Approximate insverse-free rational Krylov methods and the link with FOM and GMRES

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Introduction

This presentation is based on joint work with Stefan Güttel, Thomas Mach & Raf Vandebril.

Introduction

What has been done:

- The approximate inverse-free extended Krylov method was introduced by Mach Pranić and Vandebril (2013) and generalized to the rational case by the same authors in 2014.
- The authors illustrate the power of these methods for computing $f(A)\boldsymbol{v}$, solving matrix equations, and computing rational Ritz values.
- Jagels Mach Reichel and Vandebril (2016) showed that the inverse-free methods have a geometric convergence rate to the exact rational Krylov subspace.

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- $\Xi = (\xi_1, \ldots, \xi_{m-1}) \in \bar{\mathbb{C}} \setminus \Lambda$: tuple of poles.
- $m \ll M$: oversampling.
- Implicit approach using similarity transformations, cfr. QR-type algorithms.

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What will we see today?

FOM	Implicit similarity	Implicit equivalence	Explicit FOM
GMRES		?	Explicit GMRES

Introduction

We will require and touch upon:

- Krylov subspaces, Arnoldi, essential uniqueness, implicit Q theorem
- rational Krylov subspaces, rational Arnoldi, essential uniqueness, implicit Q theorem
- Projected counterparts
- Minimal residual conditions

Classical Krylov

$(m+1)$st order Krylov subspace for $A \in \mathbb{C}^{N\times N}$, $\boldsymbol{v} \in \mathbb{C}^N \setminus \{\mathbf{0}\}$

$$\mathcal{K}_{m+1}(A, \boldsymbol{v}) := \mathcal{R}(\boldsymbol{v}, A\boldsymbol{v}, \ldots, A^m\boldsymbol{v}).$$

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Arnoldi decomposition:

$$AV_m = V_{m+1}\underline{H}_m = V_m H_m + V_{m+1}\underline{R}_m \quad \text{with} \quad \underline{R}_m = h_{m+1,m}\underline{\boldsymbol{e}}_{m+1}\boldsymbol{e}_m^T$$

- $\mathcal{R}(V_{m+1}) = \mathcal{K}_{m+1}(A, \boldsymbol{v})$,
- $V_{m+1}\boldsymbol{e}_1 = \boldsymbol{v}/\|\boldsymbol{v}\|_2$,
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We assume throughout the talk that breakdown does not occur.If it does happen, the approximate rational Krylov method would give an exact result.

Uniqueness and implicit Q

Let $(V_{m+1}, \underline{H}_m)$ and $(\hat{V}_{m+1}, \underline{\hat{H}}_m)$ both be Arnoldi pairs for A satisfying $\boldsymbol{v}_1 = \sigma \hat{\boldsymbol{v}}_1$, $|\sigma| = 1$. Then,

$$(V_{m+1}, \underline{H}_m) = (\hat{V}_{m+1} D_{m+1}, D_{m+1}^* \underline{\hat{H}}_m D_m),$$

with D_{m+1} a unitary diagonal matrix.

$\rightarrow$ The Arnoldi pair $(V_{m+1}, \underline{H}_m)$ is determined *essentially unique* if $\boldsymbol{v}$ is fixed.

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$\rightarrow$ *One-to-one* correspondence between $\langle V_{m+1}, \underline{H}_m \rangle$ and $\mathcal{K}_{m+1}(A, \boldsymbol{v})$.

Orthogonal projected counterpart(s)

Orthogonal projection of A on $\mathcal{K}_{m+1}(A, \boldsymbol{v})$:

$$V_{m+1}^* A V_{m+1} = \left[\begin{array}{cc} \underline{H}_m & V_{m+1}^* A \boldsymbol{v}_{m+1} \end{array} \right]$$

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$$V_{m+1}^* A V_{m+1} = \begin{bmatrix} \underline{H}_m & V_{m+1}^* A \boldsymbol{v}_{m+1} \end{bmatrix}$$

Orthogonal projection of A on $\mathcal{K}_m(A, \boldsymbol{v})$:

$$V_m^* A V_m = H_m = \begin{matrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \end{matrix}$$

$\rightarrow$ unique up to similarity transformation with D_m.

