Index

ABIDE database, 260
abstract meaning representation, 205
abstract syntax tree, 281
across-dimension neighbor, 177
across-dimension representation, 179
activation functions, 47
adjacency matrix, 183, 222, 260
adjacent matrix, 18
adversarial attack, 137
air pollution, 243
air quality, 243
air quality forecasting, 243
amino acid, 251
amino acid residues, 253
AMR, 205
anti-money laundering, 248
artificial neural networks, 43
ASD, 260
AST, 281
attention mechanism, 209, 236
attribute mask, 271
attribute masking, 273
autism spectrum disorder, 260
autoencoder, 63–67, 187, 192
decoder, 65
coder, 63
regularized autoencoder, 66
undercomplete autoencoder, 65
auxiliary task, 269
backpropagation, 68–70
balance theory, 180
balanced representation, 181
batch normalization, 71
BERT, 269
betweenness centrality, 25
Bi-directional LSTM, 206
Bi-LSTM, 206, 208
binary classification, 234, 253
binary graph classification, 246
bio-chemistry, 249
bipartite graph, 33
bipartite graph embedding, 96–97
bipartite graph neural network, 176
bouncing balls, 282
cell memory, 190
centrality, 23–26
betweenness centrality, 25
degree centrality, 23
eigenvector centrality, 24
Katz centrality, 25
centrality ranking, 270
CFG, 281
charged particles, 282
chemical bonds, 254
CNN, 44, 51–59
collaborative filtering, 237
combinatorial optimization, 278
complex graph, 33–38, 93, 174–185
bipartite, 33, 96–97, 176
dynamic, 37, 103–104, 183
discrete, 38
heterogeneous, 33, 94–96, 174
hyper, 36, 101–103, 182
multi-dimensional, 34, 97–98, 177
signed, 35, 98–101, 179
computational phenotyping, 261
computer vision, 220–232
connected component, 22, 28
connected graph, 22
connectivity, 21
Context Prediction, 272
ContextLabel, 271

313
control flow graph, 281
control variate, 166
convolution operation, 52–57
convolutional layer, 52–57
convolutional neural network, 44, 51–59
  convolution operation, 52
  equivariant representation, 55
  filter, 53
  kernel, 53
  parameter sharing, 55
  sparse connection, 54
  convolutional layer, 52
  channel, 56
  stride, 56
  pooling layer, 58
  average, 58
  max, 58
CorrectedLabel, 272
cyber attacker, 244
cybersecurity, 244
cybersecurity data mining, 244
data flow graph, 281
data mining, 233–248
DDI, 255
decoder, 187, 192, 208
deep learning, 1, 43–71
deep neural networks, 43
deep Q-learning, 148
deepwalk, 77–84
degree, 19
degree centrality, 23
degree matrix, 26, 27
dependency relation, 208
DFG, 281
diameter, 23, 162
discrete dynamic graph, 38
discriminator, 198, 200
disease association prediction, 261
disease prediction, 259
DisMult factorization, 218
Distance2Clusters, 270
Distance2Labeled, 271
distributed circuit design, 283
dropedge, 268
dropout, 71
drug, 249
drug development, 249
drug discovery, 249
drug re-purposing, 250, 253
drug similarity integration, 255
drug-drug interaction, 255, 257
drug-drug interaction prediction, 255
drug-protein interaction, 257
drug-protein pair, 254
drug-target binding affinity prediction, 249, 253
drug-target interaction, 253
drug-target interaction prediction, 254
DTI, 253
dynamic graph, 37
dynamic graph embedding, 103–104
dynamic graph neural network, 183
dynamical system, 282
e-commerce, 244
e-finance, 244
ECC-filter, 194
decor, 18
decor mask, 270
decor network, 234
eigen-decomposition, 267
eigenvector centrality, 24
ELU, 48
encoder, 192, 208
ten graph, 212
  COMPLEMENT edge, 212
  COREF edge, 212
  DOC-BASED edge, 212
  MATCH edge, 212
entity-GCN, 211, 212
EvolveGCN, 183
explainable graph neural network, 277
expressive piano performance, 283
expressiveness, 273
fake news, 246
fake news detection, 246
fast gradient sign method, 142
feature engineering, 8
feature learning, 8
feature selection, 9
feedforward networks, 44–51
few-shot image classification, 229
FGSM, 142
finite Markov decision process, 148, 149
fraud detection, 248
frequency component, 112
functional MRI, 260
GAN, 196
GAT-Filter, 219
gated global pooling, 194, 200
gated recurrent unit, 63
update gate, 63
### Index

Gaussian distribution, 192
