Efficient Solutions for the Large Scale Trust Region Subproblem, TRS

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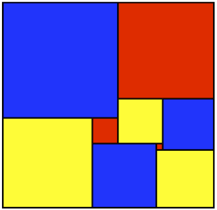


Success of Linear Models/LP/Duality

Classical Linear Program

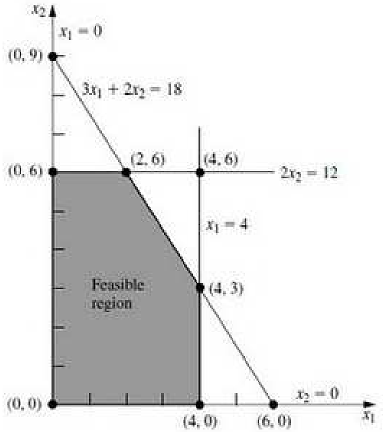
$$\text{(PLP)} \qquad \begin{array}{rll} p^* := & \min & f(y) := b^T y \\ & \text{s.t.} & g(y) := c - A^T y \leq 0 \\ & & x \in \mathbb{R}^n \end{array}$$

Strong Duality if (LP) Feasible; and Attained if Finite

$$\text{(DLP)} \qquad \begin{array}{rcl} p^* & = & d^* \\ & := & \max_{x \geq 0} \min_y L(y,x) := b^T y + x^T (c - A^T y) \\ & := & \max_{x \geq 0} \min_y c^T x + y^T (b - Ax) \\ & := & \max_{x \geq 0} \{c^T x : Ax = b, x \geq 0\} \text{ hidden constraint} \end{array}$$

Duality is behind algorithms (simplex, interior-point).

Polyhedral (so Convex) Feasible Set



Quadratic Models

Modelling NP-Hard Problems

$$\text{(MaxCut)} \qquad p^* := \begin{array}{ll} \max & q_0(x) := x^T L x \\ \text{s.t.} & x_i \in \{\pm 1\}, x \in \mathbb{R}^n \end{array}$$

(L is Laplacian matrix of the graph)
Then, equivalent quadratic constraints to ± 1 are:

$$p^* = \max\{x^T L x : x_i^2 = 1, i = 1, \ldots, n\}$$

Strong Duality Fails; No Lagrange Multiplier

Simple example:

$$\text{(P)} \qquad p^* := \begin{array}{ll} \min & f(x) := x \\ \text{s.t.} & g(x) := x^2 \leq 0 \end{array}$$

$$0 = \nabla L(x^*, \lambda) = \nabla f(x^*) + \lambda \nabla g(x^*) = 1 + \lambda 2(0) \qquad \text{impossible}$$

Quadratic Models; Trust Region Subproblem, (TRS)

"Nonconvex" quadratic minimization

$$\text{(TRS)} \qquad \begin{array}{rll} q^* = & \min & q(x) := x^T A x - 2a^T x \\ & \text{s.t.} & \|x\|^2 \le s^2, \\ & & x \in \mathbb{R}^n \end{array}$$

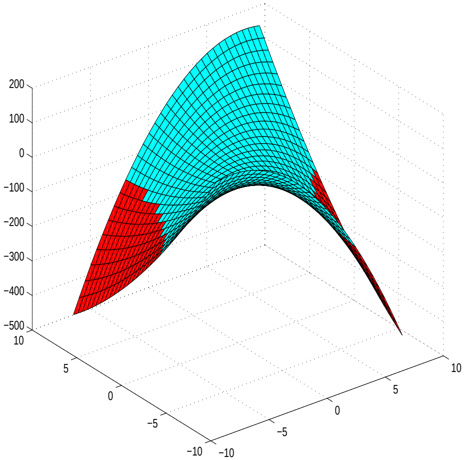
- $A \in \mathcal{S}^n$ - $n \times n$ symmetric (possibly indefinite) matrix
- $a \in \mathbb{R}^n$; $s > 0$ (TR radius);

