Krylov Subspace Recycling For Matrix Functions

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General Overview

Computational challenge : A sequence of matrix function applications on a set of vectors

$$f(\mathbf{A}^{(i)})\mathbf{b}^{(i)} \qquad i = 1, 2, \ldots, N \tag{1}$$

- Each $\mathbf{A}^{(i)} \in \mathbb{C}^{n\times n}$ is *slowly* changing.
- Each $\mathbf{b}^{(i)} \in \mathbb{C}^{n}$ is available in sequence rather than simultaneously.

Examples

- Solution to a sequence of linear systems : $\mathbf{A}^{(i)}\mathbf{x}^{(i)} = \mathbf{b}^{(i)}$.
- Solution to systems of ODE's : $\exp(\mathbf{A}^{(i)})\mathbf{b}^{(i)}$.
- Lattice QCD simulations : $\text{sign}(\mathbf{A}^{(i)})\mathbf{b}^{(i)}$.

Goal : A *Krylov subspace recycling algorithm for (1).*

What is augmentation and recycling ?

Augmentation and Recycling

- An *augmented* Krylov subspace method is a projection method which projects a problem onto the subspace $\mathcal{S}_j = \mathcal{V}_j \oplus \mathcal{U}$ where $\mathcal{V}_j$ is a Krylov subspace and $\mathcal{U}$ is an *augmentation subspace*.
- A *recycling* method is an augmented method used to treat a sequence of problems where the augmentation subspace is *recycled* from the Krylov subspace used to solve a previous problem in the sequence.

Example : Sequence of linear systems

$$\begin{aligned} \mathbf{A}^{(1)}\mathbf{x}^{(1)} = \mathbf{b}^{(1)} \qquad \to \mathcal{U}^{(1)} \to \qquad \mathbf{A}^{(2)}\mathbf{x}^{(2)} = \mathbf{b}^{(2)} \\ \to \mathcal{U}^{(2)} \to \ldots \to \mathcal{U}^{(N-1)} \to \mathbf{A}^{(N)}\mathbf{x}^{(N)} = \mathbf{b}^{(N)} \end{aligned}$$

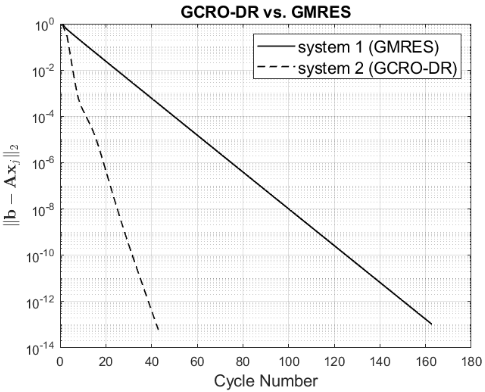


Figure – Convergence plot of two system solves using a fixed Poisson matrix $\mathbf{A} \in \mathbb{R}^{10{,}000 \times 10{,}000}$. The first system uses standard GMRES, and the second system uses the GCRO-DR algorithm with a recycling subspace $\mathcal{U}$ constructed from the first system solve ($\dim(\mathcal{U}) = 2$).

Overview

I will give a brief background :

- Matrix Functions
- Projection Methods
- Krylov Subspace Methods (Augmented and Recycled)

And then discuss recent work...

- L. Burke, A. Frommer, G. Ramirez, K. M Soodhalter - Krylov Subspace Recycling For Matrix Functions, arXiv :2209.14163 [math.NA] (2022)

A definition..

