

Contents

1	Introduction	5
1.1	Organization of this Thesis	7
2	Exploratory Data Analysis	9
2.1	Knowledge Discovery	10
2.2	Visual Data Mining	11
2.2.1	Scientific Visualization	13
2.2.2	The Process of Scientific Visualization	14
2.2.3	Classification Schemes for Scientific Data	15
2.2.4	Scientific Visualization Techniques	17
2.2.4.1	Two-Dimensional Domain	18
2.2.4.2	Three-Dimensional Domain	21
2.2.5	Color in Visualization	24
2.2.5.1	Color Fundamentals	25
2.2.5.2	Device Independent Color Spaces	26
2.2.5.3	Device Dependent Color Spaces	27
2.2.5.4	Color Scale Properties	28
2.2.5.5	Univariate Color Scales	29
2.2.5.6	Perceptually Optimized Color Mapping Techniques	30
2.2.5.7	CIELUV Color Scales Based on sRGB Color Specifications	32
2.2.5.8	Bivariate and Trivariate Color Scales	33
2.3	Image Fusion	33
2.3.1	Dimensionality Reduction	36
2.3.2	Feature Selection	38
2.3.3	Feature Extraction	38
2.4	Conclusion	40
3	Linear Transformations	41
3.1	Principal Component Analysis	42
3.1.1	Intrinsic Data Dimensionality	45
3.1.2	Eigenvector Computation Using Neural Networks	46
3.1.3	Principal Component Analysis and Image Fusion	47
3.1.4	Case Study: DCE-MRI of the Breast	49
3.1.4.1	Motivation	49
3.1.4.2	Detection and Classification of Lesions	51
3.1.4.3	Computer Aided Diagnosis	53

3.1.4.4	Material and Methods	55
3.1.4.5	Preparation of the Data	56
3.1.4.6	Experimental Results	57
3.2	Procrustes Analysis	70
3.2.1	Comparison of Point Configurations	70
3.2.2	Comparison of Subspaces	71
3.2.3	Case Study Revisited: DCE-MRI of the Breast	73
3.2.3.1	Experimental Results	73
3.3	Independent Component Analysis	77
3.3.1	Statistical Independence	78
3.3.2	Non-Gaussianity	79
3.3.3	The FastICA Algorithm	81
3.3.4	Validation of Independent Components	82
3.3.5	ICA and Image Fusion	86
3.3.6	Case Study Revisited: DCE-MRI of the Breast	88
3.3.6.1	Experimental Results	89
3.4	Conclusion	97
4	Non-Linear Transformations	99
4.1	Self-Organizing Maps	100
4.1.1	The Incremental Algorithm	101
4.1.2	Topology Preservation	103
4.1.3	Intrinsic Data Dimensionality	106
4.1.4	SOM Based Data Visualization	108
4.1.4.1	Analysis of the Structure of a Data Distribution	108
4.1.4.2	Reference Vector Based Analysis	109
4.1.4.3	SOM Calibration	109
4.1.5	Image Fusion and Self-Organizing Maps	110
4.1.6	Case Study: Screening of Synthetic Stationary-Phase Promoters	111
4.1.6.1	Motivation	111
4.1.6.2	Material and Method	112
4.1.6.3	Experimental Results	115
4.2	Hyperbolic Self-Organizing Maps	118
4.2.1	Characteristics of Hyperbolic Spaces	119
4.2.2	The Poincaré Disc Model	121
4.2.3	A Hyperbolic Lattice and a Modified Adaptation Method	121
4.2.4	Visualizing Hyperbolic Self-Organizing Maps	122
4.2.5	The Hyperbolic Self-Organizing Maps in Image Fusion	123
4.2.6	Case Study Revisited: DCE-MRI of the Breast	124
4.2.6.1	Experimental Results	124
4.3	Topographic Mapping for Proximity Data	135
4.3.1	Probabilistic Autoencoders	136
4.3.2	EM Algorithm and Deterministic Annealing for Optimization	137

4.3.2.1	An Approximation of the Optimization Scheme	138
4.3.2.2	A Hyperbolic Topographic Mapping for Proximity Data .	138
4.3.3	Case Study Revisited: DCE-MRI of the Breast	140
4.3.3.1	Material and Methods	141
4.3.3.2	Experimental Results for the Exploration of Randomly Sampled Image Sections	143
4.3.3.3	Experimental Results for Image Fusion based on Proxim- ity Data	147
4.4	Conclusion	155
5	Summary and Outlook	157
6	Appendix	161
6.1	Performance Metrics	161
	Bibliography	167