Stanford University, ICME

CME 338 Large-Scale Numerical Optimization

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Notes 2: Overview of Optimization Software

1 Optimization problems

We study optimization problems involving linear and nonlinear constraints:

NP
$$\min_{x \in \mathbb{R}^n} \operatorname{inimize} \quad \phi(x)$$
 subject to $\ell \leq \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \leq u$,

where $\phi(x)$ is a linear or nonlinear objective function, A is a sparse matrix, c(x) is a vector of nonlinear constraint functions $c_i(x)$, and ℓ and u are vectors of lower and upper bounds. We assume the functions $\phi(x)$ and $c_i(x)$ are *smooth*: they are continuous and have continuous first derivatives (gradients). Sometimes gradients are not available (or too expensive) and we use finite difference approximations. Sometimes we need second derivatives.

We study algorithms that find a *local optimum* for problem NP. Some examples follow. If there are many local optima, the starting point is important.

LP Linear Programming

min $c^T x$ subject to $\ell \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u$

MINOS, SNOPT, SQOPT

LSSOL, QPOPT, NPSOL (dense)

CPLEX, Gurobi, LOQO, HOPDM, MOSEK, XPRESS

CLP, lp_solve, SoPlex (open source solvers [7, 34, 57])

QP Quadratic Programming

min $c^T x + \frac{1}{2} x^T H x$ subject to $\ell \le \binom{x}{Ax} \le u$

MINOS, SQOPT, SNOPT, QPBLUR

LSSOL ($H = B^T B$, least squares), QPOPT (H indefinite)

CLP, CPLEX, Gurobi, LANCELOT, LOQO, MOSEK

BC Bound Constraints

min $\phi(x)$ subject to $\ell \le x \le u$

MINOS, SNOPT

LANCELOT, L-BFGS-B

LC Linear Constraints

MINOS, SNOPT, NPSOL

min $\phi(x)$ subject to $\ell \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u$

 $\min \, \phi(x) \text{ subject to } \ell \leq \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \leq u$

NC Nonlinear Constraints

MINOS, SNOPT, NPSOL

CONOPT, LANCELOT

Filter, KNITRO, LOQO (second derivatives)

IPOPT (open source solver [30])

Algorithms for finding local optima are used to construct algorithms for more complex optimization problems: *stochastic*, *nonsmooth*, *global*, *mixed integer*. Excellent examples are SCIP [53] for **MILP** and BARON [3] for **MINLP**.

2 AMPL, GAMS, NEOS

A fuller picture emerges from the list of problem types and solvers handled by the AMPL [2] and GAMS [20] modeling systems and the NEOS server [43]. NEOS is a free service

developed originally at Argonne National Laboratory and now hosted by the University of Wisconsin – Madison. It allows us to submit optimization problems in various formats (AMPL, GAMS, CPLEX, MPS, C, Fortran, ...) to be solved remotely on geographically distributed machines.

NEOS usage (Jan 1–Dec 31 of each year):

