Note: Page numbers followed by "f" indicate figures; and "t" indicate tables; and "b" indicate boxes.

•	A
A	Artificial intelligence, 1–2, 4
ABIDE. See Autism Brain Imaging Data	Artificial neural networks, 3
Exchange (ABIDE)	ASD. See Autism spectrum disorder (ASD)
Accountability, 332–333	Asymmetric data fusion, 287
gap, 332–333, 333f	Atlas-based ROIs, 320-321
Accuracy, 37–38, 313	Attention-deficit/hyperactivity disorder
score, 238, 238t	(ADHD), 124, 135–136
Activation functions, 159-160, 159f	aggression prediction in, 135-136
Activity space, 268–269	AUC. See Area under curve (AUC)
AD. See Alzheimer's disease (AD)	AUC-ROC. See Area under ROC curve
ADHD. See Attention-deficit/	(AUC-ROC)
hyperactivity disorder (ADHD)	Augmentation
ADNI. See Alzheimer's Disease	data, 259
Neuroimaging Initiative (ADNI)	simulation-based, 259-260
AE. See Autoencoders (AE)	Autism Brain Imaging Data Exchange
Agglomerative clustering (AG clustering),	(ABIDE), 133–134, 250–251
240-241	ABIDE I, 204
Aggregated voxels, 319	Autism spectrum disorder (ASD), 84, 166,
Aggregating features, 314–315	168–169, 203
Aggression prediction in ADHD, 135–136	classification of, 93
AlexNet, 173	diagnosis of, 203-205
AlphaGo model, 174	predicting depressive states, 205–206
Alzheimer's disease (AD), 4, 46, 51, 74,	predicting symptoms severity and
109, 148–149, 166, 184, 215–216,	mathematical abilities, 133–135
283-284, 330-331	pretraining and fine-tuning
diagnostic classification, 149–150	process, 204f
early detection in, 167–168	Autoencoders (AE), 24–25, 193–194, 299
multimodal neuroimaging studies with	adversarial, 198–201
deep learning in, 299–301	network, 199f
predicting cognitive decline in, 76–77	representations in latent space, 198f
predicting conversion from mild	structure, 200f
cognitive impairment to, 110–112	application to brain disorders, 201–206
prediction, 184–185	denoising, 196–197, 197f
Alzheimer's Disease Neuroimaging	method description, 194-201
Initiative (ADNI), 58, 149, 220,	sparse, 197–198
250–251	structure of, 195f
Anaconda (programming language), 345	undercomplete, 196
Analysis of variance (ANOVA),	Automated feature reduction methods,
25–27, 242	314–315
RB kernels, 129	Automated feature selection, 25-28, 26t
Aphasia. See Language impairment	embedded methods, 27–28
Area under curve (AUC), 38–39	filter methods, 25–27
Area under ROC curve (AUC-ROC),	selection methods, 34
38–39	wrapper methods, 27
00 07	

В	of machine learning to, 330–331
bac. See Balanced accuracy (bac)	in multimodal integration, 296-301
Backpropagation, 161	using neuroimaging to predicting brain
Balanced accuracy (bac), 37–38, 101, 358	age, 319–321
Bayes rule, 89	in voxel-wise encoding models, 278-279
Bayesian logistic regression, 89, 93	autoencoders application to, 201-206
Bayesian variant of sparse logistic	predicting prognosis from EHRs,
regression, 89–90	201-203
Behaviorism, 2–3	challenges in machine learning studies of
Bias, 308–309	psychiatric and neurological
problem of, 337–338	disorders, 50–55
sources in machine learning, 309–311	absence of biomarkers, 51
choice of features, 310–311	heterogeneity, 53–55
choice of machine learning	reliability of diagnosis, 52–53
algorithm, 311	cost of misclassification, 56, 57f
choice of target variable, 309–310	DNN applications to, 166–169
data processing, 311	autism spectrum disorders, 168–169
Bias—variance trade-off, 34—35	diagnostic classification in
Big data, 7–8	schizophrenia, 166–167
<u> </u>	early detection in Alzheimer's disease,
Bilingualism, 77–78 Binary Jabale, 85	167–168
Binary labels, 85	ethical tensions from using machine
Biological age score, 221	learning in, 331–338
Biomarker, 51, 329—330	challenges in interaction between
absence of, 51	humans and intelligent systems,
Biomedical data, ontology of, 335	332–333
Bipolar disorder, 94	
data fusion in, 298 Black box, 165	data security and patient privacy, 334–335
Blind source separation problem,	interpretability of machine learning
287–288, 288f	and problem of bias, 337-338
Block-wise missing data, 150	mental privacy and question of
Blood oxygen level dependent activity	"neurorights", 335-336
(BOLD activity), 267–268	ontology of biomedical data, 335
Boolean class labels, 109	transparency of machine learning,
Brain aging, 221	336-337
in schizophrenia, 132–133	linear classification model applications,
Brain atrophy, 75	91–96
Brain disorders, 283-284, 329-330	classification of ASD, 93
applications in clustering analysis,	classification of schizophrenia,
240-243	94-96
functional connectivity states	linear regression applications, 74-79
investigation in fMRI, 242-243	machine learning applications, 45
identification of cross-diagnostic	machine learning relevant to
neurocognitive profiles, 242	data-driven models and big data, 7-8
identifying disorder subtypes, 240–242	focus on prediction and
applications to, 318–323	generalizability, 6–7
using clinical variables for prognostic	group-level to individual-level
prediction, 322–323	inferences, 5
in CNNs, 184–188	recognizing heterogeneity, 8
language as marker of psychiatric and	univariate to multivariate inferences,
developmental disorders, 321–322	5–6

