Verified Computations in Optimization with Applications

Christian Jansson Denis Chaykin Christian Keil

Institute for Reliable Computing
Hamburg University of Technology

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Outline

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Benefits of Convex Optimization

Convex Optimization

- Vast number of applications in finance, engineering, ...
- Appears as subproblem in global optimization

Rockafellar (1993)

In fact the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity.

Outline

Linear Programming Applications

- Oil refinery problems
- Flap settings on aircraft
- Industrial production and allocation
- Image restoration
- Linear relaxations in global optimization

Lovasz (1980)

If one would take statistics about which mathematical problem is using up most of the computer time in the world, then (not including database handling problems like sorting and searching) the answer would probably be linear programming.

A linear program

Definition (Linear program (LP))

Find the optimal value f^* of a linear objective function $c^T x$ subject to

- linear constraints $Ax \leq a, \; Bx = b$ and
- simple bounds $\underline{x} \leq x \leq \overline{x}$.

- Set of feasible points F satisfying constraints and simple bounds
- Can be represented by the tuple $P := (c, A, a, B, b)$ and $\underline{x}, \overline{x}$
- Simple bounds may be infinite

A lower bound for the optimal value (1)

Theorem (Jansson (2004))

Given a linear program P and $\underline{x}, \overline{x}$. If $\mathbf{y} \le 0, \mathbf{z}$ satisfy

- $\exists\, y \in \mathbf{y}, z \in \mathbf{z} : c_j - (A_{:j})^T y - (B_{:j})^T z = 0$ *for free x_j, and*
- *the defects*

$$\mathbf{d}_j := c_j - (A_{:j})^T \mathbf{y} - (B_{:j})^T \mathbf{z} \begin{cases} \le 0 & \text{for} \quad -\infty < x_j \le \overline{x}_j \\ \ge 0 & \text{for} \quad \underline{x}_j \le x_j < \infty \end{cases}$$

then a lower bound for the optimal value is

$$\underline{f}^* := \inf\{a^T \mathbf{y} + b^T \mathbf{z} + \sum_{\underline{x}_j \ne -\infty} \underline{x}_j \mathbf{d}_j^+ + \sum_{\overline{x}_j \ne \infty} \overline{x}_j \mathbf{d}_j^-\}.$$

A lower bound for the optimal value (2)

- $O(n^2)$ operations for finite simple bounds, coincides with Neumaier and Shcherbina's (2004)
- Conditions not met (infinite simple bounds) $\Rightarrow$ iterate with perturbed dual constraints
- Works for interval problems **P**

An upper bound for the optimal value

- Based on idea from Krawczyk (1975) later used and modified
  Jansson (1988), Hansen and Walster (1991), Kearfott (1994)
- Enclose primal interior point
- Verifies existence of primal feasible solutions
- Works for interval problems **P**

Lurupa: verified linear programming

Lurupa

- Computes rigorous bounds for the optimal value
- Computes enclosures of near optimal, feasible points
- Generates certificates of infeasibility, unboundedness
- Computes verified condition numbers
- Postprocesses approximate solution of unmodified LP solver

LP test set

Netlib comprises $\sim$ 100 problems

- First added in 1988, latest in 1996
- 32 to 15695 variables, 27 to 16675 constraints (medium size)
- Established test set for lp algorithms
- Ordóñez and Freund (2003): 71% ill-posed

Numerical Results (unpreprocessed!)

In total 89 problems, 86 with infinite simple bounds

- 35 finite upper bounds for the optimal value

$$\text{med}(\mu(\overline{f}^*, f^*)) = 8.0e-9 \qquad \text{med}(t_{\overline{f}^*}/t_{f^*}) = 5.3$$

- 76 finite lower bounds for the optimal value

$$\text{med}(\mu(\underline{f}^*, f^*)) = 2.2e-8 \qquad \text{med}(t_{\underline{f}^*}/t_{f^*}) = 0.5$$

Outline

Semidefinite programming applications

- Control theory
- Circuit design
- Combinatorial optimization
- Robust optimization
- Signal processing
- Algebraic geometry
- Quantum chemistry
- Atom physics

A semidefinite program

Definition (Semidefinite program (SDP) block diagonal form)

Find the optimal value f^* of $\langle C_1, X_1\rangle + \cdots + \langle C_n, X_n\rangle$ subject to

$$\langle A_{11}, X_1\rangle + \cdots + \langle A_{1n}, X_n\rangle = b_1$$
$$\vdots$$
$$\langle A_{m1}, X_1\rangle + \cdots + \langle A_{mn}, X_n\rangle = b_m$$
$$X_j \succeq 0$$

- Dual constraints equivalent to Linear matrix inequality (LMI)

$$y_1 A_{1j} + \cdots + y_m A_{mj} \preceq C_j \quad \text{for } j = 1, \ldots, m$$

- Weak duality holds, strong duality complicated

Verified Error Bounds: SDP lower bound

Theorem (Jansson (2007))