Cauchy integral definition of $f(\mathbf{A})$

For the matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ with spectrum $\Lambda(\mathbf{A})$, if f is analytic in a region containing the closed contour Γ which in turn contains $\Lambda(\mathbf{A})$ in its interior, $f(\mathbf{A})$ can be defined as

$$f(\mathbf{A}) = \frac{1}{2\pi i} \int_{\Gamma} f(\sigma)(\sigma \mathbf{I} - \mathbf{A})^{-1} d\sigma.$$

As a consequence we have :

$$f(\mathbf{A})\mathbf{b} = \frac{1}{2\pi i} \int_{\Gamma} f(\sigma)(\sigma \mathbf{I} - \mathbf{A})^{-1}\mathbf{b} d\sigma.$$

Thus $f(\mathbf{A})\mathbf{b}$ contains, in its integrand, the solution $\mathbf{x}(\sigma)$ of the shifted linear system

$$(\sigma \mathbf{I} - \mathbf{A})\mathbf{x}(\sigma) = \mathbf{b}.$$

Problem

Solve $\mathbf{A}\mathbf{x} = \mathbf{b}$ where $\mathbf{A} \in \mathbb{C}^{n \times n}$ and

- $\mathbf{A}$ is only available as some function which takes a vector $\mathbf{v} \in \mathbb{C}^n$ and returns $\mathbf{v} \leftarrow \mathbf{A}\mathbf{v}$.

- Consider two j dimensional subspaces $\mathcal{V}_j, \widetilde{\mathcal{V}}_j \subset \mathbb{C}^n$, $j \ll n$.
- For an initial guess $\mathbf{x}_0$, (initial residual $\mathbf{r}_0$) compute correction $\mathbf{t}_j \in \mathcal{V}_j$ and update $\mathbf{x}_j = \mathbf{x}_0 + \mathbf{t}_j$ such that

$$\mathbf{r}_j = \mathbf{b} - \mathbf{A}\mathbf{x}_j \perp \widetilde{\mathcal{V}}_j.$$

Problem on subspace $\mathcal{V}_j$

Solve for $\mathbf{y} \in \mathbb{C}^j$, the $j \times j$ linear system

$$\widetilde{\mathbf{V}}_j^* \mathbf{A} \mathbf{V}_j \mathbf{y}_j = \widetilde{\mathbf{V}}_j^* \mathbf{r}_0.$$

- Update $\mathbf{x}_j = \mathbf{x}_0 + \mathbf{V}_j \mathbf{y}_j$.

Suitable choice of $\mathcal{V}_j$ and $\widetilde{\mathcal{V}}_j$?

The subspaces $\mathcal{V}_j$ and $\widetilde{\mathcal{V}}_j$ should be chosen such that

- It is cheap (and practical) to build a basis for $\mathcal{V}_j$ and $\widetilde{\mathcal{V}}_j$.
- The matrix $\widetilde{\mathbf{V}}_j^* \mathbf{A} \mathbf{V}_j$ is non-singular.
- $\mathcal{V}_j$ contains a good approximate solution for small j.

Common to choose $\mathcal{V}_j$ to be a Krylov subspace $\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$.

Krylov subspace $\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$

The j dimensional Krylov subspace built from the matrix $\mathbf{A}$ and vector $\mathbf{r}_0$ is defined as the subspace

$$\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0) = \text{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \ldots, \mathbf{A}^{j-1}\mathbf{r}_0\}$$

Numerically unstable to construct the Krylov matrix.

$$\mathbf{V}_j = \begin{bmatrix} \mathbf{r}_0 & \mathbf{A}\mathbf{r}_0 & \mathbf{A}^2\mathbf{r}_0 & \ldots & \mathbf{A}^{j-1}\mathbf{r}_0 \end{bmatrix}.$$

Columns become linearly dependent quickly.

