

Index

- F_1 score, 302, 311
 K -means clustering, 17, 242, 245, 351, 355
 K -nearest neighbor graph, 97
 K -nearest neighbors (KNN), 42, 90
 L^1 norm, 37, 99, 256, 340, 344
 L^2 norm, 36, 37, 54–56, 59, 67, 95, 99, 256, 266, 324, 340, 344, 356
 L^p norm for vectors, 340
 χ^2 test, 304
 δ -tolerance closed frequent pattern mining, 228, 235
 t -test, 94
accuracy, 300
AdaBoost, 81
adjacency matrix, 20, 96, 109, 238, 248, 260, 344
adjusted rand index (ARI), 314
agglomerative hierarchical clustering, 27, 29, 184
all subsequence kernel, 170, 209
all subtree kernel, 208, 211
alternating least squares, 347
alternating least squares (ALS) algorithm, 36, 55, 56, 249, 250
Apriori algorithm, 122
area under the precision-recall (AUPR), 311
area under the ROC curve (AUC), 46, 94, 308
artificial neural network, *see* layered neural network
back-propagation (BP), 67
bag of words (BOW), 119, 127, 152
Baum-Welch algorithm, 159, 166
Bayes estimation, 353
Bayes theorem, 25, 132, 353
Bayesian belief network (BBN), 32
Bayesian belief network classifier, 53
Bayesian learning, 127
Bernoulli distribution, 327
Bernoulli trial, 326
beta distribution, 328
bi-factorization, 35
bicluster, 32
biclustering, 32, 110
binary classification, 42, 117
binary tree, 27
Binomial distribution, 327
boosting, 83
bootstrap aggregating (bagging), 74
bootstrapping, 73, 296
breadth-first search (BFS), 191
candidate generation, 122, 146
canonical correlation analysis (CCA), 265, 351
canonical form, 209
case-based reasoning (CBR), 43, 90
Cholesky decomposition, 336
classification, 42, 115
closed frequent pattern mining, 235
closed frequent patternmining, 228
cluster assignment matrix, 18, 40, 101, 240, 242, 248
clustering, 4, 16, 40
collaborative matrix factorization, 288
computational linguistics, 8
conditional random field (CRF), 168
conjugate prior distribution, 133, 354
connected subgraph, 11

- constrained K -means clustering, 23, 98, 102, 244, 246, 285
context free grammar (CFG), 164
contingency table, 298
convex optimization, 346
correlation coefficient, 94, 330
covariance, 329, 363
covariance matrix, 96, 104, 269
cross-validation, 109, 296

data fusion, 13
data sparsity, 5, 8, 239
data transformation, 13
decision stump, 44, 92, 98
decision tree, 47, 63, 74, 75, 98, 116
deep learning, 70, 72
dendrogram, 27, 28, 110
depth-first search (DFS), 149, 150, 191, 221
dimensionality reduction, 92
directed acyclic graph, 33
Dirichlet distribution, 130, 131, 133, 328
discriminative model, 26, 62, 169
divisive hierarchical clustering, 27
downward closure property, 121, 146, 220, 276
drug-target interaction, 111
dynamic programming, 158, 162, 182, 184, 185, 197, 202, 277

E-commerce (electric commerce), 5, 8, 15, 121, 261, 263
eigenvalue decomposition, *see* eigenvalue problem
eigenvalue problem, 22, 23, 34, 40, 95, 97, 98, 108, 242, 260, 267, 286, 333
elastic net, 100, 256, 270
ensemble learning, 63, 64, 72
entropy, 45, 325, 331
enumeration tree, 225, 231
error rate, 301
exclusive OR (XOR), 62
Expectation and Maximization (EM) algorithm, 25, 128, 155
Expectation-Maximization (EM) algorithm, 159, 352

expected reciprocal rank (ERR), 321
feature learning, 91
feature selection, 91
feature vector, 7
feed-forward neural network, *see* layered neural network
finite mixture model (FMM), 24, 153
Fisher discriminant analysis, 351
Fisher's exact test, 304
FP-growth algorithm, 123, 147, 151
frequent itemset mining, 120, 144, 147
frequent pair mining, 275
frequent pattern mining, 120
frequent subgraph mining, 220, 226, 231
frequent subsequence mining, 145, 146, 178
frequent subtree mining, 210, 216
Frobenius norm, 341, 342
full rank, 34

