Riemannian optimization methods to compute the nearest singular pencil

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Part of "Proyecto de I+D+i PID2019-106362GB-I00 financiado por MCIN/AEI/10.13039/501100011033"

ALAMA 2024

Linear Algebra, Matrix Analysis and Applications

Universidad de Oviedo. Gijón (Asturias). 12-14 June 2024

Matrix Pencils

- This talk deals with square complex matrix pencils $A + \lambda B \in \mathbb{C}[\lambda]_1^{n\times n}$ or polynomial matrices of degree 1, where $A, B \in \mathbb{C}^{n\times n}$.
- Matrix pencils arise naturally in differential-algebraic equations and in linear time invariant control systems

$$-B\dot{x} = Ax + Fu, \qquad y = Cx \tag{1}$$

  by taking Laplace transforms.
- The pencil $A + \lambda B$ is regular if its characteristic polynomial $p(\lambda) = \det(A + \lambda B)$ is NOT identically zero. Otherwise, the pencil is singular, i.e., if $p(\lambda) = \det(A + \lambda B) \equiv 0$.
- The regularity of $A + \lambda B$ implies that a solution of (1) exists for all smooth enough controls and for consistent initial conditions.
- This existence is no longer guaranteed if the pencil $A + \lambda B$ is singular. Therefore, the distance of a regular pencil $A + \lambda B$ to a nearest singular pencil is a measure of the robustness of the problem (1).

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Problem

Given a square regular pencil $A + \lambda B \in \mathbb{C}[\lambda]_1^{n\times n}$ find a singular pencil nearest to it.

We measure the distances in Frobenius norm:

$$\|A + \lambda B\|_F := \left\| \begin{bmatrix} A & B \end{bmatrix} \right\|_F .$$

It is also possible and interesting to look for a nearest *real* singular pencil when A and B are real. The approach we present can be extended directly to the real case. We omit the details of the real case for brevity.

Problem (Refined)

Given $A + \lambda B \in \mathbb{C}[\lambda]_1^{n\times n}$, find a minimizer for the distance $\|(A + \lambda B) - (S + \lambda T)\|_F$ amongst all pencils $S + \lambda T \in \mathbb{C}[\lambda]_1^{n\times n}$ that satisfy $\det(S + \lambda T) \equiv 0$.

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Previous works (I)

- **The problem was posed for the first time by Byers, He and Mehrmann in 1998**, who collected lower and upper bounds and proposed several characterizations of the distance to singularity but could not provide an exact solution (except in very special cases) nor an efficient algorithm.

R. Byers, C. He and V. Mehrmann, Where is the nearest non-regular pencil?, Linear Algebra Appl., 285 (1998) 81–105.

- D. Kressner and M. Voigt wrote in 2015 the survey

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Since then, several works have been published on this problem. We mention the following ones:

- M. Giesbrecht, J. Haraldson and G. Labahn presented in 2017 a method based on structured perturbations of mosaic Toeplitz matrices with an asymptotic complexity of $O(n^{12})$ flops per iteration.

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- N. Guglielmi, C. Lubich and V. Mehrmann presented in 2017 an ODE-approach based on expressing the set of $n \times n$ singular pencils as those pencils whose characteristic polynomial is zero when it is evaluated in $n+1$ given distinct points.

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This method needs to compute the smallest singular value of n matrices in each iteration and therefore is slow, though it is flexible for incorporating structures and for being extended to polynomial matrices.

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Previous works (III)

- B. Das and S. Bora presented in 2023 a method based on structured perturbations of the Gantmacher's block Toeplitz matrices associated with a pencil and on a careful analysis of the properties of singular polynomial matrices.

B. Das and S. Bora, Nearest rank deficient matrix polynomials, Linear Algebra Appl., 674 (2023) 304–350.

This method is still very slow, but much more efficient than previous methods, and can be applied/extended to matrix polynomials of degree larger than 1.

