**MATH 5364 Data Mining I**

**Instructor**

Dr. Jesse Crawford Office phone: (254) 968-9536

Email: [jcrawford@tarleton.edu](mailto:jcrawford@tarleton.edu) Office: Math 332

Website: faculty.tarleton.edu/crawford

**Office Hours**

TBA

You are highly encouraged to visit my office for help.

**Course Meeting Times**

TR 6:55 – 8:10 in Math 212

**Required Materials**

*Introduction to Data Mining*, by Tan, Steinbach, and Kumar.

**Homework**

Homework will be assigned regularly and will be due a week later. It is crucial to keep up with the homework to succeed in this course.

**Grades**

Course averages will be computed as follows.

|  |  |
| --- | --- |
| **Assignment** | **% of Grade** |
| Homework | 70% |
| Final Project | 30% |

**Students with Disabilities:** It is the policy of Tarleton State University to comply with the Americans with Disabilities Act and other applicable laws. If you are a student with a disability seeking accommodations for this course, please contact Trina Geye, Director of Student Disability Services, at 254.968.9400 or [geye@tarleton.edu](mailto:geye@tarleton.edu). Student Disability Services is located in Math 201. More information can be found at [www.tarleton.edu/sds](http://www.tarleton.edu/sds) or in the University Catalog.

**Academic Integrity:** The Tarleton University Mathematics Department takes academic integrity very seriously. The usual penalty for a student caught cheating includes an F in the course. Further penalties may be imposed, including expulsion from the university.

**Catalog Description**

This course centers on the identification, exploration, and description of new patterns contained within data sets using appropriate software. Selected topics will be chosen from data exploration, classification, cluster analysis, and model evaluation and comparison.

**Student Learning Outcomes**

1. Examine raw data in order to detect data quality issues and interesting subsets or features contained within the data.
2. Transform raw data into a form appropriate for modeling.
3. Select and train appropriate models using the transformed data.
4. Measure the effectiveness of each model.
5. Draw appropriate conclusions.

