Permuted Graph Bases for Verified Computation of Invariant Subspaces

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Invariant subspaces

Definition

A subspace $U \in \mathbb{C}^{n \times k}$ is called invariant under $H \in \mathbb{C}^{n \times n}$ if Hu is in U for all u in U.

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Equivalent problem

Find $U \in \mathbb{C}^{n\times k}$ and $R \in \mathbb{C}^{k\times k}$ s.t. $HU = UR$.

Related non-Hermitian algebraic Riccati equation

Assumption $HU = UR,\ U = \begin{bmatrix} I_{k\times k} \\ X_{(n-k)\times k} \end{bmatrix},$

Solve the non-Hermitian algebraic Riccati equation (NARE)

$$F(X) := Q + XA + \tilde{A}X - XGX = 0, \qquad (1)$$

instead of finding invariant subspaces for

$$H = \begin{bmatrix} A_{k\times k} & -G_{k\times(n-k)} \\ -Q_{(n-k)\times k} & -\tilde{A}_{(n-k)\times(n-k)} \end{bmatrix}.$$

- $R = A - GX$ is the closed loop matrix associated to 1.
- A solution X of 1 is called stabilizing if the closed loop matrix R is stable.

Graph matrix and graph subspace

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$$\text{Graph matrix } \mathcal{G}(X) := \begin{bmatrix} I_{k\times k} \\ X_{(n-k)\times k} \end{bmatrix}.$$

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Almost every subspace is a graph subspace:

If $U = \begin{bmatrix} E_{k\times k} \\ A_{(n-k)\times k} \end{bmatrix}$ full column rank, E invertible then $U = \mathcal{G}(AE^{-1})E$.

Graph basis matrix

Definition

U and V full column rank matrices.
$U \sim V$ for a square invertible matrix E, $U = VE \iff$ same column space.

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U and V full column rank matrices.
$U \sim V$ for a square invertible matrix E, $U = VE \iff$ same column space.

- If $U = \begin{bmatrix} E \\ A \end{bmatrix}$, with E square invertible, $U \sim \begin{bmatrix} I \\ AE^{-1} \end{bmatrix}$ graph basis.
- $E^{-1} \longrightarrow$ danger: can be ill conditioned.

Permuted graph matrix

If E any square invertible submatrix of U, we can post–multiply by E^{-1} to enforce an identity in a subset of rows.

Example

$$U = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \\ 1 & 1 & 2 \\ 3 & 5 & 8 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 \\ 0.5 & 0.5 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 2 & 0 & 1 \end{bmatrix}.$$

We can write this as $U \sim P \begin{bmatrix} I \\ X \end{bmatrix}$, P permutation matrix.

Permuted graph matrix

If E any square invertible submatrix of U, we can post–multiply by E^{-1} to enforce an identity in a subset of rows.

Example

$$U = \begin{bmatrix} \color{red}{1} & \color{red}{2} & \color{red}{3} \\ 4 & 5 & 6 \\ \color{red}{7} & \color{red}{8} & \color{red}{9} \\ \color{red}{1} & \color{red}{1} & \color{red}{2} \\ 3 & 5 & 8 \end{bmatrix} \sim \begin{bmatrix} \color{red}{1} & \color{red}{0} & \color{red}{0} \\ 0.5 & 0.5 & 0 \\ \color{red}{0} & \color{red}{1} & \color{red}{0} \\ \color{red}{0} & \color{red}{0} & \color{red}{1} \\ 2 & 0 & 1 \end{bmatrix}.$$

We can write this as $U \sim P \begin{bmatrix} I \\ X \end{bmatrix}$, P permutation matrix.

Theorem (Knuth, '80 or earlier, Mehrmann and Poloni, '12)

Each full column rank matrix U has a permuted graph basis $P \begin{bmatrix} I \\ X \end{bmatrix}$ with $|x_{ij}| \leq 1$.