In summary:

1. **The problem is very difficult:**
   - no general solution formula exists,
   - the running time of all the numerical methods proposed so far is very high even for pencils of moderate size,
   - the number of local minima seems to increase fast with the size of the pencil, making it hard to find global minima (which in general are not unique).
2. The existing methods rely generally on either
   - ODE-based techniques or
   - structured perturbations of (potentially very large for moderate sizes) block (or mosaic) Toeplitz matrices.
3. The method in this talk uses a novel approach based on Riemannian optimization inspired in the recent work by V. Noferini and F. Poloni (2021)

V. Noferini and F. Poloni, Nearest Ω-stable matrix via Riemannian optimization, Numer. Math., 148(4) (2021) 817–851.

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- **Pros:**
  - Relatively fast $\rightarrow$ works in reasonable times for larger pencils than previous approaches (e.g. 100×100).
  - Yields competitive candidate solutions.
  - Publicly available and easy to use.
- *Current* **Cons:**
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Outline

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Reformulating the problem (I)

The main tool for the reformulation is the Generalized Schur form [Stewart, 1972] of matrix pencils, which let us split the problem in

- finding a nearest singular *upper triangular* pencil and
- solving a minimization problem over unitary matrices (justified later).

We denote by $U(n)$ the set of $n \times n$ unitary matrices.

Theorem (Generalized Schur form)

For any pair $A, B \in \mathbb{C}^{n\times n}$ there exist $Q, Z \in U(n)$ such that QAZ and QBZ are both upper triangular.

Lemma (Singular upper triangular pencil)

An upper triangular square pencil $A + \lambda B$ is singular if and only if it has at least one zero diagonal element.

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Proposition (Nearest singular upper triangular pencil)

Let $A + \lambda B \in \mathbb{C}[\lambda]_1^{n\times n}$. *Let* k *be any index such that*

$$|A_{kk}|^2 + |B_{kk}|^2 = \min_{1\leq i\leq n} \{|A_{ii}|^2 + |B_{ii}|^2\}.$$

An upper triangular singular pencil nearest to $A + \lambda B$ *is* $\mathcal{P}(A) + \lambda\mathcal{P}(B)$ *where*

$$\mathcal{P}(A)_{ij} = \begin{cases} A_{ij} & \text{if } i < j \text{ or } i = j \neq k; \\ 0 & \text{otherwise;} \end{cases} \qquad \mathcal{P}(B)_{ij} = \begin{cases} B_{ij} & \text{if } i < j \text{ or } i = j \neq k; \\ 0 & \text{otherwise;} \end{cases}$$

i.e., $\mathcal{P}(A)$ *and* $\mathcal{P}(B)$ *are obtained by setting to zero the lower triangular parts of* A *and* B*, respectively, and* A_{kk} *and* B_{kk}.

In particular, the squared distance of $A + \lambda B$ *from* $\mathcal{P}(A) + \lambda\mathcal{P}(B)$ *is*

$$\mathcal{F}(A + \lambda B) = \sum_{i>j}(|A_{ij}|^2 + |B_{ij}|^2) + \min_{1\leq i\leq n} \{|A_{ii}|^2 + |B_{ii}|^2\}.$$

Reformulating the problem (II)

Proposition (Nearest singular upper triangular pencil)

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Theorem (Nearest singular pencil via minimization over $U(n) \times U(n)$)

If $A + \lambda B \in \mathbb{C}[\lambda]_1^{n\times n}$, then the squared distance of $A + \lambda B$ to a nearest singular pencil is

$$\min_{(Q,Z)\in U(n)\times U(n)} f(Q,Z),$$

where

$$f(Q,Z) := \mathcal{F}(QAZ + \lambda QBZ) = \|(QAZ + \lambda QBZ) - (\mathcal{P}(QAZ) + \lambda \mathcal{P}(QBZ))\|_F^2.$$

Moreover, if (Q_0, Z_0) is a global minimizer of $f(Q,Z)$ over $U(n) \times U(n)$, then the pencil

$$Q_0^* \mathcal{P}(Q_0 A Z_0) Z_0^* + \lambda Q_0^* \mathcal{P}(Q_0 B Z_0) Z_0^*$$

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Proof.

