

Stanford University, Dept of Management Science and Engineering  
MS&E 318 (CME 338) Large-Scale Numerical Optimization

Instructor: Michael Saunders Spring 2009

Notes 1: **Overview**

## Course Description

The main algorithms and software for constrained optimization, emphasizing the sparse-matrix methods needed for their implementation. Iterative methods for linear equations and least squares. The simplex method. Basis factorization and updates. Interior methods. The reduced-gradient method, augmented Lagrangian methods, and SQP methods.

3 units, Grading basis ABCD/NP, about 5 homeworks, 1 project, no final.

Prerequisites: Basic numerical linear algebra, including LU, QR, and SVD factorizations, and an interest in MATLAB, sparse-matrix methods, and algorithms for constrained optimization.

## Syllabus

1. Overview (problem types, NEOS, MATLAB, TOMLAB, headlines)
2. Iterative methods for symmetric  $Ax = b$  (symmetric Lanczos process, CG, SYMMLQ, MINRES, MINRES-QLP)
3. Iterative methods for unsymmetric  $Ax = b$  and least squares (Golub-Kahan process, CGLS, LSQR, Craig, Arnoldi process, GMRES)
4. The primal simplex method (phase 1 in practice, basis factorization, updating, crash, scaling, degeneracy)
5. Basis updates (PF update, Bartels-Golub, Forrest-Tomlin, Block-LU)
6. A sparse Basis Factorization Package (LUSOL: the engine for MINOS, SQOPT, SNOPT, MILES, PATH, lp\_solve)
7. Primal-dual interior methods for LP (CPLEX, HOPDM, IPOPT, KNITRO, LOQO, MOSEK) and convex nonlinear objectives (PDCO), Basis Pursuit, BP Denoising (Lasso, LARS, Homotopy, BPdual, SPGL1)
8. The reduced-gradient method (MINOS part 1)
9. BCL methods (Augmented Lagrangians, LANCELOT)
10. LCL methods (MINOS part 2, Knossos)
11. SQP methods (NPSOL, SQOPT, SNOPT)

## 1 Optimization Problems

We study optimization problems involving linear and nonlinear constraints:

NP	$\begin{aligned} &\underset{x \in \mathbb{R}^n}{\text{minimize}} && \phi(x) \\ &\text{subject to} && \ell \leq \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \leq u, \end{aligned}$
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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  $\ell$  and  $u$  are vectors of lower and upper bounds. We assume the nonlinear 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 usually 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 (open source solvers [4, 13])

**QP** Quadratic Programming  $\min c^T x + \frac{1}{2} x^T H x$  subject to  $\ell \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u$   
 MINOS, SQOPT, SNOPT  
 LSSOL ( $H = B^T B$ , least squares), QPOPT ( $H$  indefinite)  
 CLP, CPLEX, LANCELOT, LOQO, MOSEK

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

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

**NC** Nonlinear Constraints  $\min \phi(x)$  subject to  $\ell \leq \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \leq u$   
 MINOS, SNOPT, NPSOL  
 CONOPT, LANCELOT  
 Filter, KNITRO, LOQO (second derivatives)  
 IPOPT (open source solver [11])

Algorithms for finding local optima are used to construct algorithms for more complex optimization problems: *stochastic, nonsmooth, global, mixed integer*. An excellent example for **MINLP** is BARON [3].

## 2 AMPL, GAMS, NEOS

A fuller picture emerges from the list of problem types and solvers handled by the AMPL [2] and GAMS [8] modeling systems and the NEOS server [15]. NEOS is a free service provided by Argonne National Laboratory, Illinois. It allows us to submit optimization problems in various formats (AMPL, GAMS, CPLEX, MPS, C, Fortran, ...) to be solved remotely on geographically distributed solver stations.

**Recent NEOS usage** (up to March 29, 2009):

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	66,000	BPMPD, SNOPT, CBC, BARON, CONOPT	AMPL, GAMS, C

### NEOS problem categories:

**BCO** Bound Constrained Optimization

BLMVM, L-BFGS-B, TRON

**CP** Complementarity Problems

MILES, PATH

**GO** Global Optimization

ACRS, GLCF, GLOBMIN, LGO, MLOCPSOA

**LNO** Linear Network Optimization

NETFLO, RELAX4

**LP** Linear Programming

BDMLP, BPMPD, CLP, CPLEX, FortMP, Gurobi, IPOPT, MOSEK, OOQP  
PCx, XA, XPRESS

**MILP** Mixed Integer Linear Programming

BONSAIG, CBC, CPLEX, FortMP, GLPK, MOSEK, XA, XPRESS

**MINCO** Mixed Integer Nonlinearly Constrained Optimization

BARON, Bonmin, DICOPT, MINLP, SBB

**NCO** Nonlinearly Constrained Optimization

CONOPT, DONLP2, Filter, KNITRO, IPOPT, LANCELOT,  
LOQO, MINOS, MOSEK, PATHNLP, PENNON, SNOPT

**NDO** Nondifferentiable Optimization

ACCPM, APPS, BT, DFO, NDA

**QP** Quadratic Programming

BPMPD, CPLEX, GALAHAD (QPA, QPB), LOQO, OOQP

- SDP and SOCP** Semidefinite and Second Order Cone Programming  
 CSDP, CIRCUT, DSDP, MOSEK, PENNON,  
 SDP-LR, SDPA, SDPT3, SeDuMi
- SLP** Stochastic Linear Programming  
 CPA, DECIS, MSLIP, OSLSE
- SIO** Semi-Infinite Optimization  
 NSIPS
- UCO** Unconstrained Optimization  
 CGplus, NMTR, VMLM

### 3 Interactive Optimization Systems

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

**MATLAB** [14] has an Optimization Toolbox with a selection of dense and sparse solvers (none of the above!):

```
fminbnd, fmincon, fminsearch, fminunc, fseminf
fgoalattain, fminimax
lsqlin, lsqnonneg, lsqcurvefit, lsqnonlin
bintprog, linprog, quadprog
```

**TOMLAB** [21] provides a complete optimization environment for MATLAB users. There are many problem types, many solvers (including CGO, CONOPT, CPLEX, GENO, GP, KNITRO, LGO, LSSOL, MINLP, MINOS, NLPQL, NPSOL, OQNLP, PENBMI, PENSDP, PROPT, SNOPT, SQOPT, XA, Xpress), a unified input format, automatic differentiation of M-files with MAD, an interface to AMPL, and a GUI for selecting parameters and plotting output.

