and accuracy
- $\mathrm{n}_{\text {covers }}=$ \# of tuples covered by R
- $\mathrm{n}_{\text {correct }}=$ \# of tuples correctly classified by $R$
coverage $(\mathrm{R})=\mathrm{n}_{\text {covers }} /[\mathrm{D} \mid \quad / * \mathrm{D}$ : training data set */
$\operatorname{accuracy}(R)=n_{\text {correct }} / n_{\text {covers }}$
- If more than one rule is triggered, need conflict resolution strategy are 2
- 1)Size ordering: assign the highest priority to the triggering rules that has the "toughest" requirement (i.e., with the most attribute test)
- 2)Rule ordering: this scheme prioritizes the rules before hand. Ordering may be based class based or rule based. This is known as Decision list
- 2.1 rule based: rules are organized into one long priority list, according to some measure of rule quality or by experts. Ordering may be class based or rule based.
- 2.2 Class-based ordering: classes are sorted in order of decreasing "importance".

- Each attribute-value pair along a path forms a conjunction: the leaf holds the class prediction
- Rules are mutually exclusive and exhaustive
- Example: Rule extraction from our buys_computer decision-tree

IF age $=$ young AND student $=$ no $\quad$ THEN buys_computer $=$ no
IF age $=$ young AND student $=$ yes $\quad$ THEN buys_computer $=$ yes
IF age $=$ mid-age $\quad$ THEN buys_computer $=$ yes
IF age $=$ old AND credit_rating $=$ excellent THEN buys_computer $=$ yes
IF age = young AND credit_rating $=$ fair THEN buys_computer $=$ no

## Rule Extraction from the Training Data

- Sequential covering algorithm: Extracts rules directly from training data
- Typical sequential covering algorithms: FOIL, AQ, CN2, RIPPER
- Rules are learned sequentially, each for a given class $C_{i}$ will cover many tuples of $C_{i}$ but none (or few) of the tuples of other classes
- Steps:
- Rules are learned one at a time
- Each time a rule is learned, the tuples covered by the rules are removed
- The process repeats on the remaining tuples unless termination condition, e.g., when no more training examples or when the quality of a rule returned is below a user-specified threshold
- decision-tree induction: learning a set of rules simultaneously


## Sequential Covering Algorithm

while (enough target tuples left)
generate a rule
remove positive target tuples satisfying this rule


## Rule Generation

- To generate a rule while(true)
find the best predicate $p$
if foil-gain $(p)>$ threshold then add $p$ to current rule else break



## Rule Quality Measures How to Learn-One-Rule?

- Start with the most general rule possible: condition = empty
- Adding new attributes by adopting a greedy depth-first strategy
- Picks the one that most improves the rule quality
- Rule-Quality measures: consider both coverage and accuracy
- Foil-gain (in FOIL \& RIPPER): assesses info_gain by extending condition FOIL_Gain $=$ pos' $\times\left(\log _{2} \frac{\text { pos' }}{\text { pos' }+ \text { neg' }}-\log _{2} \frac{\text { pos }}{\text { pos }+ \text { neg }}\right)$
- favors rules that have high accuracy and cover many positive tuples
- Rule pruning based on an independent set of test tuples

$$
F O I L_{-} \operatorname{Prune}(R)=\frac{p o s-n e g}{p o s+n e g}
$$

Pos/neg are \# of positive/negative tuples covered by R. If FOIL_Prune is higher for the pruned version of $R$, prune $R$

## Classification by Backpropagation

- Backpropagation: A neural network learning algorithm
- Started by psychologists and neurobiologists to develop and test computational analogues of neurons
- A neural network: A set of connected input/output units where each connection has a weight associated with it
- During the learning phase, the network learns by adjusting the weights so as to be able to predict the correct class label of the input tuples
- Also referred to as connectionist learning due to the connections between units


## Neural Network as a Classifier

- Weakness
- Long training time
- Require a number of parameters typically best determined empirically, e.g., the network topology or "structure."
- Poor interpretability: Difficult to interpret the symbolic meaning behind the learned weights and of "hidden units" in the network
- Strength
- High tolerance to noisy data
- Ability to classify untrained patterns
- Well-suited for continuous-valued inputs and outputs
- Successful on a wide array of real-world data
- Algorithms are inherently parallel
- Techniques have recently been developed for the extraction of rules from trained neural networks


## A Neuron (= a perceptron)



- The n -dimensional input vector $\mathbf{x}$ is mapped into variable $\mathbf{y}$ by means of the scalar product and a nonlinear function mapping