Algorithm Arnoldi with Modified Gram-Schmidt

Input : $\mathbf{A}$, $\mathbf{r}_0$, cycle length m
Compute $\mathbf{v}_1 \leftarrow \frac{\mathbf{r}_0}{\|\mathbf{r}_0\|}$
for $j = 1, 2, ...m$ **do**
    $\mathbf{w} \leftarrow \mathbf{A}\mathbf{v}_j$
    for $i = 1, 2, .., j$ **do**
        $h_{i,j} \leftarrow \mathbf{v}_i^* \mathbf{w}$
        $\mathbf{w} \leftarrow \mathbf{w} - h_{i,j}\mathbf{v}_i$
    end for
    $h_{j+1,j} \leftarrow \|\mathbf{w}\|_2$
    $\mathbf{v}_{j+1} \leftarrow \mathbf{w}/h_{j+1,j}$
end for

Arnoldi Relation (after j steps)

$$\mathbf{A}\mathbf{V}_j = \mathbf{V}_{j+1}\overline{\mathbf{H}}_j = \mathbf{V}_j\mathbf{H}_j + h_{j+1,j}\mathbf{v}_{j+1}\mathbf{e}_j^T$$

1

1. $\mathbf{V}_{j+1} \in \mathbb{C}^{n\times(j+1)}$, $\overline{\mathbf{H}}_j \in \mathbb{C}^{(j+1)\times j}$, $\mathbf{H}_j \in \mathbb{C}^{j\times j}$

Full Orthogonalization Method (FOM)

- We will focus on the choice $\widetilde{\mathcal{V}}_j = \mathcal{V}_j = \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$.

Problem on Krylov subspace $\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$

Solve for $\mathbf{y} \in \mathbb{C}^j$, the $j \times j$ linear system

$$\mathbf{H}_j \mathbf{y}_j = \|\mathbf{r}_0\| \mathbf{e}_1.$$

Algorithm Restarted FOM

1: **Input :** $\mathbf{A} \in \mathbb{C}^{n \times n}$, $\mathbf{b} \in \mathbb{C}^n$, $\mathbf{x} \in \mathbb{C}^n$, tolerance ϵ
2: $\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}$
3: **while** $\|\mathbf{r}\| > \epsilon$ **do**
4: Build a basis for the Krylov subspace $\mathcal{K}_j(\mathbf{A}, \mathbf{r})$ via the Arnoldi algorithm generating $\mathbf{V}_{j+1}$ and $\overline{\mathbf{H}}_j$.
5: Solve $\mathbf{H}_j \mathbf{y} = \|\mathbf{r}\| \mathbf{e}_1$ for $\mathbf{y}$.
6: $\mathbf{x} \leftarrow \mathbf{x} + \mathbf{V}_j \mathbf{y}$
7: $\mathbf{r} \leftarrow \mathbf{r} - \mathbf{V}_{j+1} \overline{\mathbf{H}}_j \mathbf{y}$
8: **end while**

Shifted Linear Systems

Shift invariance of a Krylov subspace

For any $\sigma \in \mathbb{C}$ we have

$$\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0) = \mathcal{K}_j(\sigma \mathbf{I} - \mathbf{A}, \mathbf{r}_0^{(\sigma)})$$

provided $\mathbf{r}_0 = \beta \mathbf{r}_0^{(\sigma)}$, $\beta \in \mathbb{C}$.

- Leads to a *shifted Arnoldi relation*

$$(\sigma \mathbf{I} - \mathbf{A})\mathbf{V}_j = \mathbf{V}_j(\sigma \mathbf{I} - \mathbf{H}_j) - h_{j+1}\mathbf{v}_{j+1}\mathbf{e}_j^T.$$

- Allows for efficient solution to shifted linear systems $(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{x}^{(i)} = \mathbf{b}$ over a single Krylov subspace.
- Shifted FOM approximation

$$\mathbf{x}_j^{(i)} = \|\mathbf{b}\| \mathbf{V}_j(\sigma_i \mathbf{I} - \mathbf{H}_j)^{-1}\mathbf{e}_1.$$

Arnoldi Approximation To $f(\mathbf{A})\mathbf{b}$

Recall : Cauchy integral definition of $f(\mathbf{A})$

For the matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ with spectrum $\Lambda(\mathbf{A})$, if f is analytic in a region containing the closed contour Γ which in turn contains $\Lambda(\mathbf{A})$ in its interior, $f(\mathbf{A})$ can be defined as

$$f(\mathbf{A}) = \frac{1}{2\pi i} \int_\Gamma f(\sigma)(\sigma \mathbf{I} - \mathbf{A})^{-1} d\sigma.$$

