# Advances in resource-constrained matrix Krylov methods for space-time discretizations

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*From joint works with*
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# Discretizations and heterogeneous variable setting

A given differential problem may depend on space variable and

- Time (high quality soln of heat-, wave-type equations, dynamical systems generally)
- Parameters (e.g., coefficients with uncertainty, model tuning)

Irrespective of this, discretization may lead to a component mixing via

$$\mathcal{A}x = f, \quad \mathcal{A} \in \mathbb{R}^{n\times n}$$

Solution methods: Preconditioned Krylov subspace methods (CG, MINRES, GMRES, BiCGSTAB, etc.)

As an alternative: Use a tensor space at the discretization phase

$$\mathcal{H} \times \mathcal{S}$$

with ♣ $\mathcal{H}$: spatial variables ♣ $\mathcal{S}$: time/parameter variables

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# Identity/Property-preserving algebraic formulations

Avoid the mixing

$$\Downarrow$$

$$AX + XG = F, \qquad x = \mathrm{vec}(X), \qquad f = \mathrm{vec}(F), \quad X \in \mathbb{R}^{n_A \times n_G}$$

Among the various solvers, Projection-type methods:
Assume $F = F_1 F_2^T$. Given low dim. approx spaces $\mathcal{K}_A$, $\mathcal{K}_G$, and $V_m, W_m$ their bases
let $X_m := V_m Y_m W_m^T$, $X_m \approx X$

Galerkin condition: $\quad R := AX_m + X_m G^T - F_1 F_2^T \quad \perp \quad \mathcal{K}_A \otimes \mathcal{K}_G$

$$V_m^\top R W_m = 0$$

Note: $\mathcal{K}_A$, $\mathcal{K}_G$ tiny wrto $\mathbb{K}(\mathcal{A}, f)$

The hard-to-find space is $V_m \quad \Rightarrow \quad$ Krylov space based

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# Pausing on pros and cons

Current full-orth based Krylov subspaces may be "expensive"

- "expensive" in different ways: Memory, computation, communication, etc.
- General concern :
  linear systems, eigenvalue problems, matrix function evaluations, etc.

**Imperative**

Keep the Krylov recurrence short and cheap!

# Several steps back. Short-term recurrences

Main ingredient: Krylov decomposition (Stewart, '01)

$$AU_k = U_k B_k + u_{k+1} b_{k+1}^*$$

with

- $B_k$ is $k \times k$, Rayleigh quotient
- $[U_k, u_{k+1}]$ are linearly independent, build a Krylov space (here, $b_{k+1} = \beta_{k+1} e_k$)

Procedures fitting this framework:

- Full orth Arnoldi (*)
- Truncated Arnoldi, restarted Arnoldi
- Chebyshev, Newton, ... iterations
- Nonsymmetric Lanczos

Except for (*), all methods suffer from lack/loss of orthogonality properties!

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# Towards stabilized procedures

$$AU_k = U_k B_k + u_{k+1} b_k^*$$

⋆ Let $\mathcal{J} : \mathbb{R}^{n\times(k+1)} \to \mathbb{R}^{s\times(k+1)}$ be a row selection operator with $s > k+1$

⋆ Let $\mathcal{J}(U) = QR$ be the reduced QR decomposition of the *subsampled* matrix
(see, e.g., Woodruff, '14)

**Ideal low-cost stabilization problem**

Given $U_{k+1} = [U_k, u_{k+1}]$, for some $s$ with $k+1 < s \ll n$, find $\mathcal{J}$ giving the best conditioned matrix

$$\widehat{U}_{k+1} := U_{k+1} R^{-1}$$

where $\mathcal{J}(U_{k+1}) = QR$

Unrealistic:

- Solving this problem is expensive
- Columns of $U_{k+1}$ are assumed not to be available simultaneously!

**First practical compromise**

Select $\mathcal{J}$ a priori $\Rightarrow$ random subsampling, with row selection probability $p_i$

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# A randomly subsampled Krylov decomposition

Let $\widehat{U}_k = U_k R_k^{-1}$

**Randomized Krylov decomposition v.1** (Palitta, Schweitzer, Simoncini, '23)

It holds that

$$\mathcal{J}(A\widehat{U}_k) = \mathcal{J}(\widehat{U}_k)(\widehat{B}_k + d_k e_k^*) + q_{k+1}\chi_k e_k^*, \quad q_{k+1} \perp \mathcal{J}(\widehat{U}_k)$$

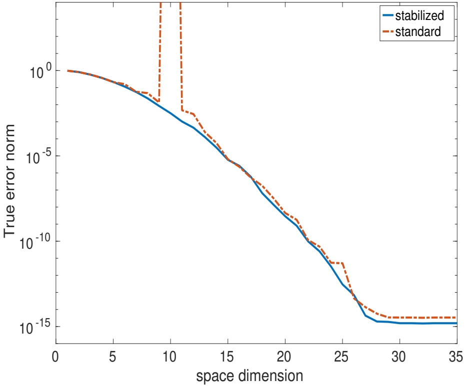
1. $\widehat{B}_k + d_k e_k^*$ rank-one modification (last column) of $\widehat{B}_k = R_k^{-1} B_k R_k$
2. Randomized Krylov decomposition corresponds to $\mathcal{J}^*\mathcal{J}$-orthogonalization of original Krylov decomposition

# A simple example. Matrix function evaluation.

$$\exp(A)v \approx \widehat{U}_k \exp(\widehat{B}_k + d_k e_k^*) e_1 \chi_0$$

$n = 4900$, $s = 200$ – similar results for $s = 80$ ($k_{\max}$=40)

Nonsymmetric Lanczos iteration:



# Carrying on

Why non-symmetric Lanczos iterations?

