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# Multilabel Classification

Problem Analysis, Metrics and  
Techniques

 Springer

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Problem Analysis, Metrics and Techniques

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*To my family*

Francisco Herrera

*To María Jesús, my beloved life partner*

Francisco Charte

*To my family*

Antonio J. Rivera

*To Jorge, my beloved life partner*

María J. del Jesus

# Preface

The huge growth of information stored everywhere, from mobile phones to datacenter servers, as well as the large user base of many Internet services, such as social networks and online services for publishing music, pictures, and videos, demands automated systems for categorizing and labeling all this information. A common characteristic of texts published in news sites and blogs, videos, images, and pieces of music is that all of them can be assigned to multiple categories at once. Hence, the need to have algorithms able to adequately classify the data assigning it the proper labels.

Multilabel classification is a data mining area that encompasses several tasks specific for this type of data, including custom metrics aimed to characterize multilabel datasets and also to evaluate results, specialized preprocessing methods able to solve the peculiarities of multilabeled data, and also specific classification algorithms qualified for learning from this type of data, among others. Most of these techniques are pretty new and many of them are still in development.

Multilabel classification is a topic which has generated a notable interest in late years. Beside its multiple applications to classify different types of online information, it is also useful in many other areas, such as genomic and biology. Consequently, the demand for multilabel techniques is constantly growing. This book will guide the reader to the discovery of all aspects of multilabel classification.

Based on the experience of the authors after several years focused on multilabel learning techniques, this book reviews the specificities of this kind of classification, including all the custom metrics and techniques designed to deal with it, and provides a comprehensive reference for anyone interested in the field.

After portraying the context that multilabel classification belongs to, in the introduction, a formal definition of this problem along with a broad view on how it has been faced and the fields it has been applied to are provided in the second chapter. The third one is devoted to introducing most of the publicly available multilabel use cases, as well as the metrics defined to characterize and evaluate them. Chapters 4–6 review multilabel classification methods grouping them into three groups, depending on the approach followed to tackle the task, data

transformation, method adaptation, or the use of ensembles. Two of the most relevant obstacles in working with multilabel data, high dimensionality and class imbalance, are discussed in Chaps. 7 and 8. Chapter 9 introduces several software tools and frameworks aimed to ease the work with multilabel data, including obtaining this kind of datasets, performing exploratory analysis and conducting experiments.

Although multilabel learning is still in an early development stage with respect to other data mining techniques, the amount of proposed algorithms, most of them classification methods, is impressive. In the foreseeable future, it predictably will further expand to additional application fields, and the volume of new techniques grows almost every day.

The intended audience of this book are developers and engineers aiming to apply multilabel techniques to solve different kinds of real-world problems, as well as researchers and students needing a comprehensive review on multilabel literature, methods, and tools. In addition to the text itself, the authors supply the readers with a software repository containing data, code, and links, along with two R packages as tools to work with multilabel data.

We wish to thank all our collaborators of the research groups “Soft Computing and Intelligent Information Systems” and “Intelligent Systems and Data Mining.” We are also thankful to our families for their helpful support.

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# Contents

<b>1</b>	<b>Introduction</b>	1
1.1	Overview	1
1.2	The Knowledge Discovery in Databases Process	2
1.3	Data Preprocessing	3
1.4	Data Mining	6
1.4.1	DM Methods Attending to Available Data	6
1.4.2	DM Methods Attending to Target Objective	7
1.4.3	DM Methods Attending to Knowledge Representation	8
1.5	Classification	11
1.5.1	Binary Classification	11
1.5.2	Multiclass Classification	12
1.5.3	Multilabel Classification	13
1.5.4	Multidimensional Classification	14
1.5.5	Multiple Instance Learning	14
	References	15
<b>2</b>	<b>Multilabel Classification</b>	17
2.1	Introduction	17
2.2	Problem Formal Definition	18
2.2.1	Definitions	18
2.2.2	Symbols	18
2.2.3	Terminology	19
2.3	Applications of Multilabel Classification	19
2.3.1	Text Categorization	20
2.3.2	Labeling of Multimedia Resources	20
2.3.3	Genetics/Biology	21
2.3.4	Other Application Fields	21
2.3.5	MLDs Repositories	22