Thus the Arnoldi approximation can be derived via

$$\begin{aligned} f(\mathbf{A})\mathbf{b} = \frac{1}{2\pi i} \int_\Gamma f(\sigma)\mathbf{x}(\sigma) d\sigma &\approx \|\mathbf{b}\| \mathbf{V}_j \frac{1}{2\pi i} \int_\Gamma f(\sigma)(\sigma \mathbf{I} - \mathbf{H}_j)^{-1} d\sigma \mathbf{e}_1 \\ &= \|\mathbf{b}\| \mathbf{V}_j f(\mathbf{H}_j) \mathbf{e}_1. \end{aligned}$$

- Need to develop a recycled shifted FOM for linear systems

$$(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{x}^{(i)} = \mathbf{b}.$$

- Take an approximation from some Krylov subspace $\mathbf{t}_j^{(i)} \in \mathcal{V}_j$ and an *augmentation subspace* $\mathbf{s}_j^{(i)} \in \mathcal{U}$.

$$\mathbf{x}_j^{(i)} = \mathbf{V}_j \mathbf{y}_j^{(i)} + \mathbf{U}\mathbf{z}^{(i)} \qquad \mathbf{y}_j^{(i)} \in \mathbb{C}^j, \mathbf{z}^{(i)} \in \mathbb{C}^k$$

- Use a well known residual projection framework which describes augmented Krylov subspace methods in terms of solving a projected problem. Impose

$$\mathbf{r}_j^{(i)} = \mathbf{b} - (\sigma_i \mathbf{I} - \mathbf{A})(\mathbf{V}_j \mathbf{y}_j^{(i)} + \mathbf{U}\mathbf{z}^{(i)}) \perp \widetilde{\mathcal{V}}_j + \widetilde{\mathcal{U}}$$

- This yields the following linear system for $\mathbf{z}_j^{(i)}$ and $\mathbf{y}_j^{(i)}$:

$$\begin{bmatrix} \widetilde{\mathbf{U}}^*(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{U} & \widetilde{\mathbf{U}}^*(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{V}_j \\ \widetilde{\mathbf{V}}_j^*(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{U} & \widetilde{\mathbf{V}}_j^*(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{V}_j \end{bmatrix} \begin{bmatrix} \mathbf{z}_j^{(i)} \\ \mathbf{y}_j^{(i)} \end{bmatrix} = \begin{bmatrix} \widetilde{\mathbf{U}}^*\mathbf{b} \\ \widetilde{\mathbf{V}}_j^*\mathbf{b} \end{bmatrix}$$

- A block LU factorization to eliminate the bottom left block allows us to express $\mathbf{y}_j^{(i)}$ as the solution to the problem :

Problem on subspace $\mathcal{V}_j$

Solve the linear system for $\mathbf{y}_j^{(i)}$

$$\widetilde{\mathbf{V}}_j^*(\mathbf{I} - \mathbf{Q}_{\sigma_i})(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{V}_j \mathbf{y}_j^{(i)} = \widetilde{\mathbf{V}}_j^*(\mathbf{I} - \mathbf{Q}_{\sigma_i})\mathbf{b},$$

with the projector $\mathbf{Q}_{\sigma_i} := (\sigma_i \mathbf{I} - \mathbf{A})\mathbf{U}(\widetilde{\mathbf{U}}^*(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{U})^{-1}\widetilde{\mathbf{U}}^*$.