Let $\mathcal{S}_n, \mathcal{T}_n \subset \mathbb{C}[\lambda]_1^{n\times n}$ denote the set of singular pencils and the set of singular upper triangular pencils, respectively. Then,

$$\begin{aligned}\min_{S+\lambda T\in\mathcal{S}_n} \|(A-S)+\lambda(B-T)\|_F^2 &= \min_{Q,Z\in U(n)} \min_{X+\lambda Y\in\mathcal{T}_n} \|(A-Q^*XZ^*)+\lambda(B-Q^*YZ^*)\|_F^2 \\ &= \min_{Q,Z\in U(n)} \min_{X+\lambda Y\in\mathcal{T}_n} \|(QAZ-X)+\lambda(QBZ-Y)\|_F^2 \\ &= \min_{Q,Z\in U(n)} \mathcal{F}(QAZ+\lambda QBZ).\end{aligned}$$

$\square$

Summary of the reformulation

- **Squared distance** of $A + \lambda B$ to a nearest singular upper triangular pencil is

$$\mathcal{F}(A + \lambda B) = \sum_{i>j} (|A_{ij}|^2 + |B_{ij}|^2) + \min_{1 \le i \le n} (|A_{ii}|^2 + |B_{ii}|^2).$$

- The objective function in $U(n) \times U(n)$ is

$$f(Q, Z) := \mathcal{F}(QAZ + \lambda QBZ).$$

  We are interested in finding

$$(Q_0, Z_0) \in \underset{(Q,Z) \in U(n) \times U(n)}{\operatorname{argmin}} f(Q, Z).$$

- A singular pencil nearest to $A + \lambda B$ is given by

$$Q_0^* \mathcal{P}(Q_0 A Z_0) Z_0^* + \lambda Q_0^* \mathcal{P}(Q_0 B Z_0) Z_0^*.$$

Outline

Minimizing the objective function

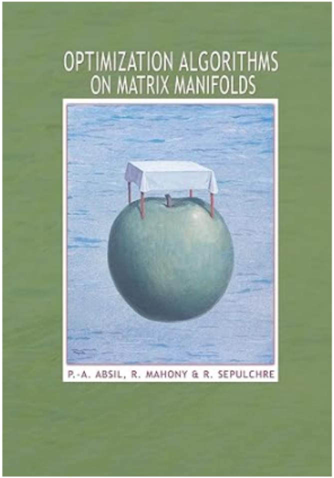
- How to find

$$(Q_0, Z_0) \in \operatorname*{argmin}_{(Q,Z)\in U(n)\times U(n)} f(Q,Z)$$

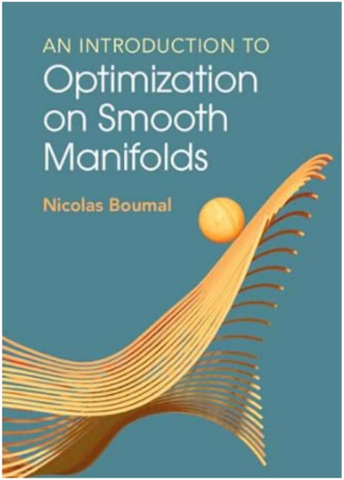
with

$$f(Q,Z) := \sum_{i>j} \left(|(QAZ)_{ij}|^2 + |(QBZ)_{ij}|^2\right) + \min_{1\le i\le n} \left(|(QAZ)_{ii}|^2 + |(QBZ)_{ii}|^2\right)?$$

Books on optimization on matrix manifolds



Princeton University Press, 2008



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- We use **MATLAB toolbox Manopt 7.1 for optimization on matrix manifolds**, in particular its `trustregions` method.

