Detecting the numerical ill posedness in delay (and ordinary) differential equations

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Distance to singularity

Consider a matrix-valued function in the form:

$$\mathcal{D}(\lambda) = f_0(\lambda) A_0 + f_1(\lambda) A_1 + \ldots + f_d(\lambda) A_d,$$

where $A_i \in \mathbb{C}^{n \times n}$ and analytic functions $f_i : \mathbb{C} \mapsto \mathbb{C}$, $i = 0, \ldots, d$.
$\mathcal{D}(\lambda)$ is regular if $\det(\mathcal{D}(\lambda)) \not\equiv 0$, otherwise it is singular.

Distance to singularity

Given a regular function $\mathcal{D}(\lambda)$, we look for the **distance to singularity**:

$$d(\mathcal{D}) = \min \{ \| [\Delta A_0, \ldots, \Delta A_d] \| \text{ such that } \widetilde{\mathcal{D}}(\lambda) = \sum_{i=0}^{d} f_i(\lambda)(A_i + \Delta A_i) \text{ is singular } \}.$$

Motivating example

Consider a system

$$E\dot{y}(t) = Ay(t) + By(t - \tau)$$
$$y(t) = \begin{pmatrix} \cos(\pi t) \\ 2 - 4t^2 \end{pmatrix}, \text{ for } t \leq 0,$$

where

$$E = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix},\ A = \begin{pmatrix} -1+\delta & \frac{1}{2} \\ 0 & -1 \end{pmatrix},\ B = \begin{pmatrix} 1+\delta & -\frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix}.$$

We consider:

- $\delta = 0$ and $\delta = 2 \times 10^{-6}$;
- $\tau = 1$ and $\tau = 10^{-5}$.

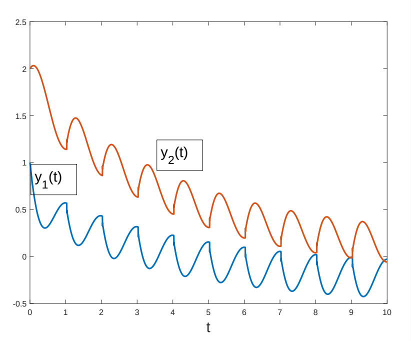
Motivating example

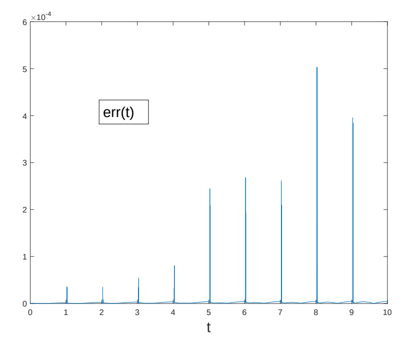
Case: $\tau = 1$.

$y(t)$: solution of the system with $\delta = 0$;

$\tilde{y}(t)$: solution of the system with $\delta = 2 \times 10^{-6}$;

$\mathrm{err}(t) := \|\tilde{y}(t) - y(t)\|$: error.



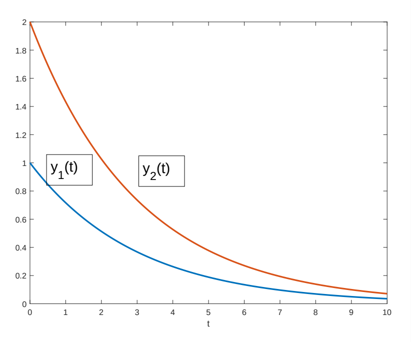


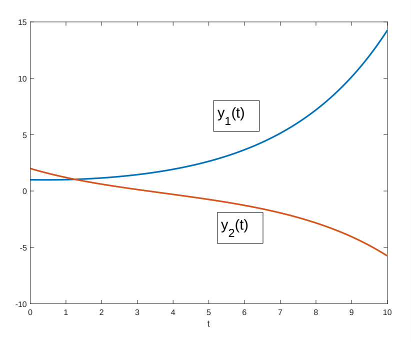
Motivating example

Case: $\tau = 10^{-5}$.

$y(t)$: solution of the system with $\delta = 0$;

$\tilde{y}(t)$: solution of the system with $\delta = 2 \times 10^{-6}$.