MKL applications, 148–153	Canonical variate, 289–290
AD, diagnostic classification of,	Canonical variate analysis (CVA), 214,
149-150	215t
PD, diagnostic classification of, 150–151	CANSAS. See Camberwell Assessment of Need Short Appraisal Schedule
psychosis, diagnostics classification of,	(CANSAS)
151–153	Care, 90–91
optimism, 55	CCA. See Canonical correlation analysis
PCA applications to, 218–221	(CCA)
healthy aging and disease process, 221	CCC. See Canonical correlation coefficient
neurological disorders, 219–221	(CCC)
psychiatric disorders, 218–219	CDI. See Communicative Development
reason for people interested in machine	Inventories (CDI)
learning, 45–50	Centroid-based clustering, 229
diagnostic evaluation, 48-49	Cerebrospinal fluid (CSF), 148-149
prediction of illness onset, 46-48	Classes, 10
prediction of outcomes, 49-50	Classical statistics, 6–7
result of machine learning applied in	statistical methods, 90-91
psychiatry and neurology, 57-59	Classification, 101
SVM applications to, 109-116	algorithms, 10
brain-based diagnostics of	function, 86
schizophrenia, 112–115	threshold, 38-39
predicting conversion from MCI to AD,	Classifier, 101
110-112	Clinical and behavioral scores, 141–142
predicting treatment response in	Clinical neuroimaging, 84, 150
depression, 115–116	Clinical translation, 47–48
SVR applications to, 131–136	Cluster validation, 230–234
aggression prediction in ADHD,	Clustering analysis, 11, 227
135–136	applications to brain disorders, 240–243
predicting deviations from "brain age" in schizophrenia, 132–133	choosing <i>K</i> with silhouette scores, 232–233
predicting symptoms severity and	with density-based spatial clustering,
mathematical abilities in ASD,	237f
133-135	K-means, 230–240
Brain imaging machine learning, 318	multipeak and uniform distributions,
Brain morphometry to classifying patients	228f
with SZ and HC, 345–347	SSE, 231–232
Brain tumor segmentation, 185–187	testing for multipeak distribution,
Brain volume measures, 75	233–234
BRATS. See Multimodal Brain Tumor	CNNs. See Convolutional neural networks
Image Segmentation Benchmark	(CNNs)
(BRATS)	"Cocktail party" problem, 287–288
By-chance heterogeneity, 260	Cognitive impairment, 148–149
C	Comma-separated values (CSV), 349
Camberwell Assessment of Need Short	Communicative Development Inventories (CDI), 322
Appraisal Schedule (CANSAS),	Competitive approach, 146–147
322–323	= = = = = = = = = = = = = = = = = = = =
Canonical correlation analysis (CCA),	Complete case analysis/listwise deletion, 255
289–290, 290f	Computational models, 3
Canonical correlation coefficient (CCC),	Computed tomography (CT), 259–260
289–290	Confidence intervals, 259

Confounding variable, 23	data-driven models, 7-8
Confounds, 261–264	data-driven unsupervised techniques,
Confusion matrix, 36–37, 37f	314-315
Control-based harmonization model, 262	efficient learning, 260
Convergence to local minima, 232	fusion, 285–291
ConvNets. See Convolutional neural	in schizophrenia and bipolar
networks (CNNs)	disorder, 298
Convolution operation, 177, 178f	harmonization, 262
Convolutional neural networks (CNNs),	prediction of, 6–7
173, 299, 321	preparation, 23
applications to brain disorders, 184–188	security, 334–335
architecture, 182–183	transformations, 34
convolutional layer, 176–181	implementing in machine learning
filter count, 180	pipeline, 34
filter size, 180	Data processing, 311–318
padding, 181	addressing high dimensionality, 314–318
stride size, 180, 180f	feature aggregation, 315–318
flexibility, 186–187	unsupervised methods, 318
fully connected layer for, 182	measuring separability between two
layers, 176–182	groups, 313–314
method description, 175–183	Dataframe, 349
structure, 174f	DBSCAN. See Density-based spatial
Cooperative approach, 146–147	clustering of applications with
Coordinate descent with early	noise (DBSCAN)
stopping, 276	DD. See Developmental dyslexia (DD)
Core object, 237–238	Decision-support system (DSS), 332–333
Core observations, 237—238	Decoder, 194–195
Cortical surface, 319–320	Deep learning (DL), 3, 157–158, 273,
Cost of misclassification, 56, 57f	285–286, 293–294, 321, 336–337
Covariance matrices, 212–213	approaches, 257
Cross-diagnostic neurocognitive profiles,	encoding models from Gabor feature
identification of, 242	space to, 271–275
Cross-validation (CV), 29–33, 106,	multimodal neuroimaging studies with
141-142, 345-347, 357-359	deep learning in AD, 299–301
feature selection scheme, 113-115	Deep neural networks (DNNs), 158,
final performance in, 36f	161–162, 166, 175, 194, 299. See also
nested, 31–32	Convolutional neural networks
parameter selection using, 131	(CNNs)
performance, 41	applications to brain disorders, 166–169
stratified, 33	hyperparameter tuning, 165–166
types, 32f	interpretability, 165
CSF. See Cerebrospinal fluid (CSF)	learning rate on weight
CSV. See Comma-separated values (CSV)	optimization, 164f
CT. See Computed tomography (CT)	loss landscape, 162f
Curse of dimensionality, 72–73, 243	overfitting, 164
CV. See Cross-validation (CV)	starting weights, multiple local minima,
CVA. See Canonical variate analysis (CVA)	and saddle points, 163–164
, , ,	structure, 159–160, 159f
D	training, 160–164
Data	Deepnet-fwRF models, 273, 274f-275f
augmentation, 259	Dendrogram, 240–241

