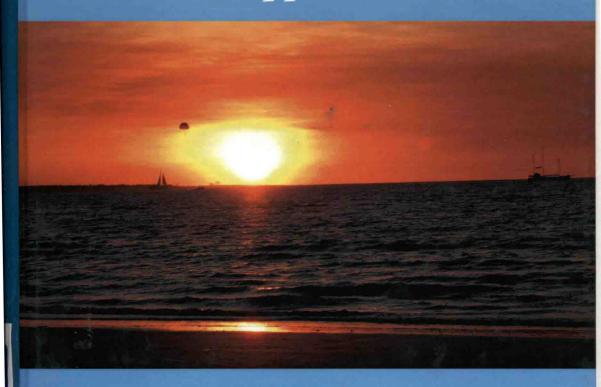
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## CONTRAST DATA MINING

Concepts, Algorithms, and Applications

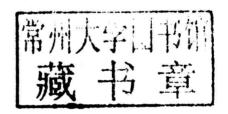


Edited by
Guozhu Dong and James Bailey



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## Concepts, Algorithms, and Applications



Guozhu Dong and James Bailey



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### CONTRAST DATA MINING

Concepts, Algorithms, and Applications

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CONTRAST DATA MINING: CONCEPTS, ALGORITHMS, AND APPLICATIONS Guozhu Dong and James Bailey



#### Dedication

To my wife Diana and my children. {G.D.}

To my wife Katherine. {J.B.}

To all contributing authors of the book and to all researchers of the contrast mining field.  $\{G.D.$  and  $J.B.\}$ 



#### **Foreword**

Contrast data mining is an important and focused subarea of data mining. Its aim is to find interesting contrast patterns that describe significant differences between datasets satisfying various contrasting conditions. The contrasting conditions can be defined on class, time, location, other "dimensions" of interest, or their combinations. The contrast patterns can represent nontrivial differences between classes, interesting changes over time, interesting trends in space, and so on.

Contrast data mining has provided, and will continue to provide, a unique angle to examine certain challenging problems and to develop powerful methodologies for solving those challenging problems, both in data mining research and in various applications. For the former, contrast patterns have been used for classification, clustering, and discriminative pattern analysis. For the latter, contrast data mining has been used in a wide spectrum of applications, such as differentiating cancerous tissues from benign ones, distinguishing structures of toxic molecules from that of non-toxic ones, and characterizing the differences on the issues discussed in the blogs on U.S. presidential elections in 2008 and those discussed in 2012. Contrast data mining can be performed on many kinds of data, including relational, vector, transactional, numerical, textual, music, image, and multimedia data, as well as complex structured data, such as sequences, graphs, and networks.

There have been numerous research papers published in recent years, on contrast mining algorithms, on applying contrast patterns in classification, clustering, and discriminative pattern analysis, and on applying contrast patterns and contrast-pattern based classification and clustering to a wide range of problems in medicine, bioinformatics, chemoinformatics, crime analysis, blog analysis, and so on. This book, edited by two leading researchers on contrast mining, Professors Guozhu Dong and James Bailey, and contributed to by over 40 data mining researchers and application scientists, is a comprehensive and authoritative treatment of this research theme. It presents a systematic introduction and a thorough overview of the state-of-the-art for contrast data mining, including concepts, methodologies, algorithms, and applications.

I have high confidence that the book will appeal to a wide range of readers, including data mining researchers and developers who want to be informed about recent progress in this exciting and fruitful area of research, scientific researchers who seek to find new tools to solve challenging problems in their

own research domains, and graduate students who want to be inspired on problem solving techniques and who want to get help with identifying and solving novel data mining research problems in various domains.

I find the book enjoyable to read. I hope you will like it, too.

Jiawei Han University of Illinois, Urbana-Champaign March 19, 2012

#### Preface

Contrasting is one of the most basic types of analysis. Contrasting based analysis is routinely employed, often subconsciously, by all types of people. People use contrasting to better understand the world around them and the challenging problems they want to solve. People use contrasting to accurately assess the desirability of important situations, and to help them better avoid potentially harmful situations and embrace potentially beneficial ones.

