Analysis of block GMRES using a new *-algebra-based approach

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Projection methods in computational mathematics

A common recipe

Generate a **finite dimensional subspace** onto which we **project** a large/infinite dimension problem arising from a mathematical model.

- Generate a “good” subspace
- Project problem onto subspace
- Solve smaller problem
- Project solution back to original space
- Often multiple levels of projection

→ Finite differences/elements/volumes

→ Integral equation discretization

→ Many iterative methods (e.g., Krylov methods, steepest descent, Gauss-Seidel)

→ Fourier- and wavelet-based approaches

Example: operator on a Hilbert space

Operator equation

Let $T \in \mathcal{L}(\mathcal{X})$ where $\mathcal{X}$ is a separable Hilbert space. We approximate the solution of

$$Tx = y$$

Discretization process (simplified setting)

We choose approximation $x_h \in \mathcal{X}_h \subset \mathcal{X}$ with $\dim \mathcal{X}_h = n < \infty$

- $\mathcal{X}_h = \mathrm{span}\{\phi_1, .\phi_2, \ldots, \phi_\mathrm{n}\} \implies x_h = \sum_{i=1}^{n} x_i \phi_i$
- Need n constraints determine x_h

$\implies$ weak formulation: find $x_h \in \mathcal{X}_h$ such that $\langle \phi_i, T x_h \rangle_{\mathcal{X}} = \langle \phi_i, y \rangle_{\mathcal{X}}$ for all i

- System of n equations (for each i) and n unknowns $\{x_i\}_i$
- Let $\mathbf{A} = \left(\langle \phi_i, T\phi_j \rangle_{\mathcal{X}} \right)_{ij}$, $\mathbf{x} = (x_i)_i$, and $\mathbf{b} = \left(\langle \phi_i, y \rangle_{\mathcal{X}} \right)_i$

Direct Methods for Solving Linear Systems

Decompose the matrix into a product of matrices.

Gaussian Elimination/LU-Decomposition

- Compute decomposition $\mathbf{A} = \mathbf{LU}$ where $\mathbf{L}$ is lower-triangular and $\mathbf{U}$ is upper-triangular
- Solve $\mathbf{LUx} = \mathbf{b} \longrightarrow \mathbf{Ux} = \mathbf{L}^{-1}\mathbf{b} \longrightarrow \mathbf{x} = \mathbf{U}^{-1}\mathbf{L}^{-1}\mathbf{b}$
- Triangular systems can be solved stably and efficiently.

When Direct Methods Are Not Appropriate

- As n gets larger, these methods do not scale well (increased communication/memory constraints)
- We may only possess a procedure which computes the product $\mathbf{v} \rightarrow \mathbf{Av}$

The Discretized Problem

Approximate the solution to a large, (often) sparse linear system,

$$\mathbf{A}\mathbf{x} = \mathbf{b} \quad \text{where} \quad \mathbf{A} \in \mathbb{R}^{n\times n} \quad \text{and} \quad n \gg 0$$

- **Sparse** means most of the matrix entries are zero.
- Amenable to fast application (e.g., FFT-based – "sparse" in some basis)
- Heirarchical matrices
- Matrices where we only have a procedure $\mathbf{v} \to \mathbf{A}\mathbf{v}$

Iterative Methods

- Generate a sequence of approximations $\{\mathbf{x}_j\}$ such that $\mathbf{x}_j \longrightarrow \mathbf{x}$
- Convergence should be rapid
- Convergence may be in the limit or not

General Framework

1. Generate two nested sequences of subspaces
$$\mathcal{K}_1 \subset \mathcal{K}_2 \subset \cdots \subset \mathcal{K}_n \quad \text{and} \quad \mathcal{L}_1 \subset \mathcal{L}_2 \subset \cdots \subset \mathcal{L}_n$$
2. $\dim \mathcal{K}_j = \dim \mathcal{L}_j = j$
3. At step j, select $\mathbf{x}_j \in \mathcal{K}_j$ such that $\mathbf{r}_j \perp \mathcal{L}_j$ where $\mathbf{r}_j = \mathbf{b} - \mathbf{A}\mathbf{x}_j$
4. Continue until $\|\mathbf{r}_j\| < \varepsilon$ where $\varepsilon > 0$ is some desired threshold.