**Sections of Primary Interest**

4 Classification: Basic Concepts, Decision Trees, and Model Evaluation 145

4.1 Preliminaries . . . . . . . . . . . . . . . . . . . . . . . . . . . . 146

4.2 General Approach to Solving a Classification Problem . . . . . 148

4.3 Decision Tree Induction . . . . . . . . . . . . . . . . . . . . . . 150

4.3.1 How a Decision Tree Works . . . . . . . . . . . . . . . . 150

4.3.2 How to Build a Decision Tree . . . . . . . . . . . . . . . 151

4.3.3 Methods for Expressing Attribute Test Conditions . . . 155

4.3.4 Measures for Selecting the Best Split . . . . . . . . . . . 158

4.3.5 Algorithm for Decision Tree Induction . . . . . . . . . . 164

4.3.6 An Example: Web Robot Detection . . . . . . . . . . . 166

4.3.7 Characteristics of Decision Tree Induction . . . . . . . . 168

4.4 Model Overfitting . . . . . . . . . . . . . . . . . . . . . . . . . . 172

4.4.1 Overfitting Due to Presence of Noise . . . . . . . . . . . 175

4.4.2 Overfitting Due to Lack of Representative Samples . . . 177

4.4.3 Overfitting and the Multiple Comparison Procedure . . 178

4.4.4 Estimation of Generalization Errors . . . . . . . . . . . 179

4.4.5 Handling Overfitting in Decision Tree Induction . . . . 184

4.5 Evaluating the Performance of a Classifier . . . . . . . . . . . . 186

4.5.1 Holdout Method . . . . . . . . . . . . . . . . . . . . . . 186

4.5.2 Random Subsampling . . . . . . . . . . . . . . . . . . . 187

4.5.3 Cross-Validation . . . . . . . . . . . . . . . . . . . . . . 187

4.5.4 Bootstrap . . . . . . . . . . . . . . . . . . . . . . . . . . 188

4.6 Methods for Comparing Classifiers . . . . . . . . . . . . . . . . 188

4.6.1 Estimating a Confidence Interval for Accuracy . . . . . 189

4.6.2 Comparing the Performance of Two Models . . . . . . . 191

4.6.3 Comparing the Performance of Two Classifiers . . . . . 192

4.7 Bibliographic Notes . . . . . . . . . . . . . . . . . . . . . . . . . 193

4.8 Exercises . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 198

5 Classification: Alternative Techniques 207

5.1 Rule-Based Classifier . . . . . . . . . . . . . . . . . . . . . . . . 207

5.1.1 How a Rule-Based Classifier Works . . . . . . . . . . . . 209

5.1.2 Rule-Ordering Schemes . . . . . . . . . . . . . . . . . . 211

5.1.3 How to Build a Rule-Based Classifier . . . . . . . . . . . 212

5.1.4 Direct Methods for Rule Extraction . . . . . . . . . . . 213

5.1.5 Indirect Methods for Rule Extraction . . . . . . . . . . 221

5.1.6 Characteristics of Rule-Based Classifiers . . . . . . . . . 223

5.2 Nearest-Neighbor classifiers . . . . . . . . . . . . . . . . . . . . 223

5.2.1 Algorithm . . . . . . . . . . . . . . . . . . . . . . . . . . 225

5.2.2 Characteristics of Nearest-Neighbor Classifiers . . . . . 226

5.3 Bayesian Classifiers . . . . . . . . . . . . . . . . . . . . . . . . . 227

5.3.1 Bayes Theorem . . . . . . . . . . . . . . . . . . . . . . . 228

5.3.2 Using the Bayes Theorem for Classification . . . . . . . 229

5.3.3 Na¨ıve Bayes Classifier . . . . . . . . . . . . . . . . . . . 231

5.3.4 Bayes Error Rate . . . . . . . . . . . . . . . . . . . . . . 238

5.3.5 Bayesian Belief Networks . . . . . . . . . . . . . . . . . 240

5.4 Artificial Neural Network (ANN) . . . . . . . . . . . . . . . . . 246

5.4.1 Perceptron . . . . . . . . . . . . . . . . . . . . . . . . . 247

5.4.2 Multilayer Artificial Neural Network . . . . . . . . . . . 251

5.4.3 Characteristics of ANN . . . . . . . . . . . . . . . . . . 255

5.5 Support Vector Machine (SVM) . . . . . . . . . . . . . . . . . . 256

5.5.1 Maximum Margin Hyperplanes . . . . . . . . . . . . . . 256

5.5.2 Linear SVM: Separable Case . . . . . . . . . . . . . . . 259

5.5.3 Linear SVM: Nonseparable Case . . . . . . . . . . . . . 266

5.5.4 Nonlinear SVM . . . . . . . . . . . . . . . . . . . . . . . 270

