

Index

- Affine map, 186
- Alpha shape, 6
 - alpha complex, 7
 - dual simplicial complex, 7
- Amino acid residue substitution rates, 78
- Approximation algorithm, 146
 - approximation ratio, 146
- Artificial neural networks, 181
 - application to cellular networks, 185
 - crop simulation modelling, 186
 - reverse engineering of gene regulatory networks, 185
 - architecture, 182
 - computational power, 183
 - feed-forward networks, 183
 - recurrent networks, 183
 - depth, 182
 - feed-forward, 182
 - function computation, 182
 - gate function, 182
 - sigmoidal, 182
 - threshold, 182
 - recurrent, 182
 - reverse engineering (learning), 184
 - loading problem, 185
 - probably-approximately-correctly learnable, 184
 - pseudo-dimension, 185
 - Vapnik-Chervonenkis dimension, 184
- Basic graph-theoretic concepts, 134
- Biomolecular networks, 103
 - phage lambda, 121
 - cooperativity, 123
 - epigenetic decision network, 121
 - lysogeny maintenance, 122
 - robustness, 124
 - state, 78
 - toggle switch, 121
- Boolean networks, 137
 - asynchronous update, 137
 - definition, 137
 - Feed-forward Boolean network, 138
 - limit cycle, 138
 - synchronous update, 137
- Cell, 133
 - eukaryotic, 133
 - prokaryotic, 133
- Chain polymer, 84, 85
 - chain growth, 85, 87, 93, 94
 - configuration, 85, 87
 - conformational entropy, 78
 - excluded volume, 87
 - generating chain polymer, 86
 - growth strategy, 84
 - loop entropy, 78
 - monomer, 85, 87, 89
 - coordinates, 87
 - self-avoiding polymer chains, 84, 87
 - self-avoiding walk, 87

- end-to-end distance, 87
- Chemical reaction, 104
- Continuous time Markov process, 78
- Decoys
 - sequence decoys, 47
 - structural decoys, 47
- Discrete chemical master equation, 105
 - ACME, 107
 - approximation, 113
 - continuous chemical master equation, 113
 - Fokker-Planck approach, 113
 - Gaussian process, 116
 - Langevin assumptions, 115
 - Langevin approach, 115
 - Poisson process, 116
 - stochastic differential equation, 113
 - Taylor expansion, 114
 - direct solution, 106
 - finite buffer, 106
 - buffer capacity, 106
 - finite buffer algorithm, 106, 121, 122
 - iBD, 107
 - independent birth-death component, 107
 - multi-finite buffer, 107
 - optimal state enumeration, 106
 - reaction network decomposition, 107
 - truncation error, 111
- Dynamical systems, 177
 - Boolean models, 180
 - communication delays, 178
 - control-theoretic concepts, 179
 - controllability, 179
 - observability, 180
 - deterministic vs. stochastic dynamics, 178
 - discrete vs. continuous state variables, 177
 - discrete vs. continuous time variables, 177
 - monotone dynamics, 193
 - algorithmic issues in computing the degree of monotonicity, 199
 - characterizations, 196
 - definition, 194
 - degree of monotonicity, 198
- Ensemble properties, 77
- Geometric constructs, 4
 - computing Delaunay tetrahedrization, 12
 - edge flip, 13
 - incremental algorithm, 12, 13
 - locally Delaunay, 13
 - computing Voronoi diagram, 14
 - discrete flow, 11
 - convex hull, 5
 - Delaunay tetrahedrization, 5
 - Delaunay triangulation, 5
 - power distance, 5
 - Voronoi cell, 4
 - Voronoi diagram, 4
 - Voronoi region, 4
- Interaction networks models, 133
 - dynamical, 135
 - continuous state, 136
 - continuous time, 136
 - differential equations model, 135
 - discrete state, 136
 - discrete time, 136
 - hybrid state, 136
 - signed graphs, 137
 - associated signed graph, 137
 - topological, 134
 - directed graphs, 134
- Ising model, 79
 - energy, 79
- Marginal distribution, 86
- Markov chain, 81
 - conditions, 81
 - aperiodicity, 82
 - irreducibility, 82
 - recurrent state, 82
 - detailed balance, 82, 84
 - property, 81
 - steady state, 82
 - time reversibility, 82
 - time reversible processes, 82
 - transition probability, 81
 - transition probability matrix, 82
- Markov process, 81
- MAX-CUT problem, 199
- Molecular species, 104
- Non-deterministic finite automata (NFA), 190
- Piece-wise linear model, 186
 - biological applications, 188
 - delta-notch protein signalling, 189
 - genetic regulatory networks, 189
 - dynamics, 187
 - PL-isomorphism, 188
 - equivalence, 187
 - piecewise-linear hybrid automata, 189
- Potential function, 29
 - assumptions, 58
 - binding free energy, 57
 - Boltzmann assumption, 34
 - Boltzmann distribution, 33
 - data dependency, 64
 - deriving parameter values, 31
 - distance and packing dependent alpha potential, 44
 - effective potential energy, 33