Gaussian kernel, 222, 260
GCN-Filter, 130, 160, 163, 182–184, 188, 216, 226, 253, 256, 266, 267
generative adversarial network, 196
generative model, 192
generator, 198, 199
GNN-Filter, 223
GNN, 106–135
GNN-Filter, 243
GPT-2, 269
Graclus, 171
gradient descent, 67, 160
graph, 1, 17, 186, 189
graph adversarial attack, 137–150
black-box attack, 140, 147–150
rewatt, 149
RL-S2V, 147
evasion attack, 139
gray-box attack, 139, 143–147
poisoning attack, 139
targeted attack, 139
untargeted attack, 139
white-box attack, 139–143
integrated gradient guided attack, 142
metattack), 145
nettack), 143
PGD topology attack, 140
graph adversarial defense, 150–159
graph adversarial training, 151–153
graph attention, 154–158
PA-GNN, 155
RGCN, 154
graph purification, 153–154
graph structural learning, 158
Pro-GNN, 158
graph classification, 41, 134
graph embedding, 75–104
community structure, 91–93
information extractor, 76
mapping function, 75
node co-occurrence, 77
node status, 89–91
structural role, 86–89
graph filter, 106, 111–127, 181, 183, 216
spatial-based graph filter, 121
ECC-Filter, 124
GAT-Filter, 123
GGNN-Filter, 125
GraphSAGE-Filter, 122
Mo-Filter, 126
MPNN-Filter, 126
spectral-based graph filter, 111–121
Cheby-Filter, 117–119
GCN-Filter, 119
graph filtering, 106, 268
graph filtering operation, 243
graph Fourier basis, 31
graph Fourier coefficient, 31, 112
Graph Fourier Transform, 30
graph Fourier transform, 112
graph generation, 193, 199
graph isomorphism, 275
graph neural network, 137, 188, 205, 225, 265, 279
graph filter, 106
graph filtering, 106
graph pooling, 107
robust, 137–159
scalable, 160–172
graph neural networks, 106–135
graph pooling, 107, 127–133
flat graph pooling, 128
average pooling, 128
gated global pooling, 128
max pooling, 128
hierarchical graph pooling, 129–133
downsampling based pooling, 129–130
supernode based pooling, 130–133
graph property prediction, 273
graph signal, 29–33, 112
graph signal processing, 29
graph spectral filtering, 111
graph to sequence learning, 205, 214
graph-focused task, 41, 109, 272
graph classification, 41
Graph-LSTM, 189
GraphSAGE-Filter, 165
GRU, 63, 184, 255
Hadamard product, 188
healthcare, 249
heterogeneous graph, 33
heterogeneous graph embedding, 94–96
heterogeneous graph neural network, 174
hidden state, 190
hierarchical softmax, 81
human action recognition, 225
human body skeleton, 225
hyperbolic geometry, 277
hyperbolic space, 277
hyperbolic tangent, 48
hyperedge, 37, 182
hypergraph, 36
hypergraph embedding, 101–103
hypergraph neural network, 182
image, 221
image captioning, 232
image classification, 227
importance sampling, 168
Inception, 269
indication matrix, 182
inference model, 192
injective operation, 276
interacting system, 282
interaction network, 282
inverse graph Fourier transform, 112
Jaccard similarity, 153
joint training, 270, 272
Katz centrality, 25
knowledge graph, 240
knowledge graph, 205, 215, 228, 230
knowledge graph completion, 217
Laplacian matrix, 26–29, 112
eigenvalue, 28
eigenvector, 28, 112
normalized, 27, 267
layer-wise sampling, 166–170
leaky ReLU, 48
ligand protein, 253
LINE, 85
linear classifier, 228
linear transformation, 223
link prediction, 40
logistic regression, 228
long short-term memory, 61–63
cell state, 61
forget gate, 62
hidden state, 61
input gate, 62
output gate, 62
LSTM, 61, 184, 189, 206, 244, 255
machine reading comprehension, 210
malicious account, 244
malicious account detection, 244, 245
matrix factorization, 240
max pooling, 195
MAXCUT, 279
maximal independent set, 279
maximum cut, 279
McCulloch-Pitts Neuron, 43
medical images, 259
medication recommendation, 261
Mento-Carlo sampling, 164
meta-gradient, 146
meta-optimization, 157
meta-path, 94, 175
meta-path schema, 95
meta-path based neighbors, 175
meta-path schema, 175
Metis, 171, 270
minimum vertex cover, 278
minmax game, 197
MIS, 279
model-level explanation, 277
molecular fingerprint, 250
molecular graph generation, 249
molecular property prediction, 249