Generalized TRS, (GTRS)

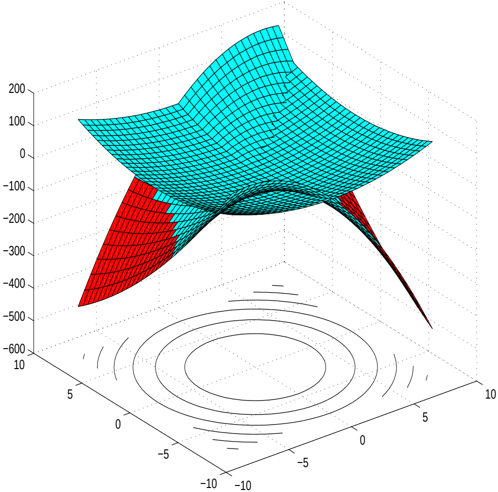
Indefinite Objective; Indefinite Two-sided Quadratic Constraint

$$\text{(GTRS)} \qquad \begin{array}{rll} q^* = & \min & q(x) := x^T A x - 2a^T x \\ & \text{s.t.} & \ell \le q_1(x) := x^T B x - 2b^T x \le u \end{array}$$

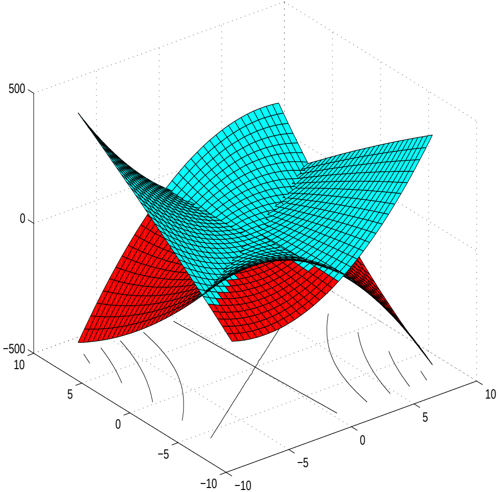
Indefinite Quadratic (Surface Plot, Saddle)



Indefinite Quadr. with Euclid. Norm Constr., TRS



Indefinite Quadr. with Indefinite Quadr. Constr., GTRS



Why Convexity Matters

R. Tyrrell Rockafellar, in SIAM Review, 1993 [9]

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

If Strong Duality Holds; We Get Implicit Convexity

if

$$\begin{aligned} p^* = d^* := \quad & \max_{\lambda \in \Lambda} \min_{x \in \Omega} & L(x, \lambda) := f(x) + \lambda^T g(x) \\ & = \max_{\lambda \in \Lambda} & \phi(\lambda) \end{aligned}$$

$\phi(\lambda)$ is concave (a minimum of functions linear in λ); therefore the dual is: concave maximization

(However, the evaluation of $\phi(\lambda)$ may be costly.)

Outline

Background

- Generalized Trust Region Subproblem and Characterizations of Optimality
- MoSo (1983) algorithm for TRS; within a primal-dual framework; handling the hard case

Duality/Exploiting Sparsity & Degeneracy/Hard Case

- Various primal-dual pairs with strong duality
- Parametric eigenvalue problem and sparsity
- Hard case is actually easiest case, with an explicit solution
- Underdetermined least squares, Numerics

Applications

Many important applications:

- forming subproblems for constrained optimization
- REGULARIZATION of ill-posed problems (inverse image denoising, Electrical impedance tomography, EIT, MRI, NMRI, MRT, CT PET...)
- theoretical applications
- **trust region (TR) methods for unconstr. min.** uses TRS formed from second order Taylor series approximation

Characterization of Optimality for TRS

Surprising: TRS (GTRS) is *on watershed* of convex/nonconvex

- a characterization of optimality of a (possibly) nonconvex problem
- second order positive semidefinite necessary conditions hold on all of $\mathbb{R}^n$

Characterization of x^* optimal for TRS (iff)