2.4	Learning from Multilabel Data . . . . .	22
2.4.1	The Data Transformation Approach. . . . .	23
2.4.2	The Method Adaptation Approach. . . . .	24
2.4.3	Ensembles of Classifiers. . . . .	25
2.4.4	Label Correlation Information. . . . .	26
2.4.5	High Dimensionality . . . . .	26
2.4.6	Label Imbalance . . . . .	27
2.5	Multilabel Data Tools . . . . .	28
	References . . . . .	29
<b>3</b>	<b>Case Studies and Metrics . . . . .</b>	<b>33</b>
3.1	Overview . . . . .	33
3.2	Case Studies . . . . .	34
3.2.1	Text Categorization . . . . .	34
3.2.2	Labeling of Multimedia Resources . . . . .	38
3.2.3	Genetics/Biology. . . . .	40
3.2.4	Synthetic MLDs . . . . .	41
3.3	MLD Characteristics . . . . .	41
3.3.1	Basic Metrics . . . . .	42
3.3.2	Imbalance Metrics. . . . .	43
3.3.3	Other Metrics . . . . .	44
3.3.4	Summary of Characterization Metrics . . . . .	45
3.4	Multilabel Classification by Example . . . . .	50
3.4.1	The ML-kNN Algorithm . . . . .	50
3.4.2	Experimental Configuration and Results . . . . .	51
3.5	Assessing Classifiers Performance . . . . .	54
3.5.1	Example-Based Metrics . . . . .	55
3.5.2	Label-based Metrics . . . . .	59
	References . . . . .	61
<b>4</b>	<b>Transformation-Based Classifiers . . . . .</b>	<b>65</b>
4.1	Introduction . . . . .	65
4.2	Multilabel Data Transformation Approaches . . . . .	66
4.3	Binary Classification Based Methods . . . . .	67
4.3.1	OVO Versus OVA Approaches. . . . .	67
4.3.2	Ensembles of Binary Classifiers . . . . .	68
4.4	Multiclass Classification-Based Methods. . . . .	69
4.4.1	Labelsets and Pruned Labelsets . . . . .	70
4.4.2	Ensembles of Multiclass Classifiers . . . . .	71
4.5	Data Transformation Methods in Practice . . . . .	72
4.5.1	Experimental Configuration . . . . .	72
4.5.2	Classification Results. . . . .	73
4.6	Summarizing Comments. . . . .	77
	References . . . . .	78

- 5 Adaptation-Based Classifiers** . . . . . 81
  - 5.1 Overview . . . . . 81
  - 5.2 Tree-Based Methods . . . . . 82
    - 5.2.1 Multilabel C4.5, ML-C4.5 . . . . . 82
    - 5.2.2 Multilabel Alternate Decision Trees, ADTBoost.MH . . . . . 82
    - 5.2.3 Other Tree-Based Proposals . . . . . 83
  - 5.3 Neuronal Network-Based Methods. . . . . 83
    - 5.3.1 Multilabel Back-Propagation, BP-MLL . . . . . 83
    - 5.3.2 Multilabel Radial Basis Function Network, ML-RBF . . . . . 84
    - 5.3.3 Canonical Correlation Analysis and Extreme Learning Machine, CCA-ELM . . . . . 85
  - 5.4 Vector Support Machine-Based Methods . . . . . 85
    - 5.4.1 MODEL-x . . . . . 85
    - 5.4.2 Multilabel SVMs Based on Ranking, Rank-SVM and SCRANK-SVM. . . . . 86
  - 5.5 Instance-Based Methods. . . . . 86
    - 5.5.1 Multilabel kNN, ML-kNN . . . . . 86
    - 5.5.2 Instance-Based and Logistic Regression, IBLR-ML . . . . . 87
    - 5.5.3 Other Instance-Based Classifiers . . . . . 87
  - 5.6 Probabilistic Methods. . . . . 88
    - 5.6.1 Collectible Multilabel Classifiers, CML and CMLF . . . . . 88
    - 5.6.2 Probabilistic Generic Models, PMM1 and PMM2 . . . . . 88
    - 5.6.3 Probabilistic Classifier Chains, PCC . . . . . 89
    - 5.6.4 Bayesian and Tree Naïve Bayes Classifier Chains, BCC and TNBCC. . . . . 89
    - 5.6.5 Conditional Restricted Boltzmann Machines, CRBM . . . . . 89
  - 5.7 Other MLC Adaptation-Based Methods . . . . . 90
  - 5.8 Adapted Methods in Practice . . . . . 91
    - 5.8.1 Experimental Configuration . . . . . 92
    - 5.8.2 Classification Results. . . . . 92
  - 5.9 Summarizing Comments. . . . . 97
  - References . . . . . 98
  