G-protein coupled receptor (GPCR), 114
gene expression, 110, 115, 119, 279
gene regulatory network, 12, 237
gene set enrichment analysis (GSEA), 113
generalization, 42, 48
generalized Rayleigh quotient, 98
generalized CCA, 268
generalized eigenvalue problem, 97, 102, 244, 267, 268, 272, 334, 351
generalized linear model, 56
generalized Rayleigh quotient, 23
generalized sequential patterns (GSP) algorithm, 146, 147
generative model, 26, 32, 62, 127, 131, 169
Gibbs sampling, 132, 354
Gini index, 309
glycan, 10, 212
gradient descent, 58, 59, 67, 68, 169
graph, 6, 9, 10, 12, 96, 109, 219
graph cut, 242
graph kernel, 229, 231
graph Laplacian, 97, 98, 241, 248, 287, 288, 344, 346

- graph learning, 237, 239
graph partitioning, 238, 240, 260
graphical model, 33, 52, 127, 131, 156, 192
greedy algorithm, 29, 31
gSpan algorithm, 221

hard margin, 85
hidden Markov model (HMM), 154
hidden Markov model (HMM), 156, 184, 186, 188, 193
hidden tree Markov model, 213
hidden tree Markov model (HTMM), 193, 206
hidden variable, *see* latent variable
hierarchical clustering, 16, 27, 110
high-throughput data, 5, 115, 237, 279
Hilbert-Schmidt norm, *see* Frobenius norm
hyperplane, 84

information, 45
information gain, 45
inner product, 89, 325, 329
inner product space, 336
invertible matrix, *see* nonsingular matrix

Jaccard index (JI), 303

Karush-Kuhn-Tucker (KKT) conditions, 256, 349
kernel K -means clustering, 101, 103, 246, 360
kernel canonical correlation analysis (KCCA), 269
kernel function, 89, 100, 103, 109, 269, 337
kernel learning, 89, 100, 109, 135, 145, 169, 211, 229, 234, 239, 274
kernel principal component analysis (kernel PCA), 107
kernel ridge regression, 103, 360
kernel trick, 100
Kullback-Leibler (KL) divergence, 331

label propagation, 250, 258, 260, 281, 287, 290
Laplacian eigenmaps, 92, 96, 247, 282
latent Dirichlet allocation (LDA), 127
latent variable, 4, 24, 127, 131, 132, 135, 153, 154, 169
layered neural network, 64, 67, 69, 72, 358
least absolute shrinkage and selection operator (LASSO), 100, 256
least squares, 347
likelihood, 58, 128
linear regression, 54, 99
linkage, 29
logistic function, *see* sigmoid function
logistic regression, 58, 60, 62, 64, 66, 67, 69, 72, 99, 169, 357
low-rank approximation, *see* matrix factorization

majority voting, 42
margin, 84
market basket, 8, 119, 121, 145
Markov blanket, 93
Markov model, 153
Markov property, 152
match kernel, 136
matrix completion, 41
matrix factorization, 34, 35, 41, 55, 56, 247, 249, 286, 290, 356
Matthew's correlation coefficient (MCC), 301
maximal frequent pattern mining, 228, 235
maximum likelihood estimation, 25, 59, 60, 128, 155, 157, 159, 351
mean, 18, 60, 324
mean average precision (MAP), 319
mean reciprocal rank (MRR), 319
metabolic network, 179
method of Lagrange multipliers, 22, 37, 86, 88, 95, 102, 104, 242, 249, 266, 271, 348
minimum cut, 243
minimum description length (MDL), 46
minimum DFS code, 222, 226, 231
mixture Markov model, 153, 154, 179
mixture pair model, 153