Year	Total jobs	Top solvers	Top inputs
2002	80,000	XpressMP, MINLP, MINOS, SNOPT, SBB	AMPL, GAMS, Fortran
2003	136,000	XpressMP, SNOPT, FortMP, MINOS, MINLP	AMPL, GAMS, Fortran
2004	148,000	MINLP, FortMP, XpressMP, PENNON, MINOS	AMPL, GAMS, Mosel
2005	174,000	Filter, MINLP, XpressMP, MINOS, KNITRO	AMPL, GAMS, Fortran
2006	229,000	Filter, MINOS, SNOPT, XpressMP, MOSEK	AMPL, GAMS, MPS
2007	551,000	SNOPT, MINLP, KNITRO, LOQO, MOSEK	AMPL, GAMS, MPS
2008	322,000	MINOS, Bonmin, KNITRO, SNOPT, IPOPT	AMPL, GAMS, CPLEX
2009	235,000	KNITRO, BPMPD, MINTO, MINOS, SNOPT	AMPL, GAMS, CPLEX
2010	236,000	KNITRO, Concorde, SNOPT, SBB, BARON	AMPL, GAMS, TSP
2011	75,000	SBB, Gurobi, filter, MINLP, XpressMP, MINTO,	GAMS, AMPL, Matlab_Binary,
		KNITRO, PATH, MINOS, MOSEK, LOQO, sdpt3	Fortran, Sparse_SDPA, MPS
2012	353,000	Gurobi, MINOS, CONOPT, SBB, KNITRO,	AMPL, GAMS, Sparse_SDPA, MPS,
		XpressMP, MINTO, SNOPT, Bonmin, Ipopt	Fortran, MOSEL, TSP, CPLEX, C
2013	1,865,000	MINOS, MINLP, KNITRO, Gurobi, Ipopt, SNOPT,	AMPL, GAMS, Sparse_SDPA, MPS,
		csdp, DICOPT, Cbc, XpressMP, MINTO, BARON	TSP, C, CPLEX, Fortran, MOSEL
2014	1,139,000	MINLP, Gurobi, filterMPEC, KNITRO, BARON,	AMPL, GAMS, TSP, Sparse_SDPA,
		MINOS, Cbc, scip, concorde, LOQO, MOSEK	MPS, C, MOSEL, FORTRAN, CPLEX
2015	645,000	MINLP, Gurobi, cbc, cplex, KNITRO, concorde,	AMPL, GAMS, TSP, MPS, LP, C,
		BARON, Bonmin, XpressMP, Couenne, MOSEK, MINOS	MOSEL, Fortran, MATLAB_BINARY
2016	1,040,000	CPLEX, Gurobi, knitro, cbc, mosek, FICO-Xpress, baron,	GAMS, AMPL, LP, MPS, TSP, MOSEL,
		Bonmin, MINOS, couenne, Ipopt, scip, concorde, CONOPT	SPARSE_SDPA, MATLAB_BINARY, C
2017	537,000	CPLEX, Gurobi, Bonmin, BARON, Knitro, Cbc,	AMPL, GAMS, MPS, LP, TSP, MOSEL,
		filterMPEC, Couenne, Ipopt, concorde, scip, MOSEK	SPARSE_SDPA, CPLEX, ZIMPL, NL
2018	701,000	CPLEX, BARON, Knitro, Gurobi, MINLP, LINDOGlobal,	AMPL, GAMS, TSP, MPS, LP,
		concorde, cbc, Couenne, Ipopt, Bonmin, MINOS, scip	SPARSE_SDPA, NL, MOSEL, MATLAB

NEOS problem categories:

 ${\bf BCO}$ Bound Constrained Optimization L-BFGS-B

COIP Combinatorial Optimization and Integer Programming BiqMac, concorde

CP Complementarity Problems Knitro, MILES, NLPEC, PATH

 \mathbf{EMP} Extended Mathematical Programming DE, JAMS

GO Global Optimization ASA, BARON, Couenne, icos, LINDOGlobal, PGAPack, PSwarm, scip

LNP Linear Network Programming RELAX4

LP Linear Programming

BDMLP, bpmpd, Clp, CPLEX, FICO-Xpress, Gurobi, MOSEK, OOQP, SoPlex80bit

MPEC Mathematical Programming with Equilibrium Constraints filterMPEC, Knitro, NLPEC

MILP Mixed Integer Linear Programming

 $Cbc,\,CPLEX,\,feaspump,\,FICO\text{-}Xpress,\,Gurobi,\,MINTO,\,MOSEK,\,proxy,\,qsopt_ex,\,scip,\,SYMPHONY$

MINCO Mixed Integer Nonlinearly Constrained Optimization

AlphaECP, BARON, Bonmin, Couenne, DICOPT, FilMINT, Knitro, LINDOGlobal, MINLP, SBB, scip

MIOCP Mixed Integer Optimal Control Problems

MUSCOD-II

NDO Nondifferentiable Optimization

condor

NCO Nonlinearly Constrained Optimization

CONOPT, filter, Ipopt, Knitro, LANCELOT, LOQO, MINOS, MOSEK, PATHNLP, SNOPT

SOCP Second-Order Conic Programming

FICO-Xpress, MOSEK

 ${\bf SIO}\;$ Semi-infinite Optimization

nsips

SDP Semidefinite Programming

csdp, penbmi, pensdp, scipsdp, SDPA, sdplr, sdpt3, sedumi

SLP Stochastic Linear Programming

bnbs, ddsip, sd

Most solvers use double-precision floating-point hardware.

For LP, SoPlex80bit mostly uses double-precision, but includes an iterative refinement procedure with rational arithmetic to obtain arbitrarily high precision [23, 22].

For LP and RLP models, GAMS now includes the QuadMINOS solver, in which hardware double-precision floating-point is replaced by software quad-precision. DQQ in the GAMS library [37, 38] shows how to combine DoubleMINOS and QuadMINOS efficiently.

For SDP, the SDPA solver on NEOS allows you to choose double-precision, quadruple-precision, octuple-precision, or variable-precision versions [54].

3 Interactive optimization systems

Several systems provide a graphical user interface (GUI) or integrated development environment (IDE) for mathematical optimization.

