The Regularized Total Least Squares Problem: Theoretical Properties and Three Globally Convergent Algorithms

Amir Beck

Faculty of Industrial Engineering and Management

Technion, Haifa, Israel

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Bibliography

The lecture is based on the three papers:

D. Sima, S. Van Huffel and G. H. Golub. **”Regularized Total Least Squares Based on Quadratic Eigenvalue Problem Solvers”** *BIT* 44(4):793–812, 2004.

A. Beck, A. Ben-Tal and and M.Teboulle. **”Finding a Global Optimal Solution for a Quadratically Constrained Fractional Quadratic Problem with Applications to the Regularized Total Least Squares”***SIMAX* 28(2):425-445, 2006.

A. Beck and M.Teboulle. **”A Convex Optimization Approach for Minimizing the Ratio of Indefinite Quadratic Functions over an Ellipsoid”***Submitted for publication*.

Total Least Squares - Review

$$\mathbf{A}\mathbf{x} \approx \mathbf{b}$$

A fixed - LS

$$\min_{\mathbf{w},\mathbf{x}} \|\mathbf{w}\|^2$$

s.t.

$$\mathbf{A}\mathbf{x} = \mathbf{b} + \mathbf{w}$$

minimal perturbation to rhs which makes this linear system consistent

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A uncertain - TLS (TLS)

$$\min_{\mathbf{w},\mathbf{E},\mathbf{x}} \|\mathbf{E}\|^2 + \|\mathbf{w}\|^2$$
s.t.
$$(\mathbf{A} + \mathbf{E})\mathbf{x} = \mathbf{b} + \mathbf{w}$$

minimal perturbation to both rhs and lhs matrix which makes the system consistent (Golub, Van Loan (80))

Another Formulation of the TLS

(Golub, Van Loan, 80)

$$(TLS) \quad \min_{\mathbf{x},\mathbf{E},\mathbf{w}} \{\|\mathbf{E}\|^2 + \|\mathbf{w}\|^2 : \mathbf{b} + \mathbf{w} = (\mathbf{A} + \mathbf{E})\mathbf{x}\} =$$

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$$= \underbrace{\min_{\mathbf{x}} \frac{\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2}{\|\mathbf{x}\|^2 + 1}}_{\text{A nonconvex optimization problem}}$$

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The solution is expressed by the singular value decomposition of the augmented matrix $(\mathbf{A}, \mathbf{b})$

Regularization of the TLS solution

- Regularization of the TLS solution is required in the case where $\mathbf{A}$ is nearly rank deficient.
- **Applications:** discretization of ill posed problems, image deblurring , medical applications, signal restoration...In these problems, TLS solution can be physically meaningless, hence regularization is needed to stabilize solution.

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Regularization Methods

- Addition of a quadratic constraint. *([Golub, Hansen & O'leary, 1999], [Guo & Renaut, 2002, 2005], [Sima, Van Huffel & Golub, 2004], [Beck, Ben-Tal & Teboulle 2006], [Beck & Teboulle 2006])*
- Addition of a quadratic penalty to the objective function [Beck & Ben-Tal 2005].
- Truncation methods. *([Fierro, Golub Hansen & O'leary, 1997], [Hansen, 1994])*.

The RTLS problem

$$\text{(RTLS):}\ \min\left\{\frac{\|\mathbf{Ax}-\mathbf{b}\|^2}{1+\|\mathbf{x}\|^2} : \|\mathbf{Lx}\|^2 \le \rho\right\}$$

- $\mathbf{L} \in \mathbb{R}^{r\times n}(r \le n)$ has full row rank.

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- The feasible set $\{\mathbf{x} : \|\mathbf{Lx}\|^2 \le \rho\}$ represents a (possibly degenerate) ellipsoid.

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- Popular choices for $\mathbf{L}$: identity matrix, an approximation of first or second order derivative.