(Gay-81 [2], More-Sorensen-83 [5])

$$\left.\begin{array}{c} (A-\lambda^* I)x^* = a, \\ A-\lambda^* I \succeq 0, \lambda^* \leq 0 \end{array}\right\} \quad \text{dual feasibility}$$

$$\|x^*\|^2 \leq s^2 \quad \text{primal feasibility}$$

$$\lambda^*(s^2 - \|x^*\|) = 0 \quad \text{complementary slackness}$$

Characterization of Optimality for (homog) GTRS

(Mild) Slater Type Constraint Qualification

$$\text{(GTRS)} \qquad q^* = \begin{array}{ll} \min & q(x) := x^T A x - 2a^T x \\ \text{s.t.} & \ell \leq q_1(x) := x^T B x \leq u \end{array}$$

$$(CQ) \qquad \exists \hat{x} \text{ s.t. } l < q_1(\hat{x}) := \hat{x}^T B \hat{x} < u$$

Characterization of x^* optimal for GTRS (iff)

(More-93 [4], Stern-W-93 [10])

$$\left.\begin{array}{c} (A - \lambda^* B) x^* = a, \\ A - \lambda^* B \succeq 0 \end{array}\right\} \qquad \text{dual feasibility}$$

$$\ell \leq {x^*}^T B x \leq u \qquad \text{primal feasibility}$$

$$\lambda^*(u - {x^*}^T B x^*) \geq 0 \geq \lambda^*({x^*}^T B x^* - \ell) \qquad \text{compl. slack.}$$

S-Lemma Yakubovich-71,73

(survey in Polik-Terlaky:07 [6] (Farkas Lemma for quadratic functions))

$f, g : \mathbb{R}^n \to \mathbb{R}$ quadratic functions
$\exists \bar{x}$ s.t. $g(\bar{x}) < 0$
then TFAE:

1. $\nexists x \in \mathbb{R}^n : f(x) < 0, g(x) \leq 0$
2. $\exists \lambda \geq 0$ s.t. $f(x) + \lambda g(x) \geq 0, \forall x \in \mathbb{R}^n$

Finsler:37 , Hestenes-McShane:40
$\{x^T Bx = 0, x \neq 0 \implies x^T Ax > 0\}$
implies
$\{\exists \lambda \geq 0, A + \lambda B \succ 0\}$

Mo-So Algorithm Framework

Recall: Opt. conditions of TRS

$$\left.\begin{array}{c}(A-\lambda^* I)x^* = a,\\ A-\lambda^* I \succeq 0, \lambda^* \leq 0\end{array}\right\}$$ dual feasibility

$$\|x^*\|^2 \leq s^2$$ primal feasibility

$$\lambda^*(s^2 - \|x^*\|) = 0$$ complementary slackness

Original view: if $A - \lambda^* I \succ 0, \lambda^* < 0$

- define: $x(\lambda) = (A-\lambda I)^{-1} a$
- <u>SOLVE</u>: $\psi(\lambda) := \|x(\lambda)\| - s = \|(A-\lambda I)^{-1} a\| - s = 0$
- maintain: $A - \lambda I \succ 0, \ \lambda \leq 0$

Less Nonlinear $\phi(\lambda)$ for Newton's Method

Newton for $\psi(\lambda) = 0$?

$A = Q\Lambda Q^T$ orthogonal diagonalization; $\gamma = Q^T a$;

$\psi(\lambda) = \|x(\lambda)\|^2 - s^2 = \sum_{j=1}^{n} \frac{\gamma_j^2}{(\lambda_j(A)-\lambda)^2} - s^2$ *highly* nonlinear in λ, in particular near $\lambda_1(A)$.

less nonlinear $\phi(\lambda)$ (Reinsch:67 [7, 8], Hebden:73 [3])

