

Index

Note: Page numbers referring to figures should be *italics* and those referring to tables should be **bold**

a

absolute error loss 8
 accelerators 452
 accuracy score 234
 ACF (autocorrelation function) 80, 81
 activation function 223, 224, 224, 227
 aeronautics 474
 affinity propagation 252, 259–262
 agglomerative algorithms 252
 AI (artificial intelligence) 1, 273, 375, 465
 alternative hypothesis 132
 analysis of variance (ANOVA) F statistic 137–140, 168
 ANN. *see* artificial neural networks
 ANOVA (analysis of variance) F statistic 137–140, 168
 api.py file 428, 443, 445, 458
 apiVersion 423
 artificial intelligence (AI) 1, 375, 465
 artificial neural networks (ANN) 175, 223–249
 backpropagation 227–230
 convolutional neural networks 230–232
 estimation of parameters 225–230
 multilayer perceptron 224–225
 multilayer perceptron neural networks 233–242
 recurrent neural networks 232–233, 233
 schematic representation of 223
 autocorrelation function (ACF) 80, 81

b

backpropagation
 binary classification 226–227
 multi-class classification 227–230
 backward difference encoding method 72–73
 backward elimination 151–153
 backward propagation of errors 226
 bag-of-words method 274, 278, 280, 296
 bash command 378

batch gradient descent 181
 batch inference 389, 415, 424–428
 Bayesian approach 76
 Bayesian encoders 58
 Bayesian machine learning models 175
 BCSS (between-cluster sum of squares) 253
 Bernoulli random variables 132
 BERT. *see* Bidirectional Encoder Representations from Transformers
 between-cluster sum of squares (BCSS) 253
 bias 4
 Bidirectional Encoder Representations from Transformers (BERT) 11, 251, 286–287
 bidirectional
 training 287
 for binary text classification using tensorflow 288–294
 functionality 287–288
 language models 287
 objective 287
 for question answering 296–297
 for text summarization 294–295
 bidirectional training approach 287
 binary classification 2, 225, 333–337
 with EstimatorQNN 338–343
 regression 351
 with SamplerQNN 343–348
 with variational quantum classifier 348–351
 binary cross-entropy 225
 as loss functions 8, 352
 binary encoding method, 64, 64–65
 binary logistic regression 202–204
 cost function 203–204
 gradient descent 204
 with Keras on TensorFlow 210–211
 binary systems 466–467
 biologically inspired systems 468–469

bottom-up clustering 252
 Box-Cox transformation 46, 47

C

Caffe2 12
 California Cooperative Oceanic Fisheries Investigations (CalCOFI) dataset 185
 Captum 12
 categorical cross-entropy loss 8
 categorical (discrete) data 17–18, 57–77
 encoding methods 57–58, 58. *see also* encoding methods
 nominal 57
 types of 57
 using hephAistos to encode 77
 workflow with continuous and 58
 CD (continuous delivery) 389, 396, 397
 CentOS 378, 397
 CERN 304
 ChatGPT 286
 Chebyshev norm 43
 chi-squared test 134–137, 168
 for feature selection 135
 percentiles of 136
 CI (continuous integration) 389, 396, 397
 class-dependent LDA 110
 classical computing 465
 classical information theory 300
 classical kernel method 307
 classical neural network 352
 classical physics 299, 470
 classical support vector machines 303
 classification accuracy 6, 327
 classification algorithms 23–31, 274
 on CPUs 14
 on GPUs 14, 24–25, 266
 support vector machine using 220–222
 class-independent LDA 110
 clustering 252–264
 Kubernetes 407–409, 416–418, 426, 435–437
 objective of 175
 techniques 252
 clustering algorithm 252–264
 affinity propagation 259–262
 DBSCAN 252, 262–264
 k-means 252–255
 mean shift clustering 252, 257–259
 mini-batch k-means 252, 255–256
 CNNs (convolutional neural networks) 12, 32, 223, 230–232, 246–249, 269, 274
 CNOT (Controlled-NOT) gate 302
 “cocktail party problem” 102