- molecular graph, 6, 11, 219, 235, 272
most likely path, 162, 185, 196
mostlikely path, 204
multinomial distribution, 131
multinomial distribution, 130, 327
multiple kernel learning, 274, 290
multiple kernel learning (MKL), 264
multiple sequence alignment (MSA), 180, 183, 184, 186
multiplicative update, 38, 39
multivariate analysis, 58
multiview learning, 13, 262
mutual information, 330

naive Bayes classifier, 51, 60, 72, 169
natural language processing, 8, 12, 119, 126, 152, 156, 163
Needleman-Wunsch algorithm, 182
network sciences, 237
node degree, 11
nonparametric distribution, 138
nonsingular matrix, 36, 37, 54, 56, 97, 332
normal distribution, 26, 60
normalized cut, 244
normalized discounted cumulative gain (nDCG), 321
normalized graph Laplacian, 244, 252, 260
normalized mutual information (NMI), 315

observable variable, 3
ordered tree Markov model, 213
ordered tree Markov model (OTMM), 198, 207
outlier, 5, 21
overfitting, 42, 55, 72, 99, 129, 130

pair model, 153
pairwise sequence alignment (PSA), 180, 184
partitional clustering, 16, 31
pattern growth, 122, 146
perceptron, 57
positive semidefinite matrix, 141
positive definite matrix, 37

positive semidefinite matrix, 56, 109, 241, 245, 334, 335
posterior distribution, 25, 131
precision-recall (PR) curve, 309
PrefixSpan algorithm, 147, 151
principal component analysis (PCA), 92, 94, 107, 110, 246, 265, 270, 351
prior distribution, 25
prior knowledge, 21, 64, 109, 130, 153, 184, 186, 231, 274
probabilistic latent semantic analysis (pLSA), 127
probabilistic model, 23, 33
probability density function (PDF), 323, 327
probability mass function (PMF), 323, 326
profile hidden Markov model (profile HMM), 184, 185
pruning, 48
pyramid match kernel, 138

rand index (RI), 313
random forest, 75
ratio cut, 244
Rayleigh quotient, 96
Rayleigh quotient, 23, 41, 103, 108, 245, 253, 286, 350
Receiver Operator Characteristic (ROC) curve, 305
recommendation, 41
recursive partitioning, 47, 74
regression, 42
regular matrix, *see* nonsingular matrix
regularization, 42, 54
regularization coefficient, 5, 37
regularization term, *see* regularizer
regularizer, 4, 36, 55, 130
relative risk, 302
reverse search, 225, 226
ridge regression, 54, 56, 103, 105
root mean square deviation (RMSD), 312

sampling with replacement, 73, 75, 323

- sampling without replacement, 323
scalability, 109
semi-structured data, 12
semi-supervised classification, 280
semi-supervised clustering, 280, 285
semi-supervised learning, 238, 279
sequence, 6, 8, 12, 115, 145
sequence classification, 118
set, 6, 7, 12
sigmoid function, 57, 65, 69, 325
single nucleotide polymorphisms (SNPs),
 116
singular matrix, 332
singular value decomposition (SVD), 36,
 96, 334
social network, 11
social network services (SNS), 237, 261,
 279
soft margin, 87
sparse learning, 37, 92, 98, 109, 239
spectral clustering, 103, 245, 248, 286,
 287, 290, 351
spectral embedding, *see* Laplacian eigen-
 maps
spectrum kernel, 170
speech recognition, 8, 12, 156, 163
squared error (loss), *see* L^2 norm
standard deviation, 324
state transition diagram, 153, 155, 156,
 193
steepest descent, 347
step function, 57
string, 8
string kernel, 169, 190
subgraph, 11, 112, 220, 231
subsequence, 8, 112, 146
substring, 8
subtree, 10, 211, 213, 231
suffix tree, 172
supervised learning, 4, 26, 42
support vector machine, 359
support vector machine (SVM), 84, 100,
 103, 291
topic model, 127
traceback, 182, 185
tree, 6, 9, 12, 191
tree grammar, 166, 187
tri-factorization, 35
unsupervised learning, 4, 16, 26
user-item matrix, 41
variance, 60, 94, 324, 361
vector, 5, 7, 15
visualization, 32
Viterbi algorithm, 163
weak learner, 84
world wide web (WWW), 237
Z-test, 304