MATLAB [39] has an Optimization Toolbox with a selection of dense and sparse solvers (none of the above!, except ktrlink uses KNITRO [31]). Matlab Version 7.2 (R2015a) has the following functions (see help optim):

fminbnd, fmincon, fminsearch, fminunc, fseminf, ktrlink

fgoalattain, fminimax

lsqlin, lsqnonneg, lsqcurvefit, lsqnonlin

fzero, fsolve

intlinprog, linprog, quadprog

TOMLAB [60] provides a complete optimization environment for MATLAB users. There are many problem types and solvers (CGO, CONOPT, CPLEX, GENO, GP, Gurobi, KNITRO, LGO, LSSOL, MINLP, MINOS, NLPQL, NLSSOL, NPSOL, OQNLP, PENBMI, PENSDP, PROPT, QPOPT, SNOPT, SQOPT, Xpress), a unified input format, automatic differentiation of M-files with MAD, an interface to AMPL, a GUI for selecting parameters and plotting output, and TomSym: a modeling language with complete source transformation.

Note: TOMLAB is available on the Stanford Linux cluster.

See http://stanford.edu/group/SOL/download.html

- CVX [11] is a MATLAB-based modeling system for convex optimization problems (and for geometric programs). It allows objectives and constraints to be specified using MATLAB syntax.
- **AIMMS** [1] includes solvers for CP, GO, LP, MILP, MINLP, NLP, QCP, QP. Its modeling language has historical connections to GAMS.
- COMSOL Optimization Lab [10] provides the LP and NLP capabilities of SNOPT to users of COMSOL Multiphysics [9]. Currently, most problem classes are handled by SNOPT. A Nelder-Mead "simplex algorithm" is included for unconstrained optimization without derivatives.

Frontline Systems [19] provides Excel spreadsheet and Visual Basic access to optimizers for many problem classes: LP, QP, SOCP, MILP, NLP, GO, NDO.

GAMS IDE [20] provides an IDE for GAMS Windows installations.

IBM ILOG CPLEX Optimization Studio [29] provides an IDE for LP, MILP, and constraint-programming applications, along with a high-level modeling language (OPL).

4 More optimization systems

We cite a few systems in order to include them in the references: COIN-OR [8], CPLEX [28], Galahad [24, 25], Gurobi [26], Lindo [33], MOSEK [41], Optizelle [44], PENOPT [50], SeDuMi [55], TFOCS [59].

5 Sparse linear systems

Underlying almost all of the optimization algorithms is the need to solve a sequence of linear systems Ax = b (where "x" is likely to be a search direction). We will study some of the linear system software below. Most codes are implemented in Fortran 77. MA57 includes an F90 interface, and newer HSL packages [27] are in F90. UMFPACK is written in C.

When A is a sparse matrix, MATLAB uses MA57 for 1dl(A) and UMFPACK for $A \setminus b$ and lu(A) (both direct methods).

If A is a sparse matrix (or a linear operator defined by a function handle), MATLAB has the following iterative methods for solving Ax = b or min $||Ax - b||_2$: bicg, bicgstab, bicgstabl, cgs, gmres, lsqr, minres, pcg, qmr, symmlq, tfqmr.

Some of the iterative solvers are available in F77, F90, and MATLAB from SOL [56]. Python and Julia implementations are provided by Orban [45]. PETSc [51] provides many direct and iterative solvers for truly large problems (C, C⁺⁺, Fortran, Python).

Direct methods factorize sparse A into a product of triangular matrices that should be sparse and well defined even if A is singular or ill-conditioned. In Matlab, [Q,R,P] = qr(A) computes sparse factors R (triangular) and Q (orthogonal) using SuiteSparseQR. With its own Matlab interface, SuiteSparseQR can keep Q in product form (which is more sparse).

LUSOL [21, 35, 36] Square or rectangular Ax = b, A = LU, plus updating

MA48 [16] Square or rectangular Ax = b, A = LU

MA57 [15] Symmetric Ax = b, $A = LDL^T$ or LBL^T (MATLAB's [L,D,P] = ldl(A))

MUMPS [42] Square Ax = b, A = LU, LDL^T or LBL^T (massively parallel)

PARDISO [49] Square Ax = b (shared memory)

SuperLU [14, 32, 58] Square Ax = b (uniprocessor or shared or distributed memory)

SuiteSparseQR [13] Rectangular sparse QR (MATLAB's [Q,R,P] = qr(A))

UMFPACK [61, 12] Square Ax = b (MATLAB's [L,U,P,Q] = lu(A))

Iterative methods regard A as a black box (a linear operator) for computing matrix-vector products Ax and sometimes $A^{T}y$ for given x and y. In Matlab, A may be a sparse matrix or a function.