Rational Krylov

Rational Krylov subspace for $A \in \mathbb{C}^{N\times N}$, $\boldsymbol{v} \in \mathbb{C}^N \setminus \{\mathbf{0}\}$, $\Xi \in \bar{\mathbb{C}}^m$

$$\mathcal{K}^{\mathrm{rat}}_{m+1}(A, \boldsymbol{v}, \Xi) := q(A)^{-1}\,\mathcal{K}_{m+1}(A, \boldsymbol{v}),$$

with $\Xi = (\xi_1, \ldots, \xi_m)$, $\xi_i \in \bar{\mathbb{C}} \setminus \Lambda$, $q(z) = \prod_{\xi_i \in \Xi \setminus \infty}(z - \xi_i)$.

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rational Arnoldi decomposition

$$AV_{m+1}\underline{K}_m = V_{m+1}\underline{L}_m$$

- $\mathcal{R}(V_{m+1}) = \mathcal{K}^{\text{rat}}_{m+1}(A, \boldsymbol{v}, \Xi)$,
- $V_{m+1}\boldsymbol{e}_1 = \boldsymbol{v}/\|\boldsymbol{v}\|_2$,
- $(\underline{L}_m, \underline{K}_m)$ proper upper Hessenberg pair,
- Pole tuple $\Xi(\underline{L}_m, \underline{K}_m) = (\ell_{21}/k_{21}, \ldots, \ell_{m+1,m}/k_{m+1,m}) = (\xi_1, \ldots, \xi_m) = \Xi$.

Rational Krylov

Uniqueness and implicit Q by Berljafa and Güttel (2015)

Let $(V_{m+1}, \underline{L}_m, \underline{K}_m)$ and $(\hat{V}_{m+1}, \hat{\underline{L}}_m, \hat{\underline{K}}_m)$ both be rational Arnoldi triplets for A satisfying $\Xi = \hat{\Xi}$ and $\boldsymbol{v}_1 = \sigma \hat{\boldsymbol{v}}_1$, $|\sigma| = 1$. Then,

$$(V_{m+1}, \underline{L}_m, \underline{K}_m) = (\hat{V}_{m+1} D_{m+1}, D_{m+1}^* \hat{\underline{L}}_m T_m, D_{m+1}^* \hat{\underline{K}}_m T_m),$$

with D_{m+1} a unitary diagonal matrix and T_m an invertible upper triangular.

→ $(V_{m+1}, \underline{L}_m, \underline{K}_m)$ is determined *essentially unique* if both Ξ and $\boldsymbol{v}$ are fixed.

→ Equivalence class $\langle V_{m+1}, \underline{L}_m, \underline{K}_m \rangle$, satisfying $\Xi\langle \underline{L}_m, \underline{K}_m \rangle = \Xi$.

→ *One-to-one* correspondence between $\langle V_{m+1}, \underline{L}_m, \underline{K}_m \rangle$ and $\mathcal{K}_{m+1}^{\text{rat}}(A, \boldsymbol{v}, \Xi)$.

Rational Krylov

Orthogonal projected counterpart(s) (Berljafa, 2017)

Orthogonal projection of A on $\mathcal{K}^{\text{rat}}_{m+1}(A, \boldsymbol{v}, \Xi)$:

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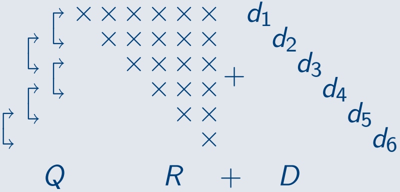
Orthogonal projection of A on $\mathcal{R}(V_{m+1}\underline{K}_m) = \mathcal{K}_m(A, q(A)^{-1}\boldsymbol{v})$:

$$(V_{m+1}\underline{K}_m)^\dagger A (V_{m+1}\underline{K}_m) = \underline{K}_m^\dagger \underline{L}_m$$

Orthogonal projected counterpart(s) (C. Meerbergen and Vandebril, 2019)

The matrix $\underline{K}_m^{\dagger}\underline{L}_m$ is of *rational Hessenberg* form:



- $C_i C_{i+1}$ if $\xi_{i+1} = \infty$
- $C_{i+1} C_i$ if $\xi_{i+1} \neq \infty$
- $d_i = \xi_i$ if $\xi_i \neq \infty$

Rational Krylov

Same idea:

- Let (A, B) be a proper Hessenberg pencil, B invertible. Then both $B^{-1}A$ and AB^{-1} are proper rational Hessenberg matrices.
- Conversely, for any proper rational Hessenberg matrix M there is a proper Hessenberg pencil (A, B) such that $M = B^{-1}A$.