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- The feasible set $\{\mathbf{x} : \|\mathbf{Lx}\|^2 \le \rho\}$ represents a (possibly degenerate) ellipsoid.
- Popular choices for $\mathbf{L}$: identity matrix, an approximation of first or second order derivative.
- A nonconvex optimization problem (the objective function is nonconvex).

Main Problem

Minimization of a ratio of indefinite quadratic functions over an Ellipsoid

$$(RQ) \quad \min\left\{\frac{f_1(\mathbf{x})}{f_2(\mathbf{x})} : \|\mathbf{L}\mathbf{x}\|^2 \le \rho\right\}$$

$$f_i(\mathbf{x}) = \mathbf{x}^T\mathbf{A}_i\mathbf{x} + 2\mathbf{b}_i^T\mathbf{x} + c_i, i = 1, 2$$

$$\mathbf{A}_i = \mathbf{A}_i^T \in \mathbb{R}^{n\times n}, \mathbf{b}_i \in \mathbb{R}^n, c_i \in \mathbb{R}, \mathbf{L} \in \mathbb{R}^{r\times n}$$

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Assumption: the problem is well defined, i.e., $f_2(\mathbf{x}) > 0$ for every $\mathbf{x}$ such that $\|\mathbf{L}\mathbf{x}\|^2 \le \rho$

First Subclass: GTRS Problems

Generalized Trust Region Subproblem (GTRS): $f_2(\mathbf{x}) \equiv 1$

$$(GTRS)\,\min\{\mathbf{x}^T\mathbf{A}_1\mathbf{x} + 2\mathbf{b}_1^T\mathbf{x} + c_1 : \|\mathbf{L}\mathbf{x}\|^2 \le \rho\}$$

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- A key subproblem in Trust Region Algorithms for unconstrained minimization problems

$$\min\{f(x) : \mathbf{x} \in \mathbb{R}^n\} \Rightarrow \mathbf{x}^{k+1} \in \underset{\|\mathbf{x}-\mathbf{x}^k\|^2 \leq \Delta}{\text{argmin}} g^k(\mathbf{x})$$

Second Subclass: RTLS Problems

Regularized Total Least Squares Problem (RTLS):

$f_1(\mathbf{x}) = \|\mathbf{Ax} - \mathbf{b}\|^2, f_2(\mathbf{x}) = \|\mathbf{x}\|^2 + 1$

$$(RTLS) \min \left\{ \frac{\|\mathbf{Ax} - \mathbf{b}\|^2}{\|\mathbf{x}\|^2 + 1} : \|\mathbf{Lx}\|^2 \leq \rho \right\}$$

- A nonconvex problem (although both the denominator and nominator are convex functions).

The iterative scheme of Sima, Van Huffel and Golub

Optimality conditions: $\mathbf{x}^*$ is a global optimal solution if and only if

$$\mathbf{x}^* \in \mathrm{argmin}\{f_2(\mathbf{x})(f(\mathbf{x}) - f(\mathbf{x}^*)) : \|\mathbf{L}\mathbf{x}\|^2 \leq \rho\}, \left(f(\mathbf{x}) \equiv \frac{f_1(\mathbf{x})}{f_2(\mathbf{x})}\right)$$

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Fixed Point Iterations:

$$\mathbf{x}^{k+1} \in \operatorname{argmin}\{f_2(\mathbf{x})(f(\mathbf{x}) - f(\mathbf{x}^k)) : \|\mathbf{L}\mathbf{x}\|^2 \le \rho\}$$

Equivalently:

$$\mathbf{x}^{k+1} \in \operatorname{argmin}\{f_1(\mathbf{x}) - f(\mathbf{x}^k) f_2(\mathbf{x}) : \|\mathbf{L}\mathbf{x}\|^2 \le \rho\}$$

Each iteration involves the solution of a nonconvex GTRS.

