
Index

- Q -process, 54, 108
 - waiting time, 56
- σ -algebra, 5
 - Borel, 8
 - generated by a random variable, 15
 - infinite product, 103
- accessible state, 50
- action functional, 200
- algebra, 282
- Arrhenius's law, 250

- backward stochastic integral, 166, 194
- Bayes's theorem, 7
- Bayesian inference, 90
- BKL algorithm, *see also* kinetic Monte Carlo
- Bochner's theorem, 19
- Boltzmann constant, 12
- Borel-Cantelli lemma, 21, 30
- Brownian bridge, 113, 136
- Brownian dynamics, 171, 234
- Brownian motion on sphere, 172
- Brownian sheet, 136

- central limit theorem, 31
- Chapman-Kolmogorov equation, 47, 55
- characteristic function, 17
- chemical master equation, 264
- chemical potential, 172, 223
- chemical reaction kinetics
 - diffusion approximation, 268
 - multiscale, 272
- closed system, 218

- colored noise, 139
- compound Poisson process, 72
- conditional expectation, 14, 239
- conditional probability, 6
- convergence
 - almost sure, 16
 - in L^p , 16
 - in distribution, 16
 - in probability, 16
 - relations, 17
- coordinate process, 103
- covariance, 9
- covariance function, 235
- Cramér's theorem, 33, 37
- cross-correlation function, 237
- cylinder set, 102

- density of states, 221
- detailed balance, 87, 176
- diffusion coefficient, 118
- diffusion process, 154
- Dirichlet form, 61
- distribution, 8
 - Bernoulli, 7, 24
 - binomial, 8, 24
 - Cauchy-Lorentz, 31
 - exponential, 11
 - Fréchet, 41
 - gamma, 72
 - Gaussian, 11
 - Gibbs, 12, 77, 89, 95, 176, 216, 221, 229, 236
 - Gumbel, 41

- normal, 11
- Poisson, 8, 24
- uniform, 10
- Weibull, 41
- distribution function, 12
- Dynkin's formula, 182
- Dyson's formula, 239
- Ehrenfest's diffusion model, 46
- Einstein relation, 234, 238
- emission matrix, 61
- ensemble
 - canonical, 218, 222, 226
 - grand canonical, 218, 222
 - isothermal-isobaric, 224
 - microcanonical, 218, 225
- entropy
 - Boltzmann, 38, 219
 - Gibbs, 219, 222
 - ideal gas, 227
 - mixing, 225
 - relative, 37
 - Shannon, 26, 43
- ergodic theorem, 52
 - Q -process, 59
 - finite Markov chain, 51
- Euler-Maruyama scheme, 157
 - strong convergence, 161
 - weak convergence, 190
- exit problem, 182, 249
- expectation, 9
- extremal statistics, 40
- Feynman-Kac formula, 180, 207
- filtration, 104
 - augmented filtration, 105, 141
- first passage time, 72
- Fisher-Tippett-Gnedenko theorem, 41
- fluctuation-dissipation relation, 234
- Fokker-Planck equation, 170
 - boundary conditions, 175
- fractional Brownian motion, 114, 136
- free energy, 39
 - Gibbs, 224
 - Helmholtz, 221
 - Landau, 223
- Gärtner-Ellis theorem, 231
- Gaussian process, 109, 242
 - characteristic function, 110
 - covariance function, 109
 - mean function, 109
- Gaussian random field, 212
- generalized Langevin equation, 234, 242
- generating function, 19
 - moment, 20
- generator, *see also* infinitesimal generator
- geometric Brownian motion, 153
- Gibbs distribution, *see also* distribution, Gibbs
- Gillespie's algorithm, *see also* stochastic simulation algorithm
- Girko's circular law, 27
- Girsanov theorem, 206, 207
- grand potential, *see also* free energy, Landau
- Green-Kubo relation, 238
- Hamilton-Jacobi equation, 255
- Hammersley-Clifford theorem, 215
- heat capacity, 222
- hidden Markov model, 61
 - backward algorithm, 65
 - Baum-Welch algorithm, 66
 - forward algorithm, 63
 - Viterbi algorithm, 64
- Hille-Yosida theorem, 287
- HMM, *see also* hidden Markov model
- holding time, 57
- i.o. set, 21
- ideal gas, 226
 - discrete, 227
- independence, 12, 13
- inequality
 - Boole, 6
 - Burkholder-Davis-Gundy, 148
 - Chebyshev, 10
 - conditional Jensen, 15
 - discrete Gronwall, 281
 - Doob's maximal, 151
 - Fenchel, 33
 - Gronwall, 281
 - Hölder, 9
 - Jensen, 10
 - martingale, 285
 - Minkowski, 9
 - Schwartz, 10
- infinitesimal generator, 55, 108, 170, 286
- information theory, 43
- internal energy, 39
- invariance principle, 120
- invariant distribution, 48, 56, 176, 271

