Cambridge University Press & Assessment 978-1-108-42578-0 - Bayesian Optimization Roman Garnett Index More Information

INDEX

Primary references and definitions are indicated in bold.

Α

a posteriori methods, 270, 272, 274 a priori methods, 270, 273 acquisition function, $\alpha(x; \mathcal{D})$, 11, 88, 94, 96, 98, 150, 247, see also expected improvement; knowledge gradient; mutual information; probability of improvement; upper confidence bound batch, $\beta(\mathbf{x}; \mathcal{D})$, 252 gradient, 158, 208 optimization, 207 action space, A, 90, 245 for batch observations, 252 for dynamic termination, 104 for multifidelity optimization, 263 for optimization with fixed budget, 91 for sequential procedures, 281 for terminal recommendation, 250 for terminal recommendations, 110 active learning, 136, 275 active search, 115, 283 adaptivity gap, 254 additive decomposition, 63, 83 aerospace engineering, applications in, 325 algorithm configuration, 246, 327 anytime algorithm, 209, 239, 248 approximate dynamic programming, 100, 150, 284 augmented Chebyshev scalarization, 274 automated machine learning (automL), 263, 328, see also hyperparameter tuning automatic relevance determination (ARD), 57, 62, 241 automobile engineering, applications in, 326 В

bandits, see multi-armed bandits batch observations, 252, 262 connection to sequential observations, 254 batch rollout, 103, 152, 154, 284, see also rollout Bayes' theorem, 7 Bayesian decision theory, 10, 89, 124 isolated decisions, 90

sequential decisions dynamic termination, 103 fixed budget, 91 multi-armed bandits, 143 Bayesian inference introduction to, 6 of objective function, 8 Bayesian information criterion, 79, 83 Bayesian neural networks, 198, 281 Bayesian Occam's razor, 71 Bayesian quadrature, 33, 278 Bayesian regret, $\mathbb{E}[r_{\tau}]$, $\mathbb{E}[R_{\tau}]$, 218, 224, 240 Bellman equation, see Bellman optimality Bellman optimality, 94, 99 beta warping, 58 BINOCULARS algorithm, 153 biology, applications in, 318 biomedical engineering, applications in, 320 Bochner's theorem, 50 branch and bound, 232, 240

C

central composite design, 76, 81 certainty equivalent, 111 characteristic length scale, see length scale chemistry, applications in, 288, 313 chemoinformatics, 314 Cholesky decomposition, 201, 258 low-rank updates, 202 civil engineering, applications in, 323 сма-es algorithm, 208 combinatorial optimization, 209 compactness of domain, 34 conditional entropy, $H[\omega \mid D]$, 115, see also entropy conditional mutual information, $I(\omega; \psi \mid \mathcal{D})$, 137, see also mutual information confidence interval, 225, 233, 237 conformational search, 315 conjugate gradients, 203 constant liar heuristic, 256 constrained optimization, 249 constraint functions, 249 unknown, 249 constraints on objective function, 36, 39, 56 continuity in mean square, 29, see also sample path continuity

Cambridge University Press & Assessment 978-1-108-42578-0 — Bayesian Optimization Roman Garnett Index More Information

354 INDEX

continuous differentiability, 31, 221 cost-aware optimization, 103, 245, 253, 265 covariance function, *see* prior covariance function cross-covariance function, **19**, 23, 24, 27, 30, 201, 264 cumulative regret, R_{τ} , 145, 214 cumulative reward, **11**, 142, 155, 215, 283 curse of dimensionality, 61, 208, 285

D

de novo design, 314 decoupled constraint observations, 252 deep kernel, 59, 61 deep neural networks, ix, 1, 59, 61, 292 density ratio estimation, 197 design and analysis of computer experiments (DACE), 290 determinantal point process, 261, 285 differentiability in mean square, 30, see also continuous differentiability differential entropy, $H[\omega]$, see entropy dilation, 56 DIRECT algorithm, 208 disjoint union, 27 drug discovery, see molecular design dynamic termination, see termination decisions

Е

early stopping, 210, 281 electrical engineering, applications in, 324 elliptical slice sampling, 38 embedding, see linear embedding, neural embedding entropy search, see mutual information entropy, $H[\omega]$, 115, see also conditional entropy environmental variables, 277 expectation propagation, 39, 182, 190, 273, 302 expected gain per unit cost, 248 expected hypervolume improvement (EHVI), 271 expected improvement, $\alpha_{\rm EI}$, 81, 95, 113, 117, 127, 151, 158, 193, 196, 199, 265, 266, 268, 286, see also simple reward augmented, 166 batch, 259 comparison with probability of improvement, 132 computation with noise, 160

alternative formulations, 163 gradient, 308 computation without noise, 159 gradient, 159 convergence, 217 modified, 154 origin, 289 worst-case regret with noise, 239, 243 expected utility, 90, 93 exploration bonus, 145 exploration vs. exploitation dilemma, 11, 83, 123, 128, 131, 133, 143, 145, 146, 148, 154, 159, 214, 293 exponential covariance function, $K_{M^{1/2}}$, 52, 219 extreme value theorem, 34

