Contents

| 1 | Deep | • Learning on Graphs: An Introduction | page 1 | |
|---|------|---|--------|--|
| | 1.1 | Introduction | 1 | |
| | 1.2 | Why Deep Learning on Graphs? | 1 | |
| | 1.3 | What Content is Covered? | 3 | |
| | 1.4 | .4 Who Should Read the Book? | | |
| | 1.5 | Feature Learning on Graphs: A Brief History | 8 | |
| | | 1.5.1 Feature Selection on Graphs | 9 | |
| | | 1.5.2 Representation Learning on Graphs | 10 | |
| | 1.6 | Conclusion | 12 | |
| | 1.7 | Further Reading | 13 | |
| | | | | |
| | PAR | T ONE FOUNDATIONS | 15 | |
| 2 | Four | ndations of Graphs | 17 | |
| | 2.1 | Introduction | 17 | |
| | 2.2 | Graph Representations | 18 | |
| | 2.3 | Properties and Measures | 19 | |
| | | 2.3.1 Degree | 19 | |
| | | 2.3.2 Connectivity | 21 | |
| | | 2.3.3 Centrality | 23 | |
| | 2.4 | Spectral Graph Theory | 26 | |
| | | 2.4.1 Laplacian Matrix | 26 | |
| | | 2.4.2 The Eigenvalues and Eigenvectors of the | | |
| | | Laplacian Matrix | 28 | |
| | 2.5 | Graph Signal Processing | 29 | |
| | | 2.5.1 Graph Fourier Transform | 30 | |
| | 2.6 | Complex Graphs | 33 | |
| | | | | |

iii

Contents

| | 2.6.1 | Heterogeneous Graphs | 33 |
|------|---------|---|----|
| | 2.6.2 | Bipartite Graphs | 33 |
| | 2.6.3 | Multi-dimensional Graphs | 34 |
| | 2.6.4 | Signed Graphs | 35 |
| | 2.6.5 | Hypergraphs | 36 |
| | 2.6.6 | Dynamic Graphs | 37 |
| 2.7 | Comp | utational Tasks on Graphs | 39 |
| | 2.7.1 | Node-focused Tasks | 39 |
| | 2.7.2 | Graph-focused Tasks | 41 |
| 2.8 | Conclu | usion | 42 |
| 2.9 | Furthe | r Reading | 42 |
| Four | dations | of Deep Learning | 43 |
| 3.1 | Introdu | uction | 43 |
| 3.2 | Feedfo | orward Networks | 44 |
| | 3.2.1 | The Architecture | 46 |
| | 3.2.2 | Activation Functions | 47 |
| | 3.2.3 | Output Layer and Loss Function | 50 |
| 3.3 | Convo | lutional Neural Networks | 51 |
| | 3.3.1 | The Convolution Operation and Convolutional | |
| | | Layer | 52 |
| | 3.3.2 | Convolutional Layers in Practice | 56 |
| | 3.3.3 | Non-linear Activation Layer | 57 |
| | 3.3.4 | Pooling Layer | 58 |
| | 3.3.5 | An Overall CNN Framework | 58 |
| 3.4 | Recuri | rent Neural Networks | 59 |
| | 3.4.1 | The Architecture of Traditional RNNs | 60 |
| | 3.4.2 | Long Short-Term Memory | 61 |
| | 3.4.3 | Gated Recurrent Unit | 63 |
| 3.5 | Autoer | ncoders | 63 |
| | 3.5.1 | Undercomplete Autoencoders | 65 |
| | 3.5.2 | Regularized Autoencoders | 66 |
| 3.6 | Trainii | ng Deep Neural Networks | 67 |
| | 3.6.1 | Training with Gradient Descent | 67 |
| | 3.6.2 | Backpropagation | 68 |
| | 3.6.3 | Preventing Overfitting | 70 |
| 3.7 | Conclu | usion | 71 |
| 3.8 | Furthe | r Reading | 72 |