CG, PCG [39, 51] Symmetric positive-definite Ax = b

SYMMLQ [46, 56, 51] Symmetric nonsingular Ax = b (may be indefinite)

MINRES, MINRES-QLP [46, 56, 51, 4, 5, 18, 6] Symmetric Ax = b (may be indefinite or singular)

GMRES [52, 51] Unsymmetric Ax = b

CGLS, LSQR, LSMR, LSRN [47, 48, 56, 51, 17, 40] Ax = b, $\min ||Ax - b||_2^2$, $\min \left\| \begin{pmatrix} A \\ \delta I \end{pmatrix} x - \begin{pmatrix} b \\ 0 \end{pmatrix} \right\|_2^2$

References

- [1] AIMMS modeling environment. http://www.aimms.com/aimms.
- [2] AMPL modeling system. http://www.ampl.com.
- [3] BARON global optimization system. http://archimedes.scs.uiuc.edu/baron/baron.html.
- [4] S.-C. Choi. Iterative Methods for Singular Linear Equations and Least-Squares Problems. PhD thesis, ICME, Stanford University, Dec 2006.
- [5] S.-C. Choi, C. C. Paige, and M. A. Saunders. MINRES-QLP: A Krylov subspace method for indefinite or singular symmetric systems. SIAM J. Sci. Comput., 33(4):1810-1836, 2011. http://stanford.edu/ group/SOL/software.html.
- [6] S.-C. Choi and M. A. Saunders. Algorithm 937: MINRES-QLP for symmetric and Hermitian linear equations and least-squares problems. ACM Trans. Math. Software, 40(2):Article 16, 12 pp., 2014. http://stanford.edu/group/SOL/software.html.
- [7] CLP open source LP, QP, and MILP solver. http://www.coin-or.org/projects/Clp.xml.
- [8] COIN-OR: Computational Infrastructure for Operations Research. http://www.coin-or.org.
- [9] COMSOL AB. http://www.comsol.com.
- [10] COMSOL Optimization Lab. http://www.comsol.com/products/optlab.
- [11] CVX: Matlab software for Disciplined Convex Programming. http://cvxr.com.
- [12] T. A. Davis. Direct Methods for Sparse Linear Systems. Fundamentals of Algorithms. SIAM, Philadelphia, 2006.
- [13] T. A. Davis. Algorithm 915, SuiteSparseQR: Multifrontal multithreaded rank-revealing sparse QR factorization. ACM Trans. Math. Software, 38(1):8:1–22, 2011.
- [14] J. W. Demmel, S. C. Eisenstat, J. R. Gilbert, X. S. Li, and J. W. H. Liu. A supernodal approach to sparse partial pivoting. SIAM J. Matrix Anal. Appl., 20(3):720-755, 1999.
- [15] I. S. Duff. MA57: a Fortran code for the solution of sparse symmetric definite and indefinite systems. ACM Trans. Math. Software, 30(2):118–144, 2004. See 1d1 in MATLAB.
- [16] I. S. Duff and J. K. Reid. The design of MA48: a code for the direct solution of sparse unsymmetric linear systems of equations. ACM Trans. Math. Software, 22(2):187–226, 1996.
- [17] D. C.-L. Fong and M. Saunders. LSMR: An iterative algorithm for least-squares problems. SIAM J. Sci. Comput., 33(5):2950–2971, 2011.
- [18] D. C.-L. Fong and M. A. Saunders. CG versus MINRES: An empirical comparison. SQU J. Sci., 17(1):44-62, 2012. http://stanford.edu/group/SOL/reports/SOL-2011-2R.pdf.
- [19] Frontline Systems, Inc. spreadsheet modeling system. http://www.solver.com.
- [20] GAMS modeling system. http://www.gams.com.
- [21] P. E. Gill, W. Murray, M. A. Saunders, and M. H. Wright. Maintaining LU factors of a general sparse matrix. Linear Algebra and its Applications, 88/89:239–270, 1987.
- [22] A. M. Gleixner, D. E. Steffy, and K. Wolter. Iterative refinement for linear programming. INFORMS J. on Computing, 28(3):449–464, 2016.
- [23] Ambros M. Gleixner. Exact and Fast Algorithms for Mixed-Integer Nonlinear Programming. PhD thesis, Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB), Technical University of Berlin, 2015.
- [24] N. I. M. Gould, D. Orban, and Ph. L. Toint. The Galahad library. http://www.galahad.rl.ac.uk/.
- [25] N. I. M. Gould, D. Orban, and Ph. L. Toint. Galahad, a library of thread-safe Fortran 90 packages for large-scale nonlinear optimization. ACM Trans. Math. Software, 29(4):373–394, 2003.
- [26] Gurobi optimization system for linear and integer programming. http://www.gurobi.com.
- [27] The HSL Mathematical Software Library. http://www.hsl.rl.ac.uk/.
- [28] IBM ILOG CPLEX optimizer. http://www-01.ibm.com/software/commerce/optimization/cplex-optimizer/.
- [29] IBM ILOG CPLEX Optimization Studio. https://www.ibm.com/developerworks/downloads/ws/ ilogcplex/.
- [30] IPOPT open source NLP solver. https://projects.coin-or.org/Ipopt.
- [31] KNITRO optimization software. https://www.artelys.com/tools/knitro.
- [32] X. S. Li and J. W. Demmel. SuperLU-DIST: A scalable distributed-memory sparse direct solver for unsymmetric linear systems. ACM Trans. Math. Software, 29(2):110-140, 2003.
- [33] Lindo Systems optimization software. http://www.lindo.com.

