# **Numerics**

1D convolutions 237 2D grid, random walk on 24 10 base estimators, bagging ensembles with 153

## A

active learning 138 Cramer-Rao lower bound 141-150 query strategies 139-141 query by committee 140-141 uncertainty sampling 139–140 variance reduction 141 Active Learning Literature Survey (Settles) 139 AdaBoost (adaptive boosting) 154 AdaGrad 243 Adam optimizer 245, 248 ADASYN (adaptive synthetic sampling) 137 adjusted Rand index (ARI) 166 AGI (artificial general intelligence) 12 algorithmic paradigms 61 algorithms, definition and purpose 3 amortized VI (variational inference) 68, 259-265 applications in MDNs 280 mixture density networks 259-265 overview of 259 approximating distribution 10, 47 ARI (adjusted Rand index) 166 arrays, searching and sorting operations on 59 artificial general intelligence (AGI) 12 arXiv papers 285 attention matrix heatmap 267 attention mechanisms, transformer architecture and 265-272

autoencoders 251–257 overview of 251–252 variational autoencoder anomaly detection in time series 253–257

## В

backpropagation 6, 9, 221, 230 backward LSTM model 233 backward pass 130 bagging (bootstrap aggregation) 151-154 batch mode classification 273 Bayes algorithms naive 93-98 variational 188-195 Bayesian inference overview of 8-9 types of 9-11 Bayesian nonparametric models 166, 213 Bayesian optimization 148-150 Bayesian regression hierarchical 111-114 linear 107–111, 117 Bellman equations 66 Bernoulli Naive Bayes algorithm 93, 96 Bernoulli RV (random variable) 16-17 bias correction 245 bidirectional LSTM architecture 233 binary classification 74 binary heap 60 binary logistic regression 139 binary random variable, mean of 50 binary search 64 binomial coefficients 65

binomial tree model 21–24 books 283–284 boosting 154–157 bootstrapping 138	deep learning algorithms 219–281 amortized variational inference 259–265 mixture density networks 259–265 overview of 259
C	attention mechanisms and transformer architecture 265–272
	autoencoders 251–257
California house pricing dataset 111	overview of 251–252
Caltech 101 dataset 230	variational autoencoder anomaly detection in time series 253–257
CART (classification and regression trees)	convolutional neural networks 225–242
algorithm 64, 104	LeNet architecture on MNIST dataset
CDF (inverse cumulative density function) method 10	226-229
Chow-Liu algorithm 201–202	ResNet image search 229-232
CIFAR-100 dataset 242	graph neural networks 273–279
cifar100 248	machine learning algorithms research 279–280
classification algorithms 73–105	modern algorithms 11–12
decision trees 98–104	multilayer perceptron 220–224
logistic regression 86–93	neural network optimizers 242–248
naive Bayes algorithm 93–98	recurrent neural nets 232–242
overview of 74	long short-term memory sequence classification 233–236
perceptron algorithm 74–80	multi-input model 237–242
support vector machine 80–86	deep learning architecture, evolution of 11
cluster centroids 134	deep learning models 9
clusters, DP (Dirichlet Process) K-means and 166	deep neural networks (DNNs) 9
CNNs (convolutional neural networks)	dense layers, for computing probability of
9, 242, 279	duplicate questions 237
LeNet architecture on MNIST dataset 226-229	density estimation 195–200
ResNet image search 229-232	kernel density estimator 195–198
coin flips, posterior distribution of 16–18	tangent portfolio optimization 198–200
competitive programming 283	dimensionality reduction 179–184
complete search 61-62	principal component analysis 179–181
computational biology, density estimation in 195	t-SNE manifold learning on images 182–184
compute_posterior function 118	Dirichlet distribution 184
computer vision (CV) 7, 279	divide and conquer 64–65
confusion matrix 75	DLVM (deep latent variable models) 68
conjugate priors 9	DNNs (deep neural networks) 9 DP (Dirichlet process) K-means 166–170
context vector 265	DP (dynamic programming) 65–67
Cramer-Rao lower bound 141–150	DP-means algorithm 170
CV (computer vision) 7, 279	dropout 222, 233
CVXOPT software package 82	duplicate questions, identifying 237
cyclic permutation property 184	dynamically resizable array 59
D	Е
data structures 58–61	FI / 11 3 140
linear 59	EI (expected improvement) 148
nonlinear 60–61	eigenvalue decomposition 180
overview of 12	eigenvectors 179  FLRO (Evidence Lower Round) 43 49 51
probabilistic 61	ELBO (Evidence Lower Bound) 43, 49, 51 EM (expectation-maximization) algorithm
decision boundary 80	171–179
decision trees 98–104, 153	empirical covariance matrix 179
deep latent variable models (DLVM) 68	Empirical variance 19