N. Boumal, B. Mishra, P. A. Absil and R. Sepulchre, Manopt, a Matlab toolbox for optimization on manifolds, The Journal of Machine Learning Research, 15(1) (2014) 1455-1459.

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- Problem is **non-convex**: computed minimum is not necessarily global.
- Manopt requires for high-efficiency that the user provides MATLAB functions for the **Riemannian gradient** and the **Riemannian Hessian** on the manifold $U(n) \times U(n)$ of the objective function.
- This requires considerable work. We omit explanations for brevity.

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- We use **MATLAB toolbox Manopt 7.1 for optimization on matrix manifolds**, in particular its `trustregions` method.

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Outline

Non-smoothness of the objective function

- The algorithm described always converged to a stationary point for a large volume of randomly generated inputs, as well as on all problems previously appeared in the literature, but
- **the objective function is not smooth**, because

$$f(Q,Z) = \sum_{i>j}(|(QAZ)_{ij}|^2 + |(QBZ)_{ij}|^2) + \min_{1\le i\le n}(|(QAZ)_{ii}|^2 + |(QBZ)_{ii}|^2).$$

- Thus, **global convergence** of the Riemannian trustregions algorithm to a stationary point **is not guaranteed**.
- Nevertheless, we have been able to prove that

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For every pencil $A+\lambda B$, the function $f(Q,Z)$ is real-differentiable at all its local minima.

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1. Smoothen the objective function via the Boltzmann operator, i.e., replace

$$\min(x_1, \ldots, x_n) \quad \longrightarrow \quad \mathcal{S}_\alpha(x_1, \ldots, x_n) = \frac{\sum_{i=1}^n x_i e^{\alpha x_i}}{\sum_{i=1}^n e^{\alpha x_i}},$$

with α negative of sufficiently large magnitude. Note that $\mathcal{S}_\alpha(x_1, \ldots, x_n) \to \min(x_1, \ldots, x_n)$ as $\alpha \to -\infty$.

2. Minimize over $U(n) \times U(n)$ each of the n everywhere smooth functions

$$f_\ell(Q, Z) = \sum_{i>j} (|(QAZ)_{ij}|^2 + |(QBZ)_{ij}|^2) + (|(QAZ)_{\ell\ell}|^2 + |(QBZ)_{\ell\ell}|^2),$$

$\ell = 1, \ldots n$, and pick as solution of our problem the one associated with the smallest minimum $f_\ell(Q_0^\ell, Z_0^\ell)$.

Each minimization subproblem $\min f_\ell(Q, Z)$ finds a nearest singular pencil with a specified (right) minimal index equal to $\ell - 1$.

These two algorithms are slower than the basic one!!!

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Outline

Numerical experiment I: Comparison with ODE-approach

- We only show results for the basic algorithm.
- First, we benchmark against the ODE-approach [Guglielmi et al., 2017].
- We use 10^3 complex random 6×6 pencils.
- Statistical comparisons with much larger pencils are not feasible because the current implementation of the ODE-approach is too slow.
- Real and imaginary parts of the matrix coefficients are drawn from $\mathcal{N}(0,1)$.

Method	Frequency of best output	Median distance	Average distance
ODE	37.3 %	1.8925	2.0601
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- For each $n = 6, 15, 30, 50$ we use 10^3 complex random $n \times n$ pencils as in Experiment I.
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- The quality of the output of the Riemannian algorithm was typically worse than that of Das-Bora algorithm for very small inputs $n = 6, 15$, but slightly better for $n = 30$ and already much better for $n = 50$.
- In terms of running time, the Riemannian algorithm outperformed Das-Bora algorithm already for $n = 15$; for $n = 50$ the difference was already striking, with a ratio of average running times ≈ 29 in favour of our method.