conditional maximum likelihood estimation 203
 configuration files, for Kubernetes 422–423, 427–428
 confusion matrix 5, 5–7
 containerization 376
 of machine learning application 443–446
 continuous delivery (CD) 389, 396, 397
 continuous integration (CI) 389, 396, 397
 continuous uniform distribution 48
 continuous variables 57, 134
 Controlled-NOT (CNOT) gate 302
 Control Plane 405
 conventional support vector machines 303
 convolutional layers 230
 convolutional neural networks (CNNs) 12, 32, 223, 230–232, 246–249, 269, 274
 CoreferenceHandler class 294
 correlation matrix 143
 cost function 8, 176, 203–204
 gradient descent to 177–181
 covariance 98
 covariance matrix 98
 covariant quantum kernels 309
 CPUs
 classification algorithms on 14
 machine learning on 13–32
 regression algorithms on 14–15, 267
 critical value 132
 cross-entropy loss function 8, 203, 225
 cross-validation score 4, 5, 234
 cryptography 473
 CUDA toolkit 11
 cuDNN libraries 11
 cumulative distribution function 43, 44, 48
 curl command 395, 433, 439
 cybersecurity 473

d

DataFrame 15
 data points 91
 data preprocessing 35
 for machine learning 36
 data rescaling method 18–19
 data scaling 36
 datasets 35
 standardization 37
 data transformation 37–50
 logistic data transformation 43
 lognormal transformation 43–44
 MaxAbsScaler 40
 MinMaxScaler 39
 to normal distribution 44–48
 normalization 42–43

- quantile transformation 48–50
 - RobustScaler 40–41
 - StandardScaler 37–38
 - using unsupervised learning 98
 - data visualization 128
 - DBSCAN (density-based spatial clustering of applications with noise) 252, 262–264
 - decision tree algorithms 4, 154
 - deep learning (DL) 1, 3
 - algorithms 88, 168
 - approaches 274
 - machine learning and. *see* machine learning
 - Red Hat OpenShift to 452–454
 - deep residual learning 11
 - default data mapping 308
 - density-based spatial clustering of applications with noise (DBSCAN) 252, 262–264
 - deployment.yaml file 438, 448
 - descriptive analysis 35
 - deviation encoding, effect of 68
 - DevOps tools 396–405, 454
 - diff()* method 85
 - discrete values 57, 202
 - distance-based models 36
 - distribution 69
 - divisive clustering algorithms 252
 - Docker Engine 377
 - Dockerfile 380–381, 383–384, 390, 393, 418, 424, 432, 443, 459
 - Docker, for machine learning 375–389
 - batch inference 424–440
 - build and run 381–389
 - containerization 376
 - Dockerfile 380–381
 - GitHub repository with 454–463
 - Cloud Kubernetes service 440–452
 - install 377–378
 - integrate machine learning models using 396–405
 - and Kubernetes. *see* Kubernetes
 - machine learning prediction in real time using 428–440
 - microservices 375–376
 - for online inference 393–394, 432–434
 - and Python APIs with Flask 389–396
 - training models 415–424
 - use of 378–379
 - Docker Hub 377
 - dummy variable 61
- e**
- EEGs (electroencephalograms) 102
 - eigenvalues 99, 110
 - eigenvectors 99, 110
 - elastic net method 157
 - electroencephalograms (EEGs) 102
 - Electronic Numerical Integrator and Computer (ENIAC) 300
 - element-wise multiplication 232
 - ELIZA program 273
 - embedded methods 22–23, 154–167, 169
 - elastic net method 157
 - lasso regression 154–156
 - ridge regression 156–157
 - tree-based algorithms 161–165
 - embedded-type feature selection 131
 - encoding functions 308, 310
 - encoding methods 57–58, 58
 - backward difference encoding method 72–73
 - binary encoding method 64, 64–65
 - frequency encoding method 65–66
 - hashing encoding 71–72
 - Helmert encoding method 58, 63–64
 - hepAIsTos encoding method 77
 - James-Stein encoding method 74–75
 - label encoding method 62
 - leave-one-out encoding 73–74
 - mean encoding 66–67, 67
 - M-estimator encoding 76
 - one-hot encoding method 61, 61–62
 - ordinal encoding method 59–60
 - probability ratio encoding 70–71
 - sum encoding method 68
 - weight of evidence method 68–70
 - ENIAC (Electronic Numerical Integrator and Computer) 300
 - equivalent docker command 423
 - error function 218
 - error rate 6
 - EstimatorQNN 338–343
 - Euclidean distance 116
 - Euclidian norm 43
 - exhaustive feature selection 153–154
 - expanding window feature 84
 - explained variance ratio 102
- f**
- feature engineering techniques 35
 - feature extraction 97–130
 - feature rescaling 36–57
 - time-related features engineering 77–88
 - work with categorical data. *see* categorical (discrete) data
 - feature extraction method 19–20, 97–130
 - advantage 97
 - with hepAIsTos 130
 - independent component analysis 102–109
 - linear discriminant analysis 110–115
 - locally linear embedding method 115–123
 - manifold learning techniques 125–130