ENN (edited nearest neighbors) 138 ensemble methods 150–159 bagging 151–154 boosting 154–157 definition 150 stacking 157–159 entropy 57, 99, 140 estep function 174 Evidence Lower Bound (ELBO) 43, 49, 51 expected improvement (EI) 148	hierarchical Bayesian regression 111–114 hierarchical regression models 107 high-dimensional parameter spaces, sampling from 14 hinge loss function 79 HMMs (hidden Markov models) 128–134 homogeneous ensembles 150 hyperparameter tuning 147–150
F  first-order Markov chain 18 Fisher information matrix 141 fit function 83, 109 fixed-size array 59 forward algorithm 129 forward KL 45 forward LSTM model 233 forward_backward function 131 Forward-backward HMM algorithm 132 fully conditional distributions 28 fully factored approximation 47	image_denoising class 52 images image denoising in Ising models 49–56 ResNet image search 229–232 t-SNE manifold learning on 182–184 imbalanced learning 134–138 oversampling strategies 136–138 undersampling strategies 134–136 IMDb movie reviews, sentiment analysis of 233 importance sampling 15, 19, 39 importance weights 36 importance_sampler class 36 information projection 45 inverse covariance estimation 202–206 IS (importance sampling) 35–41
G	Ising models, image denoising in 49–56
GAs (genetic algorithms) 210–213 gauss_conditional function 29 Gaussian mixture models 16, 171–179 expectation-maximization algorithm 171–179 overview of 171 Gaussian processes (GPs) regression 117–121 GCNs (graph convolutional networks) 273 generative models 7, 279	Jensen's inequality 46 Joint distribution 87 joint posterior distribution 43 joint probability density 128
Gibbs sampling 10, 28–31 gibbs_gauss class 29 Gini index 99–100 GMM class 174 gmm_em function 174 GMMs (Gaussian mixture models) 165, 171 GNNs (graph neural networks) 9, 273–279 GPs (Gaussian processes) regression 117–121 gradient descent 87, 108 gradient smoothing 245 graph lasso algorithm 206 greedy algorithms 62–64 grid search strategy 147	K-means algorithm 174 k-means++ 184 Kaggle competition 237 KD tree 183 KDE (kernel density estimator) 195–198 Keras/TensorFlow creating CNN Architecture with 226 image search using pretrained ResNet50 with 230 implementation 251 practical implementations using 253 kernel trick 120 kernel_func function 118
handwritten digit classification, 996	kernels 82, 214 KL (Kullback-Leibler) divergence, variational
handwritten digit classification 226	inference and 44–47