- Pros: Inherently short-term recurrence (no truncation parameter!)
- Pros: Builds same Krylov subspace as all Arnoldi-type methods
- Cons: Requires $A^T$
- Cons: Breakdown possible

Is row subsampling enough?

- Row sampling cheap and easy fix
- Row sampling is often not enough as stabilizer
- Conditioning not necessarily low

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Sketching strategies: Subspace embedding

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Sketching strategies: Subspace embedding

# Sketching strategies. Subspace embedding.

A $(1 \pm \varepsilon)$ $\ell_2$-subspace embedding for $V \in \mathbb{R}^{n \times k}$ is an operator $\mathcal{S}$ such that

$$(1-\varepsilon)\|Vx\|_2^2 \leq \|\mathcal{S}(Vx)\|_2^2 \leq (1+\varepsilon)\|Vx\|_2^2, \qquad \forall x \in \mathbb{R}^k$$

The Subsampled Randomized Hadamard Transform

A convenient such choice (Rademacher operator)

$$\mathcal{S}(v) := \frac{1}{\sqrt{sn}} PCDv, \qquad \mathcal{S}(\cdot) \text{ is an } s \times n \text{ matrix}$$

with

$D$ "rotation" (diagonal matrix from random distr. in $\{-1, 1\}$)

$C$ fast cosine transform

$P$ coordinate sampling

*See, e.g., David Woodruff (2014), Martinsson and Tropp, Acta Num. (2020)*

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# Subspace embedding in Krylov decomposition

$$\mathcal{S}(A\widehat{U}_k) = \mathcal{S}(\widehat{U}_k)(\widehat{B}_k + d_k e_k^*) + q_{k+1}\chi_k e_k^*, \quad q_{k+1} \perp \mathcal{S}(\widehat{U}_k)$$

with

$$\kappa_2(\widehat{U}_k) \le \sqrt{\frac{1+\varepsilon}{1-\varepsilon}}$$

*Contributions within the "Krylov world", Balabanov, Cortinovis, Grigori, Guettel, Kressner, Nakatsukasa, Nouy, Palitta, Schweitzer, Timsit, Tropp, etc.*

**Paradigm: Stabilize while constructing**

At each iteration $k$

- Compute next Lanczos vectors $u_k, w_k$
- Compute embedded vector $\mathcal{S}(u_k)$
- Update QR of embedded basis (i.e. stabilization matrix $R_k$)
- Update and use $\widehat{B}_k + d_k e_k^*$

Enhanced stabilitization within non-sym Lanczos:

♣ Weak biorthogonality in $U_m, V_m$ (no parameters)

♣ Strong subsampled orthogonality in $U_m$

Shared step: Two-pass strategy to recover problem solution (quick basis recostruction)

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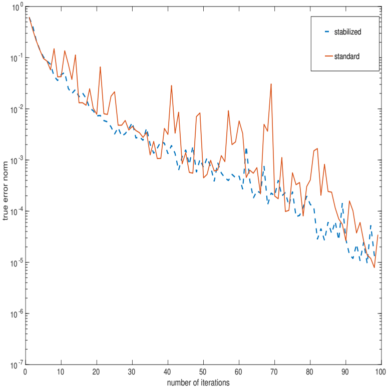
# Another example with nonsymmetric Lanczos

FD discretization of the operator

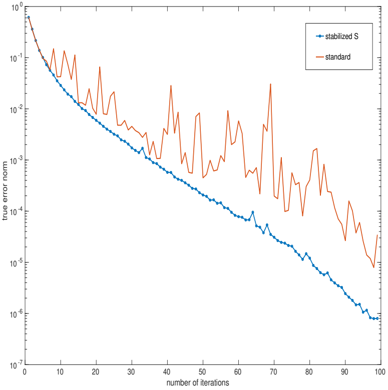
$$\mathcal{L}(u) = -(\exp(-xy)u_x)_x - (\exp(xy)u_y)_y - 100(x+y)u_y + 500u,$$

such that $n = 4900$, $v = \texttt{randn}$ (norm'd), $s = 200$

$$\exp(A^{-\frac{1}{2}})v \;\approx\; \widehat{U}_k \exp((\widehat{B}_k + d_k e_k^*)^{-\frac{1}{2}})e_1\chi_0$$




$\mathcal{J}(U_k)$




$\mathcal{S}(U_k)$

# Conclusions (so far)

- Randomized subsampling is a good compromise
- Sketching as pure stabilization procedure, for the more skeptical practitioners ;)
- Still many open issues to make sketching robust beyond "expectation"

REFERENCES


- Davide Palitta , Marcel Schweitzer , and V. Simoncini *Sketched and truncated polynomial Krylov methods: matrix equations*, arXiv:2311.16019, pp. 1-28, 2023
- Davide Palitta , Marcel Schweitzer , and V. Simoncini *Sketched and truncated polynomial Krylov methods: Evaluation of Matrix functions*, arXiv:2306.06481, pp. 1-22, 2023
- V. Simoncini and Yihong Wang *Stabilized short-term recurrences via randomized row subsampling*, in preparation, 2024.

# Lecturers of the Thirty-fourth Woudschoten Conference (October 2009)

# Howard and me at Lake Tahoe, 2011