- feature extraction method (*cont'd*)
 - principal component analysis 98–102
 - t*-Distributed Stochastic Neighbor Embedding technique 123, 123–125
- feature rescaling 36–57
 - data transformation. *see* data transformation
 - and feature selection techniques 369
 - SVM model 50–57
- feature selection method 20–23, 97, 131–169
 - embedded methods 22–23, 131, 154–167
 - filter methods 132–146
 - flow of 131
 - permutation feature importance 165–167
 - tree-based algorithms for 165
 - using GPUs 167–168
 - using hephAistos 168–169
 - wrapper methods 21–22, 146–154
- feature space 306
- filter methods 132–146
 - advantage 146
 - ANOVA F-value 137–140
 - chi-squared test 134–137
 - disadvantage 146
 - many more possibilities 146
 - Pearson correlation coefficient 140–146
 - using statistical tests 132–134
 - variance threshold 132
- fine needle aspirate (FNA) 138
- Fisher's formula 110
- .fit_transform()* method 63, 64
- Flask
 - GitHub repository with 454–463
 - Python APIs with 389–396, 428–440
- Flask-RESTful APIs 390–392, 428–431
- fMRI (functional magnetic resonance imaging) analysis 102
- FMs (foundation models) 286
- FNA (fine needle aspirate) 138
- forward stepwise selection 146, 146–150
- foundation models (FMs) 286
- frequency encoding method 65–66
- F-score 6–7
- F-test statistic 137–140
- fully connected layers 230
- functional magnetic resonance imaging (fMRI) analysis 102

g

- GABAergic interneurons 307
- Gambetta's law 465
- Gaussian distribution 44–48
 - quantile transformation with 49
- Gaussian scaling 37
- Generative Pre-Training (GPT) 286

- get_dummies* function 61
- Gibbs sampling 92
- Gini index 161
- GitHub repository 33, 294, 402
 - source code in 454–463
- glial cells 220
- GPT (Generative Pre-Training) 286
- GPUs
 - classification algorithms on 14, 24–25, 266
 - feature selection method using 167–168
 - machine learning on 13–32
 - regression algorithms on 15, 267–268
- gradient descent 177–181, 204

h

- Hadamard gate 302, 308
- ham messages 274–281
- hashing encoding methods 71–72
- head() method 255
- HelmertEncoder function 63
- Helmert encoding method 58, 63–64, 72
- hephAistos
 - categorical data 17–18
 - classification algorithms 23–31
 - data rescaling method 18–19
 - encoding method 77
 - feature extraction method 19–20, 130
 - feature selection method using 20–23, 168–169
 - function 15–32
 - installation 13–15
 - for machine learning 13–32
 - machine learning algorithms with 264–269
 - quantum algorithms with 368–372
 - time series transformation 16–17
 - time series with 88
 - training and testing datasets 15–16
- Hessian locally linear embedding (HLLE) 121, 122
- hierarchical clustering 251, 252
- Higgs boson 304
- high-performance computing 467
- Hilbert–Schmidt space 307
- Hilbert space 306
- hinge loss function 8
- HLLE (Hessian locally linear embedding) 121, 122
- Huber loss 8
- HuggingFace Pytorch transformers 294
- hybrid cloud environment 286
- hybrid quantum-classical algorithm 352
- hyperparameter optimization 303
- hyperplane 306
- hypothesis testing 132