Important formulas and notation

$$\begin{aligned}(A \otimes B)(C \otimes D) &= AC \otimes BD,\\ \operatorname{vec}(ABC) &= (C^T \otimes A)\operatorname{vec}(B),\\ \operatorname{vec}(\text{“}\mathit{uppercase}\text{”}) &= \text{“}\mathit{lowercase}\text{”},\end{aligned}$$

$\otimes$ Kronecker product of matrices,

vec Stacks columns of a matrix into a long vector.

Frechet derivative of the function F

The Frèchet derivative of F at X in the direction $E \in \mathbb{C}^{(n-k)\times k}$ is given as

$$F'(X)E = E(A - GX) + (\tilde{A} - XG)E,$$

so,

$$f'(x) = I_k \otimes (\tilde{A} - XG) + (A - GX)^T \otimes I_{n-k} \in \mathbb{C}^{k(n-k)\times k(n-k)}.$$

Standard Krawczyk operator

$$\begin{aligned} k(\tilde{x}, \mathbf{x}) &= \tilde{x} - Rf(x) + (I - R\mathbf{S})(\mathbf{x} - \tilde{x}) \\ &= \tilde{x} - Rf(x) + [I - R(I \otimes (\tilde{A} - \mathbf{X}G) + (A - G\mathbf{X})^T \otimes I)](\mathbf{x} - \tilde{x}), \end{aligned}$$

- $\mathbf{S}$ An interval matrix containing all slopes S for $x, y \in \mathbf{x}$,
- Standard choice for $\mathbf{S}$ $\mathbf{f}'(\mathbf{x})$,
- $\mathbf{f}'(\mathbf{x})$ The interval arithmetic evaluation of $f'(x)$,
- R A computed inverse of $f'(x)$ by using the standard floating point arithmetic.

Aspects of complexity

- For obtaining the matrix R, one should invert a matrix of size $k(n-k) \times k(n-k)$ cost $= \mathcal{O}(n^6)$
- The product $R\mathbf{S}$ with R full and $\mathbf{S}$ containing at least $\mathcal{O}(n)$ non-zeros per column cost $= \mathcal{O}(n^5)$!

Therefore The number of arithmetic operations needed to implement the classical Krawczyk operator is at-least $\mathcal{O}(n^5)$!

Challenge Reduce this cost to cubic.

Used tricks

Previous works involved:

- A. Frommer and B. Hashemi: Verified computation of square roots of a matrix, 2009 affine transformation for reducing wrapping effect (loses uniqueness),
- B. Hashemi: Verified computation of Hermitian (Symmetric) solutions to continuous-time algebraic Riccati matrix equation, 2012 spectral decomposition.

New work involved:

- V. Mehrmann and F. Poloni: Doubling algorithms with permuted Lagrangian graph bases, 2012 permuted graph bases (loses uniqueness).

Modified Krawczyk operator

Theorem (Rum, '83, Frommer and Hashemi, '09)

Assume that $f : D \subseteq \mathbb{C}^n \to \mathbb{C}^n$ *is continuous in* D*. Let* $\tilde{x} \in D$ *and* $\mathbf{z} \in \mathbb{IC}^n$ *be such that* $\tilde{x} + \mathbf{z} \subseteq D$*. Moreover, assume that* $\mathcal{S} \subseteq \mathbb{C}^{n \times n}$ *is a set of matrices containing all slopes* $S(\tilde{x}, y)$ *for* $y \in \tilde{x} + \mathbf{z} := \mathbf{x}$*. Finally, let* $R \in \mathbb{C}^{n \times n}$*. Denote by* $\mathcal{K}_f(\tilde{x}, R, \mathbf{z}, \mathcal{S})$ *the set*

$$\mathcal{K}_f(\tilde{x}, R, \mathbf{z}, \mathcal{S}) := \{-Rf(\tilde{x}) + (I - RS)z \ : \ S \in \mathcal{S}, z \in \mathbf{z}\}.$$