Densite hand matial about air and	Election at 00
Density-based spatial clustering of	Elastic net, 88
applications with noise (DBSCAN),	Electroencephalography (EEG), 141–142,
236—238	184, 283—284, 307—308, 329—330
comparison of K-means with, 238–240	Electronic health records (EHRs), 201–202
Density-reachable points, 237—238	deep patient model, 202f
Dependent variable, 22–23 Depression, predicting treatment response	diagnosis of ASD, 203–205
in, 115–116	predicting prognosis from, 201–203
Developmental dyslexia (DD), 322	Electronic health technology (eHealth technology), 334–335
Diagnostic and Statistical Manual of	Electrophysiological methods, 329–330
Mental Disorders (DSM), 52, 309	Embedded methods, 27–28, 105, 258
DSM-5, 52	Empirical risk
Diagnostic labels, 52–53	functional, 87
labeling method, 309	minimization, 85–87
Diagonal matrix, 213–214	loss functions, 86t
Diffusion MRI, 131–132	Encoder, 194–195
Diffusion tensor imaging (DTI), 297	Encoding models from Gabor feature
Dimension, 22–23	space, 271–275
reduction, 213–214	Enhancing Neuroimaging Genetics
Dimensionality, 22–23, 196	through Meta-analysis (ENIGMA),
curses of, 72–73, 243	250-251
of image data, 87	ENIGMA. See Enhancing Neuroimaging
reduction, 12, 24-25, 34	Genetics through Meta-analysis
Dip test, 233–234	(ENIGMA)
Discriminative mapping, 84	ENIGMA Bipolar Disorder working group
Discriminator, 199	(ENIGMA-BP), 58
Disease progression, 49	ENIGMA-BP. See ENIGMA Bipolar
DL. See Deep learning (DL)	Disorder working group
DNNs. See Deep neural networks (DNNs)	(ENIGMA-BP)
Dot products, 177	Ensemble feature selection, 113–115
Double dipping, 34	Ensemble methods, 294–296
DSM. See Diagnostic and Statistical	ε-SVR model, 125
Manual of Mental Disorders (DSM)	Euclidian distances, 243
DSS. See Decision-support system (DSS)	Event-related potentials, 319
DTI. See Diffusion tensor imaging (DTI)	Expanded Disability Status Scale (EDSS), 75
E	"Expected risk", 86
"Earlier IQ", 71–73	Explanatory variables. <i>See</i> Feature set
Early multimodal data integration, 285,	
287–291. See also Intermediate	F
multimodal integration; Late	False negatives (FN), 36
multimodal integration	False positives (FP), 36
jICA, 287–289	Family risk (FR), 322
mCCA, 289–290	FC matrices. See Functional connectivity
mCCA +jICA, 290-291	matrices (FC matrices)
EDSS. See Expanded Disability Status Scale (EDSS)	Feature engineering, 21–28, 157–158, 193, 202–203
EEG. See Electroencephalography (EEG)	dimensionality reduction, 24-25
Effect sizes, 67–68	feature extraction, 24
eHealth technology. See Electronic health	feature selection, 25–28
technology (eHealth technology)	Feature scaling, 360
EHRs. See Electronic health records (EHRs)	feature scaling/normalization, 28

Feature selection, 25–28, 105–106, 229,	G
359–360	Gabor feature space to deep learning
automated, 25–28, 26t	networks, encoding models from,
embedded methods, 105	271–275
feature scaling/normalization, 28	Gabor wavelets, 271–272
feature selection/transformation, 258	Gabor-fwRF models, 273, 274f–275f
filter methods, 105–106	GAINs. See Generative adversarial
manual, 25	imputation networks (GAINs)
method, 146–147	GANs. See Generative adversarial
wrapper methods, 106	networks (GANs)
Feature-weighted receptive field model	Gaussian mixture model (GMM), 236–237
(fwRF model), 277, 278f	comparison of <i>K</i> -means with, 238–240
Features, 101–102	Gaussian noise, 268–269
aggregation, 315–318	Gaussian prior, 89–90
extraction, 24, 357	GD. See Gradient descendant (GD)
hierarchical features, 175	General linear model (GLM), 112b
map, 177, 273	General linear regression, 70–71
reduction using ROI, 112b	Generalizability, 6–7
set, 21–23	Generalized linear model, 147–148
vector, 22–23	Generative adversarial imputation
FEP. See First episode of psychosis (FEP)	networks (GAINs), 257
Filter, 177	Generative adversarial networks (GANs),
count, 180	257, 259–260
methods, 25–27, 105–106, 258	Generative modelling, 194
size, 180	Generator, 199
sliding, 177	Genetic and epigenetic information,
First episode of psychosis (FEP), 152–153	329-330
First principal axis, 210	Genomic data, 141–142
Flatness, 126	GL-MKL. See Group lasso MKL (GL-MKL)
fMRI. See Functional magnetic resonance	GLM. See General linear model (GLM)
imaging (fMRI)	Global minima, 161–163
FN. See False negatives (FN)	GM-f model, 75
"For loop", 359, 365	GMM. See Gaussian mixture model
Forward propagation, 160	(GMM)
FP. See False positives (FP); Frontal pole	Goodness of fit, 21
(FP)	Gradient, 161–162
FR. See Family risk (FR)	Gradient descendant (GD), 160, 163-164
Fractional anisotropy, 107	Graduate Record Examinations (GRE), 67
FreeSurfer, 345–347	Grid search, 277–278
Frontal pole (FP), 135–136	GridSearchCV, 362
Functional connectivity matrices (FC	Group convolution network, 260
matrices), 166	Group lasso MKL (GL-MKL), 146-147
Functional magnetic resonance imaging	Group-level statistics, 25–27
(fMRI), 108–109, 131–132,	Group-level to individual-level
141–142, 240, 267–268, 285–286,	inferences, 5
319	Grouping criterion, 229
functional connectivity states	**
investigation in, 242–243	H
Functioning, 11	Hard clustering, 229
fwRF model. See Feature-weighted	HCs. See Healthy controls (HCs)
receptive field model (fwRF model)	Healthy aging, 218, 221