Some linear algebra tools

Calculating an approximation to $\mathbf{x} \Leftrightarrow$ calculating coefficients in a basis

We select $\mathbf{x}_j \in \mathcal{K}_j$ such that $\mathbf{r}_j \perp \mathcal{L}_j$ where $\mathbf{r}_j = \mathbf{b} - \mathbf{A}\mathbf{x}_j$

- Let $\mathbf{x}_0 = \mathbf{0}$ (wLog for simplicity here)
- $\mathbf{K}_j, \mathbf{L}_j \in \mathbb{R}^{n\times j}$ have columns spanning $\mathcal{K}_j$ and $\mathcal{L}_j$, resp.
- We must calculate $\mathbf{y}_j \in \mathbb{R}^j$ and set $\mathbf{x}_j = \mathbf{K}_j\mathbf{y}_j$
- $\Leftrightarrow \mathbf{L}_j^T\left(\mathbf{b} - \mathbf{A}\mathbf{K}_j\mathbf{y}_j\right) = \mathbf{0} \Leftrightarrow \mathbf{L}_j^T\mathbf{A}\mathbf{K}_j\mathbf{y}_j = \mathbf{L}_j^T\mathbf{b}$
- The choice of subspaces $\mathcal{K}_j, \mathcal{L}_j$ and their bases $\mathbf{K}_j, \mathbf{L}_j$ dictate effectiveness and implementability of the method

Given $\mathbf{A}$ and $\mathbf{b}$, the jth Krylov subspace is defined

$$\mathcal{K}_j(\mathbf{A}, \mathbf{b}) = \text{span}\left\{\mathbf{b}, \mathbf{A}\mathbf{b}, \ldots, \mathbf{A}^{j-1}\mathbf{b}\right\}.$$

Thus, $\mathbf{u} \in \mathcal{K}_j(\mathbf{A}, \mathbf{b})$ is such that

$$\mathbf{u} = p(\mathbf{A})\mathbf{b}$$

where $p(x)$ is a polynomial of degree less than j.

Definition

The basis $\left\{\mathbf{b}, \mathbf{A}\mathbf{b}, \ldots, \mathbf{A}^{j-1}\mathbf{b}\right\}$ is called a **Krylov basis**.

Selecting Approximations from $\mathcal{K}_j(\mathbf{A}, \mathbf{b})$

- In many Krylov subspace methods, we select $\mathbf{x}_j \in \mathcal{K}_j(\mathbf{A}, \mathbf{b})$, so that

$$\mathbf{x}_j = p_j(\mathbf{A})\mathbf{b}$$

  Why?

- The inverse $\mathbf{A}^{-1}$ of any nonsingular matrix $\mathbf{A}$ can be written as

$$\mathbf{A}^{-1} = q(\mathbf{A})$$

  where $q(x)$ is a polynomial of degree less than n.

- We want $p_j(x)$ to be a low-degree "approximation" to $q(x)\dots$

  $\rightarrow$ only need to approximate action $p_j(\mathbf{A})\mathbf{b} \approx q(\mathbf{A})\mathbf{b}$

GMRES

A General Linear System

$\mathbf{A}\left(\mathbf{x}_0 + \mathbf{t}\right) = \mathbf{b}$ with $\mathbf{A} \in \mathbb{C}^{n \times n}$, $\mathbf{b} \in \mathbb{C}^n$

- For $\mathbf{x}_0$, let $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0 \implies \mathbf{A}\mathbf{t} = \mathbf{r}_0$
- Krylov subspace: $\mathcal{K}_j := \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$.
- Choose $\mathbf{x}_j = \mathbf{x}_0 + \mathbf{t}_j$, $\mathbf{t}_j \in \mathcal{K}_j$. Let $\mathbf{r}_j = \mathbf{b} - \mathbf{A}\mathbf{x}_j$.
- GMRES - Generalized Minimum Residual Method
- For GMRES, construct $\mathbf{x}_j = \mathbf{x}_0 + \mathbf{t}_j$ such that $\mathbf{t}_j$ minimizes