Motivating example

The pencil $\lambda E - A$ is robustly regular, that is

$$\exists \lambda \in \mathbb{C}: \ \det(\lambda E - A) \neq 0.$$

But we have that:

$$F(\lambda;\tau) = \det\left(\lambda E - A - Be^{-\lambda\tau}\right) \approx 0$$

For λ such that $|\lambda\tau| \ll 1$, we have

$$A + Be^{-\lambda\tau} \approx A + B = \begin{pmatrix} 0 & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

Examples

Matrix-valued function:

$$\mathcal{D}(\lambda) = f_0(\lambda)\, A_0 + f_1(\lambda)\, A_1 + \ldots + f_d(\lambda)\, A_d, \quad A_i \in \mathbb{C}^{n\times n}$$

Few examples:

- Matrix polynomials $\mathcal{D}(\lambda) = A_0 + \lambda A_1 + \ldots + \lambda^d A_d$
  $\Rightarrow$ Differential Algebraic Equations;
- Matrix-valued quasi-polynomials $\mathcal{D}(\lambda) = \lambda A_2 + e^{-\lambda} A_1 + A_0$
  $\Rightarrow$ Delay Differential Equations.

We are interested in

$$\det(\mathcal{D}(\lambda)) \approx 0.$$

A few references

- R. Byers, C. He, V. Mehrmann, (1998), *Where is the nearest non-regular pencil?*, Linear Algebra and its Applications.
- N. Guglielmi, C. Lubich, V. Mehrmann, (2017) *On the nearest singular matrix pencil*, SIAM Journal on Matrix Analysis and Applications.
- F. Dopico, V. Noferini, L. Nyman, (2023) *A Riemannian optimization method to compute the nearest singular pencil*, arXiv.
- B. Das, S. Bora, (2023) *Nearest rank deficient matrix polynomials*, Linear Algebra and its Applications.

Robust non-singularity of the problem

We consider the following measure of non-singularity

$$\text{dist} := \min_{\Delta A_i \in \mathbb{C}^{n\times n}} \| \, [\Delta A_0, \ldots, \Delta A_d] \, \|_F$$

$$\text{subj.to } \det \left(\sum_{i=0}^{k} (A_i + \Delta A_i) f_i(\lambda) \right) \equiv 0.$$

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Two interesting cases:

- $\widetilde{\mathcal{D}}(\lambda) = \sum_{i=0}^{d} \lambda^i \, (A_i + \Delta A_i)$, matrix polynomial
  $\Rightarrow$ Analysis tool: Fundamental Theorem of the Algebra;
- $\widetilde{\mathcal{D}}(\lambda) = \sum_{i=0}^{d} f_i(\lambda) \, (A_i + \Delta A_i)$, with f_i entire
  $\Rightarrow$ Analysis tool: Maximum Modulus Theorem.

Numerically singular

Consider a (suitably normalized) matrix $A \in \mathbb{C}^{n\times n}$ and a certain threshold $\delta > 0$, larger or equal than machine precision. Let $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n$ the singular values computed in finite arithmetic. We say that r is the *numerical rank* of the matrix A if

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > \delta \geq \sigma_{r+1} \geq \ldots \geq \sigma_n.$$

Consequently, we define the matrix A *numerically singular* if the numerical rank $r < n$.

Fundamental theorem of the algebra

The scalar polynomial $\det(\mathcal{P}(\lambda) + \Delta\mathcal{P}(\lambda)) \equiv 0$ if

$$\det(\mathcal{P}(\mu_j) + \Delta\mathcal{P}(\mu_j)) = 0,$$

with distinct points μ_j, $j = 1, \ldots, m$ and $m \geq dn + 1$.

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Optimization problem (discrete version):

$$\begin{aligned} \text{dist} = \min_{\Delta A_i \in \mathbb{C}^{n\times n}} & \| \left[\Delta A_0, \ldots, \Delta A_d\right] \|_F \\ & \text{subj. to } \sigma_{\min}\left(\mathcal{P}(\mu_j) + \Delta\mathcal{P}(\mu_j)\right) = 0, \\ & \text{for } j = 1, \ldots, m. \end{aligned}$$

Fundamental theorem of the algebra

An intuitive generalization: consider the delay function

$$\begin{aligned}\mathcal{D}(\lambda) &= \lambda E - A - e^{-\tau\lambda}B \\ &\approx \lambda E - A - \left(\sum_{i=0}^{k} \frac{(-\tau\lambda)^i}{i!}\right) B.\end{aligned}$$

Fundamental theorem of the algebra

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$$\mathcal{D}(\lambda) = \lambda E - A - e^{-\tau\lambda} B$$
$$\approx \lambda E - A - \left(\sum_{i=0}^{k} \frac{(-\tau\lambda)^i}{i!} \right) B.$$

A few possible issues

- It may be not clear which k we should use;
- It may be not immediate to bound the approximation error;
- A large value of k may lead to a large amount of support points μ_i.