- empirical potential function, 30
- from optimization, 47
- functional form, 31
 - weighted linear sum, 31
- general framework, 31
 - optimization, 31
 - statistical analysis, 31
- geometric potential function, 44
- geometric view, 48
- knowledge-based effective energy function, 30
- membrane proteins, 62
- Miyazawa-Jernigan contact potential, 34
 - hydrophobic nature, 39
- non-additivity, 59
- nonlinear potential function, 52
 - derivation, 52
- optimality criterion, 50
- optimization techniques, 53
- partition function, 33, 57, 58
 - sequence dependency, 60
- physics-based potential function, 30
- probability of occupancy, 32
- protein design, 56
- protein stability, 57
- protein structure prediction, 53
- protein-protein docking prediction, 54
- reference states, 33, 42, 45, 62
 - ideal gas, 43
 - internal random model, 62
 - permutation model, 62
- Rosenblatt perceptron method, 50
- theoretical model, 32
- three-body interactions, 60
- Protein descriptors, 31
- Protein design, 47
- Protein folding, 29
 - thermodynamic hypothesis, 29
- Protein function prediction, 16
 - enzyme function prediction, 18
 - evolution of protein surfaces, 18
 - graph based methods, 16
 - matching pocket surfaces, 17
- Protein representation, 31
- Protein structure, 1
 - computing surface area, 14
 - computing volume, 14
 - packing analysis, 15
 - atom ball, 2
 - atom radius, 2
 - computing surface area, 9
 - computing volume, 9
 - Connolly's surface, 4
 - crystallography, 1
 - depressions, 11
 - distinction between voids and pockets, 11
 - electron density map, 1
 - elementary surface pieces, 4
 - experimental techniques, 1
 - fused ball model, 2
 - hard sphere model, 2
 - idealized ball model, 2
 - Lee-Richards surface, 3
 - metric measurement, 9
 - molecular surface, 4
 - nuclear magnetic resonance (NMR), 1
 - pockets, 11
 - re-entrant surfaces, 4
 - refinement, 1
 - size properties, 9
 - solvent accessible surface, 3
 - space filling model, 2
 - surface, 3
 - union of ball model, 3
 - united atom, 2
 - van der Waals radius, 2
 - voids, 4, 11
- Protein structure and function, 16
- Protein structures
 - near neighbors, 44
 - degree of near neighbors, 45
- Quadratic integer programming, 200
 - semi-definite optimization, 200
 - Cholesky decomposition, 200
 - vector program, 200
- Rare event, 79
- Reaction, 104
 - linear and nonlinear reactions, 104
 - reaction probability, 117
 - reaction rate, 104
 - intrinsic reaction rate, 104
 - reaction trajectory, 117
 - trajectory, 117
 - Markovian process, 118
 - probability of reaction trajectory, 118
- Sampling technique, 77
 - importance sampling, 85
 - bias correction, 85, 89
 - weights, 85, 86, 89
 - bias correction, 86
 - joint trial distribution, 87
 - Markov chain Monte Carlo, 83
 - Metropolis Monte Carlo, 81, 83
 - move set, 84
 - proposal function, 84
 - proposal probability, 83
 - trial function, 84
 - partial sample, 86
 - proposal distribution, 80
 - rejection sampling, 80
 - sampling distribution, 80, 85, 89
 - sequential importance sampling, 85, 89
 - sequential Monte Carlo, 84, 87

- look-ahead, 87
- partial sample, 89
- prune, 89
- resampling, 89
- resampling probability, 89
- sample variance, 89
- weights, 89
- target distribution, 79, 83–86, 89
 - decomposition, 86
 - intermediate distribution, 86, 89
 - trial distribution, 80, 85, 86
- Scoring function, 30
- Scoring matrices, 78
- Signal transduction networks, 139
 - NET-SYNTHESIS software, 142
 - biochemical evidence, 140
 - correlation between dynamic and redundancy, 152
 - data Collection, 142
 - excitatory and inhibitory influence, 139
 - genetic evidence of differential responses, 140
 - graph-theoretic notations and terminologies, 139
 - null hypothesis model, 153
 - degree distribution, 153
 - null hypothesis testing, 155
 - null model
 - bias correction, 155
 - other network reduction rules, 148
 - pharmacological evidence, 140
 - pseudo-node collapse, 147
 - random networks, 153
 - redundancy and degeneracy, 149
 - information theoretic measures, 150
 - topological measure, 151
 - reverse engineering, 155
 - combinatorial approach, 163
 - modular response analysis, 156
 - quality evaluation, 166
 - synthesis, 140
 - transitive reduction, 145
 - greedy approach, 146
- Specific biological models, 209
 - C. elegans* metabolic network, 214
 - T-LGL cell survival and death network, 215
 - ABA-induced stomatal closure network, 211
 - Drosophila segment polarity model, 209
 - Boolean, 210
 - Signal transduction, 210
 - EGFR signaling network, 212
- Stochasticity, 103
 - microstate, 104
 - Monte Carlo simulation, 117
 - probability landscape, 104, 121
 - dynamically evolving probability landscape, 108
 - GPU-based solver, 108
 - iterative solver, 108
 - matrix exponential, 108
 - phage lambda, 122
 - steady state probability landscape, 108
 - small copy numbers, 103
 - state space, 106
 - finite state projection, 110
 - Krylov subspace method, 108
 - simplification, 108
 - truncation error, 111
 - stochastic simulation, 117
 - Gillespie algorithm, 118
 - stochastic simulation algorithm, 118
 - theoretical framework, 104
 - transition rate, 105
 - transition rate matrix, 105, 108
- Stoichiometry, 104
 - stoichiometry vector, 104
- Testosterone dynamics, 174
- Topological structures of molecules, 6
 - Delaunay complex, 6
 - simplices, 6
 - simplicial complex, 6
- Two-species interaction, 207
- Uniform distribution, 87, 89