Contents

Preface XIII

List of Contributors XV

1 Entropy, Orbits, and Spectra of Graphs 1

Abbe Mowshowitz and Valia Mitsou

- 1.1 Introduction 1
- 1.2 Entropy or the Information Content of Graphs 2

١v

- 1.3 Groups and Graph Spectra 4
- 1.4 Approximating Orbits 11
- 1.4.1 The Degree of the Vertices 13
- 1.4.2 The Point-Deleted Neighborhood Degree Vector 13
- 1.4.3 Betweenness Centrality 15
- 1.5 Alternative Bases for Structural Complexity 19 References 21

2 Statistical Mechanics of Complex Networks 23

Stefan Thurner

- 2.1 Introduction 23
- 2.1.1 Network Entropies 25
- 2.1.2 Network Hamiltonians 27
- 2.1.3 Network Ensembles 28
- 2.1.4 Some Definitions of Network Measures 30
- 2.2 Macroscopics: Entropies for Networks 31
- 2.2.1 A General Set of Network Models Maximizing Generalized Entropies 32
- 2.2.1.1 A Unified Network Model 32
- 2.2.1.2 Famous Limits of the Unified Model 35
- 2.2.1.3 Unified Model: Additional Features 35
- 2.3 Microscopics: Hamiltonians of Networks Network Thermodynamics 35

VI Contents

2.3.1 2.3.2 2.4	Topological Phase Transitions 36 A Note on Entropy 37 Ensembles of Random Networks – Superstatistics 39
2.5	Conclusion 42 References 43
3	A Simple Integrated Approach to Network Complexity and Node Centrality 47 Danail Bonchev
3.1	Introduction 47
3.2	The Small-World Connectivity Descriptors 49
3.3	The Integrated Centrality Measure 52 References 53
4	Spectral Theory of Networks: From Biomolecular to Ecological Systems 55 Ernesto Estrada
4.1	Introduction 55
4.2	Background on Graph Spectra 56
4.3	Spectral Measures of Node Centrality 58
4.3.1	Subgraph Centrality as a Partition Function 60
4.3.2	Application 61
4.4	Global Topological Organization of Complex Networks 62
4.4.1	Spectral Scaling Method 63
4.4.2	Universal Topological Classes of Networks 65
4.4.3	Applications 68
4.5	Communicability in Complex Networks 69
4.5.1	Communicability and Network Communities 71
4.5.2	Detection of Communities: The Communicability Graph 73
4.5.3	Application 74
4.6	Network Bipartivity 76
4.6.1	Detecting Bipartite Substructures in Complex Networks 77
4.6.2	Application 80
4.7	Conclusion 80
	References 81
5	On the Structure of Neutral Networks of RNA Pseudoknot Structures 85
	Christian M. Reidys
5.1	Motivation and Background 85
5.1.1	Notation and Terminology 87
5.2	Preliminaries 88
5.3	Connectivity 90

- 5.4 The Largest Component 93
- 5.5 Distances in *n*-Cubes 105
- 5.6 Conclusion 110 References 111
- 6 Graph Edit Distance Optimal and Suboptimal Algorithms with Applications 113

Horst Bunke and Kaspar Riesen

- 6.1 Introduction 113
- 6.2 Graph Edit Distance 115
- 6.3 Computation of GED 118
- 6.3.1 Optimal Algorithms 118
- 6.3.2 Suboptimal Algorithms 121
- 6.3.2.1 Bipartite Graph Matching 121
- 6.4 Applications 125
- 6.4.1 Graph Data Sets 125
- 6.4.2 GED-Based Nearest-Neighbor Classification 129
- 6.4.3 Dissimilarity-Based Embedding Graph Kernels 129
- 6.5 Experimental Evaluation 132
- 6.5.1 Optimal vs. Suboptimal Graph Edit Distance 133
- 6.5.2 Dissimilarity Embedding Graph Kernels Based on Suboptimal Graph Edit Distance 136
- 6.6 Summary and Conclusions 139 References 140

7 Graph Energy 145

Ivan Gutman, Xueliang Li, and Jianbin Zhang

- 7.1 Introduction 145
- 7.2 Bounds for the Energy of Graphs 147
- 7.2.1 Some Upper Bounds 147
- 7.2.2 Some Lower Bounds 154
- 7.3 Hyperenergetic, Hypoenergetic, and Equienergetic Graphs 156
- 7.3.1 Hyperenergetic Graphs 156
- 7.3.2 Hypoenergetic Graphs 157
- 7.3.3 Equienergetic Graphs 157
- 7.4 Graphs Extremal with Regard to Energy 162
- 7.5 Miscellaneous 168
- 7.6 Concluding Remarks 169 References 170