Implicit Similarity Transformation (Mach Pranić and Vandebril, 2014)

The approximate rational Krylov method of Mach Pranić and Vandebril (2014) constructs a unitary similarity transformation to transform the Arnoldi Hessenberg matrix H_m to rational Hessenberg form:

$$Q_m^* \begin{matrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ & \times & \times & \times & \times & \times \\ & & \times & \times & \times & \times \\ & & & \times & \times & \times \\ & & & & \times & \times \end{matrix} \; Q_m = \begin{matrix} \times & \times & \times & \times & \times & \times \\ & \times & \times & \times & \times & \times \\ & & \times & \times & \times & \times \\ & & & \times & \times & \times \\ & & & & \times & \times \\ & & & & & \times \end{matrix} + \begin{matrix} d_1 & & & & & \\ & d_2 & & & & \\ & & d_3 & & & \\ & & & d_4 & & \\ & & & & d_5 & \\ & & & & & d_6 \end{matrix}$$

Remark: without changing the first row/column of $H_m \to \boldsymbol{q}_1 = \boldsymbol{e}_1$.

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$\Rightarrow$ the approximation will be accurate:

- if $|h_{m+1,m}|$ is small (exact rational Krylov if zero).
- for columns $\hat{\boldsymbol{v}}_i$ where $|q_{m,i}|$ is small.

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- *Changing the last pole :* $(A, B)Z_{n-1}$ such that $(\xi_1, \ldots, \hat{\xi}_{n-1})$.
- *Swapping consecutive poles :* $Q_{i+1}^*(A, B)Z_i$ such that $(\xi_1, \ldots, \xi_{i+1}, \xi_i, \ldots, \xi_{n-1})$.

Implicit Equivalence Transformation

We can use these two operations on the Arnoldi Hessenberg pencil (H_m, I_m):

- $\Xi(H_m, I_m) = (\infty, \ldots, \infty)$
- $(H_m, I_m)Z_{m-1}$ such that $(\infty, \ldots, \infty, \xi_1)$
- $Q^*(H_m, I_m)Z$ such that $(\xi_1, \infty, \ldots, \infty)$. Remark: $\boldsymbol{q}_1 = \boldsymbol{e}_1$.

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- $\ldots$
- $\hat{Q}^*(H_m, I_m)\hat{Z}$ such that $(\xi_1, \ldots, \xi_k, \underbrace{\infty, \ldots, \infty}_{\text{oversampling}})$

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Implicit Equivalence Transformation

$\Rightarrow$ This is mathematically equivalent to the approach of Mach Pranić and Vandebril (2014), i.e.

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Proof:

- Q_m^{sim} is essentially unique if structure and starting vector are fixed (Mach Pranić and Vandebril, 2014).
- Q_m^{eqv} is essentially unique if structure and starting vector are fixed (C. Meerbergen and Vandebril, 2019b).
- $\hat{L}_m \hat{K}_m^{-1} = Q_m^{eqv,*} H_m (Z_m Z_m^*) Q_m^{eqv}$ has the same structure as $\hat{H}_m = Q_m^{sim,*} H_m Q_m^{sim}$ (C. Meerbergen and Vandebril, 2019).

Implicit Equivalence Transformation

Main advantages over implicit similarity transformation:

- arguably easier to implement
- link with rational QZ provides further theoretical insights, e.g. placing Ritz values as poles could cause deflations.

Explicit FOM

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Explicit FOM

A third equivalent interpretation: rational Krylov within classical Krylov.

- Let $(V_{m+1}, \underline{H}_m)$ be the Arnoldi pair corresponding to $\mathcal{K}_{m+1}(A, \boldsymbol{v})$.
- Consider the rational Arnoldi triplet $(W_{k+1}, \underline{L}_k, \underline{K}_k)$ corresponding to $\mathcal{K}^{\text{rat}}_{k+1}(H_m, \boldsymbol{e}_1, (\xi_1, \ldots, \xi_k))$, $k < m$.