SOLVE: $\phi(\lambda) := \frac{1}{s} - \frac{1}{\|x(\lambda)\|} = 0$

Newton iterates $\lambda^{(k)}$ for $\phi(\lambda) = 0$; exploit Cholesky

$$\begin{aligned} \lambda^{(k+1)} &= \lambda^{(k)} \boxed{-\frac{\phi(\lambda^{(k)})}{\phi'(\lambda^{(k)})} \text{ Newton step}} \\ &= \lambda^{(k)} - \left(\frac{\|x\|}{\|y\|}\right)^2 \left(\frac{\|x\|-s}{s}\right), \end{aligned}$$

where: $A - \lambda^{(k)} I = R^T R$ (Cholesky); $R^T R x = a$; $R^T y = x$

Computing Newton direction/step Gay:81, MoSo:83

Assume $\lambda^{(k)} \leq 0$ and $A - \lambda^{(k)} I \succ 0$ (i.e. $\lambda^{(k)} < \lambda_1(A)$)

- Factor $A - \lambda^{(k)} I = R^T R$ (Cholesky factorization).
- Solve for x, $R^T R x = a$ $\quad$ ($x = x(\lambda^{(k)})$).
- Solve for y, $R^T y = x$.
- Let $\lambda^{(k+1)} = \lambda^{(k)} - \left[\frac{\|x\|}{\|y\|}\right]^2 \left[\frac{(\|x\| - s)}{s}\right]$ $\quad$ (Newton step); but, *safeguard/maintain* positive definiteness $A - \lambda^{(k+1)} I \succ 0$

Nearly linear

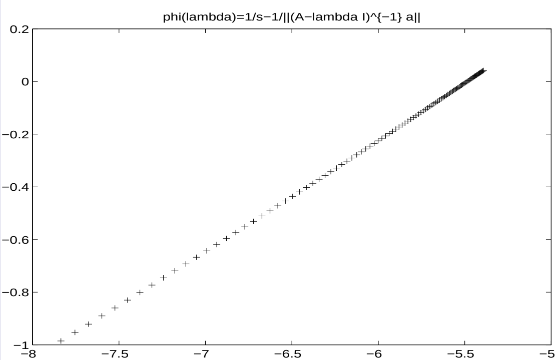


Figure: "Easy" case: $\phi(\lambda) = \frac{1}{s} - \frac{1}{||(A-\lambda I)^{\dagger}a||}$

“Easy” Case; Newton Quadr. Cvgnce from One Side

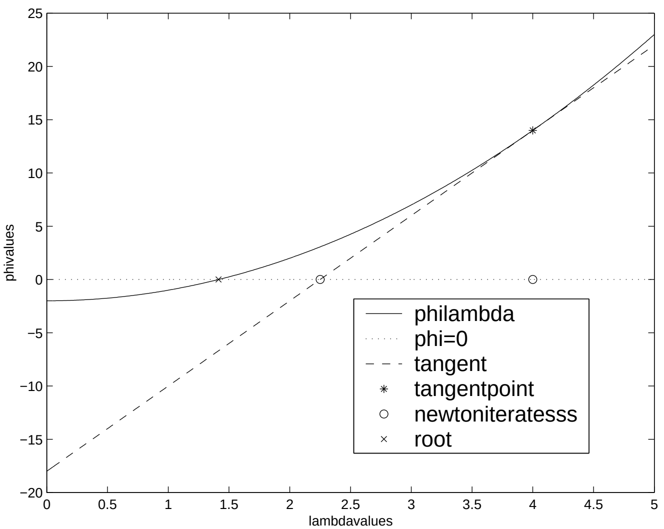


Figure: Newton’s method with the secular function, $\phi(\lambda)$.

