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Genetic regulatory networks inference : modeling, parameters estimation & model validation

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Appendix A: System Biology Toolbox review

Toolboxes

Here we give a brief overview of the contents of well-known toolboxes. The information is based on the state of affairs in 2008. For up-to-date information we refer to the webpages.

MATLAB based

<http://www.mathworks.com/>

MATLAB Optimization Toolbox Local search algorithms. Constrained non-linear optimization: trust-region. Unconstrained: quasi-Newton, Nelder-Mead.

MATLAB Genetic Algorithm and Direct Search Toolbox Extension of the Optimization toolbox. Constrained nonlinear optimisation. Global search methods: Genetic algorithms, simulated annealing.

The toolboxes above do not contain regression analysis, but implementing the Fisher Information matrix, confidence intervals and the correlation matrix is easy in MATLAB. Moreover, the Statistics Toolbox of MATLAB provides non-linear least squares fitting tools including regression analysis.

The SimBiology Toolbox of MATLAB contains sensitivity analysis and parameter estimation. If the Optimization Toolbox(es) are installed they are used, otherwise only simplex search can be used for unconstrained problems.

Public domain toolboxes based on MATLAB

SBToolbox [240,242] <http://www.sbtoolbox.org/> Only requires basic MATLAB. Box-constrained optimization. Global search methods: Simulated Annealing, SRES. Local search methods: Nelder-Mead. No regression analysis (it does contain MCA).

SSm GO toolbox [67,228] <http://www.iim.csic.es/~gingproc/ssmGO.html> Box-constrained global optimization using scatter search. Requires basic MATLAB. No regression analysis.

PottersWheel [166] <http://www.potterswheel.de/> The most complete MATLAB-based toolbox. Box-constrained optimization. Possibility to scale parameters and to fit in logarithmic parameter space. Global methods: Simulated Annealing, genetic algorithm. Local methods: Steepest descent, Quasi-Newton, Levenberg-Marquardt. Statistical analysis of estimated parameters by fit sequence (cf. [109]).

Stand-alone public domain toolboxes

COPASI [112,235] <http://www.copasi.org/> Box-constrained nonlinear optimization. Global search methods: Genetic algorithm, evolutionary programming, particle swarm optimization [136,137], SRES, simulated annealing. Local search methods: Hooke-Jeeves, Nelder-Mead, steepest descent, Levenberg-Marquardt. No regression analysis but it contains sensitivity analysis (MCA)

SBML-PET [297] Global search method: SRES. No regression analysis.