- 6 Ensemble-Based Classifiers.** . . . . . 101
  - 6.1 Introduction . . . . . 101
  - 6.2 Ensembles of Binary Classifiers. . . . . 102
    - 6.2.1 Ensemble of Classifier Chains, ECC . . . . . 102
    - 6.2.2 Ranking by Pairwise Comparison, RPC . . . . . 102
    - 6.2.3 Calibrated Label Ranking, CLR . . . . . 103
  - 6.3 Ensembles of Multiclass Classifiers . . . . . 103
    - 6.3.1 Ensemble of Pruned Sets, EPS . . . . . 103
    - 6.3.2 Random k-Labelsets, RAKEL . . . . . 104
    - 6.3.3 Hierarchy of Multilabel Classifiers, HOMER . . . . . 104
  - 6.4 Other Ensembles . . . . . 104

6.5	Ensemble Methods in Practice. . . . .	105
6.5.1	Experimental Configuration . . . . .	106
6.5.2	Classification Results. . . . .	107
6.5.3	Training and Testing Times . . . . .	110
6.6	Summarizing Comments. . . . .	111
	References . . . . .	112
<b>7</b>	<b>Dimensionality Reduction. . . . .</b>	<b>115</b>
7.1	Overview . . . . .	115
7.1.1	High-Dimensional Input Space . . . . .	116
7.1.2	High-Dimensional Output Space . . . . .	117
7.2	Feature Space Reduction . . . . .	117
7.2.1	Feature Engineering Approaches . . . . .	118
7.2.2	Multilabel Supervised Feature Selection . . . . .	119
7.2.3	Experimentation . . . . .	121
7.3	Label Space Reduction. . . . .	124
7.3.1	Sparseness and Dependencies Among Labels . . . . .	124
7.3.2	Proposals for Reducing Label Space Dimensionality . . . . .	125
7.3.3	Experimentation . . . . .	126
7.4	Summarizing Comments. . . . .	129
	References . . . . .	129
<b>8</b>	<b>Imbalance in Multilabel Datasets . . . . .</b>	<b>133</b>
8.1	Introduction . . . . .	133
8.2	Imbalanced MLD Specificities. . . . .	134
8.2.1	How to Measure the Imbalance Level . . . . .	135
8.2.2	Concurrence Among Imbalanced Labels. . . . .	136
8.3	Facing Imbalanced Multilabel Classification . . . . .	138
8.3.1	Classifier Adaptation . . . . .	138
8.3.2	Resampling Techniques . . . . .	139
8.3.3	The Ensemble Approach . . . . .	145
8.4	Multilabel Imbalanced Learning in Practice. . . . .	146
8.4.1	Experimental Configuration . . . . .	147
8.4.2	Classification Results. . . . .	147
8.5	Summarizing Comments. . . . .	150
	References . . . . .	150
<b>9</b>	<b>Multilabel Software . . . . .</b>	<b>153</b>
9.1	Overview . . . . .	153
9.2	Working with Multilabel Data. . . . .	154
9.2.1	Multilabel Data File Formats . . . . .	154
9.2.2	Multilabel Data Repositories. . . . .	155
9.2.3	The mldr.datasets Package . . . . .	157
9.2.4	Generating Synthetic MLDs . . . . .	162

9.3	Exploratory Analysis of MLDs . . . . .	162
9.3.1	MEKA. . . . .	163
9.3.2	The mldr Package . . . . .	166
9.4	Conducting Multilabel Experiments . . . . .	179
9.4.1	MEKA. . . . .	179
9.4.2	MULAN . . . . .	182
9.4.3	The RunMLClassifier Utility. . . . .	188
9.5	Summarizing Comments. . . . .	189
	References . . . . .	190
	<b>Glossary . . . . .</b>	<b>193</b>

