Chapter 8. Classification: Evaluation

Meng Jiang

CSE 40647/60647 Data Science Fall 2017

Introduction to Data Mining

Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- **Model Evaluation and Selection**
- Techniques to Improve Classification Accuracy: Ensemble Methods

Model Evaluation and Selection

- Evaluation metrics: How can we measure accuracy? Other metrics to consider?
- Use **validation test set** of class-labeled tuples instead of training set when assessing accuracy
- Methods for estimating a classifier's accuracy:
  - Holdout method
  - Cross-validation

Classifier Evaluation Metrics: Confusion Matrix

Confusion Matrix:

Actual class\Predicted class	C_1	$\neg C_1$
C_1	**True Positives (TP)**	**False Negatives (FN)**
$\neg C_1$	**False Positives (FP)**	**True Negatives (TN)**

Example of Confusion Matrix:

Actual class\Predicted class	buy_computer = yes	buy_computer = no	Total
buy_computer = yes	**6,954**	**46**	7,000
buy_computer = no	**412**	**2,588**	3,000
Total	7,366	2,634	10,000

- Given *m* classes, an entry, $CM_{i,j}$ in a **confusion matrix** indicates # of tuples in class *i* that were labeled by the classifier as class *j*
  - May have extra rows/columns to provide totals

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	C	¬C	
C	**TP**	**FN**	**P**
¬C	**FP**	**TN**	**N**
	P’	**N’**	**All**

- **Classifier Accuracy,** or recognition rate: percentage of test set tuples that are correctly classified

Accuracy = (TP + TN)/All

- **Error rate:** *1 – accuracy*, or

Error rate = (FP + FN)/All

- **Class Imbalance Problem**:
  - One class may be *rare*, e.g. fraud, or HIV-positive
  - Significant *majority of the negative class* and minority of the positive class
  - **Sensitivity**: True Positive recognition rate
    - **Sensitivity = TP/P**
  - **Specificity**: True Negative recognition rate
    - **Specificity = TN/N**

Classifier Evaluation Metrics: Precision and Recall, and F-measures

- **Precision**: exactness: what % of tuples that the classifier labeled as positive are actually positive

$$precision = \frac{TP}{TP + FP}$$

- **Recall:** completeness – what % of positive tuples did the classifier label as positive?

$$recall = \frac{TP}{TP + FN}$$

- Comment:
  - Perfect score is 1.0
  - Inverse relationship between precision & recall
- ***F*** **measure** (or ***F*****-score):** harmonic mean of precision and recall
  - In general, it is the weighted measure of precision & recall

$$F = \frac{1}{\alpha \cdot \frac{1}{P} + (1-\alpha) \cdot \frac{1}{R}} = \frac{(\beta^2 + 1)PR}{\beta^2 P + R}$$

Assigning β times as much weight to recall as to precision)

- ***F1-measure (balanced F-measure)***
  » That is, when β = 1, $F_1 = \frac{2PR}{P + R}$

Classifier Evaluation Metrics: Example

Actual Class\Predicted class	cancer = yes	cancer = no	Total	Recognition(%)
cancer = yes	**90**	**210**	300	30.00 (*sensitivity*)
cancer = no	**140**	**9,560**	9,700	98.56 (*specificity*)
Total	230	9,770	10,000	96.40 (*accuracy*)