Projected problem

The framework then describes this problem as equivalent to applying the following projection method :

Find $\mathbf{t}_j^{(i)} \in \mathcal{V}_j$ as an approximate solution corresponding to shift σ_i for the projected and shifted linear system

$$(\mathbf{I} - \mathbf{Q}_{\sigma_i})(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{x}^{(i)} = (\mathbf{I} - \mathbf{Q}_{\sigma_i})\mathbf{b} \tag{2}$$

such that $\mathbf{r}_j^{(i)} = (\mathbf{I} - \mathbf{Q}_{\sigma_i})(\mathbf{b} - (\sigma_i \mathbf{I} - \mathbf{A})\mathbf{t}_j^{(i)}) \perp \widetilde{\mathcal{V}}_j$.

- Requires basis for projected Krylov subspace

$$\mathcal{K}_j((\mathbf{I} - \mathbf{Q}_{\sigma_i})(\sigma_i \mathbf{I} - \mathbf{A}), (\mathbf{I} - \mathbf{Q}_{\sigma_i})\mathbf{b}).$$

- Shift invariance no longer holds.
  $\Longrightarrow$ Requires separate Krylov space for each σ_i
  $\Longrightarrow$ Not practical.

Equivalence to the unprojected problem

Find $\mathbf{t}_j^{(i)} \in \mathcal{V}_j$ as an approximate solution corresponding to shift σ_i for the shifted linear system

$$(\sigma_i \mathbf{I} - \mathbf{A})\mathbf{x}^{(i)} = \mathbf{b}$$

such that $\mathbf{r}_j^{(i)} = \mathbf{b} - (\sigma_i \mathbf{I} - \mathbf{A})\mathbf{t}_j^{(i)} \perp (\mathbf{I} - \mathbf{Q}_{\sigma_i})^* \widetilde{\mathcal{V}}_j$.

- Requires only a basis for $\mathcal{K}_j(\mathbf{A}, \mathbf{b})$.
  $\implies$ Shift invariance still holds.
  $\implies$ Practical to implement.

General outline

- Build basis for $\mathcal{K}_j(\mathbf{A}, \mathbf{b})$.
- Solve for $\mathbf{y}_j^{(i)}$ on $\mathcal{K}_j(\mathbf{A}, \mathbf{b})$.
- Compute $\mathbf{z}^{(i)}$ using $\mathbf{y}_j^{(i)}$.
- Update $\mathbf{x}_j^{(i)} = \mathbf{V}_j \mathbf{y}_j^{(i)} + \mathbf{U}\mathbf{z}^{(i)}$.

rsFOM method for linear systems

- Choose $\mathcal{V}_j = \widetilde{\mathcal{V}}_j = \mathcal{K}_j(\mathbf{A}, \mathbf{b})$ and $\widetilde{\mathcal{U}} = \mathcal{U}$.

Problem for each $\mathbf{y}_j^{(i)}$ on the Krylov subspace $\mathcal{K}_j(\mathbf{A}, \mathbf{b})$

Solve the linear system

$$(\mathbf{V}_j^*(\mathbf{I} - \mathbf{Q}_{\sigma_i})\mathbf{V}_{j+1}(\sigma_i\bar{\mathbf{I}} - \overline{\mathbf{H}}_j))\mathbf{y}_j^{(i)} = \mathbf{V}_j^*(\mathbf{I} - \mathbf{Q}_{\sigma_i})\mathbf{b}$$

- Never want to explicitly construct projector $(\mathbf{I} - \mathbf{Q}_{\sigma_i})$.
- Only implicitly compute product via

$$\mathbf{V}_j^*(\mathbf{I}-\mathbf{Q}_{\sigma_i})\mathbf{V}_{j+1}(\sigma_i\bar{\mathbf{I}}-\overline{\mathbf{H}}_j) = \sigma_i\mathbf{I}-\mathbf{H}_j-\mathbf{K}^{(i)}\mathbf{L}^{(i)}\mathbf{M}(\sigma_i\bar{\mathbf{I}}-\overline{\mathbf{H}}_j)$$

with

$$\mathbf{K}^{(i)} = \sigma_i\mathbf{V}_j^*\mathbf{U} - \mathbf{V}_j^*\mathbf{C}$$

$$\mathbf{L}^{(i)} = (\sigma_i\mathbf{U}^*\mathbf{U} - \mathbf{U}^*\mathbf{C})^{-1}, \;\; \mathbf{M} = \mathbf{U}^*\mathbf{V}_{j+1}.$$