Then, if

$$\mathcal{K}_f(\tilde{x}, R, \mathbf{z}, \mathcal{S}) \subseteq \operatorname{int} \mathbf{z}, \tag{2}$$

the function f *has a zero* x^* *in* $\tilde{x} + \mathcal{K}_f(\tilde{x}, R, \mathbf{z}, \mathcal{S}) \subseteq \mathbf{x}$*. Moreover, if* $\mathcal{S}$ *also contains all slope matrices* $S(x, y)$ *for* $x, y \in \mathbf{x}$*, then this zero is unique in* $\mathbf{x}$*.*

The relation between slopes and derivative

Theorem

Consider NARE (1). Then, the interval arithmetic evaluation of the derivative of $f(x)$, i.e. the interval matrix $I \otimes (\tilde{A} - \mathbf{X}G) + (A - G\mathbf{X})^T \otimes I$ contains slopes $S(x, y)$ for all $x, y \in \mathbf{x}$.

Evaluate the Krawczyk operator

$$(\mathbf{K}_f(\tilde{x}, R, \mathbf{z}, \mathbf{S}) := -Rf(\tilde{x}) + (I - R\mathbf{S})\mathbf{z},$$

Then, the enclosure property of interval arithmetic displays that

$$\mathbf{K}_f(\tilde{x}, R, \mathbf{z}, \mathbf{S}) \subset \operatorname{int} \mathbf{z} \Longrightarrow \mathcal{K}_f(\tilde{x}, R, \mathbf{z}, \mathcal{S}) \subseteq \operatorname{int} \mathbf{z}.$$

Fundamental assumptions

Existence of spectral decompositions for

$$\begin{aligned} A - GX &= V_1 \Lambda_1 W_1, \qquad & V_1, W_1, \Lambda_1 &\in \mathbb{C}^{k\times k},\\ & & \Lambda_1 &= \mathrm{Diag}(\lambda_{11}, \dots, \lambda_{k1}),\\ & & V_1 W_1 &= I_k,\\ \tilde{A}^* - G^* X^* &= V_2 \Lambda_2 W_2, \qquad & V_2, W_2, \Lambda_2 &\in \mathbb{C}^{(n-k)\times(n-k)},\\ & & \Lambda_2 &= \mathrm{Diag}(\lambda_{12}, \dots, \lambda_{(n-k)2}),\\ & & V_2 W_2 &= I_{n-k}. \end{aligned}$$

Outcomes of these eigenvalue decompositions

- $f'(x) = I \otimes (\tilde{A} - XG) + (A - GX)^T \otimes I$ converted to [Frommer, Hashemi]

$$f'(x) = (V_1^{-T} \otimes W_2^*) \cdot \left(I \otimes \Big[\underbrace{W_2(\tilde{A} - XG)^* W_2^{-1}}_{\cong \Lambda_2}\Big]^* + \Big[\underbrace{V_1^{-1}(A - GX)V_1}_{\cong \Lambda_1}\Big]^T \otimes I \right) \cdot (V_1^T \otimes W_2^{-*}),$$

- $R = (V_1^{-T} \otimes W_2^*) \cdot \Delta^{-1} \cdot (V_1^T \otimes W_2^{-*})$, $\Delta = I \otimes \Lambda_2^* + \Lambda_1^T \otimes I$ diagonal,

- $$I - Rf'(x) = (V_1^{-T} \otimes W_2^*) \cdot \Delta^{-1} \cdot \left(\Delta - I \otimes [W_2(\tilde{A} - XG)^* W_2^{-1}]^* - [V_1^{-1}(A - GX)V_1]^T \otimes I\right) (V_1^T \otimes W_2^{-*}).$$

Reducing wrapping effect

New issue The problematic wrapping effect of interval arithmetic appears in several lines of the modified Krawczyk algorithm.