## A Multi-Layer Feed-Forward Neural Network



## How A Multi-Layer Neural Network Works?

- The inputs to the network correspond to the attributes measured for each training tuple
- Inputs are fed simultaneously into the units making up the input layer
- They are then weighted and fed simultaneously to a hidden layer
- The number of hidden layers is arbitrary, although usually only one
- The weighted outputs of the last hidden layer are input to units making up the output layer, which emits the network's prediction
- The network is feed-forward in that none of the weights cycles back to an input unit or to an output unit of a previous layer
- From a statistical point of view, networks perform nonlinear regression: Given enough hidden units and enough training samples, they can closely approximate any function


## Defining a Network Topology

- First decide the network topology: \# of units in the input layer, \# of hidden layers (if $>1$ ), \# of units in each hidden layer, and \# of units in the output layer
- Normalizing the input values for each attribute measured in the training tuples to [0.0-1.0]
- One input unit per domain value, each initialized to 0
- Neural networks can be used for both classification and prediction
- For classification one output unit may be used to represent two classes
- for classification and more than two classes, one output unit per class is used


## Contd.. Defining a Network Topology

- There are no clear rules for the 'best' number of hidden layer units
- NN design is a trial and error process
- Once a network has been trained and its accuracy is unacceptable, repeat the training process with a different network topology or a different set of initial weights


## Backpropagation

- Iteratively process a set of training tuples \& compare the network's prediction with the actual known target value
- For each training tuple, the weights are modified to minimize the mean squared error between the network's prediction and the actual target value
- Modifications are made in the "backwards" direction: from the output layer, through each hidden layer down to the first hidden layer, hence "backpropagation"
- Steps
- Initialize weights (to small random \#s) and biases in the network
- Propagate the inputs forward (by applying activation function)
- Backpropagate the error (by updating weights and biases)
- Terminating condition (when error is very small, etc.)


## Network Training

- The ultimate objective of training
- obtain a set of weights that makes almost all the tuples in the training data classified correctly
- Steps
- Initialize weights with random values
- Feed the input tuples into the network one by one
- For each unit
- Compute the net input to the unit as a linear combination of all the inputs to the unit
- Compute the output value using the activation function
- Compute the error
- Update the weights and the bias


## Multi-Layer Perceptron



## Backpropagation algorithm

## Input:

- D, a data set consisting of the training tuples and their associated target values
- $\quad$ L, the learning rate
- Network, a multilayer feed-forward network

Output : A trained neural network

## Method:

1. Initialize all weights and biases in network
2. while terminating condition is not satisfied \{
3. for each training tuple $X$ in $D$ \{
4. // propagate the inputs forward
5. for each input layer unit j \{
6. $\quad \mathrm{Oj}=\mathrm{lj}$; // output of an input unit is its actual input value
7. for each hidden or output layer unit j \{
8. //compute the net input of unit j w.r.t the previous
layer, i
9. $\quad O_{j}=\frac{1}{1+e^{-I_{j}}}$
$I_{j}=\sum_{i} w_{i j} O_{i}+\theta_{j}$
\} // compute the output of each unit j

## Contd. <br> Backpropagation algorithm

10. // Backpropagation errors
11. for each unit j in the output layer
12. 

$$
E r r_{j}=O_{j}\left(1-O_{j}\right)\left(T_{j}-O_{j}\right) \quad / / \text { compute the error }
$$

13. for each unit j in the hidden layers, from the last to the first hidden layer
14. $E \operatorname{Err}{ }_{j}=O_{j}\left(1-O_{j}\right) \sum_{k} E r r_{k} w_{j k}$
// compute the error w.r.t the next higher layer, k
15. for each weight wij in network \{
16. $\Delta$ wij $=(I)$ Errkwjk ; // weight increment
17. $\quad$ wij $=$ wij $+\Delta$ wij ; \} // weight update
18. for each bias $\theta \mathrm{j}$ in network \{
19. 

$\Delta \theta \mathrm{j}=(\mathrm{I})$ Errj; // bias increment
$\theta \mathrm{j}=\theta \mathrm{j}+\Delta \theta \mathrm{j}$; // bias update
21. \} \}

## Multi-Layer Perceptron

- Case updating vs. epoch updating
- Weights and biases are updated after presentation of each sample
- Deltas are accumulated into variables throughout the whole training examples and then update
- Case updating is more common (more accurate)
- Termination condition
- Delta is too small (converge)
- Accuracy of the current epoch is high enough
- Pre-specified number of epochs
- In practice, hundreds of thousands of epochs


## Example



Initial input, weight, and bias values.

| $x_{1}$ | $x_{2}$ | $x_{3}$ | $w_{14}$ | $w_{15}$ | $w_{24}$ | $w_{25}$ | $w_{34}$ | $w_{35}$ | $w_{46}$ | $w_{56}$ | $\theta_{4}$ | $\theta_{5}$ | $\theta_{6}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 0 | 1 | 0.2 | -0.3 | 0.4 | 0.1 | -0.5 | 0.2 | -0.3 | -0.2 | -0.4 | 0.2 | 0.1 |