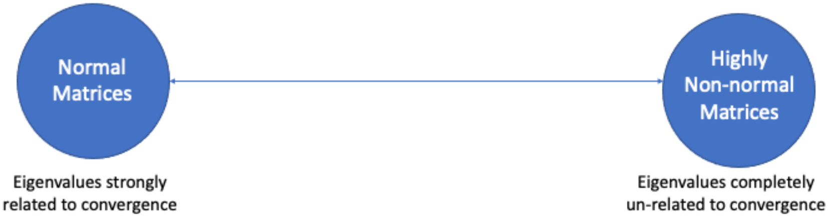
$$\min_{\mathbf{t} \in \mathcal{K}_j} \left\| \mathbf{b} - \mathbf{A}(\mathbf{x}_0 + \mathbf{t}) \right\|$$

- This is equivalent to $\mathbf{r}_j \perp \mathbf{A}\mathcal{K}_j$
- Sibling method: **Full Orthogonalization Method (FOM)** – $\mathbf{r}_j \perp \mathcal{K}_j$

Role of eigenvalues in residual convergence

GMRES polynomial minimization problem

$$
\begin{aligned}
\|\mathbf{r}_j\| &= \min_{\substack{q\in\Pi_j\\ q(0)=1}} \|q(\mathbf{A})\mathbf{r}_0\| \\
&\leq \mathcal{K}_2(\mathbf{X}) \min_{\substack{q\in\Pi_j\\ q(0)=1}} \max_{\lambda\in\sigma(\mathbf{A})} |q(\lambda)|\,\|\mathbf{r}_0\|
\end{aligned}
$$



Properties of the $\mathbf{A}$ determining residual convergence

Theorem (Greenbaum, Ptàk, and Strakoš 1996)

Given any non-increasing sequence

$$f(0) \geq f(1) \geq \cdots \geq f(n-1) > 0,$$

there exists matrices $\mathbf{A} \in \mathbb{C}^{n \times n}$ *and vectors* $\mathbf{r}_0$, $\|\mathbf{r}_0\| = f(0)$ *such that GMRES applied to* $\mathbf{At} = \mathbf{r}_0$ *produces residuals* $\mathbf{r}_k$, $\|\mathbf{r}_k\| = f(k)$ *for all* k.

An $\mathbf{A}$ *can be constructed to have any eigenvalues.*

Selected previous work analyzing GMRES/FOM

The relationship between GMRES and FOM

- Relationship of FOM/GMRES convergence: *[Walker '95], [Zhou and Walker '94], [Brown '91], [Saad '03]*
- Galerkin/norm minimizing pairs of methods (e.g., BiCG/QMR): *[Cullum '95], [Cullum and Greenbaum '96]*
- Geometric analysis: *[Eiermann and Ernst '01]*

Constructing matrices with predetermined GMRES convergence

- Any nonincreasing convergence curve is possible for GMRES: *[Greenbaum et al, 1996]*
- Parameterization of the pairs $(\mathbf{A}, \mathbf{b})$ producing specific convergence: *[Arioli et al, 1998]*
- Any Admissible Ritz/harmonic Ritz values: *[Du et al, 2017], [Tebbens and Meurant, 2012]*

What happens if one has multiple right-hand sides?

Block Krylov subspaces

- Consider: $\mathbf{A}\mathbf{X} = \mathbf{B} = \begin{bmatrix} \mathbf{b}^{(1)} & \mathbf{b}^{(2)} & \cdots & \mathbf{b}^{(s)} \end{bmatrix} \in \mathbb{C}^{n \times s}$, $s > 1$
- Let $\mathbf{X}_0 \in \mathbb{C}^{n \times s}$ and

$$\mathbf{F}_0 = \mathbf{B} - \mathbf{A}\mathbf{X}_0 = \begin{bmatrix} \mathbf{f}_0^{(1)} & \mathbf{f}_0^{(2)} & \mathbf{f}_0^{(3)} & \cdots & \mathbf{f}_0^{(s)} \end{bmatrix} \in \mathbb{C}^{n \times s}.$$