Solution Use $\hat{f}$ as a linearly transformed function instead of f:

$$\hat{f}(\hat{x}) := \left(V_1^T \otimes W_2^{-*}\right) f\left((V_1^{-T} \otimes W_2^*)\hat{x}\right),$$

$(V_1^{-T} \otimes W_2^*)\hat{x} := x$, X a solution for NARE (1). [Frommer, Hashemi]

Consequences of considering this affine transformation

- $\hat{\mathcal{S}} = \{\hat{S}(\hat{x}, \hat{y}) \ : \ \hat{x}, \hat{y} \in \hat{\mathbf{x}} := \hat{\mathring{x}} + \hat{z}\}$

$$= (V_1^T \otimes W_2^{-*}) S \left((V_1^{-T} \otimes W_2^*)\hat{x}, (V_1^{-T} \otimes W_2^*)\hat{y} \right) (V_1^{-T} \otimes W_2^*)$$
$$= (V_1^T \otimes W_2^{-*}) S(x, y) (V_1^{-T} \otimes W_2^*)$$
$$= (V_1^T \otimes W_2^{-*})(V_1^{-T} \otimes W_2^*) \cdot$$
$$\left(I \otimes [W_2(\tilde{A} - XG)^* W_2^{-1}]^* + [V_1^{-1}(A - GX)V_1]^T \otimes I \right) \cdot$$
$$(V_1^T \otimes W_2^{-*})(V_1^{-T} \otimes W_2^*)$$
$$= \left(I \otimes [\underbrace{W_2(A - XG)^* W_2^{-1}}_{\cong \Lambda_2}]^* + [\underbrace{V_1^{-1}(A - GX)V_1}_{\cong \Lambda_1}]^T \otimes I \right) \cong \Delta$$

- $\hat{R} = \Delta^{-1}$ diagonal,
- Decreasing the number of wrapping effects.

Consequence of considering this affine transformation

We compute an enclosure for $\mathcal{K}_{\hat{f}}(\hat{\check{x}}, \hat{R}, \hat{\mathbf{z}}, \hat{\mathcal{S}})$ in which

- $\hat{\check{x}} = (V_1^T \otimes W_2^{-*})\check{x}$, $\hat{\check{x}}$ an approximate solution for $\hat{f}$,
- $\check{X}$ an approximate solution for NARE (1),
- $\mathbf{Z} = W_2^* \hat{\mathbf{Z}} V_1^{-1}$.

Algorithm1: Computing an enclosure for the first term in modified Krawczyk operator

- First term $-\hat{R}\hat{f}(\hat{\check{x}}) = -\Delta^{-1}(V_1^T \otimes W_2^{-*})f(\check{x})$.
  1. Input $A, \tilde{A}, G, Q, \check{X}$;
  2. $\hat{\mathbf{F}} = Q + \check{X}A + \tilde{A}\check{X} - \check{X}G\check{X}$;
  3. $\hat{\mathbf{G}} = \mathbf{I}_{W_2}^{*}\hat{\mathbf{F}}V_1$;
  4. $\hat{\mathbf{H}} = -\hat{\mathbf{G}}./D$;
  5. Output $\hat{\mathbf{H}}$

Cost cubic.

Algorithm2: Enclosing the set of second terms in modified Krawczyk operator

- Second term $(I - \hat{R}\hat{S})\hat{z} =$
$\left(I - \Delta^{-1}\left(I \otimes [W_2(\tilde{A} - XG)^* W_2^{-1}]^* + [V_1^{-1}(A - GX)V_1]^T \otimes I\right)\right)\hat{z}.$

1. Input $\check{X}, \hat{\mathbf{Y}}$;
2. $\hat{\mathbf{M}} = W_2^* \hat{\mathbf{Y}} \mathbf{I}_{V_1}$;
3. $\hat{\mathbf{P}} = \mathbf{I}_{W_2}^* (\tilde{A} - (\check{X} + \hat{\mathbf{M}})G) W_2^*$;
4. $\hat{\mathbf{Q}} = \mathbf{I}_{V_1}^* (A - G(\check{X} + \hat{\mathbf{M}})) V_1$;
5. $\hat{\mathbf{E}} = (\Lambda_2^* - \hat{\mathbf{P}})\hat{\mathbf{Y}} + \hat{\mathbf{Y}}(\Lambda_1 - \hat{\mathbf{Q}})$;
6. $\hat{\mathbf{N}} = \hat{\mathbf{E}}./D$;
7. Output $\hat{\mathbf{N}}$.