Explicit FOM

A third equivalent interpretation: rational Krylov within classical Krylov.

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- Consider the rational Arnoldi triplet $(W_{k+1}, \underline{L}_k, \underline{K}_k)$ corresponding to $\mathcal{K}^{\text{rat}}_{k+1}(H_m, \boldsymbol{e}_1, (\xi_1, \ldots, \xi_k))$, $k < m$.

Then, combining $AV_m = V_m H_m + V_{m+1} \underline{R}_m$ and $H_m W_{k+1} \underline{K}_k = W_{k+1} \underline{L}_k$, we get:

Explicit FOM

A third equivalent interpretation: rational Krylov within classical Krylov.

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$$\Rightarrow A\check{V}_{k+1}\underline{K}_k = \check{V}_{k+1}\underline{L}_k + V_{m+1}\underline{\check{R}}_m, \quad \text{with} \quad \underline{\check{R}}_m = \boldsymbol{e}_{m+1}\boldsymbol{e}_m^T W_{k+1}\underline{K}_k.$$

Explicit FOM

It follows from the uniqueness of rational Arnoldi triplets (Berljafa and Güttel, 2015) that:

$$\hat{V}_{k+1}^{eqv} \equiv \hat{V}_{k+1}^{sim} \equiv \check{V}_{k+1}^{FOM}.$$

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Where is the link with the Full Orthogonalization Method?

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Where is the link with the Full Orthogonalization Method?

To compute $(W_{k+1}, \underline{L}_k, \underline{K}_k)$, we solve shifted-linear systems $(H_m - \xi I_m)\boldsymbol{x}_m = \boldsymbol{b}_m$!

Explicit GMRES

GMRES extension: Solve shifted least-squares problems instead:

$$\min_{\boldsymbol{x}_m \in \mathbb{C}^m} \|\underline{\boldsymbol{b}} - (\underline{H}_m - \xi \underline{I}_m)\boldsymbol{x}_m\|_2$$

The resulting algorithm computes:

$$A\breve{V}_{k+1}\underline{\breve{K}}_k = \breve{V}_{k+1}\underline{\breve{L}}_k + V_{m+1}\underline{\breve{R}}_m$$

- For $i = 1, \ldots, k+1$,

$$V_{m+1}\breve{\boldsymbol{r}}_i \perp (A - \xi_i I)\mathcal{K}_m(A, \boldsymbol{v})$$

- $\mathrm{rank}(\underline{\breve{R}}_m) = \#$ distinct poles in Ξ

Implicit GMRES

- We know how to do it using a pole swapping method if there is only a *single* finite pole.
- From the normal equations for the shifted Hessenberg LS problem, we get that:

$$\tilde{H}_m = H_m + |h_{m+1,m}|^2 \boldsymbol{f}_m^{\xi} \boldsymbol{e}_m^T,$$

with $\boldsymbol{f}_m^{\xi} = (H_m - \xi_1 I_m)^{-*} \boldsymbol{e}_m$

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- From the normal equations for the shifted Hessenberg LS problem, we get that:

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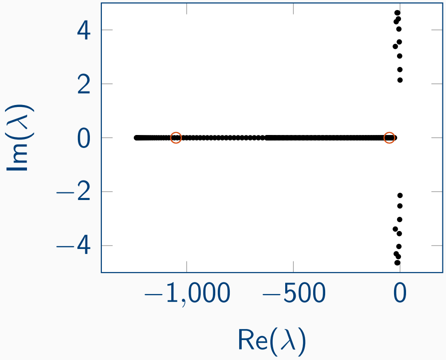
  with $\boldsymbol{f}_m^{\xi} = (H_m - \xi_1 I_m)^{-*} \boldsymbol{e}_m$
- Placing the pole ξ_1 in $(\tilde{H}_m, I_m)$ is equivalent to an explicit GMRES approximate rational Krylov step as we enforce $V_{m+1}\check{\boldsymbol{r}}_1 \perp (A - \xi_1 I)\mathcal{K}_m(A, \boldsymbol{v})$
- This also requires a shifted linear system.