Easy/Hard Cases for TRS; Singularity of Hessian

$\lambda_1(A) = \lambda_{\min}(A) > \lambda^* \implies A - \lambda^* I \succ 0$

1. Easy case	2.(a) Hard case (case 1)	2.(b) Hard case (case 2)
$a \notin \mathcal{R}(A - \lambda_1(A)I)$ (stationarity implies $\lambda^* \neq \lambda_1(A)$, so that $\lambda^* < \lambda_1(A)$, Hessian is pos. def., nonsingular)	$a \perp \mathcal{N}(A - \lambda_1(A)I)$ but $\lambda^* < \lambda_1(A)$ (Hessian is pos. def., nonsingular)	$a \perp \mathcal{N}(A - \lambda_1(A)I)$ and $\lambda^* = \lambda_1(A)$ singular Hessian (i) $\\|(A - \lambda^* I)^\dagger a\\| = s$ or $\lambda^* = 0$ (ii) $\\|(A - \lambda^* I)^\dagger a\\| < s$, $\lambda^* < 0$

three different cases for the trust region subproblem;
two subcases (i) and (ii) for the hard case (case 2), where
$A - \lambda^* I$ is positive semidefinite, SINGULAR.
($\cdot^\dagger$ denotes Moore-Penrose gen. inverse.)

Hard Case is really easiest?

We take advantage of Lanczos algorithm in large sparse case.
Will see: hard case becomes easiest case.

$\phi(\lambda)$ in the (near) Hard Case

Newton steps (linearizations) are *"useless"*

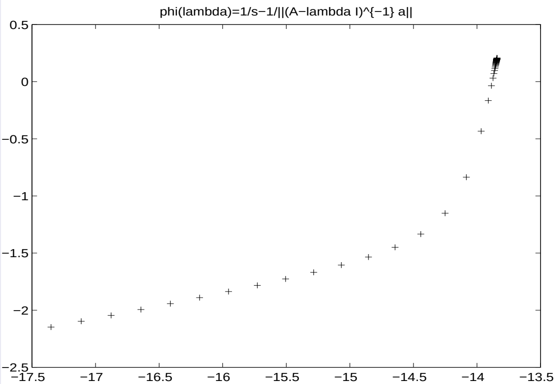


Figure: (near) hard case case: $\phi(\lambda) = \frac{1}{s} - \frac{1}{||(A-\lambda I)^{\dagger} a||}$

Towards a Parametrization for Large Sparse Case

Motivation: try to avoid Cholesky in large sparse case

Homogenization using $y_0^2 = 1$; optimal value $\mu^* =$

$$= \min_{||x||=s,\ y_0^2=1} x^tAx - 2y_0a^tx \quad \text{homogenize obj.}$$

$$= \max_t \min_{||x||=s,\ y_0^2=1} x^tAx - 2y_0a^tx + ty_0^2 - t$$

$$\geq \max_t \min_{||x||^2+y_0^2=s^2+1} x^tAx - 2y_0a^tx + ty_0^2 - t \quad \boxed{\text{**eig prob**}}$$

$$\geq \max_{t,\lambda} \min_{x,y_0} x^tAx - 2y_0a^tx + ty_0^2 - t + \lambda(||x||^2 + y_0^2 - s^2 - 1)$$

$$= \max_{r,\lambda} \min_{x,y_0} x^tAx - 2y_0a^tx + ry_0^2 - r + \lambda(||x||^2 - s^2)$$

$$= \max_\lambda \left(\max_r \min_{x,y_0} x^tAx - 2y_0a^tx + ry_0^2 - r + \lambda(||x||^2 - s^2) \right)$$

$$= \max_\lambda \min_{x,y_0^2=1} x^tAx - 2y_0a^tx + \lambda(||x||^2 - s^2)$$

$$= \mu^*,$$

equated r with $t + \lambda$.

used strong duality for TRS for last two equalities.