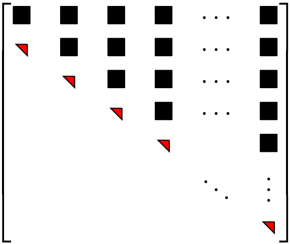
- Then we have the **block Krylov subspace**

$$\mathbb{K}_j(\mathbf{A}, \mathbf{F}_0) = \mathcal{K}_j(\mathbf{A}, \mathbf{f}_0^{(1)}) + \mathcal{K}_j(\mathbf{A}, \mathbf{f}_0^{(2)}) + \cdots + \mathcal{K}_j(\mathbf{A}, \mathbf{f}_0^{(s)}).$$

- Assumption: $\dim \mathbb{K}_j(\mathbf{A}, \mathbf{F}_0) = js$

Block Arnoldi process

- Let $\mathbf{F}_0 = \mathbf{V}_1 \mathbf{S}_0$ be a skinny QR-factorization.
- At step j, compute $\mathbf{V}_{j+1} \in \mathbb{C}^{n \times s}$
- $\mathbf{V}_{j+1}^* \mathbf{V}_{j+1} = \mathbf{I}_s$, $\mathbf{V}_{j+1}^* \mathbf{V}_i = \mathbf{0}_{s \times s}$
- $\mathbf{W}_j = \begin{bmatrix} \mathbf{V}_1, & \ldots, & \mathbf{V}_j \end{bmatrix} \in \mathbb{C}^{n \times js}$ is basis of $\mathbb{K}_j(\mathbf{A}, \mathbf{F}_0)$
- Arnoldi relation: $\mathbf{A}\mathbf{W}_j = \mathbf{W}_{j+1} \overline{\mathbf{H}}_j$
- $\overline{\mathbf{H}}_j = (\mathbf{H}_{ik})_{ik} \in \mathbb{C}^{(j+1)s \times js}$ is block upper Hessenberg
- For ■, ◥ $\in \mathbb{C}^{s \times s}$ and ◥ upper triangular

$\overline{\mathbf{H}}_j =$  $\in \mathbb{C}^{(j+1)s \times js}$

From scalars to $s \times s$ matrices

- Orthogonalization:

$$\mathbf{v} \leftarrow \mathbf{v} - \underbrace{(\mathbf{q}^*\mathbf{v})}_{\in\mathbb{C}}\mathbf{q} \qquad \text{becomes} \qquad \mathbf{V} \leftarrow \mathbf{V} - \mathbf{Q}\underbrace{(\mathbf{Q}^*\mathbf{V})}_{\in\mathbb{C}^{s\times s}}$$

- Linear combinations:

$$\mathbf{u} = \sum_{i=1}^{k} \underbrace{\alpha_i}_{\mathbb{C}} \underbrace{\mathbf{v}_i}_{\mathbb{C}^n} \qquad \text{becomes} \qquad \mathbf{U} = \sum_{i=1}^{k} \underbrace{\mathbf{V}_i}_{\mathbb{C}^{n\times s}} \underbrace{\boldsymbol{\alpha}_i}_{\mathbb{C}^{s\times s}}$$

Block GMRES and Block FOM

Block GMRES and Block FOM valid for all $s \geq 1$

- Build an orthonormal basis for $\mathbb{K}_m(\mathbf{A}, \mathbf{F}_0)$
- For block GMRES

  Compute $\mathbf{Y}_m^{(G)} = \underset{Y \in \mathbb{C}^{ms \times s}}{\operatorname{argmin}} \left\| \overline{\mathbf{H}}_m \mathbf{Y} - \mathbf{E}_1^{(m+1)} \mathbf{S}_0 \right\|_F$ [a]

  Set $\mathbf{X}_m^{(G)} = \mathbf{X}_0 + \mathbf{W}_m \mathbf{Y}_m^{(G)}$, $\mathbf{R}_m^{(G)} = \mathbf{B} - \mathbf{A}\mathbf{X}_m^{(G)}$
- For block FOM

  Compute $\mathbf{Y}_m^{(F)} = \mathbf{H}_m^{-1} \mathbf{E}_1^{[m]} \mathbf{S}_0$ [b]