Solving the GTRS problem

$$(P): \min\{\mathbf{x}^T\mathbf{B}\mathbf{x} - 2\mathbf{d}^T\mathbf{x} : \|\mathbf{L}\mathbf{x}\|^2 = \rho\}$$

Two solution approaches:

- Formulation as a Quadratic Eigenvalue problem:

$$(\lambda^2\mathbf{I} + 2\lambda\mathbf{W} + \mathbf{W}^2 - \rho\mathbf{h}\mathbf{h}^T)\mathbf{u} = 0,$$

where $\mathbf{W} = \mathbf{L}^{-T}\mathbf{B}\mathbf{L}^{-1}, \mathbf{h} = \mathbf{L}^{-T}\mathbf{d}$.

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- A dual approach:
  The dual problem:

  $$(D) \quad \max\{-\mathbf{d}^T(\mathbf{B} + \lambda\mathbf{L}^T\mathbf{L})^{-1}\mathbf{d} - \lambda\rho : \lambda \geq -\lambda_{\min}(\mathbf{L}^{-T}\mathbf{B}\mathbf{L})\}$$

  Strong duality: val(P)=val(D).

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- Question 1: Does the algorithm converge to a global optimum for (RTLS)? (RQ)?

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- In the case $r < n$, the initial vector is carefully chosen.
- Proof that any limit point of the generated sequence satisfies first order optimality conditions. No proof of global convergence.
- Numerical experiments: convergence in at most 5 iterations to a high accuracy vector.
- The numerical experiments suggest that the algorithm converges to a global optimum
- Question 1: Does the algorithm converge to a global optimum for (RTLS)? (RQ)?
- Question 2: What is the reason for the small number of iterations?

A Globally Convergent Algorithm

Dinkelbach's principal for fractional programming (67)

$$F(\alpha) = \min\{f_1(\mathbf{x}) - \alpha f_2(\mathbf{x}) : \|\mathbf{L}\mathbf{x}\|^2 \le \rho\}$$

- F is a decreasing function of α.

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Outer Bisection Algorithm (Beck, Ben-Tal, Teboulle, 06)

Initialization: α_l, α_u - lower and upper bounds on α^*.
while $\alpha_u - \alpha_l > \epsilon$ repeat
$\alpha_h = \frac{\alpha_u+\alpha_l}{2}$
If $F(\alpha_h) > 0$ then $\alpha_u = \alpha_h$, else $\alpha_l = \alpha_h$

Analysis of the Outer Bisection Algorithm

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- Extension: Nonconvex feasible set $\{m \leq \|\mathbf{L}\mathbf{x}\|^2 \leq M\}$. Usage of the hidden convexity property of problems of the form:

$$\min\{\mathbf{x}^T\mathbf{B}\mathbf{x} - 2\mathbf{d}^T\mathbf{x} : m \leq \|\mathbf{L}\mathbf{x}\|^2 \leq M\}$$

Image Deblurring Example

- **Problem: estimate a 32×32 two dimensional image obtained from the sum of three harmonic oscillations:**

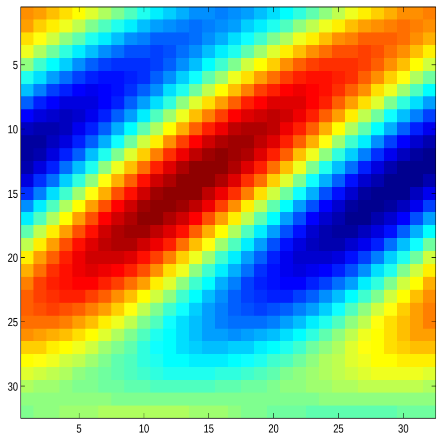
$$\mathbf{x}(\mathbf{z_1}, \mathbf{z_2}) = \sum_{\mathbf{l}=1}^{3} \mathbf{a_i} \cos(\mathbf{w_{l,1}} \mathbf{z_1} + \mathbf{w_{l,2}} \mathbf{z_2} + \phi_{\mathbf{l}}), \quad \left(\mathbf{w_{l,i}} = \frac{2\pi \mathbf{k_{l,i}}}{\mathbf{n}} \right),$$

where $1 \le \mathbf{z_1}, \mathbf{z_2} \le \mathbf{32}$, $\mathbf{k_{l,i}} \in \mathbb{Z}^2$, and $\mathbf{a_i}, \phi_{\mathbf{l}}$ given parameters.