Healthy controls (HCs), 106–107, 143–144,	Intermediate multimodal integration, 285,
217, 345–347	291–294. See also Early multimodal
using brain morphometry to classifying	data integration; Late multimodal
patients with, 345–347	integration
Heterogeneity, 53-55, 249-251	deep learning, 293–294
algorithms and procedures, 260–262	kernel-based methods, 291-292
data simulation, 251–253	Intermediate-level approaches, 256–257
recognizing, 8	International Classification of Diseases
High-dimensional data, 160, 267	(ICD), 52, 309
Hold-out method, 29	Interpretability, 165, 311-313, 318-320
Homogeneity score, 238, 238t	Interpretability of machine learning,
Human learning, 1–2	337-338
to machine learning, 2-4	Interpretation, 216–217
Hyperbolic tangent activation, 159-160	Alzheimer's disease pattern, 217f
Hyperparameters, 31, 107	Interrater reliability, 52
optimization, 360–362	Intracranial volume (ICV), 75
tuning, 32, 160, 165–166	IQ. See Intelligence quotient (IQ)
Hyperplane, 101–103, 102f, 106–107, 109, 125–126	isnull() function, 351
123-120	Ţ
I	Joint independent component analysis
	(iCA) 287 280 280f
ICA. See Independent component analysis (ICA)	(jICA), 287–289, 289f
ICD. See International Classification of	K
Diseases (ICD)	k-fold CV, 29–31
ICs. See Independent components (ICs)	K-means, 230–240, 242–243
ICV. See Intracranial volume (ICV)	algorithm, 230
Illness onset prediction, 46–48	cluster validation, 230-234
ImageNet competition. See "ImageNet	K-nearest neighbours (KNNs), 212,
Large Scale Visual Recognition	256-257
Challenge" event	Kernel, 141–142
"ImageNet Large Scale Visual Recognition	functions, 143-144
Challenge" event, 173	kernel-based data integration
Imputation methods, 253-254, 257	approaches, 285–286
"In-sample" analyses, 73	kernel-based machine learning
Indentation, 359	algorithms, 141–142
Independent component analysis	kernel-based methods, 291-292
(ICA), 24–25, 152, 242–243,	MKL, 292
287—288	unweighted simple sum of kernels, 292
Independent components (ICs), 288	linear, 141–142
Independent variables. See Feature set	methods, 104
Inference stage, 89–90	space, 127–128
Inner CV, 32, 345–347	SVR, 127–129
Input space, 268–269	trick, 71, 91, 105, 127-128, 143-144
Intelligence, 68	types, 150-151
Intelligence quotient (IQ), 67–68	KNNs. See K-nearest neighbours (KNNs)
explanation of, 73–74	Knowledge leakage, 345–347
prediction of, 73–74	0, 020
test, 70	L
Intercept, 69	Labels, 10

Language as marker of psychiatric and	limitations, 72–73
developmental disorders, 321–322	multiple regression, 71–72
Language impairment, 74, 77	prediction vs. explanation, 73–74
prediction after stroke, 77–79	scatter plots of earlier IQ, 68f
Lasso penalty, 88	simple regression, 69–70
Late multimodal integration, 285, 294–296.	Linear SVM, 83–84, 102–103
See also Early multimodal data	Linear SVR model, 135–136
integration; Intermediate multimodal	Linear ε -SVR model, 126–127
integration	Linear ν-SVR algorithm, 132–133
majority voting, 296	Local connectivity, 174-175
soft voting, 295–296	Local kernel approach, 147-148
"Later IQ", 71–73	Local minima, 163
Lateral orbitofrontal (IOFC), 135-136	IOFC. See Lateral orbitofrontal (IOFC)
Laterality index (LI), 318	Log loss, 85–86
Layer-wise structure, 159–160	Logistic activation function, 86
Learning	Logistic regression, 85–86, 141–142
rate, 161–162	LOOCV approach. See Leave-one-out
decay, 161–162	cross-validation approach (LOOCV
types, 9	approach)
Leave-one-out cross-validation approach	LOSO procedure. See Leave-one-site-out
(LOOCV approach), 29-31, 30f,	procedure (LOSO procedure)
77–78	Loss function, 85–86, 160–161, 268–269
Leave-one-site-out procedure (LOSO	Loss landscape, 161–162
procedure), 94	Low signal-to-noise ratio, 258–259
Leave-one-subject-out cross-validation,	Lower-dimensional space, 196
134-135	Lp-norm MKL, 146–147
154 155	Ep 1101111 14111E, 110 117
	Ep norm vines, 110 117
LI. See Laterality index (LI) Linear classification models, 83–84	M
LI. See Laterality index (LI)	M
LI. See Laterality index (LI) Linear classification models, 83–84	
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87	M Machine learning, 1–2, 4–5, 21, 101, 231,
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning—based decision
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning—based decision support system, 55–56
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms, 145–147	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning–based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms,	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning–based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41 training, 28–35
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms, 145–147 Linear regression analysis, 67, 123–124,	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning–based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41 training, 28–35
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms, 145–147 Linear regression analysis, 67, 123–124, 268–269	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning–based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms, 145–147 Linear regression analysis, 67, 123–124, 268–269 applications to brain disorders, 74–79 predicting cognitive decline in AD, 76–77	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning–based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41 training, 28–35 pipeline implementing in tutorial, 346f
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms, 145–147 Linear regression analysis, 67, 123–124, 268–269 applications to brain disorders, 74–79 predicting cognitive decline in AD,	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning–based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41 training, 28–35 pipeline implementing in tutorial, 346f post hoc analysis, 41–42
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms, 145–147 Linear regression analysis, 67, 123–124, 268–269 applications to brain disorders, 74–79 predicting cognitive decline in AD, 76–77	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning–based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41 training, 28–35 pipeline implementing in tutorial, 346f post hoc analysis, 41–42 problem formulation, 22–23
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms, 145–147 Linear regression analysis, 67, 123–124, 268–269 applications to brain disorders, 74–79 predicting cognitive decline in AD, 76–77 predicting disease progression in MS,	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning—based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41 training, 28–35 pipeline implementing in tutorial, 346f post hoc analysis, 41–42 problem formulation, 22–23 relevant to brain disorders, 5–8
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear Gaussian process models, 83–84 Linear MKL combination algorithms, 145–147 Linear regression analysis, 67, 123–124, 268–269 applications to brain disorders, 74–79 predicting cognitive decline in AD, 76–77 predicting disease progression in MS, 74–76 predicting language impairment after stroke, 77–79	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning—based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41 training, 28–35 pipeline implementing in tutorial, 346f post hoc analysis, 41–42 problem formulation, 22–23 relevant to brain disorders, 5–8 steps of standard supervised machine
LI. See Laterality index (LI) Linear classification models, 83–84 applications to brain disorders, 91–96 empirical risk minimization, 85–87 extensions to nonlinear models, 91 fundamentals and notation, 85 mapping discriminating pattern, 90–91 optimization, 88–89 probabilistic classification, 89–90 regularization, 87–88, 87t Linear classifier, 102–103 Linear discriminant analysis, 83–84 Linear Gaussian process models, 83–84 Linear kernel, 141–142 Linear MKL combination algorithms, 145–147 Linear regression analysis, 67, 123–124, 268–269 applications to brain disorders, 74–79 predicting cognitive decline in AD, 76–77 predicting disease progression in MS, 74–76 predicting language impairment after	M Machine learning, 1–2, 4–5, 21, 101, 231, 267, 329–330, 343 algorithms, 107, 360–362 applications to brain disorders, 330–331 data preparation, 23 diagnostic evaluation, 48 ethical tensions from using machine learning in brain disorders, 331–338 feature engineering, 23–28 human learning to, 2–4 machine learning–based decision support system, 55–56 methods, 123–124, 157–158, 167, 307–308 models, 249 evaluation, 36–41 training, 28–35 pipeline implementing in tutorial, 346f post hoc analysis, 41–42 problem formulation, 22–23 relevant to brain disorders, 5–8 steps of standard supervised machine learning pipeline, 22f