iv

3

| | | | Contents | v |
|---|------|----------|---|-----|
| | PAR | т тwo | METHODS | 73 |
| 4 | Gra | oh Embe | edding | 75 |
| | 4.1 | Introdu | uction | 75 |
| | 4.2 | Graph | Embedding on Simple Graphs | 77 |
| | | 4.2.1 | Preserving Node Co-occurrence | 77 |
| | | 4.2.2 | Preserving Structural Role | 86 |
| | | 4.2.3 | Preserving Node Status | 89 |
| | | 4.2.4 | Preserving Community Structure | 91 |
| | 4.3 | Graph | Embedding on Complex Graphs | 93 |
| | | 4.3.1 | Heterogeneous Graph Embedding | 94 |
| | | 4.3.2 | Bipartite Graph Embedding | 96 |
| | | 4.3.3 | Multi-dimensional Graph Embedding | 97 |
| | | 4.3.4 | Signed Graph Embedding | 98 |
| | | 4.3.5 | Hypergraph Embedding | 101 |
| | | 4.3.6 | Dynamic Graph Embedding | 103 |
| | 4.4 | Conclu | ision | 104 |
| | 4.5 | Furthe | r Reading | 105 |
| 5 | Grap | oh Neura | al Networks | 106 |
| | 5.1 | Introdu | action | 106 |
| | 5.2 | The G | eneral GNN Frameworks | 108 |
| | | 5.2.1 | A General Framework for Node-focused Tasks | 108 |
| | | 5.2.2 | A General Framework for Graph-focused Tasks | 109 |
| | 5.3 | Graph | Filters | 111 |
| | | 5.3.1 | Spectral-based Graph Filters | 111 |
| | | 5.3.2 | Spatial-based Graph Filters | 121 |
| | 5.4 | Graph | Pooling | 127 |
| | | 5.4.1 | Flat Graph Pooling | 128 |
| | | 5.4.2 | Hierarchical Graph Pooling | 129 |
| | 5.5 | Parame | eter Learning for Graph Neural Networks | 133 |
| | | 5.5.1 | Parameter Learning for Node Classification | 133 |
| | | 5.5.2 | Parameter Learning for Graph Classification | 134 |
| | 5.6 | Conclu | ision | 135 |
| | 5.7 | Furthe | r Reading | 136 |
| 6 | Robi | ıst Grap | h Neural Networks | 137 |
| | 6.1 | Introdu | action | 137 |
| | 6.2 | Graph | Adversarial Attacks | 137 |
| | | 6.2.1 | Taxonomy of Graph Adversarial Attacks | 138 |
| | | 6.2.2 | White-box Attack | 140 |
| | | 6.2.3 | Gray-box Attack | 143 |

| Contents |
|----------|
|----------|

| | | 6.2.4 | Black-box Attack | 147 |
|---|-------|----------|---|-----|
| | 6.3 | Graph | Adversarial Defenses | 150 |
| | | 6.3.1 | Graph Adversarial Training | 151 |
| | | 6.3.2 | Graph Purification | 153 |
| | | 6.3.3 | Graph Attention | 154 |
| | | 6.3.4 | Graph Structure Learning | 158 |
| | 6.4 | Conclu | ision | 159 |
| | 6.5 | Further | r Reading | 159 |
| 7 | Scala | ble Gra | ph Neural Networks | 160 |
| | 7.1 | Introdu | action | 160 |
| | 7.2 | Node-v | wise Sampling Methods | 164 |
| | 7.3 | Layer- | wise Sampling Methods | 166 |
| | 7.4 | Subgra | ph-wise Sampling Methods | 170 |
| | 7.5 | Conclu | ision | 172 |
| | 7.6 | Further | r Reading | 172 |
| 8 | Grap | oh Neura | al Networks on Complex Graphs | 174 |
| | 8.1 | Introdu | iction | 174 |
| | 8.2 | Hetero | geneous Graph Neural Networks | 174 |
| | 8.3 | Biparti | te Graph Neural Networks | 176 |
| | 8.4 | Multi-o | dimensional Graph Neural Networks | 177 |
| | 8.5 | Signed | Graph Neural Networks | 179 |
| | 8.6 | Hyperg | graph Neural Networks | 182 |
| | 8.7 | Dynam | nic Graph Neural Networks | 183 |
| | 8.8 | Conclu | ision | 185 |
| | 8.9 | Further | r Reading | 185 |
| 9 | Beyo | nd GNN | s: More Deep Models on Graphs | 186 |
| | 9.1 | Introdu | action | 186 |
| | 9.2 | Autoer | coders on Graphs | 187 |
| | 9.3 | Recurr | ent Neural Networks on Graphs | 189 |
| | 9.4 | Variati | onal Autoencoders on Graphs | 191 |
| | | 9.4.1 | Variational Autoencoders for Node Represen- | |
| | | | tation Learning | 193 |
| | | 9.4.2 | Variational Autoencoders for Graph Generation | 193 |
| | 9.5 | Genera | ative Adversarial Networks on Graphs | 196 |
| | | 9.5.1 | Generative Adversarial Networks for Node | |
| | | | Representation Learning | 197 |
| | | 9.5.2 | Generative Adversarial Networks for Graph | |
| | | | Generation | 199 |
| | 9.6 | Conclu | ision | 200 |

vi

| | | Contents | vii |
|-----|-----------------|----------|-----|
| 9.7 | Further Reading | | 200 |