  Set $\mathbf{X}_m^{(F)} = \mathbf{X}_0 + \mathbf{W}_m \mathbf{Y}_m^{(F)}$, $\mathbf{R}_m^{(F)} = \mathbf{B} - \mathbf{A}\mathbf{X}_m^{(F)}$

[a] $\mathbf{E}_1^{(m+1)} \in \mathbb{C}^{(m+1)s \times s}$ has appropriate columns of an identity matrix

[b] $\mathbf{E}_1^{[m]} \in \mathbb{C}^{ms \times s}$ has appropriate columns of an identity matrix

Pros and cons of block Krylov methods

Pros

- Constraining residuals over larger subspaces
  - $\rightarrow$ Leads to convergence in fewer iterations
- Block matrix-vector product has more efficient data movement characteristics

Cons

- More operations per iteration
- Increased operation cost thought to not justify by increase in convergence rate
- Interactions between systems makes analysis more difficult

Renewed interest in block methods in HPC setting necessitates new analysis to extend existing non-block results to block Krylov subspace case

Selected previous work on analysis of block GMRES

- Convergence analysis: [Simoncini and Gallopoulos; 1997]
- Block Grade: [Gutknecht and Schmelzer; 2009]
- Relationship to block FOM and characterization of stagnation [S.; 2017]
- *-algebra framework [Frommer, Lund, Szyld; 2017]

The *-algebra framework

We follow [Frommer et al 2017] and consider the problem over *-algebra $\mathbb{S}$ of complex $s \times s$ matrices. We define a framework of corresponding objects and operations over $\mathbb{C}$ and over $\mathbb{S}$.

- $\mathbf{A} \in \mathbb{C}^{ns \times ns} \to \mathbf{A} \in \mathbb{S}^{n \times n}$
- $\mathbf{B} \in \mathbb{C}^{ns} \to \mathbf{B} \in \mathbb{S}^{n}$
- $\mathbb{K}_j(\mathbf{A}, \mathbf{B}) = \text{blockspan}\{\mathbf{B}, \mathbf{AB}, \ldots, \mathbf{A}^{j-1}\mathbf{B}\}$
- $\sum_{i=1}^{j} \mathbf{V}_i \, \mathbf{D}_i, \quad \mathbf{D}_i \in \mathbb{C}^{s \times s}$ is a block linear combination
- $\{\mathbf{V}_1, \ldots, \mathbf{V}_j\}$ is the basis of this subspace

System and right-hand side can be extended, without loss of generality, such that dimension is a multiple of s.

The *-algebra framework - definitions

standard	block
$\mathbb{C}$	$\mathbb{S} = \mathbb{C}^{s\times s}$
$\mathbb{R}^+$	$\mathbb{S}^+ \ldots$ upper-Δ with positive diag. entries
$\mathbb{R}_0^+$	$\mathbb{S}_0^+ \ldots$ upper-Δ with nonnegative diag. entries
0	singular $s \times s$ matrix (zero divisors!)
1	I

The *-algebra framework - properties I

standard	block
$a, b \in \mathbb{C}$	$\mathbf{A}, \mathbf{B} \in \mathbb{S}$
$\lvert a \rvert = \sqrt{a^* a} \in \mathbb{R}_0^+$	$\lvert \mathbf{A} \rvert = \sqrt{\mathbf{A}^* \mathbf{A}} \equiv \mathrm{cholUT}(\mathbf{A}^* \mathbf{A}) \in \mathbb{S}_0^+$
$\lvert a \rvert \in \mathbb{R}^+ \iff a \neq 0$	$\lvert \mathbf{A} \rvert \in \mathbb{S}^+ \iff \mathbf{A}$ nonsingular