Given an SDP $P = (A_{ij}, b, C_j)$ and approximate $\tilde{y} \in \mathbb{R}^m$. Let

$$\mathbf{D}_j := C_j - \sum_{i=1}^{m} \tilde{y}_i A_{ij}, \ \underline{d}_j \leq \lambda_{\min}(\mathbf{D}_j) \text{ (measures violations)}$$

$$l_j \geq \text{ number of negative eigenvalues of } \mathbf{D}_j.$$

If the optimal X_j satisfies the primal boundedness qualification $\lambda_{\max}(X_j) \leq \overline{x}_j \in \mathbb{R}_+ \cup \{+\infty\}$, then a lower bound for the optimal value is

$$f_p^* \geq b^T \tilde{y} + \sum_{j=1}^{n} l_j \underline{d}_j^- \overline{x}_j =: \underline{f}_p^* \text{ , where } \underline{d}_j^- = \min(0, \underline{d}_j)$$

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VSDP: Verified Semi-Definite Programming

MATLAB software package by Jansson using INTLAB (Rump)

- Verified lower and upper bounds of the optimal value
- Proves existence of feasible solutions, also for LMI's
- Provides rigorous certificates of infeasibility
- Facilitates to solve approximately the problem by using different well-known semidefinite programming solvers (SDPT3, SDPA)
- Can handle several formats
- Allows the use of interval data

SDP test set

SDPLIB

- 92 problems out of control and system theory, truss topology design, graph partitioning, max cut, ...
- Wide range of sizes (6 to 7000 constraints, dimension of X: 13 to 7000 $\Rightarrow$ up to $\approx$ 24 million variables)
- Freund, Ordóñez, and Toh (2006): 32 out of 80 problems ill-posed

Numerical results

Using SDPT3

- Approximate solver runs out of memory for two very large problems
- Median of guaranteed relative accuracy: $7.0 \cdot 10^{-7}$
- Median $(\underline{t}/t) = 0.085$
- Median $(\bar{t}/t) = 1.99$
- $\bar{f}_d^* = +\infty$ for 32 ill-posed problems, reflecting zero distance to primal infeasibility
- Finite bounds and strong duality proved for all other problems, with exception of `hinf2`
- 7 warnings from SDPT3, 3 warnings for well-posed problems $\Rightarrow$ not reflecting difficulty of the problems

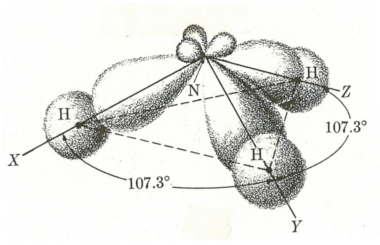
Electronic structure calculations

Electrons

(i) do not move around nucleus in circular orbits

(ii) may exist at any arbitrary point

(iii) more frequently exist in regions described by probability amplitudes, wave functions $\Psi(r, t)$



Electronic distribution in NH_3 molecule (Ammonia)

with unitary time evolution

$$\hbar \frac{\partial}{\partial t} \Psi = H \Psi,$$ Schrödinger's Equation,

H Hamiltonian (operator corresponding to energy)

Electronic structure calculations

- Challenging, large-scale problem in atomic physics: ground-state-energy of molecules (smallest eigenvalue of Hamiltonian H)
- ground-state-energy can be computed from an SDP (Coleman 1987, . . . , Fukuda et. al to appear in Math. Programming) that is ill-conditioned
- Nakata et. al (J. Chem. Phys. 2001) report numerical inaccuricies → need for verification

Electronic structure calculations example

Ammonia *NH*3

- N = 10 electrons, r = 16, m = 2964
- size of block matrices: 8, 8, 8, 8, 28, 28, 64, 28, 28, 64, 128, 64, 64, 56, 224, 224, 56, 736, 736, 224, 224
- ground-stage energy: 67.92487 eV

Using SDPA as approximate solver:

- approximate relative accuracy: $4.9906e - 009$
- guaranteed relative accuracy: $1.2502e - 007$
- times: $\tilde{t} = 6.59h, \bar{t} = 0.54h, \underline{t} = 6.67h$

Electronic structure calculations results

- VSDP solved all but the largest molecule problems ($m > 7000$, more than 2.5 million variables) due to SDPA and SDPT3 being aborted after 3 days of computation
- D.Chaykin implements a C++ code for verified results using SDPARA for solving the problems with $m > 5000$ and $n > 1500$

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Summary

Cheap rigorous error bounds available for

- ill-conditioned and even ill-posed convex problems
- rigorous error bounds for convex relaxations in global optimization

- Neumaier and Shcherbina 2004, MILP
- Jansson 2004, LP and Convex Programming
- Keil and Jansson 2006, NETLIB LP library
- Jansson, Chaykin and Keil 2007, SDP
- Jansson 2005, Ill-posed SDP