i

IBM Cloud Container Registry 446, 447, 450
 IBM Cloud Kubernetes service 440–452
 IBM Power System 452
 IBM Quantum framework 310, 318
 ICA (independent component analysis) 102–109
 identity function 223
 independent component analysis (ICA) 102–109
 independent variables 70
 inference.py script 382–384, 387, 388–389, 424–426
 information value (IV) 69
 integer encoding method 59
 integrate machine learning models 396–405
 intercept-only model 137
 internal network 410–414
 interneuron phenotypes 307
 interneurons 219–220
 interquartile range (IQR) 40, 41
 inverse document frequency 278
 inverse linear correlation 140
 IQR (interquartile range) 40, 41
 IV (information value) 69

j

James-Stein encoding method 74–75
 Jenkins 389, 400
 installation 397–399
 integrate machine learning models using 396–405
 scenario implementation 399–405
 JupyterLab 13
 Jupyter Notebooks 13, 33, 77, 98, 182, 353, 379

k

KDE (kernel density estimation) 257
 Keras 12, 167
 binary logistic regression with 210–211
 logistic regression with 208–210
 kernel density estimation (KDE) 257
 kernel functions 212, 217, 303, 306
 kernel trick. *see* kernel function
 k-fold cross-validation 4
 k-means clustering algorithm 252–255
 k-nearest neighbors (KNN) 274
 imputation method 93–97
 permutation feature importance with 165–166
 KNN. *see* k-nearest neighbors
 Kubeadm installation 434–435
 kubectrl 453
 kubelet 405
 kube-proxy 405
 Kubernetes
 application to 448–452

 batch inference 424–428
 CLI 442
 cluster 407–409, 416–418, 424, 426, 435–437
 commands to delete 424
 configuration files for 422–423, 427–428
 containerized machine learning model to 437–440
 distribution 376
 initialization and internal network 410–414
 installation 406–407, 415–416
 internal network 417
 Jobs 415
 kubectrl 453
 machine learning with 405–414
 OpenShift and 453–454
 Python APIs with 428–440
 service on Public Cloud 440–452
 training models 415–424
 virtual machines 415
 vocabulary 405–406
 Kubernetes Dashboard 452
 Kullback–Leibler divergence 123
 kustomization.yaml file 439, 450

l

label encoding method 62, 130
 Lagrange multipliers 213
 lag variables 79–82
 language modeling 287
 Large Models, Large Language Models (LMs/LLMs) 286
 LDA (linear discriminant analysis) 7, 110–115, 381, 430, 431
 learning algorithm 177
 learning styles, for machine learning 2–9
 methods 9
 reinforcement learning 9
 semi-supervised learning 9
 supervised learning. *see* supervised learning
 unsupervised learning 9
 least absolute shrinkage and selection operator (lasso)
 regression 154–156, 169
 leave-one-out encoding method 73–74
 linear algorithms 131
 linear discriminant analysis (LDA) 7, 110–115, 381, 430, 431
 linear interpolation 91–92
 linear regression 68, 137, 176–202
 gradient descent to cost function 177–181
 implementation 182–202
 math 176–177
 multiple 185–202
 univariate 182–185
 linear support vector classification algorithm 157
 LLE (locally linear embedding) method 115–123
 L-Measure 219