The *-algebra framework - properties II

standard	block
$\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$	$\mathbf{X}, \mathbf{Y} \in \mathbb{S}^n (= \mathbb{C}^{ns \times s})$
$\langle \mathbf{x}, \mathbf{y} \rangle \equiv \mathbf{y}^* \mathbf{x} \in \mathbb{C}$	$\langle\langle \mathbf{X}, \mathbf{Y} \rangle\rangle \equiv \mathbf{Y}^* \mathbf{X} \in \mathbb{S}$
$\langle \mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{y}, \mathbf{x} \rangle^*$	$\langle\langle \mathbf{X}, \mathbf{Y} \rangle\rangle = \langle\langle \mathbf{Y}, \mathbf{X} \rangle\rangle^*$
$\langle \mathbf{x}a, \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle a$	$\langle\langle \mathbf{X}\mathbf{A}, \mathbf{Y} \rangle\rangle = \langle\langle \mathbf{X}, \mathbf{Y} \rangle\rangle \mathbf{A}$
$\langle \mathbf{x}, \mathbf{y}a \rangle = a^* \langle \mathbf{x}, \mathbf{y} \rangle$	$\langle\langle \mathbf{X}, \mathbf{Y}\mathbf{A} \rangle\rangle = \mathbf{A}^* \langle\langle \mathbf{X}, \mathbf{Y} \rangle\rangle$
$\Vert \mathbf{x} \Vert \equiv \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle} \in \mathbb{R}_0^+$	$\vert\vert\vert \mathbf{X} \vert\vert\vert \equiv \sqrt{\langle\langle \mathbf{X}, \mathbf{X} \rangle\rangle} \in \mathbb{S}_0^+$
$\langle \mathbf{x}, \mathbf{y} \rangle = \Vert \mathbf{x} \Vert \, \Vert \mathbf{y} \Vert \cos \theta_{\mathbf{x},\mathbf{y}}$	$\langle\langle \mathbf{X}, \mathbf{Y} \rangle\rangle = \vert\vert\vert \mathbf{Y} \vert\vert\vert^* \mathbf{U} \, \mathrm{diag}(c_i) \mathbf{V}^* \vert\vert\vert \mathbf{X} \vert\vert\vert$

Block Arnoldi revisited

- Let $\mathbf{F}_0 = \mathbf{V}_1\mathbf{S}_0$; $\mathbf{V}_1 \in \mathbb{S}^n$ and $\mathbf{S}_0 = |||\mathbf{F}_0||| \in \mathbb{S}^+$
- The **block Arnoldi process** is generally performed in terms of $\langle\langle\cdot,\cdot\rangle\rangle$
- $\mathbf{W}_j = \begin{bmatrix}\mathbf{V}_1, & \ldots, & \mathbf{V}_j\end{bmatrix} \in \mathbb{S}^{n\times j}$ has orthonormal columns
- Arnoldi relation: $\mathbf{A}\mathbf{W}_j = \mathbf{W}_{j+1}\overline{\mathbf{H}}_j$
- $\overline{\mathbf{H}}_j = (\mathbf{H}_{ik})_{ik} \in \mathbb{S}^{(j+1)\times j}$ is upper Hessenberg
- For $\blacksquare \in \mathbb{S}$ and $\text{◥} \in \mathbb{S}^+$

$$\overline{\mathbf{H}}_j = \begin{bmatrix} \blacksquare & \blacksquare & \blacksquare & \blacksquare & \cdots & \blacksquare \\ \text{◥} & \blacksquare & \blacksquare & \blacksquare & \cdots & \blacksquare \\ & \text{◥} & \blacksquare & \blacksquare & \cdots & \blacksquare \\ & & \text{◥} & \blacksquare & \cdots & \blacksquare \\ & & & \text{◥} & & \blacksquare \\ & & & & \ddots & \vdots \\ & & & & & \text{◥} \end{bmatrix}$$

Peak-plateau relationship between blFOM and blGMRES

Proposition (Kubínová and S. 2020)

The blGMRES and blFOM residuals satisfy:

$$\langle\langle \mathbf{R}_k^F, \mathbf{R}_k^F \rangle\rangle^{-1} = \langle\langle \mathbf{R}_k^G, \mathbf{R}_k^G \rangle\rangle^{-1} - \langle\langle \mathbf{R}_{k-1}^G, \mathbf{R}_{k-1}^G \rangle\rangle^{-1}.$$

Applying this relation recursively, we obtain

$$\langle\langle \mathbf{R}_k^G, \mathbf{R}_k^G \rangle\rangle^{-1} = \sum_{i=0}^{k} \langle\langle \mathbf{R}_i^F, \mathbf{R}_i^F \rangle\rangle^{-1}.$$