tunes 0 12 0f	mHoalth tochnology Cos Mobile health
types, 9–13, 9f	mHealth technology. See Mobile health
reinforcement learning, 13	technology (mHealth technology)
semisupervised learning, 12	Mild cognitive impairment (MCI), 4,
supervised learning, 9–11	46–47, 76, 110–111, 149, 168, 299
unsupervised learning, 11–12	to AD, 110–112
MAE. See Mean absolute error (MAE)	A-priori regions of interest, 111f
Magnetic resonance imaging (MRI),	feature reduction using ROI, 112b
22–23, 47, 72, 85, 124, 176, 218, 257–259, 307–308, 329–330,	Min-max scaling, 28 Mini-Mental State Examination (MMSE), 76
345–347	Missing at random (MAR), 254
acquisition techniques, 131–132	Missing completely at random (MCAR),
Major depressive disorder (MDD),	254
106–107	Missing data, 249, 251
Manhattan distances, 243	algorithms and procedures, 253–257
MANOVA. See Multivariate analysis of	mechanism and model, 254
variance (MANOVA)	simulation, 251–253
Manual feature selection, 25	Missing not at random (MNAR), 254
Mapping discriminating pattern, 90–91	MKL. See Multi-kernel learning (MKL);
MAR. See Missing at random (MAR)	Multiple kernel learning (MKL)
Markov chain Monte Carlo methods,	MLM. See Multivariate linear models
89–90	(MLM)
Mass-univariate methods, 5–6	MMD. See Maximum mean discrepancy
Mathematics, 1–2	(MMD)
Matplotlib, 344–345, 347–348, 352–353	MMSE. See Mini-Mental State
Max pooling layer, 182, 182f	Examination (MMSE)
Maximum margin principle, 143–144	MNAR. See Missing not at random
Maximum mean discrepancy (MMD), 150	(MNAR)
MCAR. See Missing completely at random	MNI. See Montreal Neurological Institute
(MCAR)	(MNI)
mCCA. See Multimodal canonical	Mobile health technology (mHealth
correlation analysis (mCCA)	technology), 334–335
MCCA. See Multiset canonical correlation	Mobility measures, 334–335
analysis (MCCA)	Model
mCCAR. See Multimodal canonical	averaging, 259
correlation analysis with reference	class, 268–269
(mCCAR)	coefficients, 362
MCI. See Mild cognitive impairment	fitting, 272—273
(MCI)	selection, 32
MDD. See Major depressive disorder	Model evaluation, 36–41
(MDD)	classification, 36–40
Mean absolute error (MAE), 40	accuracy, 37–38 multiclass classification, 39–40
Mean rule, 145 Mean squared error (MSE), 40	ROC and area under curve, 38–39
Mean/median/mode imputation, 256	sensitivity/true positive rate/recall, 38
Measurements, 309–313	specificity/true negative rate, 38
instruments, 307–308	regression, 40–41
suboptimal, 310–311	Model training, 28–35
Medial orbitofrontal (mOFC), 135–136	bias-variance trade-off, 34–35
Medial prefrontal cortex (mPFC), 135–136	cross-validation, 29–33
Medial temporal lobe (MTL), 216	implementing data transformations in
Mental imagery, 279	machine learning pipeline, 34
Mental privacy, 335–336	training and test sets, 29