F

factor graph, 37 Fano's inequality, 231 feasible region, \mathcal{F} , 249 figure of merit, *see* acquisition function fill distance, δ_x , 238 Fourier transform, 50, 53, 236 freeze-thaw Bayesian optimization, 281 fully independent training conditional (FITC) approximation, 207

G

Gauss-Hermite quadrature, 172, 258 gradient, 309 Gaussian process (GP), $GP(f; \mu, K)$, 8, 16, 95, 124, see also prior mean function; prior covariance function approximate inference, 35, see also sparse spectrum approximation; sparse approximation classification, 41, 283 computation of policies with, 157 continuity, 28 credible intervals, 18 differentiability, 30 exact inference, 19 additive Gaussian noise, 20, 23 computation, 201 derivative observations, 32 exact observation, 22 interpretation of posterior moments, 21 joint, see joint Gaussian process marginal likelihood $p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta})$, 72, 202, 220

CAMBRIDGE

Cambridge University Press & Assessment 978-1-108-42578-0 — Bayesian Optimization Roman Garnett Index More Information

INDEX 355

gradient, 307 maxima, existence and uniqueness, 33 mixture, 38, 75, 193 model assessment, selection, and averaging, 67 modeling, 45 posterior predictive distribution, 25, 157, 208 gradient, 307 sampling, 18 gene design, 319 generalized additive models, 63 generalized linear models, 41 GLASSES algorithm, 152 global reward, 113, 117, 129, 172, see also knowledge gradient GP-SELECT algorithm, 285 Gram matrix, $K(\mathbf{x}, \mathbf{x})$, 17, 49 grid search, 3, 240

Η

Hamiltonian Monte Carlo (HMC), 75 Heine–Borel theorem, 30 heteroskedastic noise, 4, 23, 166 Hölder continuity, 35, 221, 240 horizon, 93, 125, 151, 245, 254 hubris of youth, ix human–computer interfaces, 329 hyperband algorithm, 282 hyperparameter tuning, 1, 61, 109, 263, 267, 291, 327 hyperparameters, θ , 68, *see also* length scale; output scale unknown, effect of convergence, 241

I

ill-conditioning, 203 incumbent value, ϕ^* , 128, 159, 251 inducing values, v, 205 infill function, see acquisition function information capacity, γ_{τ} , 221, 225, 229, 233, 237 bounds, 222 information gain, 115, 117, 135, 180, 187, see also mutual information initialization, 210 instantaneous regret, $\rho_{ au}$, 214, 241 integrated expected conditional improvement, 251 intrinsic dimensionality, 61 inverse problems, 318, 319 isotropy, 50, 54

iterative numerical methods, 203 Iverson bracket, xiii

J

joint Gaussian process, 27, 267, see also cross-covariance function between function and gradient, 30 exact inference, 28 for multifidelity modeling, 264 marginals, 27

Κ

kernel, see prior covariance function kernel, see prior covariance function kernel kernel, 83 knowledge gradient, α_{KG} , 113, **129**, 172, 193, 266, 276, see also global reward batch, 259 computation, 172 discrete domain, 173 gradient, 310 KGCP approximation, 175 origin, 290 Kolmogorov extension theorem, 16 kriging believer heuristic, 256 Kullback–Leibler divergence, $D_{\text{KL}}[p \parallel q]$, 115, 137, 206

L

Laplace approximation, 39, 41, 76, 79, 83, 301 learning curve, 281 length scale, 54, 56, 69, see also automatic relevance determination likelihood, 7, see also observation model marginal, see marginal likelihood limited lookahead, see lookahead line search methods, 285 linear covariance function, K_{LIN} , 54 linear embedding, 58, 62, 209 linear scalarization, 274 linear transformations of domain, 55, 56, 62 of Gaussian processes, 33, see also Bayesian quadrature; joint Gaussian process: between function and gradient Lipschitz continuity, 227, 240, 258 local optimization, 285 local optimum, conditioning a Gaussian process on a, 36, 182 local penalization, 257 lookahead, 101, 125, 150, 284, see also one-step lookahead; two-step lookahead