5.5.5 Characteristics of SVM . . . . . . . . . . . . . . . . . . 276

5.6 Ensemble Methods . . . . . . . . . . . . . . . . . . . . . . . . . 276

5.6.1 Rationale for Ensemble Method . . . . . . . . . . . . . . 277

5.6.2 Methods for Constructing an Ensemble Classifier . . . . 278

5.6.3 Bias-Variance Decomposition . . . . . . . . . . . . . . . 281

5.6.4 Bagging . . . . . . . . . . . . . . . . . . . . . . . . . . . 283

5.6.5 Boosting . . . . . . . . . . . . . . . . . . . . . . . . . . . 285

5.6.6 Random Forests . . . . . . . . . . . . . . . . . . . . . . 290

5.6.7 Empirical Comparison among Ensemble Methods . . . . 294

5.7 Class Imbalance Problem . . . . . . . . . . . . . . . . . . . . . 294

5.7.1 Alternative Metrics . . . . . . . . . . . . . . . . . . . . . 295

5.7.2 The Receiver Operating Characteristic Curve . . . . . . 298

5.7.3 Cost-Sensitive Learning . . . . . . . . . . . . . . . . . . 302

5.7.4 Sampling-Based Approaches . . . . . . . . . . . . . . . . 305

5.8 Multiclass Problem . . . . . . . . . . . . . . . . . . . . . . . . . 306

5.9 Bibliographic Notes . . . . . . . . . . . . . . . . . . . . . . . . . 309

5.10 Exercises . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 315

6 Association Analysis: Basic Concepts and Algorithms 327

6.1 Problem Definition . . . . . . . . . . . . . . . . . . . . . . . . . 328

6.2 Frequent Itemset Generation . . . . . . . . . . . . . . . . . . . 332

6.2.1 The Apriori Principle . . . . . . . . . . . . . . . . . . . 333

6.2.2 Frequent Itemset Generation in the Apriori Algorithm . 335

6.2.3 Candidate Generation and Pruning . . . . . . . . . . . . 338

6.2.4 Support Counting . . . . . . . . . . . . . . . . . . . . . 342

6.2.5 Computational Complexity . . . . . . . . . . . . . . . . 345

6.3 Rule Generation . . . . . . . . . . . . . . . . . . . . . . . . . . 349

6.3.1 Confidence-Based Pruning . . . . . . . . . . . . . . . . . 350

6.3.2 Rule Generation in Apriori Algorithm . . . . . . . . . . 350

6.3.3 An Example: Congressional Voting Records . . . . . . . 352

6.4 Compact Representation of Frequent Itemsets . . . . . . . . . . 353

6.4.1 Maximal Frequent Itemsets . . . . . . . . . . . . . . . . 354

6.4.2 Closed Frequent Itemsets . . . . . . . . . . . . . . . . . 355

6.5 Alternative Methods for Generating Frequent Itemsets . . . . . 359

6.6 FP-Growth Algorithm . . . . . . . . . . . . . . . . . . . . . . . 363

6.6.1 FP-Tree Representation . . . . . . . . . . . . . . . . . . 363

6.6.2 Frequent Itemset Generation in FP-Growth Algorithm . 366

6.7 Evaluation of Association Patterns . . . . . . . . . . . . . . . . 370

6.7.1 Objective Measures of Interestingness . . . . . . . . . . 371

6.7.2 Measures beyond Pairs of Binary Variables . . . . . . . 382

6.7.3 Simpson’s Paradox . . . . . . . . . . . . . . . . . . . . . 384

6.8 Effect of Skewed Support Distribution . . . . . . . . . . . . . . 386

6.9 Bibliographic Notes . . . . . . . . . . . . . . . . . . . . . . . . . 390

6.10 Exercises . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 404

7 Association Analysis: Advanced Concepts 415

7.1 Handling Categorical Attributes . . . . . . . . . . . . . . . . . 415

7.2 Handling Continuous Attributes . . . . . . . . . . . . . . . . . 418

7.2.1 Discretization-Based Methods . . . . . . . . . . . . . . . 418

7.2.2 Statistics-Based Methods . . . . . . . . . . . . . . . . . 422

7.2.3 Non-discretization Methods . . . . . . . . . . . . . . . . 424

7.3 Handling a Concept Hierarchy . . . . . . . . . . . . . . . . . . 426

7.4 Sequential Patterns . . . . . . . . . . . . . . . . . . . . . . . . . 429

7.4.1 Problem Formulation . . . . . . . . . . . . . . . . . . . 429

7.4.2 Sequential Pattern Discovery . . . . . . . . . . . . . . . 431

7.4.3 Timing Constraints . . . . . . . . . . . . . . . . . . . . . 436