| | DAD | | 202 |
|---|------|--|-----|
| • | PAR | THREE APPLICATIONS | 203 |
| 0 | Grap | h Neural Networks in Natural Language Processing | 205 |
| | 10.1 | Introduction | 205 |
| | 10.2 | Semantic Role Labeling | 206 |
| | 10.3 | Neural Machine Translation | 208 |
| | 10.4 | Relation Extraction | 209 |
| | 10.5 | Question Answering | 210 |
| | | 10.5.1 The Multi-hop QA Task | 211 |
| | 10.6 | 10.5.2 Entity-GCN | 212 |
| | 10.6 | Graph to Sequence Learning | 214 |
| | 10.7 | Graph Neural Networks on Knowledge Graphs | 215 |
| | | 10.7.1 Graph Filters for Knowledge Graphs | 216 |
| | | 10.7.2 Transforming Knowledge Graphs to Simple | |
| | | Graphs | 217 |
| | | 10.7.3 Knowledge Graph Completion | 217 |
| | 10.8 | Conclusion | 218 |
| | 10.9 | Further Reading | 218 |
| | Grap | h Neural Networks in Computer Vision | 220 |
| | 11.1 | Introduction | 220 |
| | 11.2 | Visual Question Answering | 220 |
| | | 11.2.1 Images as Graphs | 221 |
| | | 11.2.2 Images and Questions as Graphs | 223 |
| | 11.3 | Skeleton-based Action Recognition | 225 |
| | 11.4 | Image Classification | 227 |
| | | 11.4.1 Zero-shot Image Classification | 228 |
| | | 11.4.2 Few-shot Image Classification | 229 |
| | | 11.4.3 Multi-label Image Classification | 230 |
| | 11.5 | Point Cloud Learning | 231 |
| | 11.6 | Conclusion | 232 |
| | 11.7 | Further Reading | 232 |
| | Grap | h Neural Networks in Data Mining | 233 |
| | 12.1 | Introduction | 233 |
| | 12.2 | Web Data Mining | 233 |
| | | 12.2.1 Social Network Analysis | 234 |
| | | 12.2.2 Recommender Systems | 237 |
| | 12.3 | Urban Data Mining | 241 |
| | | | |

Contents

| | | 12.3.1 Traffic Prediction | 241 |
|----|------|--|-----|
| | | 12.3.2 Air Quality Forecasting | 243 |
| | 12.4 | Cybersecurity Data Mining | 244 |
| | | 12.4.1 Malicious Account Detection | 244 |
| | | 12.4.2 Fake News Detection | 246 |
| | 12.5 | Conclusion | 247 |
| | 12.6 | Further Reading | 247 |
| 13 | Grap | h Neural Networks in Biochemistry and Healthcare | 249 |
| | 13.1 | Introduction | 249 |
| | 13.2 | Drug Development and Discovery | 249 |
| | | 13.2.1 Molecule Representation Learning | 250 |
| | | 13.2.2 Protein Interface Prediction | 251 |
| | | 13.2.3 Drug-Target Binding Affinity Prediction | 253 |
| | 13.3 | Drug Similarity Integration | 255 |
| | 13.4 | Polypharmacy Side Effect Prediction | 256 |
| | 13.5 | Disease Prediction | 259 |
| | 13.6 | Conclusion | 260 |
| | 13.7 | Further Reading | 261 |
| | | | |

| | PAR | ΓFOUR ADVANCES | 263 |
|----|------|---|-----|
| 14 | Adva | nced Topics in Graph Neural Networks | 265 |
| | 14.1 | Introduction | 265 |
| | 14.2 | Deeper Graph Neural Networks | 266 |
| | | 14.2.1 Jumping Knowledge | 268 |
| | | 14.2.2 DropEdge | 268 |
| | | 14.2.3 Pairnorm | 268 |
| | 14.3 | Exploring Unlabeled Data via Self-supervised Learning | 268 |
| | | 14.3.1 Node-focused Tasks | 269 |
| | | 14.3.2 Graph-focused Tasks | 272 |
| | 14.4 | Expressiveness of Graph Neural Networks | 273 |
| | | 14.4.1 Weisfeiler-Lehman Test | 274 |
| | | 14.4.2 Expressiveness | 275 |
| | 14.5 | Conclusion | 277 |
| | 14.6 | Further Reading | 277 |
| 15 | Adva | nced Applications in Graph Neural Networks | 278 |
| | 15.1 | Introduction | 278 |
| | 15.2 | Combinatorial Optimization on Graphs | 278 |
| | 15.3 | Learning Program Representations | 280 |

viii

| | Contents | ix |
|--------------|--|-----|
| 15.4 | Reasoning Interacting Dynamical Systems in Physics | 282 |
| 15.5 | Conclusion | 283 |
| 15.6 | Further Reading | 283 |
| | | |
| Bibliography | | |
| Index | | |