knapsack problem 62

hash table 60

Markov chain for page rank 18–19

Metropolis-Hastings sampling 32–35

KNN (K nearest neighbors) bagging ensemble 153 KNN classifiers 153 KNN regression 115–117	overview of 9–11, 15–19 posterior distribution of coin flips 16–18 self-avoiding random walk 24–28 MDNs (mixture density networks) 259–265 mean of binary random variable 50
L	mean-field approximation 47–48
12 regularization 233 Lagrangian objective function 81	mean-field factorization 11 mean-variance analysis 198 meta-classifier 157
latent states 128 LDA (latent Dirichlet allocation) 187–195 overview of 187–188 variational Bayes 188–195	meta-regressor 157 MH (Metropolis-Hastings) sampling 10, 32–35 mh_gauss class 33 MI (mutual information) maximization 56–57
Least confident definition 140 LeCun, Yann 226 LeNet architecture 226–229	mixture density networks 12 ML (machine learning) algorithms 3–13 Bayesian inference
leveraging model structure 68 likelihood function 117 linear classifier 74	overview of 8–9 types of 9–11 deep learning 11–12
linear data structures 59 linear regression 107 linked lists 59	implementing 12–13 data structures 12 problem-solving paradigms 12–13
log likelihood 86–87, 178 log partition function 45	mathematical concepts 7–8 reasons to learn from scratch 7 research
loss functions 88, 156, 260 low-dimensional spaces, sampling from 10 LR (logistic regression) 86–93, 160 LSTM (long short-term memory) sequence	deep learning 279–280 sampling methods and variational inference 67–68
classification 233-236	supervised learning algorithms 160–161 unsupervised learning 214 research conferences 285
M	types of 4–7
M-projection (moment projection) 46 machine learning algorithms. See ML algorithms MAP (maximum a posteriori) estimates 171 maps 60 marginal likelihood 45 marginal probability 130 Markov chain for page rank 18–19 Markov models 124–134	using divide and conquer paradigm 64 ML (maximum likelihood) 171 MLP (multilayer perceptron) 220–224 MNIST dataset, LeNet architecture on 226–229 model selection Bayesian optimization 148–150 hyperparameter tuning 147–150 modern deep learning algorithms 11 momentum parameter 243
hidden Markov models 128–134 page rank algorithm 125–128	MRF (Markov random field) 49 MSE (mean squared error) 107
masked attention 269	mstep function 174
Max margin strategy 140 max-pooling operations 226, 237	multi-input model 237–242 multiclass classification 74
maximum likelihood (ML) 171	multidimensional distribution 28
MCMC (Markov chain Monte Carlo) 14–42	multihead attention 268
binomial tree model 21-24	multivariate Gaussian distribution 28, 41
comparison with variational inference 67 estimating pi 19–21	N
Gibbs sampling 28–31 importance sampling 35–41	naive Bayes algorithm 93-98

narrow ÁI 12

natural language processing (NLP) 7, 280, 285

nearest neighbor portfolio weights 198 nearest neighbors approximation methods 116 Nesterov Momentum 243, 248 neural model capacity, increasing 248 neural network optimizers 242–248 NLL (negative log likelihood) 87 NLP (natural language processing) 7, 280, 285 NMI (normalized mutual information) 166 nonlinear data structures 60–61 nonnegative matrix factorization 214 normalizing constant 9

## 0

objective function 6 Occam's razor principle 147 optimal latent state sequence 131 optimization algorithms 220 optimum approximating distribution 50 OSS (one-sided selection) method 135 output constraints 260 overfitting 222, 248 oversampling strategies 136–138

## P

page rank algorithm Markov chain for 18–19 supervised learning 125–128 parallel ensemble methods 150 parallel processing 237 parallelizing Monte Carlo algorithms 67 PCA (principal component analysis) 138, 179–181, 230 perceptron algorithm 74-80, 160 Perceptron binary classifier confusion matrix 79 perceptron classifier 74 perceptron update rule 80 perplexity hyperparameter 184 PGM (probabilistic graphical models) 9 pi, estimating 19–21 pool-based sampling 139 pooled graphical models 111 positional encodings 268 posterior distribution 8–9, 16–18, 117 power method algorithm 126–127 precision-recall plot 76 predict function 83, 109 principal component analysis (PCA) 138, 179–181, 230 probabilistic data structures 61 probabilistic graphical models (PGM) 9, 68 problem-solving paradigms 61–67 complete search 61–62

divide and conquer 64–65 dynamic programming 65–67 greedy 62–64 overview of 12–13

## Q

QBC (query by committee) 140–141 quadratic dual optimization program 81–82 query strategies 139–141 query by committee 140–141 uncertainty sampling 139–140 query\_by\_committee function 143 queues 59

#### R

random forests 153 random oversampling 136 random search strategy 147 random undersampling 134 random walk Metropolis algorithm 35 random walk square distance 27 random walk, self-avoiding 24–28 RBF (radial basis function) kernel 82, 118, 121 reconstruction error 179 regression algorithms 106–122 Bayesian linear regression 107–111 Gaussian processes regression 117–121 hierarchical Bayesian regression 111–114 K nearest neighbors regression 115-117 overview of 107 regression models 107 regularized loss function 80 research conferences 284–285 computer vision 285 machine learning 285 natural language processing 285 theoretical computer science 285 ResNet image search 229-232 RFC (random forest classifier) 148 ridge\_reg class 109 RL (reinforcement learning) 66 RMSProp 244-245 RNA-seq data 196 RNA-Seq density estimate 198 RNNs (recurrent neural networks) 9, 232–242 long short-term memory sequence classification 233–236 multi-input model 237-242 Robbins-Monro conditions 87 ROC (receiver operating characteristic) plot 76 run-time complexity 3