Parametric Eigenvalue Problem

$$\max_t \boxed{\min_{||x||^2+y_0^2=s^2+1} x^tAx - 2y_0a^tx + ty_0^2} - t$$

$$k(t) := (s^2+1)\lambda_1(D(t)) - t \qquad D(t) = \begin{bmatrix} t & -a^t \\ -a & A \end{bmatrix}$$

An Unconstrained dual problem to (TRS)

$$\max_t k(t) \qquad \text{(concave max)}$$

$k'(t) = (s^2 + 1)y_0(t)^2 - 1$

If $\lambda_1(D(t))$ is simple

- $y(t)$ normalized eigenvector for $\lambda_1(D(t))$
- $y(t) = \begin{pmatrix} y_0(t) \\ x(t) \end{pmatrix}$
- $$\frac{1}{y_0(t)}\|x(t)\| = s \text{ if, and only if, } k'(t) = 0$$

Linear Primal-Dual SDP Pair

From parametric eigenvalue problem

$$(DSDP) \qquad \begin{array}{rll} \mu^* = & \max_{\lambda,t} & (s^2+1)\lambda - t \\ & \text{s.t.} & D(t) \succeq \lambda I \qquad (\lambda_{\min}(D(t)) \geq \lambda) \end{array}$$

(with $\lambda \leq 0$ for inequality constraint TRS)

$$(PSDP) \qquad \begin{array}{rll} \mu^* = & \min & \operatorname{trace} D(0)X \\ & \text{s.t.} & \operatorname{trace} X = s^2+1 \\ & & X_{11} = 1 \\ & & X \succeq 0 \end{array}$$

$$X \cong \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T$$

Hard Case is Easiest Case: Shift and Deflation

If $\lambda_{\min} < 0$ use $A \leftarrow A - \lambda_{\min}(A)$

- hard case (case 2) happens only when $\lambda^* = \lambda_{\min}(A) < 0$
- $A \succeq 0$ after the shift (objective changes by a constant)

Lemma Fortin-W:03 [1]

$A = \sum_{i=1}^{n} \lambda_i(A) v_i v_i^T = Q \Lambda Q^T$
orthogonal spectral decomposition of A; with $\gamma_i = (Q^T a)_i$

$$\begin{aligned} S_1 &= \{i : \gamma_i \neq 0, \lambda_i(A) > \lambda_{\min}(A)\} \\ S_2 &= \{i : \gamma_i = 0, \lambda_i(A) > \lambda_{\min}(A)\} \\ S_3 &= \{i : \gamma_i \neq 0, \lambda_i(A) = \lambda_{\min}(A)\} \\ S_4 &= \{i : \gamma_i = 0, \lambda_i(A) = \lambda_{\min}(A)\} \end{aligned}$$

For $k = 1, 2, 3, 4,$: $A_k = \sum_{i \in S_k} \lambda_i(A) v_i v_i^T$
Then:

Lemma Conclusions

1. If $S_3 \neq \emptyset$ (easy case), then (x^*, λ^*) solves TRS iff (x^*, λ^*) solves TRS when A is replaced by $A_1 + A_3$.
2. If $S_3 = \emptyset$ (hard case), let $i_0 = 1 \in S_4$, then
   (x^*, λ^*) solves TRS iff
   (x^*, λ^*) solves TRS when A is replaced by
   $\boxed{A_1 + \lambda_{i_0}(A) v_{i_0} v_{i_0}^T.}$ (DEFLATE)
3. Let $x(\lambda^*) = (A - \lambda^* I)^\dagger a$, then (x^*, λ^*), where $x^* = x(\lambda^*) + z, z \in \mathcal{N}(A - \lambda^* I)$ and $\|x^*\| = s$ solves TRS iff $(x(\lambda^*), \lambda^* - \lambda_{\min}(A))$ solves TRS when A is replaced by $A - \lambda_{\min}(A) I$.
4. If $\lambda_{\min}(A) \geq 0$, then (x^*, λ^*) solves TRS iff
   (x^*, λ^*) solves TRS when A is replaced by
   $A + \sum_{i \in S_4} \alpha_i v_i v_i^T$, with $\alpha_i \geq 0$. (DEFLATE all in S_4)

Shift/Deflate: Solve Hard Case Explicitly

Summary - sometimes you get !lucky!