**AIMMS** [1] includes solvers for LP, MILP, MINLP, NLP, QCP, QP. Its modeling language has historical connections to GAMS.

**GAMS IDE** [8] provides an IDE for GAMS PC installations.

**Frontline Systems** [7] provides Excel spreadsheet and Visual Basic access to optimizers for many problem classes: LP, QP, MILP, NLP, GO, NDO.

**ILOG OPL Studio** [10] is a further IDE for LP, MILP, and constraint-programming applications, based on a C-like modeling language.

**COMSOL Optimization Lab** [6] provides the LP and NLP capabilities of SNOPT to users of COMSOL Multiphysics and COMSOL Script [5] (a language closely related to MATLAB). Currently, most problem classes are handled by SNOPT. A Nelder-Mead “simplex algorithm” is included for unconstrained optimization without derivatives.

### 4 More Optimization Systems

Several optimization systems have been mentioned already. We cite a few more here in order to include them in the references below:

Gurobi [9], Lindo [12], PENOPT [17], SeDuMi [19].

## 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*,  $\Delta x$ ).

We will study some of the following software for linear systems. Most are implemented in Fortran 77. MA57 includes an F90 interface. UMFPACK is written in C. Some of the iterative solvers are available in F77, F90, and MATLAB from SOL [20]. Note that PETSc [18] provides many direct and iterative solvers for truly large problems.

*Direct methods* factorize  $A$  into a product of triangular matrices that should be sparse and well defined even if  $A$  is singular or ill-conditioned.

**LUSOL** [27] Square or rectangular  $Ax = b$ ,  $A = LU$ , plus updating

**MA48** [26] Square or rectangular  $Ax = b$ ,  $A = LU$

**MA57** [25] Symmetric  $Ax = b$ ,  $A = LDL^T$  or  $LBLE^T$  (may be indefinite)

**UMFPACK** [22, 23] Square  $Ax = b$  (used for MATLAB's  $[L,U,P,Q] = \text{lu}(A)$ )

**SuperLU** [24, 28] Square  $Ax = b$  (parallel: shared or distributed memory)

**PARDISO** [16] Symmetric or unsymmetric  $Ax = b$  (parallel: shared memory)

*Iterative methods* regard  $A$  as a “black box” for computing matrix-vector products  $Ax$  and/or  $A^T y$  for given  $x$  and  $y$ .

**CG, PCG** [14, 18] Symmetric positive-definite  $Ax = b$

**SYMMLQ** [29, 20, 18] Symmetric nonsingular  $Ax = b$  (may be indefinite)

**MINRES** [29, 20, 18] Symmetric  $Ax = b$  (may be indefinite and/or singular)

**GMRES** [32, 18] Unsymmetric  $Ax = b$

**CGLS, LSQR** [30, 31, 20, 18]  $Ax = b$ ,  $\min \|Ax - b\|_2^2$ ,  $\min \left\| \begin{pmatrix} A \\ \delta I \end{pmatrix} x - \begin{pmatrix} b \\ 0 \end{pmatrix} \right\|_2^2$

## 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] CLP open source LP, QP, and MILP solver. <http://www.coin-or.org/faqs.html>.
- [5] COMSOL AB. <http://www.comsol.com>.
- [6] COMSOL Optimization Lab. <http://www.comsol.com>.
- [7] Frontline Systems, Inc. spreadsheet modeling system. <http://www.solver.com>.
- [8] GAMS modeling system. <http://www.gams.com>.
- [9] Gurobi optimization system for linear and integer programming. <http://www.gurobi.com>.
- [10] ILOG OPL Studio modeling environment. <http://www.ilog.com/products/oplstudio>.
- [11] IPOPT open source NLP solver. <https://projects.coin-or.org/Ipoppt>.
- [12] Lindo Systems optimization software. <http://www.lindo.com>.

- [13] lp\_solve open source LP and MILP solver. [http://groups.yahoo.com/group/lp\\_solve/](http://groups.yahoo.com/group/lp_solve/).
- [14] MATLAB matrix laboratory. <http://www.mathworks.com>.
- [15] NEOS server for optimization. <http://www-neos.mcs.anl.gov>.
- [16] PARDISO parallel sparse solver. <http://www.pardiso-project.org>.
- [17] PENOPT optimization systems for nonlinear programming, bilinear matrix inequalities, and linear semidefinite programming. <http://www.penopt.com>.
- [18] PETSc toolkit for scientific computation. <http://www.mcs.anl.gov/petsc>.
- [19] SeDuMi optimization system for linear programming, second-order cone programming, and semidefinite programming. <http://sedumi.ie.lehigh.edu>.
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- [21] TOMLAB optimization environment for MATLAB. <http://tomopt.com>.
- [22] UMFPACK solver for sparse  $Ax = b$ . <http://www.cise.ufl.edu/research/sparse/umfpack>.
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