Precision = 90/230 = 39.13%

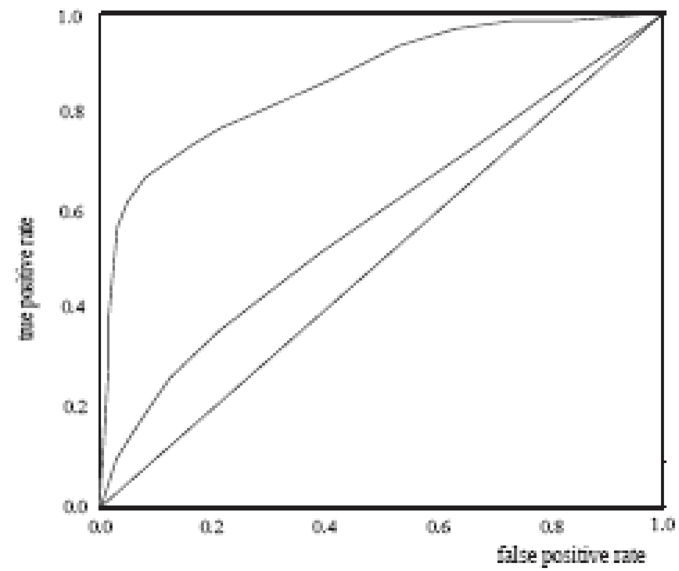
Recall = 90/300 = 30.00%

Evaluating Classifier Accuracy: Holdout & Cross-Validation Methods

- **Holdout method**
  - Given data is randomly partitioned into two independent sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
  - Random sampling: a variation of holdout
    - Repeat holdout k times, accuracy = avg. of the accuracies obtained
- **Cross-validation** (*k*-fold, where k = 10 is most popular)
  - Randomly partition the data into *k mutually exclusive* subsets, each approximately equal size
  - At *i*-th iteration, use D_i as test set and others as training set
  - Leave-one-out: *k* folds where *k* = # of tuples, for small sized data
  - ***Stratified cross-validation***: folds are stratified so that class dist. in each fold is approx. the same as that in the initial data

Model Selection: ROC Curves

- ROC (Receiver Operating Characteristics) curves: for visual comparison of classification models
- Originated from signal detection theory
- Shows the **trade-off between the true positive rate and the false positive rate**
- The area under the ROC curve is a measure of the accuracy of the model
- Rank the test tuples in decreasing order: the one that is most likely to belong to the positive class appears at the top of the list
- **The closer to the diagonal line (i.e., the closer the area is to 0.5), the less accurate is the model**



- **Vertical axis represents the true positive rate**
- **Horizontal axis rep. the false positive rate**
- The plot also shows a diagonal line
- **A model with perfect accuracy will have an area of 1.0**

Issues Affecting Model Selection

- **Accuracy**
  - classifier accuracy: predicting class label
- **Speed**
  - time to construct the model (training time)
  - time to use the model (classification/prediction time)
- **Robustness**: handling noise and missing values
- **Scalability**: efficiency in disk-resident databases
- **Interpretability**
  - understanding and insight provided by the model
- Other measures, e.g., goodness of rules, such as decision tree size or compactness of classification rules

Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Model Evaluation and Selection
- **Techniques to Improve Classification Accuracy: Ensemble Methods**

Ensemble Methods: Increasing the Accuracy

- Ensemble methods
  - Use a **combination of models** to increase accuracy
  - Combine a series of k learned models, M_1, M_2, …, M_k, with the aim of creating an improved model M*
- Popular **ensemble methods**
  - Bagging: averaging the prediction over a collection of classifiers
  - Boosting: weighted vote with a collection of classifiers
  - **Ensemble: combining a set of heterogeneous classifiers**

Bagging

- Analogy: Diagnosis based on multiple doctors' majority vote
- Training
  - Given a set D of d tuples, at each iteration i, a training set D_i of d tuples is sampled with replacement from D
  - A classifier model M_i is learned for each training set D_i
- Classification: classify an unknown sample **X**
  - Each classifier M_i returns its class prediction
  - The bagged classifier M* counts the votes and assigns the class with the most votes to **X**
- Prediction: can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple
- Accuracy: Proved improved accuracy in prediction
  - Often significantly better than a single classifier derived from D
  - For noise data: not considerably worse, more robust

Boosting

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - **Weights** are assigned to each training tuple
  - A series of k classifiers is iteratively learned
  - After a classifier M_i is learned, the weights are updated to allow the subsequent classifier, M_{i+1}, to **pay more attention to the training tuples that were misclassified** by M_i
  - The final **M* combines the votes** of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- Boosting algorithm can be extended for numeric prediction
- Comparing with **bagging**: **Boosting** tends to have **greater accuracy**, but it also risks **overfitting** the model to misclassified data

Ensemble: Adaboost (Freund and Schapire, 1997)

- Given a set of *d* class-labeled tuples, $(\mathbf{X_1}, y_1), \ldots, (\mathbf{X_d}, y_d)$
- Initially, all the weights of tuples are set the same (1/d)
- Generate k classifiers in k rounds. At round i,
  - Tuples from D are sampled (with replacement) to form a training set D_i of the same size
  - Each tuple's chance of being selected is based on its weight
  - A classification model M_i is derived from D_i
  - Its error rate is calculated using D_i as a test set
  - If a tuple is misclassified, its weight is increased, o.w. it is decreased
- Error rate: $err(\mathbf{X_j})$ is the misclassification error of tuple $\mathbf{X_j}$. Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_{j}^{d} w_j \times err(\mathbf{X_j})$$