Contrasting involves the comparison of one dataset against another. The datasets may represent data of different time periods, spatial locations, or classes, or they may represent data satisfying different conditions. Contrasting is often employed to compare cases with a desirable outcome against cases with an undesirable one, for example comparing the benign and diseased tissue classes of a cancer, or comparing students who graduate with university degrees against those who do not. Contrasting can identify patterns that capture changes and trends over time or space, or identify discriminative patterns that capture differences among contrasting classes or conditions.

Traditional methods for contrasting multiple datasets were often very simple so that they could be performed by hand. For example, one could compare the respective feature means, compare the respective attribute-value distributions, or compare the respective probabilities of simple patterns, in the datasets being contrasted. However, the simplicity of such approaches has limitations, as it is difficult to use them to identify specific patterns that offer novel and actionable insights, and identify desirable sets of discriminative patterns for building accurate and explainable classifiers.

Contrast data mining, a special and focused area of data mining, develops concepts and algorithmic tools to help us overcome the limitations of those simple approaches. Recently, especially in the last dozen or so years, a large number of research papers on the concepts and algorithms of contrast data mining, and a large number of papers on successful applications of contrast mining in a wide range of scientific and business domains, have been reported. However, those results were only available in widely scattered places. This book presents the results in one place, in a comprehensive and coordinated fashion, making them more accessible to a wider spectrum of readers.

The importance and usefulness, and the diversified nature of contrast mining, have been indicated not only by the large number of papers, but also by the many names that have been used for *contrast patterns*. For example, the following names have been used: change pattern, characterization rule,

class association rule, classification rule, concept drift, contrast set, difference pattern, discriminative association, discriminative interaction pattern, discriminative pattern, dissimilarity pattern, emerging pattern, gradient pattern, group difference, unusual subgroups, and generalized contrast patterns such as fuzzy/disjunctive emerging patterns and contrast inequalities/regressions.

This book is focused on the mining and utilization of contrast patterns. It is divided into seven parts.

Part I, Preliminaries and Measures on Contrasts, contains two chapters, on preliminaries and on statistical measures for contrast patterns, respectively.

Part II, Contrast Mining Algorithms, contains five chapters: Chapters 3 and 4 are on mining emerging patterns using tree-based structures or tree-based searches, and using Zero-Suppressed Binary Decision Diagrams, respectively. Chapter 5 is on efficient direct mining of selective discriminative patterns for classification. Chapter 6 is on mining emerging patterns from structured data, such as sequences and graphs. Chapter 7 is on incremental maintenance of emerging patterns.

Part III, Generalized Contrasts, Emerging Data Cubes, and Rough Sets, contains three chapters: Chapter 8 is on more expressive contrast patterns (such as disjunctive/fuzzy emerging patterns, and contrast inequalities). Chapter 9 is on emerging data cube representations for OLAP data mining. Chapter 10 relates jumping emerging patterns with rough set theory.

Part IV, Contrast Mining for Classification and Clustering, contains four chapters: Chapter 11 gives an overview and analysis of contrast pattern based classification. Chapter 12 is on using emerging patterns in outlier and rare-class prediction. Chapter 13 is on enhancing traditional classifiers using emerging patterns. Chapter 14 presents CPC — Contrast Pattern Based Clustering Algorithm — together with a brief discussion on the CPCQ clustering quality index, which is based on the quality, abundance, and diversity of contrast patterns.

Part V, Contrast Mining for Bioinformatics and Chemoinformatics, contains five chapters: Chapter 15 is on emerging pattern based rules characterizing subtypes of leukemia. Chapter 16 is on discriminating gene transfer and microarray concordance analysis. Chapter 17 is on mining optimal emerging patterns when there are thousands of genes or features. Chapter 18 is on the theory and applications of emerging chemical patterns. Chapter 19 is on emerging molecule patterns as structural alerts for computational toxicology.

Part VI, Contrast Mining for Special Application Domains, contains five chapters: Chapter 20 is on emerging patterns and classification for spatial and image data. Chapter 21 is on geospatial contrast mining with applications on vegetation, biodiversity, and election-voting analysis. Chapter 22 is on mining emerging patterns for activity recognition. Chapter 23 is on emerging pattern based prediction of heart diseases and powerline safety. Chapter 24 is on emerging pattern based crime spots analysis and rental price prediction.