7.4.4 Alternative Counting Schemes . . . . . . . . . . . . . . 439

7.5 Subgraph Patterns . . . . . . . . . . . . . . . . . . . . . . . . . 442

7.5.1 Graphs and Subgraphs . . . . . . . . . . . . . . . . . . . 443

7.5.2 Frequent Subgraph Mining . . . . . . . . . . . . . . . . 444

7.5.3 Apriori -like Method . . . . . . . . . . . . . . . . . . . . 447

7.5.4 Candidate Generation . . . . . . . . . . . . . . . . . . . 448

7.5.5 Candidate Pruning . . . . . . . . . . . . . . . . . . . . . 453

7.5.6 Support Counting . . . . . . . . . . . . . . . . . . . . . 457

7.6 Infrequent Patterns . . . . . . . . . . . . . . . . . . . . . . . . . 457

7.6.1 Negative Patterns . . . . . . . . . . . . . . . . . . . . . 458

7.6.2 Negatively Correlated Patterns . . . . . . . . . . . . . . 458

7.6.3 Comparisons among Infrequent Patterns, Negative Patterns,

and Negatively Correlated Patterns . . . . . . . . 460

7.6.4 Techniques for Mining Interesting Infrequent Patterns . 461

7.6.5 Techniques Based on Mining Negative Patterns . . . . . 463

7.6.6 Techniques Based on Support Expectation . . . . . . . . 465

7.7 Bibliographic Notes . . . . . . . . . . . . . . . . . . . . . . . . . 469

7.8 Exercises . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 473

8 Cluster Analysis: Basic Concepts and Algorithms 487

8.1 Overview . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 490

8.1.1 What Is Cluster Analysis? . . . . . . . . . . . . . . . . . 490

8.1.2 Different Types of Clusterings . . . . . . . . . . . . . . . 491

8.1.3 Different Types of Clusters . . . . . . . . . . . . . . . . 493

8.2 K-means . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 496

8.2.1 The Basic K-means Algorithm . . . . . . . . . . . . . . 497

8.2.2 K-means: Additional Issues . . . . . . . . . . . . . . . . 506

8.2.3 Bisecting K-means . . . . . . . . . . . . . . . . . . . . . 508

8.2.4 K-means and Different Types of Clusters . . . . . . . . 510

8.2.5 Strengths and Weaknesses . . . . . . . . . . . . . . . . . 510

8.2.6 K-means as an Optimization Problem . . . . . . . . . . 513

8.3 Agglomerative Hierarchical Clustering . . . . . . . . . . . . . . 515

8.3.1 Basic Agglomerative Hierarchical Clustering Algorithm 516

8.3.2 Specific Techniques . . . . . . . . . . . . . . . . . . . . . 518

8.3.3 The Lance-Williams Formula for Cluster Proximity . . . 524

8.3.4 Key Issues in Hierarchical Clustering . . . . . . . . . . . 524

8.3.5 Strengths and Weaknesses . . . . . . . . . . . . . . . . . 526

8.4 DBSCAN . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 526

8.4.1 Traditional Density: Center-Based Approach . . . . . . 527

8.4.2 The DBSCAN Algorithm . . . . . . . . . . . . . . . . . 528

8.4.3 Strengths and Weaknesses . . . . . . . . . . . . . . . . . 530

8.5 Cluster Evaluation . . . . . . . . . . . . . . . . . . . . . . . . . 532

8.5.1 Overview . . . . . . . . . . . . . . . . . . . . . . . . . . 533

8.5.2 Unsupervised Cluster Evaluation Using Cohesion and

Separation . . . . . . . . . . . . . . . . . . . . . . . . . 536

8.5.3 Unsupervised Cluster Evaluation Using the Proximity

Matrix . . . . . . . . . . . . . . . . . . . . . . . . . . . . 542

8.5.4 Unsupervised Evaluation of Hierarchical Clustering . . . 544

8.5.5 Determining the Correct Number of Clusters . . . . . . 546

8.5.6 Clustering Tendency . . . . . . . . . . . . . . . . . . . . 547

8.5.7 Supervised Measures of Cluster Validity . . . . . . . . . 548

8.5.8 Assessing the Significance of Cluster Validity Measures . 553

8.6 Bibliographic Notes . . . . . . . . . . . . . . . . . . . . . . . . . 555

8.7 Exercises . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 559

9 Cluster Analysis: Additional Issues and Algorithms 569

9.1 Characteristics of Data, Clusters, and Clustering Algorithms . 570