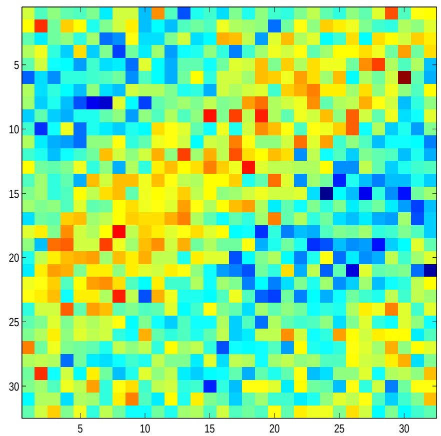
- The image is blurred by atmospheric turbulence blur which results with a highly noisy image (see Fig. B).
- We ran algorithms and show the results for:
  • RLS with standard regularization ($\mathbf{L} = \mathbf{I}$).
  • RLS with $\mathbf{L}$ as a discrete approximation of the Laplace operator, which is standard in image processing .
  • TTLS and our algorithm RTLSC.

Results for Regularization Solvers: RLS

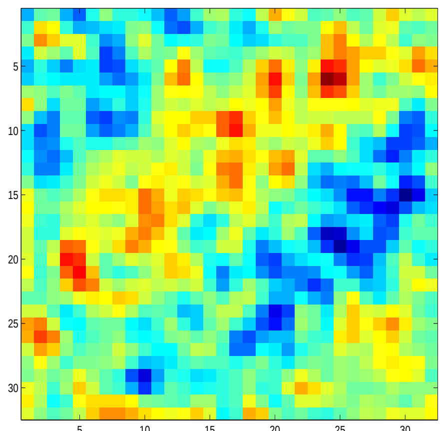
(A) True Image



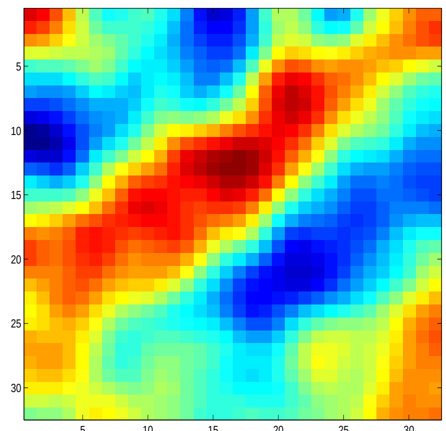