Generalization of the ordering of $\mathbb{R}_0^+$

Generalize the ordering of nonnegative real numbers $\mathbb{R}_0^+$ to upper triangular matrices with nonnegative diagonal entries $\mathbb{S}_0^+$ as follows:

$$|\mathbf{A}| \prec |\mathbf{B}| \iff \mathbf{A}^*\mathbf{A} \overset{\text{Löwner}}{\prec} \mathbf{B}^*\mathbf{B},$$
$$|\mathbf{A}| \preceq |\mathbf{B}| \iff \mathbf{A}^*\mathbf{A} \overset{\text{Löwner}}{\preceq} \mathbf{B}^*\mathbf{B}.$$

Peak-plateau result has some nontrivial consequences for the convergence behavior of blGMRES. In particular, the ordering of the residual norms

bIGMRES residual norm ordering

Theorem (Kubínová and S. 2020)

The bIGMRES residuals satisfy

$$|||\mathbf{R}_0||| \succeq |||\mathbf{R}_1^G||| \succeq \cdots \succeq |||\mathbf{R}_{n-1}^G||| \succeq 0.$$

Definition (Admissible convergence sequence)

Any sequence $\{\mathbf{F}_k\}_{k=0}^{n-1} \subset \mathbb{S}^+$ that satisfies

$$\mathbf{F}_0 \succeq \mathbf{F}_1 \succeq \cdots \succeq \mathbf{F}_{n-1} \succ 0$$

is called an admissible convergence sequence.

Note: One can construct non-trivial examples of inadmissible sequences where the individual column norms decrease monotonically

Prescribing convergence of blGMRES

Theorem (Kubínová and S. 2020)

Let $\{\mathbf{F}_k\}_{k=0}^{n-1} \subset \mathbb{S}^+$ *be an admissible convergence sequence. The following are equivalent:*

- *Residuals of blGMRES(*$\mathbf{A}$,$\mathbf{B}$*) satisfy* $|||\mathbf{R}_k^G||| = \mathbf{F}_k \,\forall\, k$
- *The* $\mathbf{A}$ *and* $\mathbf{B}$ *satisfy*

$$\mathbf{A} = \mathbf{W}\hat{\mathbf{R}}\hat{\mathbf{H}}\mathbf{W}^* \quad \textit{and} \quad \mathbf{B} = \mathbf{W}\mathbf{G},$$

where $\mathbf{W}$ *is unitary,* $\hat{\mathbf{R}} \in \mathbb{S}^{n\times n}$ *nonsing., upper block* Δ*,*

$$\hat{\mathbf{H}} = \begin{pmatrix} 0 & & & \langle\langle \mathbf{B}, \mathbf{W}_n \rangle\rangle^{-1} \\ I & \ddots & & -\langle\langle \mathbf{B}, \mathbf{W}_1 \rangle\rangle \langle\langle \mathbf{B}, \mathbf{W}_n \rangle\rangle^{-1} \\ & \ddots & 0 & \vdots \\ & & I & -\langle\langle \mathbf{B}, \mathbf{W}_{n-1} \rangle\rangle \langle\langle \mathbf{B}, \mathbf{W}_n \rangle\rangle^{-1} \end{pmatrix},$$

and the blocks of $\mathbf{G}$ *are* $\sqrt{\langle\langle \mathbf{F}_{k-1}, \mathbf{F}_{k-1} \rangle\rangle - \langle\langle \mathbf{F}_k, \mathbf{F}_k \rangle\rangle}$

All solvents are possible

Choosing $\hat{\mathbf{R}}$ as

$$\hat{\mathbf{R}} \equiv \hat{\mathbf{H}}^{-1}\mathbf{C}.$$

we can make $\mathbf{A}$ similar to any block companion matrix $\mathbf{C}$.