Cost cubic.

Algorithm3: Computation of an interval matrix $\mathbf{X}$ containing at least one stabilizing solution of NARE (1)

1. Compute approximations V_1, W_1, Λ_1 and V_2, W_2, Λ_2 for the eigenvalue decompositions of
2. $A - GX$ and $\tilde{A}^* - G^*X^*$ in floating point, resp;
3. {Take `eig.m` from MATLAB, e.g. };
4. Compute an approximate solution $\check{X}$ of NARE (1) in floating point when $H = [A \;\; -G; -Q \;\; -\tilde{A}]$;
5. {Take `nare.m` from MATLAB, e.g.};
6. Compute $D = \overline{\mathrm{diag}(\Lambda_2)}[1,1,\ldots,1]_{1\times k} + [1,1,\ldots,1]^T_{1\times n-k}(\mathrm{diag}(\Lambda_1))^T$;
7. Compute interval matrices $\mathbf{I}_{V_1}$ and $\mathbf{I}_{W_2}$ containing V_1^{-1} and W_2^{-1}, resp;
8. {Take `verifylss.m` from INTLAB, e.g.};
9. Compute the interval matrix $\hat{\mathbf{H}}$ with $-\hat{R}\hat{f}(\hat{\check{x}}) \in \hat{\mathbf{H}}$, where $\hat{\mathbf{H}}$ is obtained from Algorithm1;

Algorithm3: Computation of an interval matrix $\mathbf{X}$ containing at least one stabilizing solution of NARE (1)

9. Put $k = 0$ and $\hat{\mathbf{Z}} = \hat{\mathbf{H}}$;
10. **For** $k = 1, \ldots, k_{\max}$ **do**
11. Put $\hat{\mathbf{Y}} := \square(0, \hat{\mathbf{Z}} \cdot [1-\epsilon, 1+\epsilon]);$ $\{\epsilon$ -inflation$\}$
12. Compute $\hat{\mathbf{N}}$ using $\check{X}, \hat{\mathbf{Y}}$ in Algorithm 2;
13. **If** $\hat{\mathbf{K}} := \hat{\mathbf{H}} + \hat{\mathbf{N}} \subset \operatorname{int} \hat{\mathbf{Y}}$ **then** $\{$successful$\}$
14. $\hat{\mathbf{R}} = \hat{\mathbf{K}}$;
15. break;
16. **end if**;

Algorithm3: Computation of an interval matrix $\mathbf{X}$ containing at least one stabilizing solution of NARE (1)

17. $\hat{\hat{\mathbf{Z}}} = \hat{\mathbf{Y}} \cap \hat{\mathbf{K}}$;
18. Comput $\hat{\hat{\mathbf{N}}}$ as in Algorithm2 using $\hat{\hat{\mathbf{Z}}}$ instead of $\hat{\hat{\mathbf{Y}}}$;
19. **If** $\hat{\hat{\mathbf{K}}} = \hat{\mathbf{H}} + \hat{\hat{\mathbf{N}}} \subset \operatorname{int} \hat{\hat{\mathbf{Z}}}$ **then** {successful}
20. $\hat{\mathbf{R}} = \hat{\hat{\mathbf{K}}}$;
21. break;
22. **end if**;
23. $\hat{\mathbf{Z}} = \hat{\mathbf{Z}} \cap \hat{\hat{\mathbf{K}}}$;
24. **end for**;
25. $\mathbf{X} := \check{X} + W_2^* \hat{\mathbf{R}} \mathbf{I}_{V_1}$;
26. Output $\mathbf{X}$.