Class label $=1$

## Example

Initial input, weight, and bias values.

| $x_{1}$ | $x_{2}$ | $x_{3}$ | $w_{14}$ | $w_{15}$ | $w_{24}$ | $w_{25}$ | $w_{34}$ | $w_{35}$ | $w_{46}$ | $w_{56}$ | $\theta_{4}$ | $\theta_{5}$ | $\theta_{6}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 1 | 0.2 | -0.3 | 0.4 | 0.1 | -0.5 | 0.2 | -0.3 | -0.2 | -0.4 | 0.2 | 0.1 |

## $I_{j}=\sum_{i} w_{i j} O_{i}+\theta_{j}$



## $E r r_{j}=O_{j}\left(1-O_{j}\right)\left(T_{j}-O_{j}\right)$



The net input and output calculations.

| Unit $j$ | Net input, $I_{j}$ | Output, $O_{j}$ |
| :--- | :--- | :--- |
| 4 | $0.2+0-0.5-0.4=-0.7$ | $1 /\left(1+e^{0.7}\right)=0.332$ |
| 5 | $-0.3+0+0.2+0.2=0.1$ | $1 /\left(1+e^{-0.1}\right)=0.525$ |
| 6 | $(-0.3)(0.332)-(0.2)(0.525)+0.1=-0.105$ | $1 /\left(1+e^{0.105}\right)=0.474$ |



| Unit $j$ | Err $_{j}$ |
| :--- | :--- |
| 6 | $(0.474)(1-0.474)(1-0.474)=0.1311$ |
| 5 | $(0.525)(1-0.525)(0.1311)(-0.2)=-0.0065$ |
| 4 | $(0.332)(1-0.332)(0.1311)(-0.3)=-0.0087$ |

## Example

Initial input, weight, and bias ralues.
 $\begin{array}{llllllllllllll}1 & 0 & 1 & 0.2 & -0.5 & 0.4 & 0.1 & -0.5 & 0.2 & -0.3 & -0.2 & -0.4 & 0.2 & 0.1\end{array}$


## Weight or bias

| $w_{46}$ | $-0.3+(0.9)(0.1311)(0.332)=-0.261$ |
| :--- | :--- |
| $w_{56}$ | $-0.2+(0.9)(0.1311)(0.525)=-0.138$ |
| $w_{14}$ | $0.2+(0.9)(-0.0087)(1)=0.192$ |
| $w_{15}$ | $-0.3+(0.9)(-0.0065)(1)=-0.306$ |
| $w_{24}$ | $0.4+(0.9)(-0.0087)(0)=0.4$ |
| $w_{25}$ | $0.1+(0.9)(-0.0065)(0)=0.1$ |
| $w_{34}$ | $-0.5+(0.9)(-0.0087)(1)=-0.508$ |
| $w_{35}$ | $0.2+(0.9)(-0.0065)(1)=0.194$ |
| $\theta_{6}$ | $0.1+(0.9)(0.1311)=0.218$ |
| $\theta_{5}$ | $0.2+(0.9)(-0.0065)=0.194$ |
| $\theta_{4}$ | $-0.4+(0.9)(-0.0087)=-0.408$ |

## Backpropagation and I nterpretability

- Efficiency of backpropagation: Each epoch (one iteration through the training set) takes $\mathrm{O}(|\mathrm{D}| *$ w), with |D| tuples and w weights, but \# of epochs can be exponential to $n$, the number of inputs, in the worst case.


## Network Pruning and Rule Extraction

- Network pruning
- Fully connected network will be hard to articulate
- $N$ input nodes, $h$ hidden nodes and m output nodes lead to $h(m+N)$ weights
- Pruning: Remove some of the links without affecting classification accuracy of the network
- Extracting rules from a trained network
- Discretize activation values; replace individual activation value by the cluster average maintaining the network accuracy
- Enumerate the output from the discretized activation values to find rules between activation value and output
- Find the relationship between the input and activation value
- Combine the above two to have rules relating the output to input


## Network Pruning and Rule Extraction

- Sensitivity analysis: assess the impact that a given input variable has on a network output. The knowledge gained from this analysis can be represented in rules


## What Is Prediction?

- (Numerical) prediction is similar to classification
- construct a model
- use model to predict continuous or ordered value for a given input
- Prediction is different from classification
- Classification refers to predict categorical class label
- Prediction models continuous-valued functions
- Major method for prediction: regression
- model the relationship between one or more independent or predictor variables and a dependent or response variable
- Regression analysis
- Linear and multiple regression
- Non-linear regression
- Other regression methods: generalized linear model, Poisson regression, log-linear models, regression trees