S	supervised learning algorithms 123–162
	active learning 138–147
SA (simulated annealing) 206–210	Cramer-Rao lower bound 141–150
sampling methods, variational inference and	query strategies 139–141
67–68	variance reduction 141
scalable machine learning 160	ensemble methods 150-159
self-attention 268	bagging 151–154
self-avoiding random walk 24–28	boosting 154–157
self-supervised learning 6	stacking 157–159
semi-supervised technique in self-training 146	imbalanced learning 134–138
sensor placement 63	oversampling strategies 136–138
Seq2Seq 232, 265	undersampling strategies 134–136
Seq2Vec 232	machine learning algorithms research 160–161
sequence classification 219	Markov models 124–134
sequence similarity 220	hidden Markov models 128–134
sequential data, encoding and decoding 232	page rank algorithm 125–128
sequential ensemble methods 150	model selection
Sequential Monte Carlo (SMC) 67	
Settles, Burr 139	Bayesian optimization 148–150
SGD (stochastic gradient descent) 87, 92, 242	hyperparameter tuning 147–150
sigmoid activation function 234, 237	SVM (support vector machine) 80–86, 148, 160
similarity between objects, measuring 82	SVM quadratic program 83
simulated annealing implementation 207	synthetic minority oversampling technique
SMC (Sequential Monte Carlo) 67	(SMOTE) 136–138
SMOTE (synthetic minority oversampling	
technique) 136–138	T
softmax function 220	
software implementation 58–69	t-SNE (t-distributed stochastic neighbor
data structures 58–61	embedding) manifold learning 182–184
linear 59	tangent portfolio optimization 198–200
nonlinear 60–61	Tomek links algorithm 134, 136
probabilistic 61	trace identity 174
machine learning algorithms research 67-68	tractable distribution 10
problem-solving paradigms 61–67	transformer architecture, attention
complete search 61–62	mechanisms and 265-272
divide and conquer 64–65	transition probability 124
dynamic programming 65–67	tree-based models 98
greedy 62–64	true posterior 47
sparse precision matrix 203	two-state Markov model 124
spectral GCN 273	
Spektral Keras/Tensorflow library 274	U
stacking 157–159	0
stacks 59	LICE (upper confidence bound) 148
state transition matrix 18	UCB (upper confidence bound) 148
stationary distribution 9, 125–126	uncertainty sampling 139–140
stochastic gradient descent (SGD) 87, 92, 242	underfitting 222
stochastic matrices 18	undersampling strategies 134–136
Stochastic Monte Carlo methods 67	unsupervised learning algorithms 165–215
stock clusters 203, 206	density estimation 195–200
stream-based sampling 139	kernel density estimator 195–198
streaming Monte Carlo 67	tangent portfolio optimization 198–200
structure learning 201–206	dimensionality reduction 179–184
Chow-Liu algorithm 201–202	principal component analysis 179–181
inverse covariance estimation 202-206	t-SNE manifold learning on images 182–184
simulated annealing 206–210	Dirichlet process K-means 166-170

unsupervised learning algorithms (continued)
Gaussian mixture models 171-179
expectation-maximization algorithm 171-17
overview of 171
genetic algorithms 210-213
latent Dirichlet allocation 187–188
overview of 187–188
variational Bayes 188-195
machine learning algorithms research 214
structure learning 201–206
Chow-Liu algorithm 201–202
inverse covariance estimation 202–206
simulated annealing 206-210
3

#### V

VAE (variational autoencoder) anomaly detection in time series 253–257 variance reduction 141 variational Bayes algorithm 188–195 variational free energy 45
Vec2Seq 232
VI (variational inference) 43–57
amortized 259–265
mixture density networks 259–265
overview of 259
image denoising in Ising models 49–56
KL divergence and 44–47
mean-field approximation 47–48
mutual information maximization 56–57
overview of 9–11
sampling methods and 67–68
Viterbi algorithm 131
viterbi function 131

## W

weak learners, converting to strong learners 154 weight decay 222 wireless communications scenario 56