Cambridge University Press & Assessment 978-1-108-42578-0 — Bayesian Optimization Roman Garnett Index More Information

356 INDEX

low-dimensional structure, 58, 61, 62, 209, 294 low-discrepancy sequence, 177, 211, 239 lower regret bounds Bayesian regret with noise, 230 Bayesian regret without noise, 240 worst-case regret with noise, 236 worst-case regret without noise, 239 Löwner order, **22**, 48

M

Mahalanobis distance, 48, 57, 297 manifold Gaussian process, 59, 61 marginal likelihood, $p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta})$, 71 materials science, applications in, 263, 313 Matérn covariance function, $K_{\rm M}$, **51**, 124, 221, 238, 241 matrix calculus convention, xiii maximum a posteriori inference, see model selection maximum information gain, see information capacity max-value entropy search, α_{MES} , 187 for multiobjective optimization, 273 gradient, 191 mean function, see prior mean function mechanical engineering, applications in, 325 model assessment, 45, 67, 70, see also model posterior model averaging, 74, 116 in acquisition function, 192 multiple model structures, 79 model evidence, see marginal likelihood model posterior, $p(\theta \mid D)$, 71 model prior, $p(\theta)$, 70 model selection, 73, 329 multiple model structures, 79 model space, see model structure model structure, \mathcal{M} , 68, see also hyperparameters posterior, $Pr(\mathcal{M} \mid \mathcal{D})$, 79 prior, $Pr(\mathcal{M})$, 78 search, 81 model, $p(\mathbf{y} \mid \mathbf{x})$, 68 molecular design, 62, 209, 283, 313 molecular fingerprint, 314 Monte Carlo sampling, 37, 75, 84, 181, 187, 258, 273 multi-armed bandits, 141 infinite-armed, 144 optimal policy, 143 origin, 292

multifidelity optimization, 26, **263**, 321 multiobjective optimization, 26, **269** multitask optimization, **266** mutual information, $I(\omega; \psi)$, 116, **135**, 291, *see also* information gain; conditional mutual information with $f_{,}^{*} \alpha_{f^{*}}$, 140, 187, 193, 266, 291, *see also* output-space predictive entropy search; max-value entropy search with $x_{,}^{*} \alpha_{x^{*}}$, 139, 180, 193, 266, 291, *see also* predictive entropy search myopic approximation, *see* lookahead

N

nats, xiii needle in a haystack analogy, 216, 236, 239, 240 neural architecture search, 328 neural embedding, 59, 61, 209 neural networks, 198 no U-turn sampler (NUTS), 76 nonmyopic policies, 150, 284, 294 no-regret property, 145, 215 Nyström method, 207

0

objective function posterior, $p(f \mid D)$, 9, 74, 92, see also Gaussian process: exact inference, approximate inference model-marginal, see model averaging objective function prior, p(f), 8, see also Gaussian process observation costs, 104 unknown, 245 observation model, $p(y \mid x, \phi)$, 4 additive Gaussian noise, 4, 23, 69, 78, 157 additive Student-t noise, 36, 38, 41, 282 exact observation, 4, 22 for unknown costs, 246 observation noise scale, σ_n , 4, 23, 69, 78, 157, 203, 222 one-step lookahead, 94, 102, 126, 171, 245, 247, 251, 252, 283, 289 cost-aware optimization, 106 with cumulative reward, 155 with global reward, see knowledge gradient with information gain, see mutual information

CAMBRIDGE

Cambridge University Press & Assessment 978-1-108-42578-0 — Bayesian Optimization Roman Garnett Index More Information

INDEX 357

with simple reward, see expected improvement optimal design, 287 optimal policy batch observations, 253 computational cost, 99, 125, 284 generic, 245 multi-armed bandits, 143 sequential optimization, 98 optimism in the face of uncertainty, 145 optimization policy, 3, see also acquisition function; grid search; optimal policy; random search; Thompson sampling optimal, see optimal policy Ornstein-Uhlenbeck (OU) process, 52, 174, 290 output scale, 55, 69, 242 output-space predictive entropy search, $\alpha_{\rm OPES}$, 187 gradient, 311