Part VII, Survey of Other Papers, contains one chapter: Chapter 25 gives

an overview of results on contrast mining and applications, with a focus on papers not already cited in the other chapters of the book. The chapter incudes citations of papers that present algorithms on mining changes and model shift, on mining conditional contrasts, on mining niche patterns, on discovering holes and bumps, on discovering changes and emerging trends in tourism and in music, on understanding retail customer behavior, on using patterns to analyze and improve genetic algorithms, on using patterns to preserve privacy and protect network security, and on summarizing knowledge level differences between datasets.

The 25 chapters of this book were written by more than 40 authors who conduct research in a diverse range of disciplines, including architecture engineering, bioinformatics, biology, chemoinformatics, computer science, lifescience informatics, medicine, and systems engineering and engineering management. The cited papers of the book deal with topics in much wider range of disciplines. It is also interesting to note that the book's authors are from a dozen countries, namely Australia, Canada, China, Cuba, Denmark, France, Germany, Japan, Korea, Poland, Singapore, and the USA.

The 25 chapters demonstrate many useful and powerful capabilities of contrast mining. For example, contrast patterns can be used to characterize disease classes. They can capture discriminative gene group interactions, and can help define interaction based importance of genes, for cancers. They can be used to build accurate and explainable classifiers that perform well for balanced classification as well as for imbalanced classification, to perform outlier detection, to enhance traditional classifiers, to serve as feature sets of traditional classifiers, and to measure clustering quality and to construct clusters without distance functions. They can be used in compound selection for drug design and in molecule toxicity analysis, in crime spot analysis and in heart disease diagnosis, in rental price prediction and in powerline safety analysis, in activity recognition, and in image and spatial data analysis. In general, contrast mining is useful for diversified application domains involving many different data types.

A very interesting virtue of contrast mining is that contrast-pattern aggregation based classification can be effective when very few, as few as three, training examples per class are available. This virtue is especially useful for situations where training data may be hard to obtain, for instance for drug lead selection. Another interesting characteristic is that length statistics of minimal jumping emerging patterns can be used to detect outliers, allowing the use of one number as a measure to detect intruders. Using such a minimal model is advantageous, since it is hard for intruders to discover and emulate the model of the normal user in order to evade detection. A third interesting trait of contrast mining is the ability to use the collective quality and diversity of contrast patterns to measure clustering quality and to form clusters, without relying on a distance function, which is often hard to define appropriately in clustering-like exploratory data analysis. As you read the chapters of the

book, you will notice many other powerful aspects of contrast patterns, which make them very useful in solving many challenging problems.

Perhaps the most important contribution of contrast mining will come when we no longer need to use the naive Bayes or similar simplifying approaches to handle the challenge of high dimensional data, when we have developed the methodology to systematically analyze, and accurately use, sets of multi-feature contrast patterns instead. We believe that contrast mining has made useful progress in this direction, and we hope that results reported in this book will help researchers make progress on this important problem. Success in this direction will have a large impact on the understanding and handling of intrinsically complex processes, such as complex diseases whose behaviors are influenced by the interaction of multiple genetic and environmental factors.

We envision that, in the not too distant future, the field of contrast data mining will become mature. Then, other disciplines such as biology, medicine, and physics will refer to contrast mining and use methods from the contrast mining toolbox, in the same way that they now use methods such as logistic regression and PCA. We also foresee that, as the world moves towards ubiquitous computing, people may some day have a *contrasting app* on their iPhone-like device, which, when pointed at two types of things, can answer the question "in what ways do these two types differ?"

This book demonstrates that contrast mining has been a fruitful field for research on data mining methodology and for research on utilizing contrast mining to solve real-life problems. There are still many interesting research questions that deserve our attention, both in developing contrast mining methodology within the realm of computer science and in utilizing contrast mining to solve challenging problems in domains outside of computer science. Let us join together in exploring the concepts, algorithms, techniques, and applications of contrast data mining, to quickly realize its full potential.

Guozhu Dong, Wright State University James Bailey, The University of Melbourne March 2012

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