Stanford University, Management Science & Engineering (and ICME)

MS&E 318 (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:

$$\text{NP} \qquad \underset{x\in\mathbb{R}^n}{\text{minimize}} \quad \phi(x) \qquad \text{subject to} \quad \ell \le \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \le u,$$

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 $\qquad \min c^Tx$ subject to $\ell \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$
- MINOS, SNOPT, SQOPT
- LSSOL, QPOPT, NPSOL (dense)
- CPLEX, Gurobi, LOQO, HOPDM, MOSEK, XPRESS
- CLP, lp_solve, SoPlex (open source solvers [7, 34, 54])

QP Quadratic Programming $\qquad \min c^Tx + \frac{1}{2}x^THx$ subject to $\ell \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$
- MINOS, SQOPT, SNOPT, QPBLUR
- LSSOL ($H = B^TB$, least squares), QPOPT (H indefinite)
- CLP, CPLEX, Gurobi, LANCELOT, LOQO, MOSEK

BC Bound Constraints $\qquad \min \phi(x)$ subject to $\ell \le x \le u$
- MINOS, SNOPT
- LANCELOT, L-BFGS-B

LC Linear Constraints $\qquad \min \phi(x)$ subject to $\ell \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$
- MINOS, SNOPT, NPSOL

NC Nonlinear Constraints $\qquad \min \phi(x)$ subject to $\ell \le \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \le u$
- 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 [50] 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 [41]. 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, KNITRO, PATH, MINOS, MOSEK, LOQO, sdpt3	GAMS, AMPL, Matlab_Binary, Fortran, Sparse_SDPA, MPS
2012	353,000	Gurobi, MINOS, CONOPT, SBB, KNITRO, XpressMP, MINTO, SNOPT, Bonmin, Ipopt	AMPL, GAMS, Sparse_SDPA, MPS, Fortran, MOSEL, TSP, CPLEX, C
2013	1,865,000	MINOS, MINLP, KNITRO, Gurobi, Ipopt, SNOPT, csdp, DICOPT, Cbc, XpressMP, MINTO, BARON	AMPL, GAMS, Sparse_SDPA, MPS, TSP, C, CPLEX, Fortran, MOSEL
2014	1,139,000	MINLP, Gurobi, filterMPEC, KNITRO, BARON, MINOS, Cbc, scip, concorde, LOQO, MOSEK	AMPL, GAMS, TSP, Sparse_SDPA, MPS, C, MOSEL, FORTRAN, CPLEX
2015	645,000	MINLP, Gurobi, cbc, cplex, KNITRO, concorde, BARON, Bonmin, XpressMP, Couenne, MOSEK, MINOS	AMPL, GAMS, TSP, MPS, LP, C, MOSEL, Fortran, MATLAB_BINARY
2016	1,040,000	CPLEX, Gurobi, knitro, cbc, mosek, FICO-Xpress, baron, Bonmin, MINOS, couenne, Ipopt, scip, concorde, CONOPT	GAMS, AMPL, LP, MPS, TSP, MOSEL, SPARSE_SDPA, MATLAB_BINARY, C
2017	537,000	CPLEX, Gurobi, Bonmin, BARON, Knitro, Cbc, filterMPEC, Couenne, Ipopt, concorde, scip, MOSEK	AMPL, GAMS, MPS, LP, TSP, MOSEL, SPARSE_SDPA, CPLEX, ZIMPL, NL

NEOS problem categories:

BCO Bound Constrained Optimization
L-BFGS-B

COIP Combinatorial Optimization and Integer Programming
BiqMac, concorde

CP Complementarity Problems
Knitro, MILES, NLPEC, PATH

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-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

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 will soon offer the QUADMINOS solver, in which hardware double-precision floating-point is replaced by software quad-precision.

For SDP, the SDPA solver on NEOS allows you to choose double-precision, quadruple-precision, octuple-precision, or variable-precision versions [51].

3 Interactive optimization systems

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

MATLAB [37] 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 [57] 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 [39], Optizelle [42], PENOPT [47], SeDuMi [52], TFOCS [56].

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 `ldl(`A`)` and UMFPACK for $A\backslash b$ 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 [53]. PETSc [48] provides many direct and iterative solvers for truly large problems.

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

PARDISO [46] Square $Ax = b$ (shared memory)

SuperLU [14, 32, 55] Square $Ax = b$ (uniprocessor or shared or distributed memory)

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

UMFPACK [58, 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 [37, 48] Symmetric positive-definite $Ax = b$

SYMMLQ [43, 53, 48] Symmetric nonsingular $Ax = b$ (may be indefinite)

MINRES, MINRES-QLP [43, 53, 48, 4, 5, 18, 6] Symmetric $Ax = b$ (may be indefinite or singular)

GMRES [49, 48] Unsymmetric $Ax = b$

CGLS, LSQR, LSMR, LSRN [44, 45, 53, 48, 17, 38] $Ax = b$, $\min \|Ax - b\|_2^2$, $\min \left\| \begin{pmatrix} A \\ \delta I \end{pmatrix} x - \begin{pmatrix} b \\ 0 \end{pmatrix} \right\|_2^2$

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