Recycled FOM For Functions Of Matrices r(FOM)^2

rsFOM solution given via

$$\mathbf{x}_j^{(i)} = \mathbf{V}_j \mathbf{y}_j^{(i)} + \mathbf{U}(\sigma_i \mathbf{U}^* \mathbf{U} - \mathbf{U}^* \mathbf{C})^{-1} \mathbf{U}^* (\mathbf{b} - \mathbf{V}_{j+1}(\sigma_i \bar{\mathbf{I}} - \overline{\mathbf{H}}_j)\mathbf{y}_j^{(i)}.$$

Sub into integral expression of $f(\mathbf{A})\mathbf{b}$ and treat via quadrature to obtain..

Augmented FOM approximation for $f(\mathbf{A})\mathbf{b}$

$$\begin{aligned} \widetilde{f}_j = & \mathbf{V}_j \sum_{\ell=1}^{n_{quad}} \omega_\ell f(z_\ell) \mathbf{y}_j^{(\ell)} \\ & + \mathbf{U} \sum_{\ell=1}^{n_{quad}} \omega_\ell f(z_\ell)(z_\ell \mathbf{U}^* \mathbf{U} - \mathbf{U}^* \mathbf{C})^{-1} \mathbf{U}^* (\mathbf{b} - \mathbf{V}_{j+1}(z_\ell \bar{\mathbf{I}} - \overline{\mathbf{H}}_j)\mathbf{y}_j^{(\ell)}), \end{aligned}$$

where z_ℓ and ω_ℓ are quadrature nodes and weights respectively.

Algorithm r(FOM)^2

Input : $\mathbf{A} \in \mathbb{C}^{n \times n}$, $\mathbf{b} \in \mathbb{C}^{n}$, scalar function f, $\mathbf{U} \in \mathbb{C}^{n \times k}$, $\mathbf{C} = \mathbf{AU}$, Arnoldi cycle length j, nodes z_ℓ and weights ω_ℓ
Build a basis for $\mathcal{K}_j(\mathbf{A}, \mathbf{b})$ to generate $\mathbf{V}_{j+1}$ and $\overline{\mathbf{H}}_j$
Set $\mathbf{t}_1 = 0 \in \mathbb{C}^j$, $\mathbf{t}_2 = 0 \in \mathbb{C}^k$
for $\ell = 1, .., n_{quad}$ **do**
  $\mu \leftarrow \omega_\ell f(z_\ell)$
  Solve $(z_\ell \mathbf{I} - \mathbf{H}_j - \mathbf{K}^{(\ell)} \mathbf{L}^{(\ell)} \mathbf{M}(z_\ell \bar{\mathbf{I}} - \overline{\mathbf{H}}_j))\mathbf{y} = \mathbf{V}_j^* (\mathbf{I} - \mathbf{Q}_{z_\ell})\mathbf{b}$
  $\mathbf{t}_1 \leftarrow \mathbf{t}_1 + \mu\, \mathbf{y}$
  $\mathbf{t}_2 \leftarrow \mathbf{t}_2 + \mu\, (z_\ell \mathbf{U}^* \mathbf{U} - \mathbf{U}^* \mathbf{C})^{-1} (\mathbf{U}^* \mathbf{b} - \mathbf{U}^* \mathbf{V}_{j+1} (z_\ell \bar{\mathbf{I}} - \overline{\mathbf{H}}_j)\mathbf{y})$
end for
$\widetilde{f}_1 \leftarrow \mathbf{V}_j \mathbf{t}_1 + \mathbf{U}\mathbf{t}_2$
Update $\mathbf{U}$ and $\mathbf{C}$