LMs/LLMs (Large Models, Large Language Models) 286
 l2 norm 43
 locally linear embedding (LLE) method 115–123
 local tangent space alignment (LTSA) 121
 loc method 255
 logistic data transformation 43
 logistic function 202
 logistic regression 202–211
 binary 202–204, 210–211
 with Keras on TensorFlow 208–210
 multinomial. *see* multinomial logistic regression
 with sklearn 205–208
 log loss 8
 lognormal cumulative distribution functions 43, 44
 lognormal transformation 43
 log transformation 44
 long short-term memory (LSTM) 233, 242–246
 loss functions 7–9, 203, 225–226
 binary cross-entropy as 352
 L2 regularization (ridge regression) 156–157
 LSTM (long short-term memory) 233, 242–246
 LTSA (local tangent space alignment) 121

m

machine learning (ML) 1. *see also* machine learning algorithms
 application 443–446
 data preprocessing for 36
 Docker. *see* Docker, for machine learning
 feature engineering. *see* feature engineering techniques
 goal 4
 handling missing values in 88–97
 hepHAIstos for running. *see* hepHAIstos, for machine learning
 learning styles for 2–9
 models 392–393, 431–432, 454–463
 production. *see* production, machine learning in
 Python tools for 9–13
 quantum advantage for 303
 quantum computing and. *see* quantum computing
 Red Hat OpenShift to 452–454
 workflow 2
 machine learning algorithms 94
 artificial neural networks 223–249
 with hepHAIstos 264–269
 linear regression 176–202
 logistic regression 202–211
 many more algorithms to explore 249–251
 in quantum computing. *see* quantum machine learning
 rule-based 176
 support vector machine 211–222
 unsupervised 251–264
 machine learning operations (MLOps) 396–405
 MAE (mean of the absolute errors) 8
 magnetoencephalograms (MEGs) 102
 Mahalanobis distance transformation 318, 327
 make_blobs() function 253
 manifold learners 116
 MAR (missing at random) 92
 Masked Language Modeling (MLM) 287, 288
 math 176–177
 matplotlib 10, 101
 MaxAbsScaler 40, 57
 maximum-margin hyperplane 212, 306
 max-norm 43
 MCAR (missing completely at random) 92
 mean 37, 37
 imputation 90
 mean encoding methods 66–67, 67
 mean of the absolute errors (MAE) 8
 mean shift clustering 252, 257–259
 mean squared error (MSE) 8
 median imputation 90
 MEGs (magnetoencephalograms) 102
 M-estimator encoding methods 76
 method(s)
 backward difference encoding 72–73
 bag-of-words 274, 278, 280, 296
 binary encoding 64, 64–65
 data rescaling 18–19
 diff() 85
 elastic net 157
 embedded. *see* embedded methods
 encoding. *see* encoding methods
 feature extraction. *see* feature extraction method
 feature selection. *see* feature selection method
 filter 132–146
 head() 255
 KNN imputation 93–97
 loc 255
 quantum kernel 307
 regularization 154
 shift() 79
 weight of evidence 68–70
 wrapper. *see* wrapper methods
 MICE (multivariate imputation by chained equation)
 imputations 92–93, 93
 microservice approach 375–376
 mini-batch k-means clustering algorithm 252, 255–256
 Minkowski norm 43
 MinMaxScaler 39, 57, 120
 misclassification rate 6
 missing at random (MAR) 92
 missing completely at random (MCAR) 92