## Linear Regression

- Linear regression: involves a response variable y and a single predictor variable x

$$
y=w_{0}+w_{1} x
$$

where $w_{0}$ ( $y$-intercept) and $w_{1}$ (slope) are regression coefficients

- Method of least squares: estimates the best-fitting straight line

$$
w_{1}=\frac{\sum_{i=1}^{|p|}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{\sum_{i=1}^{|0|}\left(x_{i}-\bar{x}\right)^{2}} \quad w_{0}=\bar{y}-w_{1} \bar{x}
$$

- Multiple linear regression: involves more than one predictor variable
- Training data is of the form $\left(\mathbf{X}_{1}, y_{1}\right),\left(\mathbf{X}_{2}, y_{2}\right), \ldots,\left(X_{|D|}, y_{|D|}\right)$
- Ex. For 2-D data, we may have: $y=w_{0}+w_{1} x_{1}+w_{2} x_{2}$
- Solvable by extension of least square method or using SAS, S-Plus
- Many nonlinear functions can be transformed into the above


## Nonlinear Regression

- Some nonlinear models can be modeled by a polynomial function
- A polynomial regression model can be transformed into linear regression model. For example,

$$
y=w_{0}+w_{1} x+w_{2} x^{2}+w_{3} x^{3}
$$

convertible to linear with new variables: $x_{2}=x^{2}, x_{3}=x^{3}$

$$
y=w_{0}+w_{1} x+w_{2} x_{2}+w_{3} x_{3}
$$

- Other functions, such as power function, can also be transformed to linear model
- Some models are intractable nonlinear (e.g., sum of exponential terms)
- possible to obtain least square estimates through extensive calculation on more complex formulae


## Other Regression-Based Models

- Generalized linear model:
- Foundation on which linear regression can be applied to modeling categorical response variables
- Variance of $y$ is a function of the mean value of $y$, not a constant
- Logistic regression: models the prob. of some event occurring as a linear function of a set of predictor variables
- Poisson regression: models the data that exhibit a Poisson distribution
- Log-linear models: (for categorical data)
- Approximate discrete multidimensional prob. distributions
- Also useful for data compression and smoothing
- Regression trees and model trees
- Trees to predict continuous values rather than class labels


## Accuracy and Error Measures

## Classifier Accuracy Measures

|  | $C_{1}$ | $C_{2}$ |
| :---: | :---: | :---: |
| $C_{1}$ | True positive | False negative |
| $\mathrm{C}_{2}$ | False positive | True negative |


| classes | buy_computer = yes | buy_computer = no | total | recognition(\%) |
| :---: | :---: | :---: | :---: | :---: |
| buy_computer = yes | 6954 | 46 | 7000 | 99.34 |
| buy_computer = no | 412 | 2588 | 3000 | 86.27 |
| total | 7366 | 2634 | 10000 | 95.52 |

- Accuracy of a classifier $M$, acc( $M$ ): percentage of test set tuples that are correctly classified by the model M
- Error rate (misclassification rate) of $M=1$ - acc( $M$ )
- Given m classes, $\mathrm{CM}_{\mathrm{i}, \mathrm{j}}$, an entry in a confusion matrix, indicates \# of tuples in class $i$ that are labeled by the classifier as class $j$
- Alternative accuracy measures (e.g., for cancer diagnosis) sensitivity $=\mathrm{t}-\mathrm{pos} /$ pos $\quad / *$ true positive recognition rate */
specificity $=\mathrm{t}-\mathrm{neg} / \mathrm{neg} \quad / *$ true negative recognition rate */
precision $=\mathrm{t}-\mathrm{pos} /(\mathrm{t}-\mathrm{pos}+\mathrm{f}-\mathrm{pos})$
accuracy $=$ sensitivity $* \operatorname{pos} /($ pos + neg $)+$ specificity $*$ neg/(pos + neg $)$
- This model can also be used for cost-benefit analysis


## Predictor Error Measures

- Measure predictor accuracy: measure how far off the predicted value is from the actual known value
- Loss function: measures the error between $y_{i}$ and the predicted value $y_{i}{ }^{\prime}$
- Absolute error: $\left|y_{i}-y_{i}^{\prime}\right|$
- Squared error: $\left(y_{i}-y_{i}^{\prime}\right)^{2}$
- Test error (generalization error): the average loss over the test set
- Mean absolute error: $\frac{\sum_{i=1}^{d}\left|y_{i}-y_{i}^{\prime}\right|}{d}$ Mean squared error: $\frac{\sum_{i=1}^{d}\left(y_{i}-y_{i}^{\prime}\right)^{2}}{{ }^{d} d}$
 Popularly use (square) root mean-square error, similarly, root relative squared error


## End of Unit-3