(B) Observation



(C) RLS with $\mathbf{L} = \mathbf{I}$

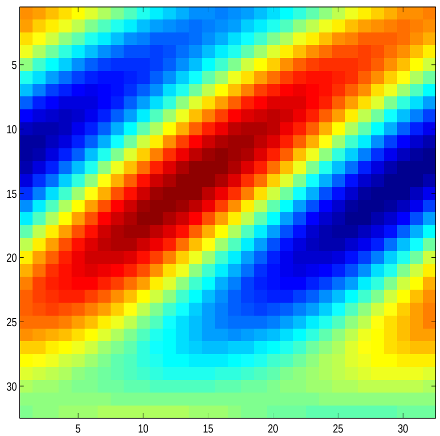


(D) RLS with Laplace operator

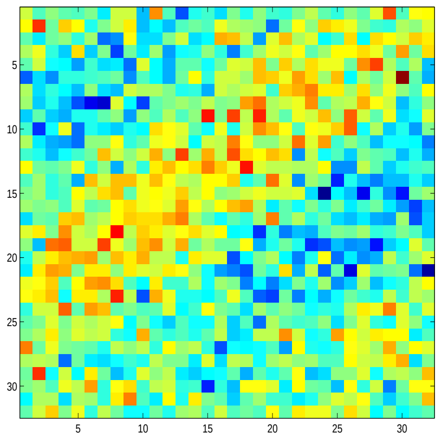


Results for Regularization Solvers: TTLS and RTLSC

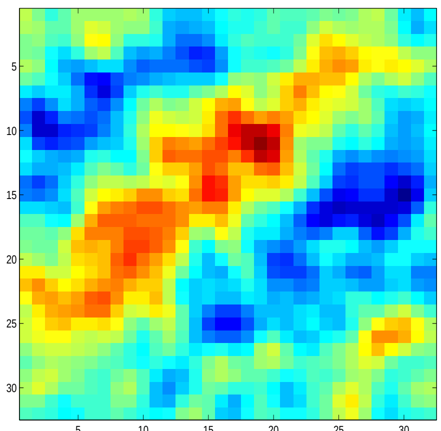
(A) True Image



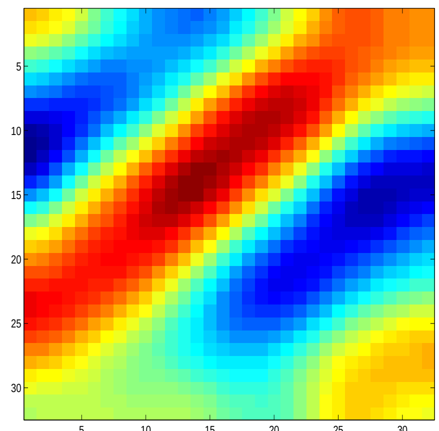
(B) Observation



(E) TTLS

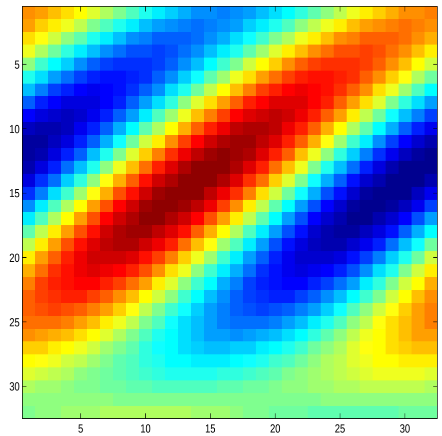


(F) Our Algorithm: RTLSC

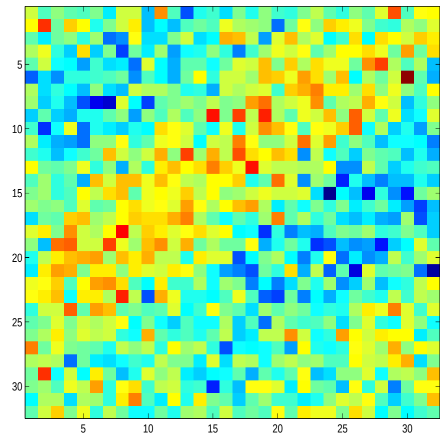


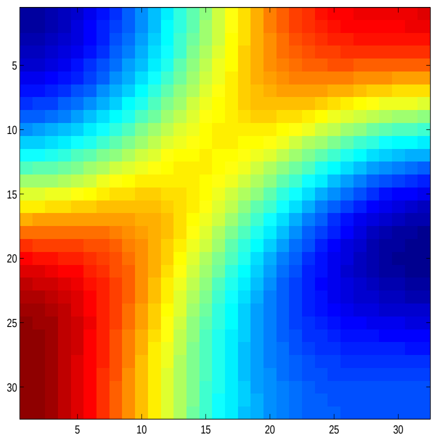
First three iterations of algorithm RTLSC