Maximum Modulus Theorem

Choose a bounded subset Ω with boundary $\partial\Omega$ and impose

$$\max_{\lambda \in \partial\Omega} \left| \det\left(\widetilde{\mathcal{D}}(\lambda) \right) \right| = 0,$$

where $\tilde{D}(\lambda) = \sum_{i=0}^{k} (A_i + \Delta A_i) f_i(\lambda)$. Then we get that

$$\max_{\lambda \in \bar{\Omega}} \det\left(\widetilde{\mathcal{D}}(\lambda) \right) = 0.$$

Maximum Modulus Theorem

Choose a bounded subset Ω with boundary $\partial\Omega$ and impose

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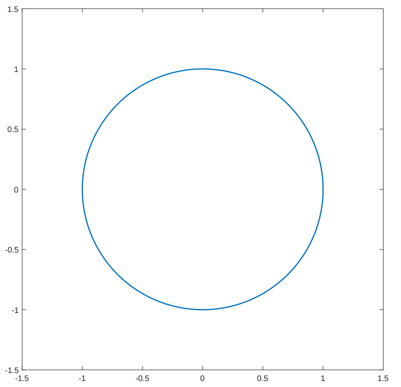
$$\max_{\lambda \in \bar{\Omega}} \det\left(\widetilde{\mathcal{D}}(\lambda)\right) = 0.$$

Idea: consider a suitable bounded subset $\Omega \subseteq \mathbb{C}$:

$$\begin{aligned} \text{dist} = \min_{\Delta A_i \in \mathbb{C}^{n \times n}} & \| [\Delta A_0, \ldots, \Delta A_d] \|_F \\ \text{subj.to } & \left| \det\left(\widetilde{\mathcal{D}}(\lambda)\right) \right| \equiv 0 \text{ for } \lambda \in \partial\Omega. \end{aligned}$$

Outline of the method

- Choose $f(\lambda) = \det\left(\widetilde{\mathcal{D}}(\lambda)\right)$;
- Choose as Ω a complex disk;



Choice of the points

Theorem (Trefethen et al. 2014): Let f be analytic in $\Omega_R = \{z \in \mathbb{C} : |z| \leq R\}$ for some $R > 1$. Consider $p(z)$ polynomial interpolant of degree $m-1$ at the points

$$z_k = e^{\frac{2\pi \mathbf{i}}{m} j}, \quad j = 1, \ldots, m.$$

Then for any ρ with $1 < \rho < R$, the polynomial approximation has accuracy

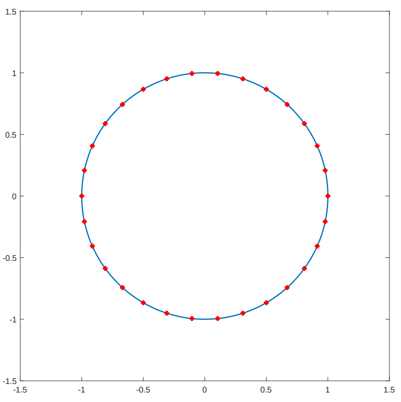
$$|p(z) - f(z)| = \begin{cases} O\left(\rho^{-m}\right), & |z| \leq 1, \\ O\left(|z|^m \rho^{-m}\right), & 1 \leq |z| < \rho. \end{cases}$$

Where:

$$|p(z) - f(z)| \approx \left| \frac{1}{2\pi \mathbf{i}} \int_{\zeta \in \partial \Omega_R} \zeta^{-m-1} f(\zeta)\, d\zeta \right|.$$

Outline of the method

- Choose $f(\lambda) = \det\left(\widetilde{\mathcal{D}}(\lambda)\right)$;
- Choose as Ω the unit disk;
- Choose a set of points $\left\{e^{2\pi\mathbf{i}\frac{j}{m}}\right\}$, $j = 1, \ldots, m$.
- Choose number m of points according to:



$$\left|\frac{1}{2\pi\mathbf{i}}\int_{|\zeta|=1}\zeta^{-m-1}\det(\zeta)\,d\zeta\right| \leq \text{tol}.$$