# Acronyms

ACO	Ant colony optimization
ADT	Alternative decision trees
ANN	Artificial neural network
API	Application programing interface
ARFF	Attribute-Relation File Format
AUC	Area under the ROC curve
BCC	Bayesian classifier chains
BID	Binary datasets
BoW	Bag of words
BR	Binary relevance
CC	Classifier chains
CCA	Canonical correlation analysis
CDE	ChiDep ensemble
CL	Compressed labeling
CLR	Calibrated label ranking
CML	Collectible multilabel
CMLPC	Calibrated pairwise multilabel perceptron
CRAN	Comprehensive R Archive Network
CRF	Conditional random fields
CS	Compressed sensing
CSV	Comma-separated values
CT	Classifier trellis
CV	Cross-validation
CVIR	Coefficient of variation for the average imbalance ratio ( <i>MeanIR</i> )
CVM	Core vector machine
DLVM	Dual-layer Voting Method
DM	Data mining
DT	Decision trees
ECC	Ensemble of classifier chains
ELM	Extreme learning machine
EML	Ensemble of multilabel learners

EPS	Ensemble of pruned sets
FN	False negatives
FP	False positives
IBL	Instance-based learning
IR	Imbalance ratio or information retrieval depending on the context
JDK	Java Development Kit
JRE	Java Runtime Environment
KDD	Knowledge discovery in databases
KDE	Kernel dependency estimation
kNN	k-nearest neighbors
LDA	Linear discriminant analysis
LP	Label powerset
LSI	Latent semantic indexing
MAP	Maximum a posteriori probabilities
MCD	Multiclass datasets
MIR	Mean imbalance ratio
MLC	Multilabel classification
MLD	Multilabel dataset
MLP	Multilayer perceptron
OVA	One-vs-all
OVO	One-vs-one
PCA	Principal component analysis
PCC	Probabilistic classifier chains
PCT	Predictive clustering tree
PMM	Probabilistic mixture models
PS	Pruned sets
PSO	Particle swarm optimization
QCLR	QWeighted calibrated label ranking
RAkEL	Random k-labelsets
RBFN	Radial basis function network
RBM	Restricted Boltzmann machine
RF-PCT	Random forest of predictive clustering trees
ROC	Receiver operating characteristic
ROS	Random over-sampling
RPC	Ranking by pairwise comparison
RUS	Random under sampling
SOM	Self-organizing map
SVD	Single-value decomposition
SVM	Support vector machine
SVN	Support vector network
TF/IDF	Term frequency/inverse document frequency
TN	True negatives
TP	True positives

# Chapter 1

## Introduction

**Abstract** This book is focused on multilabel classification and related topics. Multilabel classification is one specific type of classification, classification being one of the usual tasks in the data mining field. Data mining itself can be seen as a step into a broad process, the discovery of new knowledge from databases. The goal of this first chapter is to introduce all these concepts, aiming to set the working context for the topics covered in the following ones. A global outline to this respect is given in Sect. 1.1. Section 1.2 provides an overview of the whole Knowledge Discovery in Databases process. Section 1.3 introduces the essential preprocessing tasks. Then, the different learning styles in use nowadays are explained in Sect. 1.4, and lastly multilabel classification is introduced in comparison with other traditional types of classification in Sect. 1.5.

### 1.1 Overview

The technological progress in late years has propelled the availability of huge amounts of data. Storage and communication capabilities have grown exponentially, increasing the needs to automatically process all these data. Due to this fact, machine learning techniques have acquired considerable relevance. In particular, the automatic classification of all kind of digital information, including texts, photos, music and videos, is in growing demand. Multilabel classification is the field where methods to perform this task, labeling resources into several non-exclusive categories, are studied and proposed.

This book presents a review of multilabel classification procedures and related techniques, including the analysis of obstacles specifically tied to this class of methods. Experimentation results from the most relevant proposals are also provided. The goal of this first chapter is to set the context multilabel classification belongs to. It starts from the wide view of the whole Knowledge Discovery in Databases (KDD) process, then narrowing the focus until nonstandard classification methods, where multilabel classification is introduced.