- missing_method 97
- missing not at random (MNAR) 92
- missing values handling, in machine learning 88–97
 - KNN imputation method 93–97
 - linear interpolation 91–92
 - multivariate imputation by chained equation 92–93, 93
 - row or column removal 89–90
 - statistical imputation 90–91
- ML. *see* machine learning
- MLLE (modified locally linear embedding) 121, 122
- MLM (Masked Language Modeling) 287, 288
- MLOps (machine learning operations) 396–405
- MLP 224–225
- MLP neural networks 233–242, 395, 430, 433–434
- MNAR (missing not at random) 92
- MNIST dataset 12
- mode imputation 90
- model-building process 131
- modified locally linear embedding (MLLE) 121, 122
- monolithic approach 375
- Monte Carlo simulations 473
- Moore’s law 465, 467
- MSE (mean squared error) 8
- multi-class classification 2, 227–230
- multinomial logistic regression 154, 204
 - applied to fashion MNIST 204–210
- multiple linear regression 176, 181, 185–202
 - with Keras on TensorFlow 196–202
 - with scikit-learn 188–191
 - with *statsmodels*, 192–193
 - with TensorFlow 193–196
- multivariate imputation by chained equation (MICE)
 - imputations 92–93, 93
- n**
- namespace.yaml file 437
- NaN (Not a Number) 80
- natural language generation (NLG) 274
- natural language processing (NLP) 97, 251, 273
 - BERT. *see* Bidirectional Encoder Representations from Transformers
 - deep learning approaches 274
 - domain of 296
 - messages as spam or ham 274–281
 - neural approaches 274
 - sentiment analysis 281–286
 - statistical approaches 274
 - symbolic approach 274
 - tools and libraries for 273
- Natural Language Toolkit (NLTK) 273, 274
- natural language understanding (NLU) 274
- negative log-likelihood loss 203
- NeuralNetworkClassifier 337, 338, 343, 348
- neural network multilayer perceptron 233–242, 381, 395, 430, 431
- NeuralNetworkRegressor 337
- neural networks 27, 175, 224
 - layers 224
- neural NLP approaches 274
- NeuroM 219
- neuronal classification 307
- neuron morphology 219, 307, **327**
- new-app command 462
- Next Sentence Prediction (NSP) technique 288
- NLG (natural language generation) 274
- NLP. *see* natural language processing
- NLTK (Natural Language Toolkit) 273, 274
- NLU (natural language understanding) 274
- nodes 405
- nominal categorical data 57
- non-Gaussian processes 102, 103, 105
- nonlinear support vector machines 216, 216–217, 217
- nonlinear SVM 306
- nonparametric quantile transformation 48
- normal distribution (Gaussian distribution) 44–48
 - quantile transformation with 49
- normalization 36, 42–43
- normal probability distribution
 - right-tailed test with 133
 - two-sided test with 133
- norms, concept of 42
- Not a Number (NaN) 80
- not fully linearly separable data 214–216
- NSP (Next Sentence Prediction) technique 288
- null hypothesis 132
- numerical variable 57
- Numpy 10, 242
- o**
- objective function 36
- one-hot encoding method 61, 61–62
- one-hot vector 204
- one-to-one process 220
- one-to-rest process 220
- online inference 393–394, 428–440
- Open Java Development Kit (OpenJDK) 397
- OpenShift 376, 453
 - cluster instance 455–463
 - and Kubernetes 453–454
 - Red Hat 452–454
 - web console 460
- OpenShift Enterprise 457

- open-source world 12
- optimal fitting 3
- optimal hyperplane 212
- ordinal categorical data 57
- OrdinalEncoder class 60
- ordinal encoding method 59–60
- ordinal logistic regression 204
- ordinary least squares linear regression 160
- overfitting 3, 3–4, 131

p

- PACF (partial autocorrelation function) 80, 81
- pandas 10, 58, 59, 242
 - one-hot encoding method 61
 - ordinal encoding method 59
- partial autocorrelation function (PACF) 80, 81
- partitional clustering 251
- PauliFeatureMap 308
- Pauli-X gate 302
- Pauli-Y gate 302
- Pauli-Z gate 302
- PCA (principal component analysis) 9, 62, 98–102, 104, 106
- Pearson correlation coefficient 20, 140–146, 168
- pegasos algorithms 28, 333, 369
- pegasos QSVC 333–337
- penalization methods 154
- p-norm 43
- Pods 405, 411, 414, 438
- Poisson model 93
- polylogarithmic function 306
- pooling layers 230
- port 8888, 379
- precision score 6, 234
- pre-trained models 286
- primal optimization problem 213
- principal cells 219
- principal component analysis (PCA) 9, 62, 98–102, 104, 106
- probability distribution 225
- probability ratio encoding 70–71
- probability value (*p*-value) 132, 137
- production, machine learning in
 - DevOps to MLOPS 396–405
 - Docker containers for 375–389
 - Kubernetes. *see* Kubernetes
 - in real time using Docker and Python 389–396
- punctuation 274
- p*-value (probability value) 132, 137
- Python APIs
 - with Flask 389–396, 428–440
 - with Kubernetes 428–440
- Python ecosystem 380