mOFC. See Medial orbitofrontal (mOFC)	Multiset canonical correlation analysis
Montreal Neurological Institute (MNI),	(MCCA), 113–115
215-216	Multivariable regression model, 75
mPFC. See Medial prefrontal cortex (mPFC)	Multivariate analysis of variance (MANOVA), 5–6
MRI. See Magnetic resonance imaging	Multivariate approach, 5–6
(MRI)	Multivariate linear models (MLM), 214,
MS. See Multiple sclerosis (MS)	218–219, 221
MSE. See Mean squared error (MSE)	Multivoxel pattern analysis (MVPA),
MTL. See Medial temporal lobe (MTL)	108-109
Multiclass classification, 39-40	**
Multicollinearity, 72	N
Multimodal Brain Tumor Image	Natural images, 176
Segmentation Benchmark (BRATS),	Nested cross-validation, 31–32
186	"Neural convergence" theories, 77–78
Multimodal canonical correlation analysis	Neuroanatomical age, 133–134
(mCCA), 287, 289–290, 291f	Neurocognitive profiles, 240, 242
mCCA + jICA, 290–291, 292f	Neuroethics, 335–336
Multimodal canonical correlation analysis	Neuroimaging, 5–6, 329–331, 335–336,
with reference (mCCAR), 298	356
Multimodal diagnostic system, 113–115	data, 148–149
Multimodal integration, 283–284, 286f	to predicting brain age, 319–321
application to brain disorders, 296–301	SVM in, 108–109
data fusion in schizophrenia and	techniques, 283–284, 284f
bipolar disorder, 298	Neurological disorders, 218–221, 250, 331
multimodal neuroimaging studies with deep learning in AD, 299–301	challenges in machine learning studies 50–55
multimodal studies with kernel-based	Neurology, 50
and ensemble methods, 297–298	NeuroMiner, 343
early multimodal data integration,	Neuropsychologically normal cluster, 242
287–291	"Neurorights", 335–336
intermediate multimodal integration,	Neuroscience, 1–2
291–294	Noise, 268–269, 308–309
late multimodal integration, 294-296	sources in machine learning, 309–311
Multimodal machine learning studies,	choice of features, 310–311
286–287	choice of machine learning
Multimodality approach, 46-47	algorithm, 311
Multiparametric maps, 221	choice of target variable, 309–310
Multipeak distribution, testing for,	data processing, 311
233–234	distribution, 268–269
alternatives to K-means, 236–240	Nonlinear function, 181
main drawbacks of K-means, 234-236	Nonlinear mapping, 91, 271
Multiple kernel learning (MKL), 141-148,	Nonlinear MMD mapping function, 150
142f, 292, 293f	Nonlinear models, extensions to, 91
advanced MKL methods, 147-148	Nonlinear relationship, 269
applications to brain disorders, 148-153	Nonlinear ε-SVR, 128
linear MKL combination algorithms,	Nonlinearity layer for CNNs, 181
145-147	Normalization, 360
Multiple local minima, 163–164	Numerical Operations score, 134–135
Multiple regression, 71–72	Numpy, 344–345, 347–348
Multiple sclerosis (MS), 74	"Nurture" theory, 68–69
predicting disease progression in, 74-76	-

O	PLS. See Partial least squares (PLS)
OASIS database. See Open Access Series of	pMCI. See Progressive MCI (pMCI)
Studies database (OASIS database)	pNC. See Progressive normal controls
OLS. See Ordinary least squares (OLS)	(pNC)
Omic data, 212	Pooling, 250–251
Open Access Series of Studies database	layer for CNNs, 182
(OASIS database), 150	pooled sample of controls, 262
Optimal hyperplane, 143–144	Positive and Negative Syndrome Scale
Optimization, 88–89	(PANSS), 312–313, 323
Ordinary least squares (OLS), 70	Positron emission tomography (PET),
"Out-of-sample" analyses, 73	148-149, 167-168
Overfitting, 6–7, 24, 34–35, 103–104,	Post hoc analysis, 41–42, 364–368
108–109, 164	identifying most informative features,
,	41-42
P	significance testing, 41
Padding, 181, 181f	PPMI. See Parkinson's Progression
Pairwise deletion, 255–256	Markers Initiative (PPMI)
Pandas, 344–345, 347–348	Pretraining, 194, 201
PANSS. See Positive and Negative	Principal component analysis (PCA), 12,
Syndrome Scale (PANSS)	24-25, 132-133, 194, 209-210, 209f,
Parameter selection using cross-	215t, 216f-217f, 242-243, 314-315,
validation, 131	318, 321
Parkinson's disease (PD), 148–149, 219	applications to brain disorders, 218–221
diagnostic classification of, 150–151	based MLM analysis, 222f
Parkinson's Progression Markers	dimension reduction and variance,
Initiative (PPMI), 58, 150–151	213–214
Pars orbitalis (Pars Orb), 135–136	data, analysis, and results, 215–216
Partial least squares (PLS), 214, 215t	dataset with dementia patients,
Pathlib module, 347–348	215–217
Patient	for discriminative analyses, 219f
future disease, 203	extensions of, 214
	interpretation, 216–217
privacy, 334–335 Patient Health Questionnaire depression	method description, 212–217
<u> •</u>	singular value decomposition and
scale (PHQ-8 depression scale), 205–206	covariance matrices, 212–213
	rank-1 decomposition, 211f
PCA. See Principal component analysis	Probabilistic approaches, 84, 89–90
(PCA)	Probabilistic classification, 89–90
PD. See Parkinson's disease (PD) PDAT. See Probable dementia of	
	Probable dementia of Alzheimer type (PDAT), 110–111
Alzheimer type (PDAT)	
Pearson correlation coefficient, 25–27	Prognostic prediction, using clinical
Penalized linear models, 87, 89–90	Prognostic prediction, using clinical variables for, 322–323
Penalized logistic regression, 83–84	
Penalized regression methods, 84	Progressive normal controls (nNC), 168
Permutation testing, 41, 364–365	Progressive normal controls (pNC), 168 PRoNTo, 343
PET. See Positron emission tomography	
(PET)	Psychiatric disorders, 49, 218–219, 250,
PHQ-8 depression scale. See Patient	331
Health Questionnaire depression	challenges in machine learning studies, 50–55
scale (PHQ-8 depression scale)	Psychiatry, 50
Pixel space, 268—269	Psychology, 1–2
Plateau, 34–35	1 5 y C1 10 10 g y, 1 2