VIII Contents

8	Generalized Shortest Path Trees: A Novel Graph Class by Example
	of Semiotic Networks 175
	Alexander Mehler
8.1	Introduction 175
8.2	A Class of Tree-Like Graphs and Some of Its Derivatives 178
8.2.1	Preliminary Notions 178
8.2.2	Generalized Trees 180
8.2.3	Minimum Spanning Generalized Trees 186
8.2.4	Generalized Shortest Path Trees 190
8.2.5	Shortest Paths Generalized Trees 193
8.2.6	Generalized Shortest Paths Trees 195
8.2.7	Accounting for Orientation: Directed Generalized Trees 198
8.2.8	Generalized Trees, Quality Dimensions,
	and Conceptual Domains 204
8.2.9	Generalized Forests as Multidomain Conceptual Spaces 208
8.3	Semiotic Systems as Conceptual Graphs 212
	References 218
9	Applications of Graph Theory in Chemo- and Bioinformatics 221
	Dimitris Dimitropoulos, Adel Golovin, M. John, and Eugene Krissinel
9.1	Introduction 221
9.2	Molecular Graphs 222
9.3	Common Problems with Molecular Graphs 223
9.4	Comparisons and 3D Alignment of Protein Structures 225
9.5	Identification of Macromolecular Assemblies
	in Crystal Packing 229
9.6	Chemical Graph Formats 231
9.7	Chemical Software Packages 232
9.8	Chemical Databases and Resources 232
9.9	Subgraph Isomorphism Solution in SQL 232
9.10	Cycles in Graphs 235
9.11	Aromatic Properties 236
9.12	Planar Subgraphs 237
9.13	Conclusion 238
	References 239
10	Structural and Functional Dynamics in Cortical and Neuronal
	Networks 245
	Marcus Kaiser and Jennifer Simonotto
10.1	Introduction 245
10.1.1	Properties of Cortical and Neuronal Networks 246
10.1.1.1	Modularity 247
10.1.1.2	Small-World Features 247

- 10.1.1.3 Scale-Free Features 248
- 10.1.1.4 Spatial Layout 250
- 10.1.2 Prediction of Neural Connectivity 252
- 10.1.3 Activity Spreading 254
- 10.2 Structural Dynamics 255
- 10.2.1 Robustness Toward Structural Damage 255
- 10.2.1.1 Removal of Edges 256
- 10.2.1.2 Removal of Nodes 257
- 10.2.2 Network Changes During Development 258
- 10.2.2.1 Spatial Growth Can Generate Small-World Networks 258
- 10.2.2.2 Time Windows Generate Multiple Clusters 259
- 10.3 Functional Dynamics 260
- 10.3.1 Spreading in Excitable Media 260
- 10.3.1.1 Cardiac Defibrillation as a Case Study 261
- 10.3.1.2 Critical Timing for Changing the State of the Cardiac System 261
- 10.3.2 Topological Inhibition Limits Spreading 262
- 10.4 Summary 264 References 266
- 11 Network Mapping of Metabolic Pathways 271
 - Qiong Cheng and Alexander Zelikovsky
- 11.1 Introduction 271
- 11.2 Brief Overview of Network Mapping Methods 273
- 11.3 Modeling Metabolic Pathway Mappings 275
- 11.3.1 Problem Formulation 277
- 11.4 Computing Minimum Cost Homomorphisms 277
- 11.4.1 The Dynamic Programming Algorithm for Multi-Source Tree Patterns 278
- 11.4.2 Handling Cycles in Patterns 280
- 11.4.3 Allowing Pattern Vertex Deletion 281
- 11.5 Mapping Metabolic Pathways 282
- 11.6 Implications of Pathway Mappings 285
- 11.7 Conclusion 291 References 291
- 12 Graph Structure Analysis and Computational Tractability of Scheduling Problems 295
 - Sergey Sevastyanov and Alexander Kononov
- 12.1 Introduction 295
- 12.2 The Connected List Coloring Problem 296
- 12.3 Some Practical Problems Reducible to the CLC Problem 298
- 12.3.1 The Problem of Connected Service Areas 298
- 12.3.2 No-Idle Scheduling on Parallel Machines 300