Outline of the method

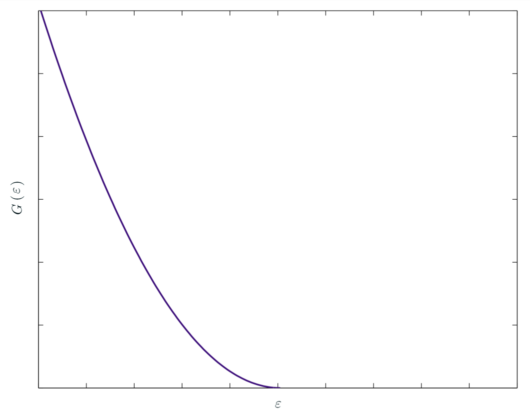
Optimization problem (discrete version):

$$\text{dist} = \min_{\Delta A_i \in \mathbb{C}^{n\times n}} \|[\Delta A_0, \ldots, \Delta A_d]\|_F$$
$$\text{subj. to } \sigma_{\min}\left(\widetilde{\mathcal{D}}(\mu_j)\right) = 0,$$
$$\text{for } \mu_j = e^{2\pi i \frac{j}{m}},\ j = 1, \ldots, m.$$

Consider $[\Delta A_0, \ldots, \Delta A_d] = \varepsilon\,[\Delta_0, \ldots, \Delta_d]$, of norm ε and the functional

$$G_\varepsilon\left(\Delta_0, \ldots, \Delta_d\right) = \frac{1}{2}\sum_{i=1}^{m} \sigma_{\min}^2\left(\widetilde{\mathcal{D}}(\mu_j)\right).$$

A two step method



- **Inner iteration**: fix the norm ε and solve the problem $G(\varepsilon) = \min_{\Delta_0,\dots,\Delta_d} G_\varepsilon(\Delta_0, \dots, \Delta_d)$;
- **Outer iteration**: tune the value ε in order to find the smallest zero ε^* of $G(\varepsilon)$.

Inner iteration

Lemma: Let $\Delta_0(t), \ldots, \Delta_d(t) \in \mathbb{C}^{n\times n}$ be a smooth path of matrices, with derivatives $\dot{\Delta}_0(t), \ldots, \dot{\Delta}_d(t)$. Then $G_\varepsilon\left(\Delta_0(t), \ldots, \Delta_d(t)\right)$ is differentiable and

$$\frac{d}{dt} G_\varepsilon\left(\Delta_0, \ldots, \Delta_d\right) = \varepsilon \mathrm{Re}\left\langle \left[M_0, \ldots, M_d\right], \left[\dot{\Delta}_0, \ldots, \dot{\Delta}_d\right]\right\rangle,$$

where for $i = 0, \ldots, d$

$$M_i = \sum_{j=1}^{m} \sigma_j \bar{f}_i(\mu_j) u_j v_j^H,$$

where $\sigma_j = \sigma_{\min}\left(\widetilde{\mathcal{D}}(\mu_j)\right)$ and u_j, v_j are the left and right singular vectors associated with σ_j.

Here we denote: $\langle X, Y\rangle = \mathrm{trace}\left(X^H Y\right)$.

Inner iteration

The (local) minimizers of the functional are the stationary points of the constrained gradient system for the functional G_ε:

$$\dot{\Delta}_i = -M_i + \eta \Delta_i, \quad i = 0, \ldots, d,$$

where η is chosen such that

$$\operatorname{Re} \left\langle \left[\dot{\Delta}_0, \ldots, \dot{\Delta}_d \right], [\Delta_0, \ldots, \Delta_d] \right\rangle = 0.$$

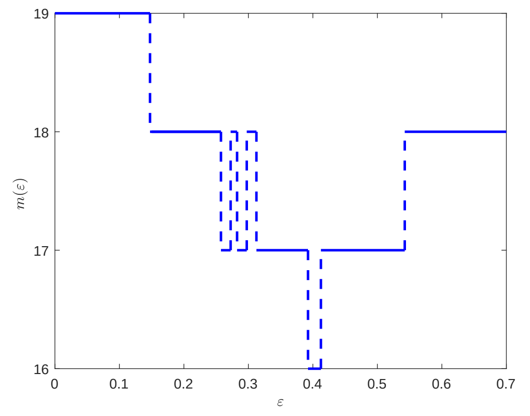
Remark

If $m \ll n$, we have a low-rank property on M_i.