Algorithm4: Verified computation of solution of NARE (1) using permuted graph bases

1. Input $A, \tilde{A}, G, Q$;
2. Compute an approximate solution X of NARE (1) in floating point when
3. $H = [A \ \ -G; \ -Q \ \ -\tilde{A}]$;
4. {Take `nare.m` from MATLAB};
5. Compute a permutatiom matrix P and Y such that $\begin{bmatrix} I \\ X \end{bmatrix} = P^T \begin{bmatrix} I \\ Y \end{bmatrix} R$; P permutation and $|y_{ij}| \leq 1$;
6. {Take `canBasisFromSubspace` from MATLAB} [Poloni, 12];
7. $\mathrm{PHP}^T = \begin{bmatrix} A_p & -G_p \\ -Q_p & -\tilde{A}_p \end{bmatrix}$;
8. Compute **Y** by Algorithm 3;

Algorithm4: Verified computation of solution of NARE (1) using permuted graph bases

9. $\begin{bmatrix} \mathbf{U}_1 \\ \mathbf{U}_2 \end{bmatrix} = P^T \begin{bmatrix} \mathbf{I} \\ \mathbf{Y} \end{bmatrix}$;
10. $\mathbf{X} = \mathbf{U}_2 / \mathbf{U}_1$;
11. Output **X**.

Algorithm5: Computing an interval matrix **U** containing at least one invariant subspace of H

1. Input $H = [A \;\; -G; \;\; -Q \;\; -\tilde{A}]$;
2. 2. Use Algorithm 4 for finding **Y**;
3. Put $\mathbf{U} = P^T \begin{bmatrix} \mathbf{I} \\ \mathbf{Y} \end{bmatrix}$;
4. Output **U**.

- Examples in fluid queues generated by `mriccatix.m` [B. Iannazzo] for NAREs whose coefficients form an M-matrix. Example from [CH Guo 2001]

$$N = 4$$

α	time(s)	mr	mrp	arp
0	-			
0.5	0.028449	1.0270e-15	9.2839e-15	4.8572e-15
0.99	0.032010	1.1732e-15	2.3503e-14	7.1739e-15

$$N = 50$$

α	time(s)	mr	mrp	arp
0	-			
0.5	0.100178	1.8890e-12	9.5237e-10	3.6791e-11
0.99	0.098313	1.0934e-12	9.0440e-11	2.0001e-11

$N = 120$

α	time(s)	mr	mrp	arp
0	-			
0.5	0.577645	1.4977e-11	2.6043e-09	7.2504e-10
0.99	-			

Example from [Bai, Guo, Xu 2006]

$N = 4$

α	time(s)	mr	mrp	arp
0	0.035132	1.7045e-16	2.2970e-14	4.6834e-15
0.5	0.036441	2.4257e-16	2.9750e-14	6.4049e-15
0.99	0.032630	1.8352e-16	1.8581e-14	4.3609e-15

$N = 50$

α	time(s)	mr	mrp	arp
0	0.101496	1.9303e-15	0.7835	9.4636e-08
0.5	0.162545	3.0240e-15	0.4497	1.4641e-07
0.99	0.098980	3.6224e-15	0.9427	3.1007e-07

$N = 110$

α	time(s)	mr	mrp	arp
0	-			
0.5	0.451587	8.1046e-15	0.5054	2.5093e-07
0.99	0.437653	1.1425e-14	0.6875	4.5676e-07

Example from [Juang, Lin, 1999]

$N = 4$

α	time(s)	mr	mrp	arp
0	-			
0.5	0.028168	3.8858e-16	1.5963e-15	8.6762e-16
0.99	0.023996	5.2403e-14	3.8371e-14	3.0541e-14

$N = 40$

α	time(s)	mr	mrp	arp
0	-			
0.5	0.048736	2.0373e-14	8.5094e-14	1.3595e-14
0.99	0.046778	2.0397e-12	1.1240e-12	7.9844e-13

$N = 400$

α	time(s)	mr	mrp	arp
0	-			
0.5	4.534196	3.9607e-13	1.5318e-12	2.1952e-13
0.99	5.039913	2.8733e-11	1.4644e-11	8.8724e-12

$N = 1000$

α	time(s)	mr	mrp	arp
0	-			
0.5	63.691614	9.2215e-13	3.5582e-12	4.1113e-13
0.99	76.882187	5.2028e-11	2.6716e-11	1.4962e-11

Conclusions?

Thanks for your attention!