molecular representation, 251
molecular representation learning, 249
molecule, 249
MPNN-Filter, 251
multi-dimensional graph, 34
multi-dimensional graph embedding, 97–98
multi-dimensional graph neural network, 177
multi-hop QA, 210
multi-label image classification, 230
multi-modal graph, 257
multi-relational link prediction, 257
multivariate Gaussian distribution, 154
MVC, 278
N-body, 282
natural code sequence, 281
natural language generation, 214
natural language processing, 205–219
NCS, 281
negative edge, 180
negative sampling, 83
neighbor, 20, 162
balanced, 180
temporal, 226
unbalanced, 180
neighborhood expansion, 162
neighborhood explosion, 162, 163, 165
neural machine translation, 205, 208
NLG, 214
NLP, 205–219
node, 18
node annotation, 279
node classification, 39, 133, 279
node property, 270
node representation, 11, 222
node representation learning, 187, 193, 197
node-focused task, 39, 108, 269
link prediction, 40
node classification, 39
node-wise sampling, 164–166
node2vec, 84
non-isomorphic graph, 275
online social media, 246
over smoothing, 266
pairnorm, 268
pairwise distance, 270
PairwiseAttSim, 271
parse tree, 205
path, 21
  balanced, 180
  unbalanced, 180
perceptron, 43
phenotypic measure, 260
point clouds, 231
polypharmacy, 256
polypharmacy side effect, 257
polypharmacy side effect prediction, 256
pooling layer, 58
positive edge, 180
pre-trained model, 269
probabilistic graph, 195
program representation, 280
projected gradient descent, 141
protein, 250, 251
protein interface, 253
protein interface prediction, 250, 251
protein-protein interaction, 257
pseudo label, 271
QA, 210
question answering, 205, 210
question dependent graph, 222
random walk, 77, 172
  biased, 89
  meta-path based, 95
receptor protein, 253
recommender system, 237–241
Rectifier, 47
recurrent neural network, 59–63, 184, 189
reinforcement learning, 147, 150, 280
  action, 148, 150
  reward, 148, 150
  state, 148, 150
  state transition dynamics, 150
relation extraction, 205, 209
ReLU, 48
representation learning, 10
rewiring operation, 149
RNN, 59, 184, 209, 255
sample-level explanation, 277
scalability, 160
scene graph generation, 232
SDN, 283
self-supervised learning, 268, 269
semantic embedding, 228
semantic relation, 281
semantic role labeling, 205–208
semi-supervised classification, 245
sequence model, 243
SGD, 158, 161
shortest path, 23, 234
side information, 237
sigmoid, 48
signed graph, 35
signed graph embedding, 98–101
signed graph neural network, 179
singular value decomposition, 154
skeleton-based action recognition, 225
skipgram, 11
social influence, 234
social influence prediction, 234
social network, 234, 240
social network analysis, 234
social relation, 240
social representation learning, 235
software defined networks, 283
software vulnerability detection, 281
spammer detection, 244
spamming message, 244
spatial domain, 29, 112
spatial relation, 241
spatial temporal graph, 226
spectral domain, 30
spectral graph theory, 26
SRL, 206–208
SSL, 269
stochastic gradient, 166
stochastic gradient descent, 158, 161
subgraph, 22, 171
subgraph-wise sampling, 170–172
surrogate model, 144
SVD, 154
syntactic dependency tree, 205, 207, 209, 223
syntactic relation, 281
temporal distance, 226
temporal relation, 243, 244
time series, 241
traffic flow, 241
Index

traffic forecasting, 241
traffic network, 242
traffic prediction, 241
trail, 21
TransR, 239
travelling salesman problem, 278
tree, 189
Tree-LSTM, 189
TSP, 278
two-stage training, 269, 272
unbalanced representation, 181
undirected graph, 18
unlabeled data, 268
urban data mining, 241
user-item interaction, 240
VAE, 191
variable misuse detection, 281
variational autoencoder, 191, 283
VGG, 269
visual question answering, 220
vqa, 220
walk, 21
web data mining, 233–237
weight regularization, 71
Weisfeiler-Lehman graph isomorphism test, 274
WIKIHOP, 210
within-dimension neighbor, 177
within-dimension representation, 179
WL test, 274
word embedding, 11
word2vec, 11
zero-shot image classification, 228