Lemma (Kubínová and S. 2020)

Assume that $\mathbf{A}$ *is of the form* $\mathbf{A} = \mathbf{W}\hat{\mathbf{R}}\hat{\mathbf{H}}\mathbf{W}^*$. *Then, for any sequence* $\mathbf{C}_0, \ldots, \mathbf{C}_n$, $\mathbf{C}_k \in \mathbb{S}$, $k = 0, \ldots, n-1$, $\mathbf{C}_0$ *nonsingular, there exists* $\hat{\mathbf{R}}$, *such that* $\mathbf{A}$ *is similar to*

$$\mathbf{C} = \begin{pmatrix} \mathbf{0} & & & \mathbf{C}_0 \\ \mathbf{I} & \ddots & & \mathbf{C}_1 \\ & \ddots & 0 & \vdots \\ & & \mathbf{I} & \mathbf{C}_{n-1} \end{pmatrix}.$$

Specifying solvents (i.e., "block eigenvalues")

- $\mathbf{C}$ is the block companion matrix to

$$\mathbf{M}(\lambda) = \mathbf{I}\lambda^n - \sum_{j=0}^{n-1} \mathbf{C}_k \lambda^k = \prod_{i=1}^{n} (\mathbf{I}\lambda - \mathbf{S}_k)$$

- "Block eigenvalues" $\mathbf{S}_k \in \mathbb{S}$ are called *solvents*.
- Eigenvalues of the solvents $\mathbf{S}_k \in \mathbb{S}$, $k = 1, \ldots, n$, are also the eigenvalues of $\mathbf{C}$
- Prescribing solvents is however stronger than prescribing just the scalar eigenvalues,
  - → since there are multiple block companion matrices similar to each other

Interpretation: more right-hand sides can reduce predictive value of the eigenvalues

Specifying Ritz solvents

We can specify Ritz solvents $\mathbf{C}_k^{(j)}$ (solvents of $\mathbf{H}_j$, $j = 1, 2, \ldots$).

$$\text{Let} \quad \mathbf{U} = \begin{bmatrix} I & -\mathbf{C}_0^{(1)} & -\mathbf{C}_0^{(2)} & \cdots & -\mathbf{C}_0^{(n-1)} \\ & I & -\mathbf{C}_1^{(2)} & \cdots & \vdots \\ & & \ddots & \ddots & \vdots \\ & & & I & -\mathbf{C}_{n-2}^{(n-1)} \\ & & & & I \end{bmatrix}^{-1}$$

and

$$\mathbf{D}_\Sigma = \operatorname{diag}\left(I, \Sigma_1, \Sigma_1\Sigma_2, \ldots, \prod_{k=1}^{n-1} \Sigma_k \right) \in \left(\mathbb{S}^+\right)^{n\times n}.$$

Then $\mathbf{A} = \mathbf{W}\mathbf{D}_\Sigma\mathbf{U}\mathbf{C}\mathbf{U}^{-1}\mathbf{D}_\Sigma^{-1}\mathbf{W}^*$ has the specified solvents, produces the specified Ritz solvents during block Arnoldi, and $\mathbf{W}\mathbf{E}_1 = \mathbf{V}_1$ should be our chosen starting vector (normalized)

Conclusions

We provided:

- an explicit peak-plateau relation for blFOM and blGMRES;
- an explicit characterization of admissible convergence behavior of blGMRES;

and showed that:

- any admissible convergence behavior is also attainable by blGMRES;
- arbitrary spectral properties of $\mathbf{A}$ can be enforced, while preserving the convergence behavior.

Conclusion: the *-algebra approach is a correct way to analyse block Krylov subspace method behavior.

Future work

- handling of linear dependence
  - $\rightarrow$ $\mathbf{V}_{j+1}$ is rank-deficient $\iff$ $|||\mathbf{V}_{j+1}|||$ is singular
  - $\rightarrow$ Zero-divisors complicate the analysis
- analysis of restarted block GMRES
- iterative methods for systems over *-algebras.
- analyze other block-level structural characteristics of matrices and matrix algorithms
  - $\rightarrow$ Understanding of "geometric" relationships of elements of the *-algebra as well as of vectors and systems built from them

References

Results in this talk are available in two papers

- **Kubínová and S.** *Prescribing convergence behavior of block Arnoldi and GMRES*, SIMAX, 2020
- **S.** *Stagnation of block GMRES and its relationship to block FOM*, ETNA, 2017

For more information: `http://math.soodhalter.com`

Thank you! Questions?