- [34] lp_solve open source LP and MILP solver. http://groups.yahoo.com/group/lp_solve/.
- [35] LUSOL sparse matrix package. http://stanford.edu/group/SOL/software.html.
- [36] LUSOL mex interface (Nick Henderson, ICME, Stanford University). https://github.com/nwh/lusol_mex, 2011.
- [37] D. Ma, M. A. Saunders, and S. Dirkse. dqq.gms: Warm-starting quad-precision MINOS in GAMS, 2017. https://www.gams.com/latest/gamslib_ml/libhtml/gamslib_dqq.html.
- [38] D. Ma, L. Yang, R. M. T. Fleming, I. Thiele, B. O. Palsson, and M. A. Saunders. Reliable and efficient solution of genome-scale models of Metabolism and macromolecular Expression. Sci. Rep., 7, Article number: 40863, http://rdcu.be/oCpn, 2017.
- [39] MATLAB matrix laboratory. http://www.mathworks.com.
- [40] X. Meng, M. A. Saunders, and M. W. Mahoney. LSRN: a parallel iterative solver for strongly over- or underdetermined systems. SIAM J. Sci. Comput., 36(2):C95-C118, 2014.
- [41] MOSEK Optimization Software. http://www.mosek.com/.
- [42] MUMPS: a multifrontal massively parallel sparse direct solver. http://mumps.enseeiht.fr/.
- [43] NEOS server for optimization. http://www.neos-server.org/neos/.
- [44] Optizelle: An open source library for general-purpose nonlinear optimization. http://www.optimojoe.com/products/optizelle/.
- [45] D. Orban. Optimization software. http://dpo.github.io/software/.
- [46] C. C. Paige and M. A. Saunders. Solution of sparse indefinite systems of linear equations. SIAM J. Numer. Anal., 12:617–629, 1975.
- [47] C. C. Paige and M. A. Saunders. LSQR: An algorithm for sparse linear equations and sparse least squares. ACM Trans. Math. Software, 8(1):43-71, 1982a.
- [48] C. C. Paige and M. A. Saunders. Algorithm 583; LSQR: Sparse linear equations and least-squares problems. ACM Trans. Math. Software, 8(2):195–209, 1982b.
- [49] PARDISO parallel sparse solver. http://www.pardiso-project.org.
- [50] PENOPT optimization systems for nonlinear programming, bilinear matrix inequalities, and linear semidefinite programming. http://www.penopt.com.
- [51] PETSc toolkit for scientific computation. http://www.mcs.anl.gov/petsc.
- [52] Y. Saad. Iterative Methods for Sparse Linear Systems. SIAM, Philadelphia, second edition, 2003.
- [53] SCIP mixed integer programming solver. http://scip.zib.de/.
- [54] SDPA on the NEOS Server. https://neos-server.org/neos/solvers/sdp:SDPA/SPARSE_SDPA.html.
- [55] SeDuMi optimization system for linear programming, second-order cone programming, and semidefinite programming. http://sedumi.ie.lehigh.edu.
- [56] SOL downloadable software. http://stanford.edu/group/SOL/software.html.
- [57] SoPlex linear programming solver. http://soplex.zib.de/.
- [58] SuperLU software for sparse unsymmetric systems. http://crd.lbl.gov/~xiaoye/SuperLU/.
- [59] TFOCS: Templates for First-Order Conic Solvers. http://cvxr.com.
- [60] TOMLAB optimization environment for MATLAB. http://tomopt.com.
- [61] UMFPACK solver for sparse Ax = b. http://faculty.cse.tamu.edu/davis/suitesparse.html.