

## Numerical linear algebra and optimization tools for bioinformatics

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Computational models often require the solution of large systems of linear equations  $Ax = b$  or least-squares problems  $Ax \approx b$  or more challenging optimization problems involving sparse matrices. For example, modeling biochemical reaction networks may depend on determining the rank of a large stoichiometric matrix, and on accurate solution of large multiscale linear programs, as in Flux Balance Analysis (FBA) and Flux Variability Analysis (FVA). Thermodynamically feasible fluxes can be obtained by solving similar optimization problems with a negative entropy objective function. We describe general-purpose algorithms and software that have provided efficient and reliable solutions for important problems in systems biology, and are likely to find broader application. In particular we mention sparse LU/QR factorizations and quad-MINOS, a quadruple-precision version of our large-scale constrained optimizer.