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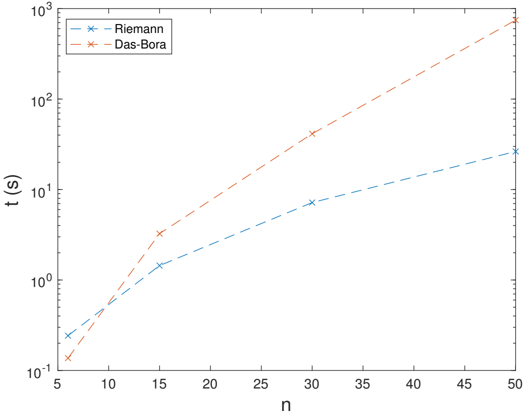
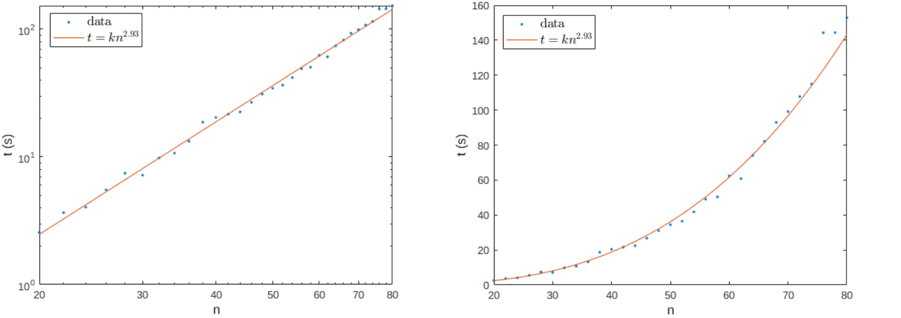


Comparison of the running time between the Riemannian method and the Das-Bora algorithm for $n \in \{6, 15, 30, 50\}$. Running times were measured using MATLAB R2023a on an Intel Core i5-12600K.

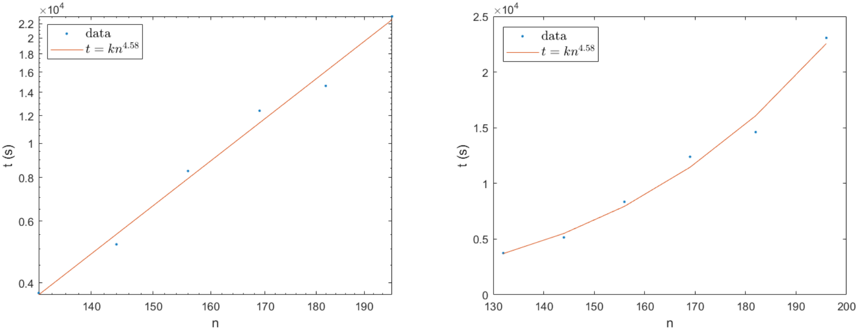
For each n, we generate random $n \times n$ pencils as before, and measure the running time.



Average running time (of 50 runs) in logarithmic scale (left) and linear scale (right) for $20 \le n \le 80$. The least squares fit yields approximately

$$t = k\, n^{2.93},$$

where $k \approx 3.8310 \times 10^{-4}$. We used MATLAB R2023a and an Intel Core i5-12600K Processor.



Average running time (of 24 runs) in logarithmic scale (left) and linear scale (right) for $130 \leq n \leq 200$. The least squares fit yields approximately

$$t = k\, n^{4.58},$$

where $k \approx 7.3423 \cdot 10^{-7}$. We used MATLAB R2023a and its internal parallelization with 24 processes on a 2x12 core Xeon E5 2690 v3 2.60GHz. The computational resources were provided by the Aalto Science-IT project.

Outline

- We have described a novel algorithm to compute the nearest singular pencil to a given one, based on Riemannian optimization.
- The new method makes it practically feasible, for the first time, to solve the problem for pencils of moderate size, say, a few hundreds rows-columns.
- The Riemannian method does better than other methods in terms of the quality of the output when the size of the problem is not very small.
- Furthermore, the performance is also very favourable to the new algorithm in terms of computational time.

Conclusions

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