- eigenpair $\lambda_{\min}(A) = \lambda_1(A), v_1$ found; large sparse case; so, assume possible hardcase: $\boxed{\lambda_1(A) < 0 \text{ and } v_1^T a = 0}$
- !we have $\lambda_1(A)$! so shift: $A \leftarrow A - \lambda_{\min}(A) I \succeq 0$; !optimum unchanged, objective value changed by $\lambda_1 s^2$!.
- !we have v_1, $v_1^T a = 0$! so deflate: $A \leftarrow A + \alpha_1 v v^T$, $\|A\| > \alpha_1 >> 0$; (repeat deflation if needed, i.e as long as $\boxed{\lambda_{\min}(A) = 0 \text{ and } v^T a = 0}$) !objective value/optima unchanged!.
- if $v^T a \neq 0$, then continue with TRS algorithm, i.e. hard case (case 1); otherwise, $A \succ 0$, so (using prec. conj grad.) calculate $\bar{x} = A^{-1} a$; if $\|x(\lambda^*)\| > s$, then continue with TRS algorithm, i.e. hard case (case 1); otherwise $\|x(\lambda^*)\| \leq s$, then we have hard case (case 2) and !we have an explicit solution : $\|x^*\| = \|\bar{x} + \beta v_1\| = s$, !since $v_1 \in \mathcal{N}(A - \lambda^* I)$!.

cputime in the hard case (*case 2*)

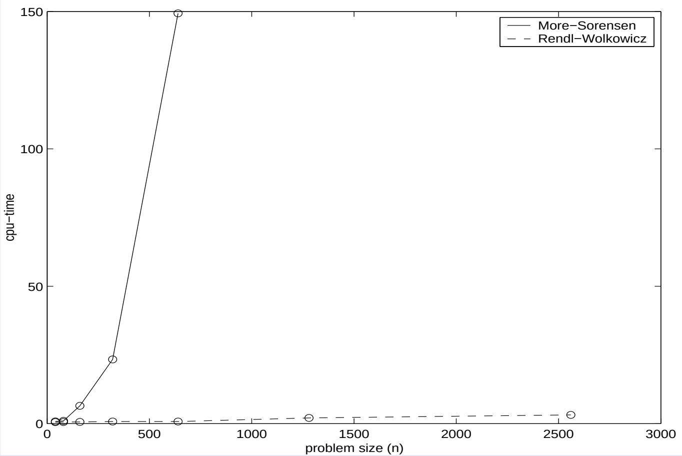


Figure: cputime in the hard case (*case 2*)

log of cputime in the hard case (*case 2*)

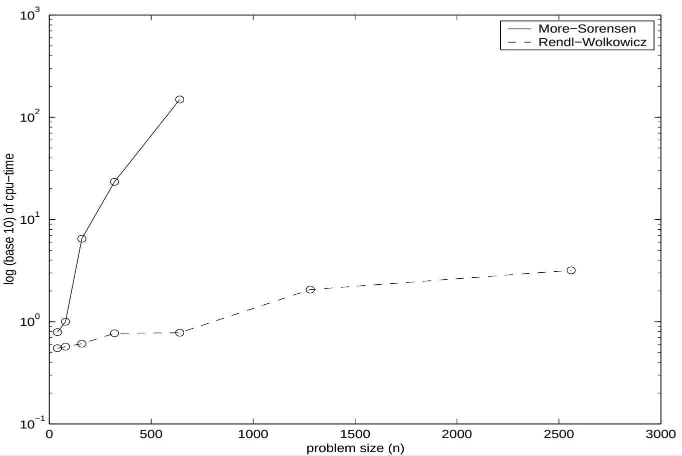


Figure: log of cputime in the hard case (*case 2*)

Conclusion

Importance of Duality/Convexity; Exploit Singularity

- The TRS (quadratic objective, one quadratic constraint) is an *implicit* convex problem.
- Convexity allows one to exploit the special structure of the dual along with information from the primal problem.
- Singularity is usually an indication of difficulty/ill-posedness. However, if the structure is well known, then one can often exploit singularity to improve the algorithm.

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Thanks for your attention!

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