- Python language 472
- Python tools 9–13
 - data manipulation with 10
 - Cloud Kubernetes service 440–452
 - JupyterLab 13
 - Jupyter Notebook 13
 - Keras 12
 - libraries 10–13
 - PyTorch 12
 - scikit-learn 10
 - TensorFlow 10–12, 288
- PyTorch 12, 168, 352

q

- qGAN (quantum generative adversarial network) 352–368
- Qiskit 304, 305
- Qiskit Runtime 305–306
- QKA (quantum kernel alignment) 27, 309, 328
- QKE (quantum kernel estimation) 307
- QNNs (quantum neural networks) 303, 337–351
- QPU. *see* quantum processing units
- QSVC 333–337
- QSVM 304, 306
- qualitative variables 35
- quantile function 48
- quantile transformation 48–50
- quantitative variables 35
- quantum computing 474
 - algorithms with hephAistos 368–372
 - characteristics of 305
 - mechanics 299
 - 127-qubit superconducting 305
 - Pegasus QSVC 333–337
 - potential use cases for 304
 - QNN. *see* quantum neural networks
 - quantum Generative Adversarial Network 352–368
 - quantum kernel machine learning 306–327
 - quantum kernel training 328–333
 - quantum machine learning 303–306
- quantum feature mapping 311
- quantum gates 302
- quantum generative adversarial network (qGAN) 352–368
- quantum information theory 300
- quantum kernel alignment (QKA) 27, 309, 328
- quantum kernel estimation (QKE) 307
- quantum kernel machine learning 306–327
- quantum kernel methods 307
- QuantumKernelTrained.fit method 309, 328
- QuantumKernelTrainer 309
- quantum kernel training 328–333
- quantum machine learning 303–306