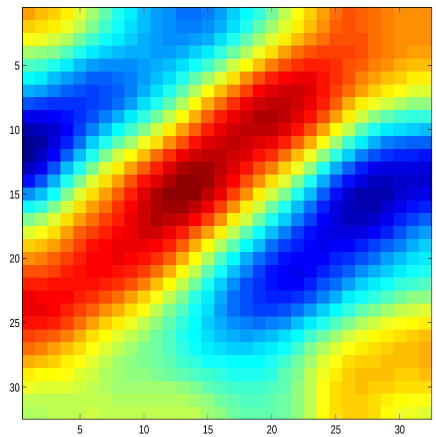
(A) True Image

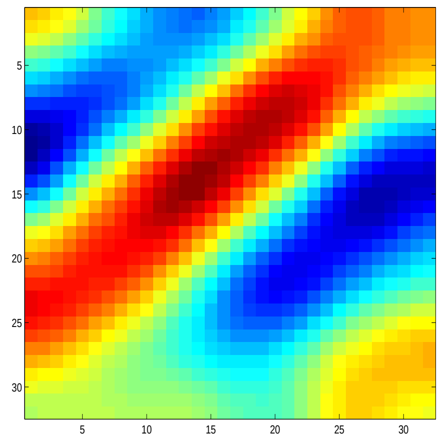


(B) Observation









An Empirical Observation and Some Questions...

Thousands of simulations suggest that both methods converge very quickly to a global minimum

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- What is the theoretical rate of convergence of the iterative scheme?
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- Hidden convexity...

Underlying Assumption

Assumption:

$$\exists \eta \geq 0 : \begin{pmatrix} \mathbf{A}_2 & \mathbf{b}_2 \\ \mathbf{b}_2^T & c_2 \end{pmatrix} + \eta \begin{pmatrix} \mathbf{L}^T\mathbf{L} & \mathbf{0} \\ \mathbf{0} & -\rho \end{pmatrix} \succ \mathbf{0}. \quad (1)$$

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- Implies that the problem is well-defined ($f_2(\mathbf{x}) > 0$ for every $\mathbf{x}$ such that $\|\mathbf{L}\mathbf{x}\|^2 \leq \rho$).
- Automatically satisfied for the RTLS problem ($\eta = 0$).
- Satisfied for the GTRS problem if $r = n$.

$$\mathbf{A} \succeq \mathbf{B} \Leftrightarrow \mathbf{A} - \mathbf{B} \textbf{ PSD}$$

$$\mathbf{A} \succ \mathbf{B} \Leftrightarrow \mathbf{A} - \mathbf{B} \textbf{ PD}$$

Attainability of the minimum

The minimum is not always attained. For example,

$$\min_{x_1,x_2}\left\{f(x_1,x_2)=\frac{5-4x_1+2x_1^2+x_2^2+x_1x_2}{1+x_1^2+x_2^2+x_1x_2}:x_1^2\leq 1\right\}.$$

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The infimum not attained since

$$f(x_1,x_2)=1+\frac{(x_1-2)^2}{1+x_1^2+x_2^2+x_1x_2}>1.$$

Attainability of the minimum

Attainability Condition: Either the feasible set if compact or

$$\lambda_{\min}(\mathbf{M}_1, \mathbf{M}_2) < \lambda_{\min}(\mathbf{F}^T\mathbf{A}_1\mathbf{F}, \mathbf{F}^T\mathbf{A}_2\mathbf{F}),$$

where

$$\mathbf{M}_1 = \begin{pmatrix} \mathbf{F}^T\mathbf{A}_1\mathbf{F} & \mathbf{F}^T\mathbf{b}_1 \\ \mathbf{b}_1^T\mathbf{F} & c_1 \end{pmatrix}, \mathbf{M}_2 = \begin{pmatrix} \mathbf{F}^T\mathbf{A}_2\mathbf{F} & \mathbf{F}^T\mathbf{b}_2 \\ \mathbf{b}_2^T\mathbf{F} & c_2 \end{pmatrix}$$

and **F** is an $n \times (n-r)$ matrix whose columns form an orthonormal basis for the null space of L.

- Weak inequality is always satisfied.
- (B-, T-, 06) The minimum is attained under the above assumption. Mathematical tools: recession function and sets.
- A generalization of the attainability condition for the unconstrained TLS problem : $\sigma_{\min}(\mathbf{A}, \mathbf{b}) < \sigma_{\min}(\mathbf{A})$.