- invariant measure, 48
- Ising model, 88, 228, 243
- isolated system, 218
- Itô integral, 140
- Itô isometry, 141, 143
- Itô process, 145
- Itô-Taylor expansion, 156
- Itô's formula, 145, 147
 - discrete, 160
- jump chain, 57
- jump matrix, 57
- jump time, 57
- Kac-Zwanzig model, 240
- Karhunen-Loève expansion, 112
- kinetic Monte Carlo, 91
- Kolmogorov equation
 - backward, 55, 175, 179, 268
 - forward, 55, 171, 264
- Kolmogorov's continuity theorem, 129
- Kolmogorov's extension theorem, 104
- Kullback-Leibler distance, *see also*
 - entropy, relative
- Langevin dynamics, *see also* Langevin equation
- Langevin equation, 153, 233
- Laplace lemma, 34, 279
 - single-sided, 42
- Laplacian matrix, 61
- large deviation theory, 32, 33, 250, 280
- large volume limit, 266
- law of large numbers, 241
 - strong, 30
 - weak, 4, 29
- law of mass action, 263
- Legendre-Fenchel transform, 33, 224, 230, 249
- Lévy's continuity theorem, 19
- likelihood function, 62, 90
- limit theorem, 29
- linear response theory, 236
 - admittance, 238
- Markov chain
 - coarse-graining, 69
 - communicate, 50
 - continuous time, 53, 54
 - discrete time, 46
 - embedded, 57
 - irreducible, 49, 58
 - lumpable, 69
 - primitive, 51
 - reducible, 49
 - reversible, 60
 - stationary, 47
 - time reversal, 59
- Markov process, 106
 - homogeneous in time, 107
 - transition density, 107
 - transition function, 106
 - transition kernel, 107, 126, 179
- Markov random field, 214
- martingale, 148, 151, 284
- maximum entropy principle, 242
- maximum likelihood estimate, 65, 90
- MCMC, *see also* Metropolis algorithm
- mean, 7, 9
- mean first passage time, 183, 249
- measurable
 - \mathcal{F} -measurable, 8, 14
- measurable space, 5, 282
- Mercer's theorem, 111
- metastability, 246
- Metropolis algorithm, 87
 - Gibbs sampling, 89
 - Glauber dynamics, 88
 - Metropolis-Hastings, 90
- Milstein scheme, 158
- minimum action path, 252, 256
- minimum energy path, *see also*
 - minimum action path
- moment, 9, 20
 - exponential, 32
- Monte Carlo integration, 76
- Monte Carlo method, 32
- Mori-Zwanzig formalism, 238
- multilevel Monte Carlo method, 162
- network, 67
 - chemical reaction, 263
 - community structure, 69
- numerical SDEs
 - strong convergence, 159
 - weak convergence, 159, 190
- open system, 218
- order statistics, 26, 72
- Ornstein-Uhlenbeck process, 113, 114, 152, 177, 193
- OU process, *see also*
 - Ornstein-Uhlenbeck process
- over-damped dynamics, 242

- partition function, 12, 221
 - grand, 223
- path integral, 203, 252
- Perron-Frobenius theorem, 50, 230
- phase transition, 231
- Poisson process, 53, 109
 - waiting time, 54
- posterior probability, 7
- pressure, 225
- prior probability, 7
- probability current density, 172
- probability density function, 9
- probability distribution
 - continuous, 8
 - discrete, 7
- probability measure, 5
 - absolutely continuous, 9
- probability space, 5

- quadratic variation, 127
- quasipotential, 254, 256
 - global, 259
 - local, 259

- Radon-Nikodym derivative, 9
- random field, 209
- random number generation, 77
 - acceptance-rejection, 82
 - Box-Muller, 81
 - composition, 81
 - inverse transformation, 79
 - linear congruential generator, 78
 - squeezing acceptance-rejection, 97
- random telegraph process, 185
- random variable, 8
- random vector, 9
- random walk, 46, 118
 - arcsine law, 120
- rare events, 245
- rate function, 33, 39
- reaction rate equation, 262
- reflection principle, 131
- resistor network, 72
- response function, 237
- Runge-Kutta scheme, 158

- semigroup, 108, 178, 286
 - Feller, 179
 - spectral theory, 183
- simple function, 141
- simulated annealing, 94
 - convergence, 96
- simulated tempering, 92
- Smoluchowski equation, 172
- spectral radius, 49
- SSA, *see also* stochastic simulation
 - algorithm
- stable laws, 26, 32
- stationary distribution, *see also*
 - invariant distribution
- stationary measure, *see also* invariant
 - measure
- Stirling's formula, 3
- stochastic differential equation
 - averaging, 185, 275
 - chemical reaction, 265
 - existence and uniqueness, 149
- stochastic matrix, 47
- stochastic process, 102
 - adapted, 105
 - modification, 128
- stochastic simulation algorithm, 57, 266
 - nested SSA, 276
- stoichiometric matrix, 263
- stopping time, 105
- Stratonovich integral, 154
- string method, 253
- strong Markov property, 58, 285

- tau-leaping algorithm, 269
- thermodynamic average, 12, 89
- transfer matrix, 230
- transition kernel, *see also* Markov
 - process, transition kernel
- transition path, 247, 258
- transition probability matrix, 47, 49,
 - 55, 61
- transition rate, 249
- transition state, 247, 260

- uncorrelated random variables, 9

- variance, 7, 9
- variance identity, 26
- variance reduction, 83
 - antithetic variable, 97
 - control variates, 86
 - importance sampling, 84
 - Rao-Blackwellization, 86
 - stratified sampling, 97

- white noise, 139
- Wick's theorem, 26
- Wiener chaos expansion, 132
- Wiener measure, 200

Wiener process, 117, 121, 125
 absorbing wall, 131
 finite-dimensional distribution, 125
 generator, 126
 local law of the iterated logarithm,
 129
 properties, 127
 reflecting barrier, 130
Witten Laplacian, 185
WKB analysis, 248