quantum mapping function 307

quantum mechanics 470

development of 300

fundamental equation of 300

notion of 299

quantum neural networks (QNNs) 337–351

quantum processing units (QPUs) 13–32

classification algorithms 27

quantum state space 303

quantum systems 469–474

qubits 300, 302, 469–474, 470

connectivity, 305

r

radial basis function (RBF) kernel 14

random forest algorithm 161–162

RBAC (role-based access control) 453

RBF (radial basis function) kernel 14

recall score 6, 234

receiver operating characteristic curve (ROC AUC) 147

reciprocal transformation 46

rectified linear unit (ReLU) 223

recurrent neural networks (RNNs) 29, 30–31, 87, 232–233, 233, 268–269, 274

long short-term memory (LSTM) 242–246

Red Hat 378, 397

Red Hat OpenShift 452–454

container platform 454–463

regression algorithms

binary classification 351

on CPUs 14–15, 267

on GPUs 15, 267–268

regression models 2, 93

with an ϵ -insensitive tube, 218

support vector machine using 222

regularization methods 154

reinforcement learning 9

ReLU (rectified linear unit) 223

residual error 93

residual variance 93

responsibility matrix 260

RGB model 230, 230

ridge regression 156–157

right-tailed test 133

RMSE (root-mean-squared error) 177, 183

RNNs. *see* recurrent neural networks

RobustScaler 40–41, 57

role-based access control (RBAC) 453

rolling window features 82–83

root-mean-squared error (RMSE) 177, 183

R-squared score 183

rule-based machine learning algorithms 176

s

SamplerQNN 338, 343–348

scaling 36

Schrödinger equation 300, 471

scikit-learn 10, 21, 36, 43, 58, 112

digits dataset using 123

Gaussian distribution using 49

GitHub repository with 454–463

locally linear embedding using 118

logistic regression with 205–208

multiple linear regression with 188–191

naive Bayes with 280

support vector machines using 220–222

SciPy 10, 134

Seaborn 10

self-supervised learning 287

semi-supervised learning 9

sentiment analysis 281–286

sequential forward selection (SFS) 148

service_port.yaml file 449–450

service.yaml file 438, 449

SFS (sequential forward selection) 148

SGD optimizer 26, 267

shift() method 79

Shor algorithm 473

sigmoid function 202, 202, 223, 227

simple linear regression model 137, 177

simple word count 274

sklearn. *see* scikit-learn

skorch 12

slack variable 215

softmax function 204

softmax loss 8

SOTA (State-of-the-Art) models 286

spam messages 274–281

Spearman's rank correlation 134

.spec.template 423

squared deviation 102

squared error loss 8

square root transformation 45

standard deviation 37, 37, 98

standardization 36, 37, 110

StandardScaler 37–38, 57, 100, 130

State-of-the-Art (SOTA) models 286

statistical imputation 90–91

statistical learning 1, 223

statistical NLP approaches 274

statistical tests 132–134

stochastic gradient descent 181, 226, 227, 232

storage systems 466

sudo command 400

sum encoding method 68

summation 223
 superposition 300, 301
 supervised learning 2–9, 110
 algorithms 2
 confusion matrix 5, 5–7
 k-fold cross-validation 4
 loss functions 7–9
 objectives 2
 overfitting and underfitting 3, 3–4
 train/test split 4–5
 support vector machines (SVM) 36, 50–57, 211–222, 212
 application 219–222
 classical 303
 conventional 303
 linearly separable data 212, 212–214
 nonlinear 216, 216–217, 217
 not fully linearly separable data 214–216
 for regression 217–219, 218
 using linear kernel 280
 using sklearn for regression 222
 support vectors 306
 SVC Loss 309
 SVM. *see* support vector machines
 Swiss Roll manifold 116
 symbolic NLP approaches 274
 target encoding 66

t

t-Distributed Stochastic Neighbor Embedding (t-SNE)
 technique 123, 123–125
 TensorFlow 10–12, 167
 BERT for binary text classification using 288–294
 Keras on. *see* Keras
 multiple linear regression with 193–196
 Python 288
 term frequency-inverse document frequency (TF-IDF) 278
 text summarization, BERT for 294–295
 TF-IDF (term frequency-inverse document frequency) 278
 three-dimensional space 115
 time-related features engineering 77–88
 date-related features 79
 expanding window feature 84
 lag variables 79–82
 rolling window features 82–83
 time series data 85
 time series 77
 with hephAistos 88
 transformation 16–17
 trends and seasonal components 85
 time transformation 88
 tokens 274

top-down clustering 252
 TorchConnector 352
 “TotalGrayVol” data 36
 TrainableFidelityQuantumKernel 309
 training Job 415
 training model 376
 Kubernetes Cluster 424
 Python application 418–422
 train.py file 381–382, 387, 390, 392, 418, 420, 428, 431, 443, 445, 457
 train/test split 4–5
 tree-based algorithms 36, 57, 161–165
 t-SNE (*t*-Distributed Stochastic Neighbor Embedding)
 technique 123, 123–125
 two-dimensional complex vector space 301
 two-sided test 133

U

Ubuntu 377
 underfitting 3, 3–4
 uniform distribution 49
 unit vector normalization 42–43
 univariate linear regression 176, 182–185, 196
 univariate tests 131
 universal approximation theorem 225
 unrestricted model 137
 unsupervised machine learning 9
 algorithms 110, 251–264
 clustering algorithms 252–264
 data transformation using 98
 methods 1

V

Vagrantfile 407, 408, 409
 variance 4, 98
 variance threshold 132, 168
 variational quantum classifier (VQC) 337, 338, 348–351
 variational quantum regressor (VQR) 337
 vector norms 42
 video games, types of 57
 virtual machines (VMs) 376, 415, 434
 VMs (virtual machines) 376, 415, 434
 VQC (variational quantum classifier) 337, 338, 348–351
 VQR (variational quantum regressor) 337

W

Ward 252
 wave mechanics 299, 300, 470
 wave-particle duality 299
 “wave-particle duality” 299
 WCSS (within-cluster sum of squares) 253

- weight of evidence (WoE) method 68–70
- within-cluster sum of squares (WCSS) 253
- WoE (weight of evidence) method 68–70
- wrapper methods 21–22, 131, 146–154,
168–169
 - backward elimination 151–153
 - exhaustive feature selection 153–154
 - forward stepwise selection 146, 146–150

y

- YAML files 437–439
- Yeo-Johnson transformation 47

z

- ZFeatureMap 308
- Z-score normalization 37
- ZZFeatureMap 308, 318