## 1.2 The Knowledge Discovery in Databases Process

The daily activity of millions of users, working and interacting with businesses and institutions, is digitally recorded into databases known as Online Transaction Processing systems. This has led to the availability of huge amounts of data in all kinds of corporations, no matter whether they are small or big companies. Extracting useful knowledge from these data by manual means is extremely difficult, if not impossible. This is why Data Mining (DM) techniques are increasing their popularity as an automatic way of getting the knowledge hidden in the data. This knowledge can be very valuable to support decision-making systems, to describe the structure of the information, to predict future data, and so on.

DM is a very-well-known and solid discipline nowadays, usually seen as one of the steps in the process known as KDD. In [14], KDD is defined as a non-trivial process of identifying valid, novel, potentially useful, and ultimately understandable patterns in data. These patterns would be the result obtained at the end of the process and can be of disparate nature as will be explained below.

Extracting new and useful insights from a database is a process that can be divided into multiple stages. These have been schematically represented in the diagram in Fig. 1.1. The starting point should be understanding the domain the problem belongs to, specifying the goals to achieve. From here, the following steps would be:

1. **Data gathering and integration:** The data needed to accomplish the established objectives can reside in heterogeneous sources, such as relational databases, spreadsheets, comma-separated value files. Once all the data have been gathered,

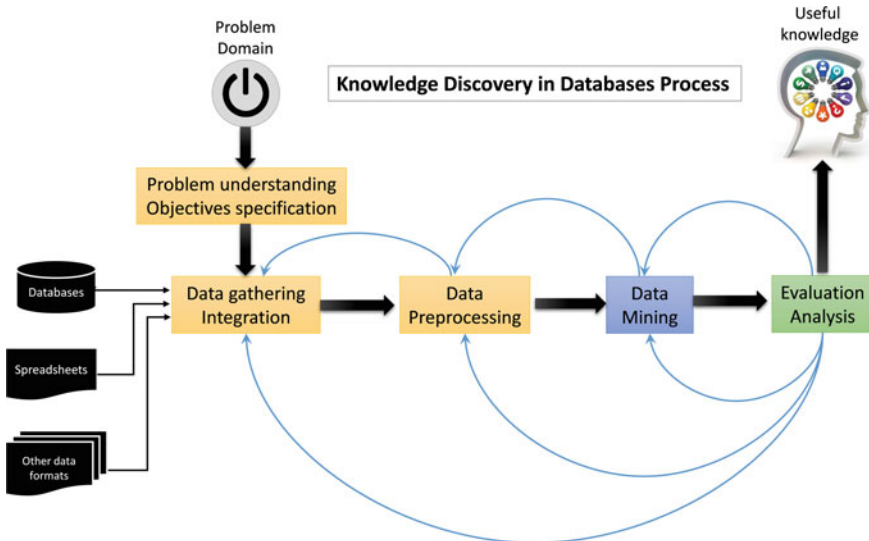


Fig. 1.1 The steps the KDD process is usually divided into

it has to be correctly integrated in a common representation, suitable for next steps in the pipeline.

2. **Data Preprocessing:** Some of the information gathered from data sources can be inconsistent and/or irrelevant. Differences in scales, noise presence, and other anomalies have to be adequately addressed through cleaning methods. By removing unimportant data, only the useful and truly relevant information is selected for further steps. In addition, depending on its nature, several preprocessing methods for data reduction can be applied to data. All of them aim to prepare the data in order to ease the learning conducted in the next phase.
3. **Data Mining:** This is the most known step in the KDD process, and some authors [19] view it as the main stage in the KDD process. Working with the data previously integrated, cleaned, selected and transformed, a DM algorithm has to be chosen to learn from this data. Depending on the objectives set at the beginning, the algorithm can be aimed to group the data samples according to some attributes, learn a model able to automatically classify new samples, etc. In Sect. 1.4 a general overview of DM tasks is provided.
4. **Evaluation and analysis:** The results obtained from the previous step have to be evaluated and analyzed. Interpreting them will assist the user to achieve the desired goals, also easing the overall problem understanding. This would be the useful and non-trivial knowledge extracted from the data.

As the diagram in Fig. 1.1 denotes, all the steps in the KDD process can jump backwards into the pipeline, depending on different conditions. As a consequence, each stage can be applied several times until a certain status is met, aiming to improve data quality in each iteration.