- The weight of classifier M_i's vote is $\log \frac{1 - error(M_i)}{error(M_i)}$

Summary

- Classification: Extracting models describing important data classes
- Effective and scalable methods
  - **Decision tree induction**, **Naive Bayesian classification**, and many other classification methods
- Evaluation metrics:
  - **Accuracy, sensitivity, specificity, precision, recall, *F* measure, and F_β measure**
  - Stratified k-fold cross-validation is recommended for accuracy estimation
- Ensemble: Bagging and boosting can be used to increase overall accuracy by learning and combining a series of individual models
  - **Adaboost**
- **No single method has been found to be superior over all others for all data sets**

References

- C. Apte and S. Weiss. Data mining with decision trees and decision rules. Future Generation Computer Systems, 13, 1997
- P. K. Chan and S. J. Stolfo. Learning arbiter and combiner trees from partitioned data for scaling machine learning. KDD'95
- A. J. Dobson. An Introduction to Generalized Linear Models. Chapman & Hall, 1990.
- R. O. Duda, P. E. Hart, and D. G. Stork. Pattern Classification, 2ed. John Wiley, 2001
- U. M. Fayyad. Branching on attribute values in decision tree generation. AAAI'94.
- Y. Freund and R. E. Schapire. A decision-theoretic generalization of on-line learning and an application to boosting. J. Computer and System Sciences, 1997.
- J. Gehrke, R. Ramakrishnan, and V. Ganti. Rainforest: A framework for fast decision tree construction of large datasets. VLDB'98.
- J. Gehrke, V. Gant, R. Ramakrishnan, and W.-Y. Loh, BOAT -- Optimistic Decision Tree Construction. SIGMOD'99.
- T. Hastie, R. Tibshirani, and J. Friedman. The Elements of Statistical Learning: Data Mining, Inference, and Prediction. Springer-Verlag, 2001.
- T.-S. Lim, W.-Y. Loh, and Y.-S. Shih. A comparison of prediction accuracy, complexity, and training time of thirty-three old and new classification algorithms. Machine Learning, 2000

References (cont.)

- J. Magidson. The Chaid approach to segmentation modeling: Chi-squared automatic interaction detection. In R. P. Bagozzi, editor, Advanced Methods of Marketing Research, Blackwell Business, 1994
- M. Mehta, R. Agrawal, and J. Rissanen. SLIQ : A fast scalable classifier for data mining. EDBT'96
- T. M. Mitchell. Machine Learning. McGraw Hill, 1997
- S. K. Murthy, Automatic Construction of Decision Trees from Data: A Multi-Disciplinary Survey, Data Mining and Knowledge Discovery 2(4): 345-389, 1998
- J. R. Quinlan. Induction of decision trees. Machine Learning, 1:81-106, 1986.
- J. R. Quinlan. C4.5: Programs for Machine Learning. Morgan Kaufmann, 1993.
- J. R. Quinlan. Bagging, boosting, and c4.5. AAAI'96.
- R. Rastogi and K. Shim. **Public: A decision tree classifier that integrates building and pruning**. VLDB'98
- J. Shafer, R. Agrawal, and M. Mehta. **SPRINT : A scalable parallel classifier for data mining**. VLDB'96
- J. W. Shavlik and T. G. Dietterich. **Readings in Machine Learning**. Morgan Kaufmann, 1990
- P. Tan, M. Steinbach, and V. Kumar. **Introduction to Data Mining**. Addison Wesley, 2005
- S. M. Weiss and C. A. Kulikowski. **Computer Systems that Learn: Classification and Prediction Methods from Statistics, Neural Nets, Machine Learning, and Expert Systems**. Morgan Kaufman, 1991
- S. M. Weiss and N. Indurkhya. **Predictive Data Mining**. Morgan Kaufmann, 1997
- I. H. Witten and E. Frank. **Data Mining: Practical Machine Learning Tools and Techniques**, 2ed. Morgan Kaufmann, 2005