Psychosis	ROC. See Receiving operating curve
diagnostics classification of, 151-153	(ROC)
multimodal studies with kernel-based	ROIs. See Regions of interests (ROIs)
and ensemble methods in, 297-298	Root mean squared error (RMSE), 40
Python, 344–345	Rostral anterior cingulate cortex (rACC), 135–136
R	rsfMRI. See Resting state fMRI (rsfMRI)
R-squared approach (R ² approach), 41	g
R ² approach. See R-squared approach	S
(R ² approach)	Saddle points, 163–164
rACC. See Rostral anterior cingulate cortex	Sample code, 347–368
(rACC)	data preparation, 349–357
Radial basis function kernels (RBF	class imbalance, 352
kernels), 129	confounding variables, 352-356
Radical behaviorism, 2–3	feature set and target, 356-357
RBF kernels. See Radial basis function	loading data, 349–351
kernels (RBF kernels)	missing data, 351-352
read_csv() function, 349	feature engineering, 357–360
Receiving operating curve (ROC), 38–39	importing libraries, 347–348
Receptive field, 174–175, 178, 180, 277	model evaluation, 363–364
Recursive feature elimination (RFE), 106,	model training, 360-362
113-115	organizing workspace, 348-349
algorithm, 27	post hoc analysis, 364–368
Regions of interests (ROIs), 109, 144, 318,	problem formulation, 349
320-321	results, 368
feature reduction using, 112b	setting random seed, 348
Regression, 40–41	Scaling/normalization, 34
algorithm, 11	Schizophrenia (SZ), 309, 345-347
analysis, 123	using brain morphometry to classifying
coefficients, 90-91	patients with, 345–347
MAE, 40	brain-based diagnostics of, 112-115
models, 67–69, 74	classification of, 94–96, 166–167
MSE, 40	data fusion in, 298
R ² approach, 41	predicting deviations from "brain age" in,
RMSE, 40	132–133
Regularization, 87–88, 87t, 258, 268–269	"School ranking", 71–72
penalty, 27–28	Scikit-learn (sklearn), 344–345, 347–348,
techniques, 27–28	361
Reinforcement learning, 2–3, 13, 101	SD. See Standard deviation (SD)
"Relevance vector machine", 89–90	Seaborn, 344–345, 347–348
Reliability, 308–309, 319	Searchlight approach, 113
of diagnosis, 52–53	Searchlight MVPA approach, 113
ReLU function's gradient, 181	Second principal axis, 209f, 210
Representation learning methods,	Seizure detection, 187–188
193–194	Semisupervised learning, 12, 101, 228–229
Response mechanism or model, 254	Sensitivity (sens), 358
Resting state fMRI (rsfMRI), 113–115	sensitivity/true positive rate/recall, 38
RFE. See Recursive feature elimination	Separability, 315–316
(RFE)	measurement between two groups, 313–314
Ridge regression, 87 RMSE. See Root mean squared error	Sequential feature selection methods,
(RMSE)	113–115

Shapiro–Wilk test, 354–355	Stable MCI (sMCI), 168
Shared agency, 332–333	Stable normal controls (sNC), 168
Sigmoid function, 181	Stacked feature maps, 178, 179f
Significance testing, 41	Standard deviation (SD), 360
Silhouette scores, choosing <i>K</i> with,	Starting weights, 163–164
232-233	State-of-the-art machine learning
Similar-go-together principle, 267-268	approaches, 3
Similarity metric, choice of, 229	Statistical methods, 67, 147–148
Simple models, 258	Statistical Parametric Mapping software
Simple regression, 69–70	(SPM12), 215–216
Simplest loss function, 85	Statistical tests, 23
Simulation-based augmentation, 259-260	Statistics, 1–2
Single dot product, 177, 177f	Step-by-step tutorial, 343-344
Single neuroimaging technique, 283–284	using brain morphometry to classifying
Single Photon Emission Computerized	patients with SZ and HC, 345-347
Tomography (SPECT), 150-151	installing Python and main libraries,
Single-nucleotide polymorphism (SNP),	344-345
297, 307-308	sample code, 347–368
Singular value decomposition (SVD),	Stimulus, 275–276
212-213	Stratified cross-validation
sklearn. See Scikit-learn (sklearn)	(Stratified CV), 33
Small sample sizes, 249, 251	Stride size, 180, 180f
algorithms and procedures, 257–260	Stroke, predicting language impairment
data simulation, 251–253	after, 77—79
sMCI. See Stable MCI (sMCI)	Structural equation modeling, 287
sMRI. See Structural magnetic resonance	Structural magnetic resonance imaging
imaging (sMRI)	(sMRI), 72, 141–142, 167–168,
sNC. See Stable normal controls (sNC)	185-186, 283-284, 307-308, 319
Snippets, 345	Structural neuroimaging, 74
SNP. See Single-nucleotide polymorphism	Structural regularization, 276–278
(SNP)	Structured sparsity, 94
Sociability measures, 334–335	"Suboptimal" measurements, 310-311
Soft clustering, 229	Sum of squared error (SSE), 231–232
Soft margin, 103–104	Supervised learning, 9–11, 21, 22f, 101.
Soft voting, 295–296	See also Unsupervised learning
Softmax function, 160	classification, 10
Space-feature separability, 277	models, 309-310
Sparse penalties, 88	regression, 11
Sparsity, 84, 88	Support vector machine (SVM), 83–84, 88,
constraint, 197	94–96, 101–104, 123, 141–142, 157,
Spatial invariance, 175	212, 285–286, 292, 322
Specificity (spec), 358	applications to brain disorders, 109–116
specificity/true negative rate, 38	model, 345–347, 361–362
SPECT. See Single Photon Emission	in neuroimaging, 108–109
Computerized Tomography	stages, 104–108
(SPECT)	evaluating SVM performance, 107–108
Speech comprehension, 77	feature selection, 105–106
Speech production, 77	training and testing classifier, 106–107
SPM12. See Statistical Parametric Mapping	Support vector regression (SVR), 123,
software (SPM12)	125–126
SSE. See Sum of squared error (SSE)	applications to brain disorders, 131–136