Choice of the number of support points

The number of points $m(\varepsilon)$ may change at each iteration

$$\left| \frac{1}{2\pi\mathbf{i}} \int_{|\zeta|=1} \zeta^{-m(\varepsilon)-1} \det(\zeta,\varepsilon) d\zeta \right| \leq \text{tol}.$$



Structured distance to singularity

Consider a subset $\mathcal{S}$ in $\mathbb{C}^{(d+1)n \times n}$ of matrices and $\mathcal{F}(\lambda)$ with coefficients $[A_d, \ldots, A_0] \in \mathcal{S}$.

Structured distance to singularity

The structured distance to singularity for $\mathcal{F}(\lambda)$ is the

$$d_{\text{sing}}^{\mathcal{S}}(\mathcal{F}(\lambda)) = \min \{ \| [\Delta A_d, \ldots, \Delta A_0] \|_F \text{ such that } [\Delta A_d, \ldots, \Delta A_0] \in \mathcal{S} \text{ and } \mathcal{F}(\lambda) + \Delta\mathcal{F}(\lambda) \text{ is singular} \}.$$

A few interesting examples

Possible structures on the matrix-valued functions:

- Fixed coefficients: for a set $I \subseteq \{0, \dots, d\}$, $|I| \leq d$, we have $\Delta A_i \equiv 0$, $i \in I$;
- Linear structure (e.g. sparsity pattern): $\Delta A_i \in \mathcal{S}_i \subseteq \mathbb{C}^{n \times n}$;
- Collective structure: for instance palindromic properties $\left\{[\Delta A_d, \dots, \Delta A_0] : \Delta A_{d-i} = \Delta A_i^H, \text{ for } i = 0, \dots, d\right\}$.

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The (local) minimizers of the functional are the stationary points of the ODE system:

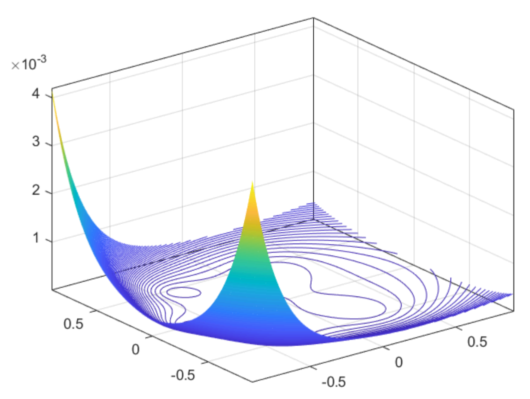
$$\dot{\Delta}_i = -\Pi_{\mathcal{S}_i}\left(M_i\right) + \eta \Delta_i,$$

where $\Pi_{\mathcal{S}} : \mathbb{C}^{(d+1)n \times n} \mapsto \mathcal{S}$ projection onto the structure.

Delay matrix-valued function

Imposing sparsity pattern on:

$$\mathcal{D}(\lambda) = \lambda E - A - e^{-\lambda} B$$
$$= -\lambda I_3 - \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ a_0 & a_1 & a_2 \end{bmatrix} - e^{-\lambda} \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ b_0 & b_1 & b_2 \end{bmatrix}$$



Case of matrix polynomials

Example: `mirror` from `nlevp` package:

- quartic $\lambda^4 A_4 + \ldots + \lambda A_1 + A_0$;
- size 9×9;
- degree of the determinant is 27;
- impose sparsity pattern.

	Max. Mod.	Th. Alg deg = 36	Th. Alg. deg = 27
Distance	4.1989×10^{-4}	4.1492×10^{-4}	4.1633×10^{-4}
Num. points	12	37	28
Time	38.89994	1.842×10^{2}	1.4623×10^{2}
Iter.	8	16	16
Max. $\sigma_{\min}$	7.1749×10^{-6}	1.1105×10^{-5}	9.9890×10^{-6}

T. Betcke, N.J. Higham, V. Mehrmann, C. Schröder, F. Tisseur.
NLEVP: A Collection of Nonlinear Eigenvalue Problems, 2013.

Conclusions

Conclusions

- We propose a novel approach for matrix-valued functions;
- We are able to treat structured perturbations;
- The method involves a limited amount of support points;
- The method can be also employed to accelerate the computation for matrix polynomials.

- **M. Gnazzo**, N. Guglielmi. On the numerical approximation of the distance to singularity for matrix-valued functions. *arXiv*, 2023.
- **M. Gnazzo**, N. Guglielmi. Computing the closest singular matrix polynomial. *arXiv*, 2023.