

Contents

<i>Preface</i>	vii
<i>Acknowledgments</i>	ix
1. Introduction and Basic Concepts	1
1.1 Pattern Recognition	1
1.2 Learning Methodology	3
1.3 Statistical and Structural Pattern Recognition	6
1.4 Dissimilarity Representation for Pattern Recognition	9
1.5 Summary and Outline	12
2. Graph Matching	15
2.1 Graph and Subgraph	17
2.2 Exact Graph Matching	19
2.3 Error-tolerant Graph Matching	27
2.4 Summary and Broader Perspective	32
3. Graph Edit Distance	35
3.1 Basic Definition and Properties	37
3.1.1 Conditions on Edit Cost Functions	39
3.1.2 Examples of Edit Cost Functions	41
3.2 Exact Computation of GED	44
3.3 Efficient Approximation Algorithms	46
3.3.1 Bipartite Graph Matching	47
3.3.2 Graph Edit Distance Computation by Means of Munkres' Algorithm	52

3.4	Exact vs. Approximate Graph Edit Distance – An Experimental Evaluation	55
3.4.1	Nearest-Neighbor Classification	55
3.4.2	Graph Data Set	56
3.4.3	Experimental Setup and Validation of the Meta Parameters	57
3.4.4	Results and Discussion	58
3.5	Summary	63
4.	Graph Data	65
4.1	Graph Data Sets	66
4.1.1	Letter Graphs	66
4.1.2	Digit Graphs	68
4.1.3	GREC Graphs	71
4.1.4	Fingerprint Graphs	74
4.1.5	AIDS Graphs	77
4.1.6	Mutagenicity Graphs	78
4.1.7	Protein Graphs	79
4.1.8	Webpage Graphs	81
4.2	Evaluation of Graph Edit Distance	83
4.3	Data Visualization	92
4.4	Summary	95
5.	Kernel Methods	97
5.1	Overview and Primer on Kernel Theory	97
5.2	Kernel Functions	98
5.3	Feature Map vs. Kernel Trick	104
5.4	Kernel Machines	110
5.4.1	Support Vector Machine (SVM)	110
5.4.2	Principal Component Analysis (PCA)	117
5.4.3	k -Means Clustering	122
5.5	Graph Kernels	125
5.6	Experimental Evaluation	129
5.7	Summary	131
6.	Graph Embedding Using Dissimilarities	133
6.1	Related Work	135
6.1.1	Graph Embedding Techniques	135

6.1.2	Dissimilarities as a Representation Formalism . . .	137
6.2	Graph Embedding Using Dissimilarities	139
6.2.1	General Embedding Procedure and Properties . . .	139
6.2.2	Relation to Kernel Methods	142
6.2.3	Relation to Lipschitz Embeddings	144
6.2.4	The Problem of Prototype Selection	146
6.3	Prototype Selection Strategies	148
6.4	Prototype Reduction Schemes	157
6.5	Feature Selection Algorithms	163
6.6	Defining the Reference Sets for Lipschitz Embeddings . .	170
6.7	Ensemble Methods	171
6.8	Summary	173
7.	Classification Experiments with Vector Space Embedded Graphs	175
7.1	Nearest-Neighbor Classifiers Applied to Vector Space Embedded Graphs	176
7.2	Support Vector Machines Applied to Vector Space Embedded Graphs	181
7.2.1	Prototype Selection	181
7.2.2	Prototype Reduction Schemes	192
7.2.3	Feature Selection and Dimensionality Reduction .	195
7.2.4	Lipschitz Embeddings	205
7.2.5	Ensemble Methods	210
7.3	Summary and Discussion	214
8.	Clustering Experiments with Vector Space Embedded Graphs	221
8.1	Experimental Setup and Validation of the Meta parameters	222
8.2	Results and Discussion	226
8.3	Summary and Discussion	231
9.	Conclusions	235
Appendix A	Validation of Cost Parameters	247
Appendix B	Visualization of Graph Data	255
Appendix C	Classifier Combination	259

Appendix D	Validation of a k -NN classifier in the Embedding Space	263
Appendix E	Validation of a SVM classifier in the Embedding Space	273
Appendix F	Validation of Lipschitz Embeddings	277
Appendix G	Validation of Feature Selection Algorithms and PCA Reduction	289
Appendix H	Validation of Classifier Ensemble	293
Appendix I	Validation of Kernel k -Means Clustering	295
Appendix J	Confusion Matrices	305
	<i>Bibliography</i>	309
	<i>Index</i>	329