X Contents

12.3.3	Scheduling of Unit Jobs on a p-Batch Machine 301
12.4	A Parameterized Class of Subproblems of the CLC Problem 302
12.5	Complexities of Eight Representatives of Class $CLC(X)$ 304
12.5.1	Three NP-Complete Subproblems 304
12.5.2	Five Polynomial-Time Solvable Subproblems 305
12.6	A Basis System of Problems 317
12.7	Conclusion 320
	References 322
13	Complexity of Phylogenetic Networks:
	Counting Cubes in Median Graphs and Related Problems 323
	Matjaž Kovše
13.1	Introduction 323
13.2	Preliminaries 324
13.2.1	Median Graphs 325
13.2.1.1	Expansion Procedure 328
13.2.1.2	The Canonical Metric Representation
	and Isometric Dimension 328
13.3	Treelike Equalities and Euler-Type Inequalities 330
13.3.1	Treelike Eequalities and Euler-Type Inequalities
	for Median Graphs 330
13.3.1.1	Cube-Free Median Graphs 332
13.3.1.2	<i>Q</i> ₄ -Free Median Graphs 333
13.3.1.3	Median Grid Graphs 333
13.3.2	Euler-Type Inequalities for Quasi-Median Graphs 334
13.3.3	Euler-Type Inequalities for Partial Cubes 335
13.3.4	Treelike Equality for Cage-Amalgamation Graphs 336
13.4	Cube Polynomials 337
13.4.1	Cube Polynomials of Cube-Free Median Graphs 339
13.4.2	Roots of Cube Polynomials 340
13.4.2.1	Rational Roots of Cube Polynomials 340
13.4.2.2	Real Roots of Cube Polynomials 341
13.4.2.3	Graphs of Acyclic Cubical Complexes 341
13.4.2.4	Product Median Graphs 342
13.4.3	Higher Derivatives of Cube Polynomials 342
13.5	Hamming Polynomials 343
13.5.1	A Different Type of Hamming Polynomial
	for Cage-Amalgamation Graphs 344
13.6	Maximal Cubes in Median Graphs of Circular Split Systems 345
13.7	Applications in Phylogenetics 346
13.8	Summary and Conclusion 347
	References 348

14	Elementary Elliptic (R, q)-Polycycles 351 Michel Deza, Mathieu Dutour Sikirić, and Mikhail Shtogrin
14.1	Introduction 351
14.2	Kernel Elementary Polycycles 355
14.3	Classification of Elementary ({2, 3, 4, 5}, 3)-Polycycles 356
14.4	Classification of Elementary $(\{2, 3\}, 4)$ -Polycycles 359
14.5	Classification of Elementary ({2,3}, 5)-Polycycles 359
14.6	Conclusion 361
	Appendix 1: 204 Sporadic Elementary ({2,3,4,5},3)-Polycycles 364 Appendix 2: 57 Sporadic eLementary ({2,3},5)-polycycles 371 References 375
15	Optimal Dynamic Flows in Networks and Algorithms for Finding Them 377
	Dmitrii Lozovanu and Maria Fonoberova
15.1	Introduction 377
15.2	Optimal Dynamic Single-Commodity Flow Problems and Algorithms for Solving Them 378
15.2.1	The Minimum Cost Dynamic Flow Problem 378
15.2.2	The Maximum Dynamic Flow Problem 380
15.2.3	Algorithms for Solving the Optimal Dynamic Flow Problems 380
15.2.4	The Dynamic Model with Flow Storage at Nodes 384
15.2.5	The Dynamic Model with Flow Storage at Nodes
	and Integral Constant Demand–Supply Functions 384
15.2.6	Approaches to Solving Dynamic Flow Problems
	with Different Types of Cost Functions 386
15.2.7	Determining the Optimal Dynamic Flows in Networks
	with Transit Functions That Depend on Flow and Time 390
15.3	Optimal Dynamic Multicommodity Flow Problems
	and Algorithms for Solving Them 392
15.3.1	The Minimum Cost Dynamic Multicommodity
	Flow Problem 392
15.3.2	Algorithm for Solving the Minimum Cost Dynamic
	Multicommodity Flow Problem 394
15.4	Conclusion 398
	References 398
16	Analyzing and Modeling European R&D Collaborations: Challenges and Opportunities from a Large Social Network 401 Michael J. Barber, Manfred Paier, and Thomas Scherngell
16.1	Introduction 401
16.2	Data Preparation 402

16.3 Network Definition 404

- XII Contents
 - 16.4 Network Structure 405
 - 16.5 Community Structure 407
 - 16.5.1 Modularity 408
 - 16.5.2 Finding Communities in Bipartite Networks 409
 - 16.6 Communities in the Framework Program Networks 409
 - 16.6.1 Topical Profiles of Communities 411
 - 16.7 Binary Choice Model 413
 - 16.7.1 The Empirical Model 413
 - 16.7.2 Variable Construction 415
 - 16.7.2.1 The Dependent Variable 415
 - 16.7.2.2 Variables Accounting for Geographical Effects 415
 - 16.7.2.3 Variables Accounting for FP Experience of Organizations 415
 - 16.7.2.4 Variables Accounting for Relational Effects 416
 - 16.7.3 Estimation Results 417
 - 16.8 Summary 420 References 421

17 Analytic Combinatorics on Random Graphs 425

Michael Drmota and Bernhard Gittenberger

- 17.1 Introduction 425
- 17.2 Trees 426
- 17.2.1 The Degree Distribution 429
- 17.2.2 The Height 430
- 17.2.3 The Profile 431
- 17.2.4 The Width 434
- 17.3 Random Mappings 436
- 17.4 The Random Graph Model of Erdős and Rényi 438
- 17.4.1 Counting Connected Graphs with Wright's Method 438
- 17.4.2 Emergence of the Giant Component 440
- 17.5 Planar Graphs 445 References 449

Index 451