Support vector regression (SVR) (Continued) graphic representation of linear ε -SVR	Two-dimension (2D) distributions, 228–229
models, 125f	grid structure, 176
kernel SVR, 127–129	Typically developed controls (TDC), 93
linear ε-SVR model, 126–127	Typically developing children (TD
parameter selection using cross-	children), 322
validation, 131	U
V-SVR model, 129–131	
SVD. See Singular value decomposition	U-Net, 187
(SVD) SVM See Support vector machine (SVM)	UK Biobank, 8, 250–251, 259 Uncorrelated PANSS Score Matrix
SVM. See Support vector machine (SVM) SVR. See Support vector regression (SVR)	(UPSM), 323
Symmetric data fusion, 287	Underfitting, 34–35
Systematic heterogeneity, 260	Unsupervised dimensionality reduction,
SZ. See Schizophrenia (SZ)	321
22. 300 Seta20pTaetaa (22)	Unsupervised learning, 11–12, 101.
T	See also Supervised learning
t-tests, 25-27	cluster analysis, 11
filtering, 113–115	dimensionality reduction, 12
T1-weighted MR images, 133-134	Unsupervised methods, 318
T1-weighted structural MRI,	Unweighted simple sum of kernels, 292,
131-132	293f
T2-weighted structural MRI, 131–132	v-SVR model, 129–130
tanh function, 181	UPSM. See Uncorrelated PANSS Score
Target variable, 22–23	Matrix (UPSM)
Targeted question, 257–258	V
Task, 22–23	•
TD children. See Typically developing	Validation, 32. See also Cross-validation
TD children. See Typically developing children (TD children)	Validation, 32. See also Cross-validation (CV)
TD children. See Typically developing children (TD children) TDC. See Typically developed controls	Validation, 32. <i>See also</i> Cross-validation (CV) cluster, 230–234
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC)	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory),
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF)	Validation, 32. <i>See also</i> Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267—268 3D CNN model, 299	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP)	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders,
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP) Tractography, 135–136 Training, 32 procedure, 268–269	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders, 278–279 encoding models from Gabor feature space to deep learning networks,
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP) Tractography, 135–136 Training, 32 procedure, 268–269 regularization, 275–276	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders, 278–279 encoding models from Gabor feature space to deep learning networks, 271–275
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP) Tractography, 135–136 Training, 32 procedure, 268–269 regularization, 275–276 set, 29	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders, 278–279 encoding models from Gabor feature space to deep learning networks, 271–275 fitting encoding model
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP) Tractography, 135–136 Training, 32 procedure, 268–269 regularization, 275–276 set, 29 Transfer learning, 259, 263	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders, 278–279 encoding models from Gabor feature space to deep learning networks, 271–275 fitting encoding model structural regularization, 276–278
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP) Tractography, 135–136 Training, 32 procedure, 268–269 regularization, 275–276 set, 29 Transfer learning, 259, 263 Transparency of machine learning,	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders, 278–279 encoding models from Gabor feature space to deep learning networks, 271–275 fitting encoding model structural regularization, 276–278 training regularization, 275–276
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP) Tractography, 135–136 Training, 32 procedure, 268–269 regularization, 275–276 set, 29 Transfer learning, 259, 263 Transparency of machine learning, 336–337	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders, 278–279 encoding models from Gabor feature space to deep learning networks, 271–275 fitting encoding model structural regularization, 276–278
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP) Tractography, 135–136 Training, 32 procedure, 268–269 regularization, 275–276 set, 29 Transfer learning, 259, 263 Transparency of machine learning, 336–337 Treatment response, 49	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders, 278–279 encoding models from Gabor feature space to deep learning networks, 271–275 fitting encoding model structural regularization, 276–278 training regularization, 275–276 Voxels, 108–109
TD children. See Typically developing children (TD children) TDC. See Typically developed controls (TDC) Test set, 29 TF. See True negatives (TF) Theory-driven approaches, 7 This-then-that principle, 267–268 3D CNN model, 299 Tikhonov regularization. See Ridge regression Top-down approaches, 7 TP. See True positives (TP) Tractography, 135–136 Training, 32 procedure, 268–269 regularization, 275–276 set, 29 Transfer learning, 259, 263 Transparency of machine learning, 336–337	Validation, 32. See also Cross-validation (CV) cluster, 230–234 Vapnik-Chervonenkis theory (VC theory), 125 Variance, 213–214 VGG model, 182–183 VGG16 model, 182–183, 183f "Vibration" effects, 91–92 Voxel-based gray matter density (VBM), 319–321 Voxel-wise encoding models, 267–278 applications to brain disorders, 278–279 encoding models from Gabor feature space to deep learning networks, 271–275 fitting encoding model structural regularization, 276–278 training regularization, 275–276

Ward's linkage, 240–241 Weighting function, 147–148 Weights, 145 of kernels, 150–151 WM-f model, 75 Wrapper methods, 27, 106, 258 Y Yale—Brown Obsessive—Compulsive Scale (Y-BOCS), 241—242

Z z-score normalization, 28