9.1.1 Example: Comparing K-means and DBSCAN . . . . . . 570

9.1.2 Data Characteristics . . . . . . . . . . . . . . . . . . . . 571

9.1.3 Cluster Characteristics . . . . . . . . . . . . . . . . . . . 573

9.1.4 General Characteristics of Clustering Algorithms . . . . 575

9.2 Prototype-Based Clustering . . . . . . . . . . . . . . . . . . . . 577

9.2.1 Fuzzy Clustering . . . . . . . . . . . . . . . . . . . . . . 577

9.2.2 Clustering Using Mixture Models . . . . . . . . . . . . . 583

9.2.3 Self-Organizing Maps (SOM) . . . . . . . . . . . . . . . 594

9.3 Density-Based Clustering . . . . . . . . . . . . . . . . . . . . . 600

9.3.1 Grid-Based Clustering . . . . . . . . . . . . . . . . . . . 601

9.3.2 Subspace Clustering . . . . . . . . . . . . . . . . . . . . 604

9.3.3 DENCLUE: A Kernel-Based Scheme for Density-Based

Clustering . . . . . . . . . . . . . . . . . . . . . . . . . . 608

9.4 Graph-Based Clustering . . . . . . . . . . . . . . . . . . . . . . 612

9.4.1 Sparsification . . . . . . . . . . . . . . . . . . . . . . . . 613

9.4.2 Minimum Spanning Tree (MST) Clustering . . . . . . . 614

9.4.3 OPOSSUM: Optimal Partitioning of Sparse Similarities

Using METIS . . . . . . . . . . . . . . . . . . . . . . . . 616

9.4.4 Chameleon: Hierarchical Clustering with Dynamic

Modeling . . . . . . . . . . . . . . . . . . . . . . . . . . 616

9.4.5 Shared Nearest Neighbor Similarity . . . . . . . . . . . 622

9.4.6 The Jarvis-Patrick Clustering Algorithm . . . . . . . . . 625

9.4.7 SNN Density . . . . . . . . . . . . . . . . . . . . . . . . 627

9.4.8 SNN Density-Based Clustering . . . . . . . . . . . . . . 629

9.5 Scalable Clustering Algorithms . . . . . . . . . . . . . . . . . . 630

9.5.1 Scalability: General Issues and Approaches . . . . . . . 630

9.5.2 BIRCH . . . . . . . . . . . . . . . . . . . . . . . . . . . 633

9.5.3 CURE . . . . . . . . . . . . . . . . . . . . . . . . . . . . 635

9.6 Which Clustering Algorithm? . . . . . . . . . . . . . . . . . . . 639

9.7 Bibliographic Notes . . . . . . . . . . . . . . . . . . . . . . . . . 643

9.8 Exercises . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 647

10 Anomaly Detection 651

10.1 Preliminaries . . . . . . . . . . . . . . . . . . . . . . . . . . . . 653

10.1.1 Causes of Anomalies . . . . . . . . . . . . . . . . . . . . 653

10.1.2 Approaches to Anomaly Detection . . . . . . . . . . . . 654

10.1.3 The Use of Class Labels . . . . . . . . . . . . . . . . . . 655

10.1.4 Issues . . . . . . . . . . . . . . . . . . . . . . . . . . . . 656

10.2 Statistical Approaches . . . . . . . . . . . . . . . . . . . . . . . 658

10.2.1 Detecting Outliers in a Univariate Normal Distribution 659

10.2.2 Outliers in a Multivariate Normal Distribution . . . . . 661

10.2.3 A Mixture Model Approach for Anomaly Detection . . . 662

10.2.4 Strengths and Weaknesses . . . . . . . . . . . . . . . . . 665

10.3 Proximity-Based Outlier Detection . . . . . . . . . . . . . . . . 666

10.3.1 Strengths and Weaknesses . . . . . . . . . . . . . . . . . 666

10.4 Density-Based Outlier Detection . . . . . . . . . . . . . . . . . 668

10.4.1 Detection of Outliers Using Relative Density . . . . . . 669

10.4.2 Strengths and Weaknesses . . . . . . . . . . . . . . . . . 670

10.5 Clustering-Based Techniques . . . . . . . . . . . . . . . . . . . 671

10.5.1 Assessing the Extent to Which an Object Belongs to a

Cluster . . . . . . . . . . . . . . . . . . . . . . . . . . . 672

10.5.2 Impact of Outliers on the Initial Clustering . . . . . . . 674

10.5.3 The Number of Clusters to Use . . . . . . . . . . . . . . 674

10.5.4 Strengths and Weaknesses . . . . . . . . . . . . . . . . . 674

10.6 Bibliographic Notes . . . . . . . . . . . . . . . . . . . . . . . . . 675

10.7 Exercises . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 680