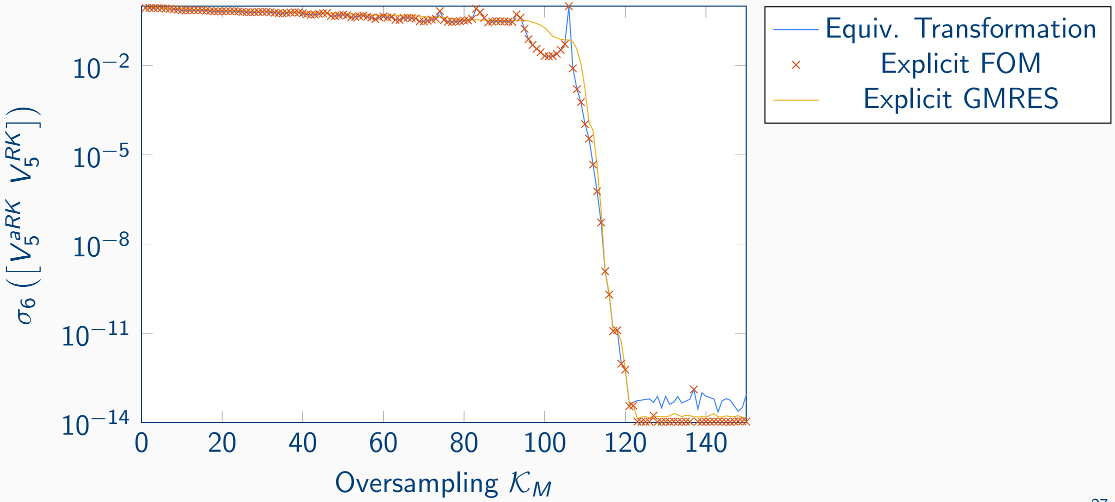
Numerical proof of concept

- Brusselator Wave Model BWM200 from MatrixMarket
- $\mathbb{R}^{200\times 200}$
- $\Xi = (-1050, -50, -1050, -50)$
- $\boldsymbol{v}$ constant entries
- $\mathcal{K}_5^{\text{rat}}(A, \boldsymbol{v}, (-1050, -50, -1050, -50))$
- $\mathcal{K}_M(A, \boldsymbol{v})$



$\bullet$: Λ, $\circ$: Ξ

Numerical proof of concept



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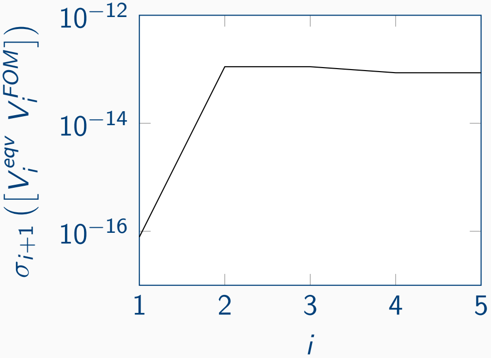

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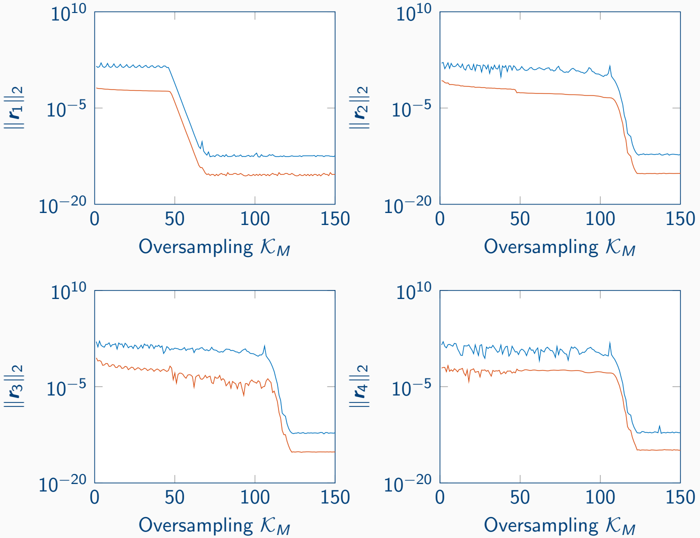

Conclusion

- We reviewed the approximate rational Krylov method of Mach Pranić and Vandebril (2014)
- We presented two equivalent algorithms: implicit pole swapping method and explicit FOM method
- Main advantages: more straightforward to implement, further theoretical insights
- We presented an extension to an explicit GMRES method

Thank you

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