Reformulation as a Nonconvex Quadratic Problem

Under the attainability condition, (RQ) can be homogenized:

$$\min_{\mathbf{z}\in\mathbb{R}^n, s\in\mathbb{R}} \left\{\varphi_1(\mathbf{z},s) : \varphi_2(\mathbf{z},s) = 1, \varphi_3(\mathbf{z},s) \leq 0\right\},$$

where

$$\begin{aligned}
\varphi_i(\mathbf{z},s) &= \mathbf{z}^T\mathbf{A}_i\mathbf{z} + 2\mathbf{b}_i^T\mathbf{z}s + c_i s^2, \quad i = 1,2,\\
\varphi_3(\mathbf{z},s) &= \|\mathbf{L}\mathbf{z}\|^2 - \rho s^2.
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S-Lemma of Polyak (98): under some mild conditions the following are equivalent for three symmetric matrices $\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3$:

(i) $\mathbf{y}^T\mathbf{R}_2\mathbf{y}=a_2, \mathbf{y}^T\mathbf{R}_3\mathbf{y}\le a_3 \Rightarrow \mathbf{y}^T\mathbf{R}_1\mathbf{y}\ge a_1.$

(ii) $\exists \alpha\in\mathbb{R}, \beta\in\mathbb{R}_+ : \mathbf{R}_1\succeq \alpha\mathbf{R}_2-\beta\mathbf{R}_3, \quad \alpha a_2\ge a_1+\beta a_3$

Semidefinite formulation of (RQ)

Under the attainability condition:

$$\begin{aligned} \max_{\beta\geq 0,\alpha,\lambda\in\mathbb{R}} \quad & \lambda \\ \text{s.t.} \quad & \begin{pmatrix} \mathbf{A}_1 & \mathbf{b}_1 \\ \mathbf{b}_1^T & c_1 \end{pmatrix} \succeq \alpha \begin{pmatrix} \mathbf{A}_2 & \mathbf{b}_2 \\ \mathbf{b}_2^T & c_2 \end{pmatrix} - \beta \begin{pmatrix} \mathbf{L}^T\mathbf{L} & \mathbf{0} \\ \mathbf{0} & -\rho \end{pmatrix}, \\ & \alpha \geq \lambda. \end{aligned}$$

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- Under the attainability condition, problem (RQ) is equivalent to a single convex semidefinite problem.
- The SDP problem can be solved efficiently via interior point methods.
- The solution of (RQ) can be extracted from the solution of the semidefinite formulation.

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Nonconvex problems that can be transformed into convex problems:

- GTRS problems: $\min\{\mathbf{x}^T\mathbf{A}_1\mathbf{x} + 2\mathbf{b}_1^T\mathbf{x} + c_1 : \|\mathbf{L}\mathbf{x}\|^2 \leq \rho\}$
- Nonconvex homogenous quadratic programming with two quadratic constraints (Polyak, 98):

$$\min\{\mathbf{x}^T\mathbf{Q}_0\mathbf{x} : \mathbf{x}^T\mathbf{Q}_1\mathbf{x} \leq \rho_1, \mathbf{x}^T\mathbf{Q}_2\mathbf{x} \leq \rho_2\}$$

- Nonconvex quadratic optimization problems with two quadratic constraints over the complex domain (Beck & Eldar, 2006):

$$\min\{f_0(\mathbf{z}) : f_1(\mathbf{z}) \leq 0, f_2(\mathbf{z}) \leq 0, \mathbf{z} \in \mathbb{C}^n\},$$

where $f_i(\mathbf{z}) = \mathbf{z}^*\mathbf{A}_i\mathbf{z} + 2\Re(\mathbf{b}_i^*\mathbf{z}) + c_i$

Back to the fixed point algorithm...

Under the attainability condition,

- The iterative scheme of Sima et al. converges to a global optimum for the general problem (RQ).

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$\Rightarrow$ three globally convergent algorithms for solving (RQ).

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Thank you for listening!