P

Parego algorithm, 275 Pareto dominance, 270 Pareto frontier, 153, 269 Pareto optimality, see Pareto frontier Parzen estimation, 197 periodic covariance function, 35, 58, 60 physics, applications in, 317 plant breeding, 1, 320 posterior distribution, 7 posterior predictive distribution, $p(y \mid x, D)$, 8, 25, 74, 92, 157, 208, 283 for multifidelity modeling, 264 for unknown costs, 246 model-marginal, see model averaging predictive entropy search, α_{PES} , 180 batch, 260 for multiobjective optimization, 273 gradient, 311 preference optimization, 282, 330 prior covariance function, K(x, x'), 17, 49, 67, see also exponential, linear, Matérn, spectral mixture, squared exponential covariance functions; automatic relevance determination addition, 60, 63 multiplication, 60 scaling, 55 warping, 56

prior distribution, 6 prior mean function, $\mu(x)$, 16, **46**, 67 concave quadratic, 48 constant, 47, 69, 124, 207 marginalization of parameter, 47, 69 impact on posterior mean, 46 linear combination of bases, 48 probability of improvement, α_{PI} , **131**, 167, 193, 196, 199 batch, 260 comparison with expected improvement, 132 computation with noise, 169 gradient, 309 computation without noise, 167 gradient, 169 convergence, 217 correspondence with upper confidence bound, 170 origin, 289 selection of improvement target, 133, 289 protein design, 319 pseudopoints, see inducing values

Q

quantile function, $q(\pi)$, 145, 165, 170

R

random embedding, 63 random forests, 196 random search, 3 reaction optimization, 288, 315 regret, 213, see also simple regret; cumulative regret; Bayesian regret; worst-case regret reinforcement learning, applications in, 322 representer points, 180, 188 reproducing kernel Hilbert space (RKHS), \mathcal{H}_K , 219, 224, 232, 242 ккнs ball, $\mathcal{H}_{K}[B]$, 220, 224, 232 RKHS norm, $\|f\|_{\mathcal{H}_K}$, 220 risk neutrality, 111, 127, 250 risk tolerance, 111 risk vs. reward tradeoff, 112, 269 robotics, applications in, 277, 282, 321 robust optimization, 277, 322 rolling horizon, 101 rollout, 102, 151, 263 batch, see batch rollout

S

 \mathcal{S} metric, 271

Cambridge University Press & Assessment 978-1-108-42578-0 — Bayesian Optimization Roman Garnett Index <u>More Information</u>

358 INDEX

safe optimization, 322 sample path continuity, 30, 34, 218, 221 scalarization, 273 second-derivative test, 36, 40 separable covariance function, 264 sequential analysis, 287 sequential experimental design, 288 sequential simulation, 255 signal variance, see output scale simple regret, r_τ, **214**, 215, 216, 230, 237 simple reward, 95, 112, 117, 127, 158, 165, 251, 284, see also expected improvement small data, 68 sparse approximation, 204 sparse spectrum approximation, 51, 178 spectral density, κ , **51**, 53 spectral measure, v, 51, 53 spectral mixture covariance function, $K_{\rm SM}$, 51, 53 spectral points, 178 sphere packing, 238 squared exponential covariance function, K_{SE}, 17, **52**, 221 stationarity, 50, 56, 58, 178, 207, 236 stochastic gradient ascent, 286 stochastic optimization, 277 stochastic process, 8, 16, see also Gaussian process structural search, 316 Student-t process, 282 sub-Gaussian distribution, 233

Т

terminal recommendations, 90, **109**, 118 termination decisions, 5, 253 optimal, 103 practical, 211 termination option, Ø, 104 Thompson sampling, **148**, 176, 181, 187, 195, 259 acquisition function view, 148 batch, 261 computation, 176 origin, 292 regret bounds Bayesian regret with noise, 229 worst-case regret with noise, 233 truncated normal distribution, $\mathcal{TN}(\phi;\mu,\sigma^2,I), 40, 159, 189, 305$ trust region methods, 285 two-step lookahead, 96, 150, 251

U

upper confidence bound, α_{UCB} , 145, 170, 195, 266 batch, 261 computation, 170 correspondence with probability of improvement, 170 gradient, 170 origin, 289 regret bounds Bayesian regret with noise, 225 worst-case regret with noise, 233, 243 selecting confidence parameter, 147 utility function for active search, 283 for constrained optimization, 250 for cost-aware optimization, 104 for isolated decisions, $u(a, \psi, D)$, 90 for multifidelity optimization, 264 for multitask optimization, 268 for optimization, u(D), 93, 109, 245, see also cumulative reward; global reward; simple reward; information gain for terminal recommendations, $v(\phi)$, 111

V

value of data, α_{τ}^* , 95, 101 value of sample information, 126 variational inference, 39, 206 virtual screening, 314 von Neumann–Morgenstern theorem, 90, 120

W

weighted Euclidean distance, 57, see also automatic relevance determination Wiener process, 174, 217, 232, 242, 290 wiggliness, 56, 198, see also length scale worst-case regret, \bar{r}_{τ} , \bar{R}_{τ} , 218, 232, 239