Although DM is considered the essential stage in KDD, most of the effort and time is usually spent in preprocessing tasks [17]. These are responsible of dealing with problems such as missing values, noise presence, outliers, feature and instance selection, and data compression. In the following, a deep analysis of preprocessing and DM tasks is provided.

### 1.3 Data Preprocessing

Once the data have been retrieved from the source it is stored into, frequently the first step is to prepare it through one or more preprocessing methods. We are generically referring here as *data preprocessing* to several integration, cleaning, transformation, and other data preparation and data reduction tasks. These methods will be run before applying any DM algorithm, easing the process of extracting some useful information.

According to the following statement from [17], data preprocessing duties can be divided into two groups entitled *data preparation* and *data reduction*. Identifying the proper preprocessing to administer to the data can improve the results obtained in

subsequent steps of the KDD process. In this section, the main preprocessing tasks are briefly introduced conforming to this grouping criteria.

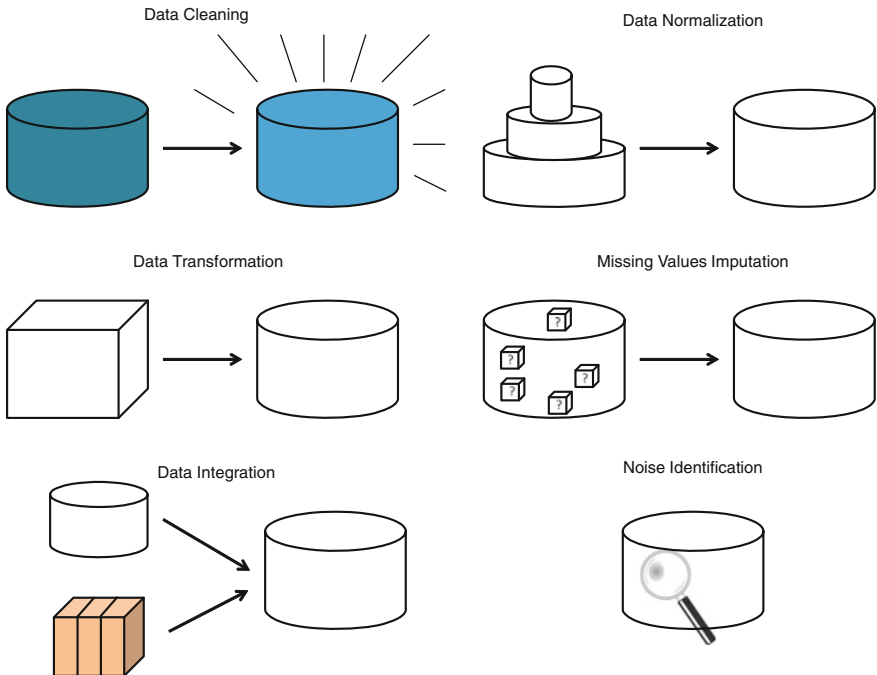
*Data preprocessing includes data preparation, compounded by integration, cleaning, normalization, and transformation of data; and data reduction tasks; such as feature selection, instance selection, and discretization. The result expected after a reliable chaining of data preprocessing tasks is a final dataset, which can be considered correct and useful for further data mining algorithms.*

*Data Preprocessing in Data Mining, Springer 2015*

Data preparation comprehend several assorted tasks, including data cleaning and normalization, dealing with missing values, addressing of noise, and extreme value detection. The main data preparation methods are depicted in Fig. 1.2 (reproduced here with authorization from [17]).

The most usual data normalizations are applied over numeric attributes. The goal is to ease the learning process of DM algorithms, normalizing the scales of values. Normalization is a simple transformation technique whose goal is to adjust the attribute values in order to share a common scale, making them proportional and comparable.

Missing values can be present in a dataset for disparate reasons. They can exist due to a failure in previous data transcription steps, or simply because someone has



**Fig. 1.2** Usual data preparation methods aimed to produce the data before applying any DM algorithm. These would be used just after the data gathering step

left empty a form item. The cleaning can consist in removing the instances with missing values or following some data imputation scheme, usually replacing the missing value by an estimation model.

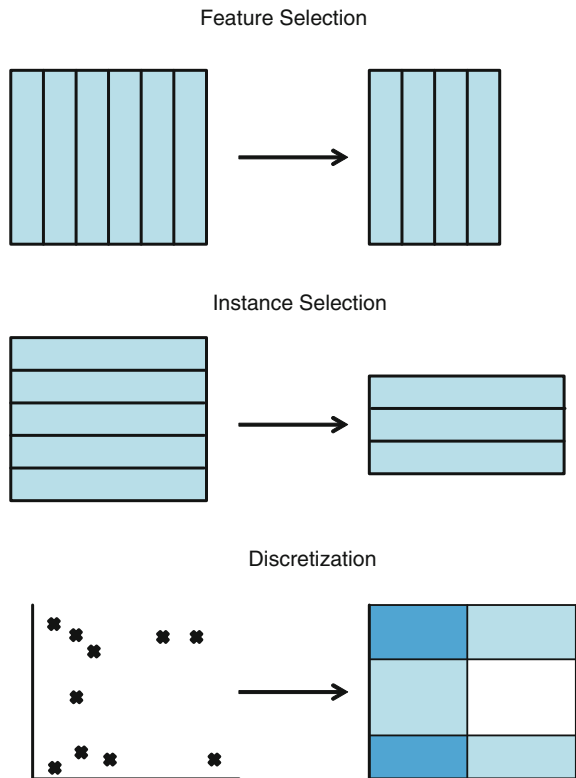
Noisy data are identified as class noise or attributes containing values which are clearly incorrect, frequently showing random variations that cannot be explained. The techniques to clean noise are similar to the ones aforementioned for missing values.

Building a model from a dataset with a large number of features or instances has a high computational cost. For this reason, data reduction techniques are among the most popular preprocessing methods. These methods can be grouped into the three categories depicted in Fig. 1.3 (reproduced here with authorization from [17]).

Feature selection algorithms aim to reduce the number of features, removing those that are redundant. Reducing the number of features usually helps in simplifying further data mining tasks.

Dimensionality reduction techniques are an alternative to explicit feature selection in some cases, creating a set of artificial features via linear or nonlinear feature combinations. Deep learning methods [24] such as Stacked Autoencoders and Restricted Boltzmann Machines can be also useful for this task.

**Fig. 1.3** Visual representation of the three categories that data reduction methods can be grouped into



The number of samples in the dataset can be reduced mainly through instance selection techniques [17]. They find the most representative instances in the dataset, selecting them as prototypes prior to applying DM algorithms.

Discretization is a process able to translate a continuous numeric value into a set of adjacent subranges, thus reducing the number of distinct values to consider. The result can be interpreted as a qualitative attribute, instead of a numeric one.

Although the discussed in this section can be considered the most common pre-processing tasks, there are a few more that can be applied when a DM algorithm cannot deal with the data in its current form. Some of them, specific to multilabel classification, will be fully described in Chap. 2.

## 1.4 Data Mining

The ultimate aim of the data preparatory phases in the KDD process is to apply some DM methods [14], whose duty would be learning from the data to produce useful knowledge. Currently, there is a large collection of proven DM algorithms available. These can be grouped attending to several criteria, depending on the data being labeled or not, the kind of result aimed for, and the model used to represent the knowledge, among others.

In this section, a brief overview of the most remarkable techniques, attending to the aforementioned three grouping standards, is provided.

### 1.4.1 *DM Methods Attending to Available Data*

The nature of the available data will affect the kind of DM methods which can be used, also determining the goals that can be set as targets of the learning process. Three main cases can be considered, as depicted in Fig. 1.4. These three categories are as follows:

- **Supervised learning:** The data instances have been previously labeled [9] by an expert in the problem domain. The DM methods can use this information to infer the knowledge needed to label new, never seen before, data instances. In this context, the *label* could be a continuous numerical value or a discrete value. The selected DM method has to work with the data in order to detect relationships between the input attributes, which determine the position of each instance in the solution space, and the target label. Supervised DM methods usually divide the dataset into two (training and test) or three (training, validation and test) disjoint subsets. The label of instances in the test set is not given to the algorithm, being used only to assess its performance.