Computational Cost Analysis

operation	arithmetic cost	how often
$\mathbf{U}^*\mathbf{U}$ and $\mathbf{U}^*\mathbf{C}$	$2k^2n$	1
$\mathbf{V}_j^*\mathbf{U}$ and $\mathbf{V}_j^*\mathbf{C}$	$2kjn$	1
$\mathbf{M} = \mathbf{U}^*\mathbf{V}_{j+1}$	$k(j+1)n$	1
$\mathbf{M}(z_\ell\mathbf{I} - \overline{\mathbf{H}}_j) := \mathbf{R}(z_\ell)$	$kj(j+1)$	n_{quad}
$\mathbf{L}(z_\ell) = (z_\ell\mathbf{U}^*\mathbf{U} - \mathbf{U}^*\mathbf{C})^{-1}$	k^3	n_{quad}
$\mathbf{L}(z_\ell)\mathbf{R}(z_\ell) =: \mathbf{S}(z_\ell)$	k^2j	n_{quad}
$\mathbf{K}(z_\ell)\mathbf{S}(z_\ell) =: \mathbf{T}(z_\ell)$	kj^2	n_{quad}
Solve for $\mathbf{y}$, system matrix is $\mathbf{T}(z_\ell)$	$\frac{1}{3}j^3$	n_{quad}
total cost : $n(2k^2 + 2jk + k(j+1)) + n_{quad}(kj(j+1) + k^3 + k^2j + kj^2 + \frac{1}{3}j^3)$		

Table – Arithmetic cost of r(FOM)^2

- The n_{quad} term in the cost is not dependent on the dominant n and thus the number of quadrature points can be increased without causing large growths in cost.

How to cheaply construct $\mathcal{U}$?

- $\mathcal{U}$ should be a space spanned by approximate eigenvectors corresponding to k smallest eigenvalues.
- Use *ritz* or *harmonic- ritz* vectors.

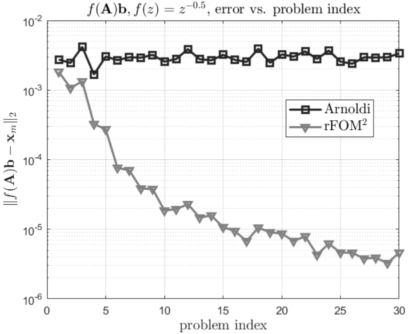
Harmonic Ritz problem

The harmonic Ritz problem for the matrix $\mathbf{A}$ with respect to the augmented Krylov subspace space $\mathcal{K}_j(\mathbf{A}, \mathbf{b}) + \mathcal{U}$ involves solving the following eigenproblem

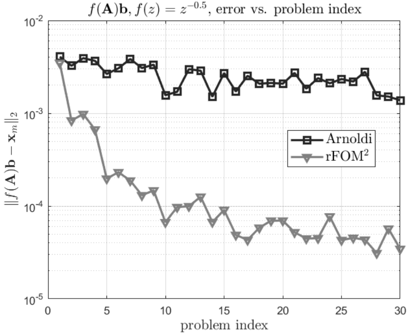
$$\overline{\mathbf{G}}_j^* \widehat{\mathbf{W}}_{j+1}^* \widehat{\mathbf{W}}_{j+1} \overline{\mathbf{G}}_j \mathbf{g}_i = \theta_i \overline{\mathbf{G}}_j^* \widehat{\mathbf{W}}_{j+1}^* \widehat{\mathbf{V}}_j \mathbf{g}_i,$$

where $\widehat{\mathbf{W}}_{j+1} = \begin{bmatrix} \mathbf{C} & \mathbf{V}_{j+1} \end{bmatrix}$ and $\overline{\mathbf{G}}_j := \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \overline{\mathbf{H}}_j \end{bmatrix}, \mathbf{D} \in \mathbb{C}^{k \times k}$.

Results



(a)



(b)

Figure – Recycling with $\epsilon = 0$ and $\epsilon = 10^{-3}$, $j = 50$ Arnoldi iterations, recycle subspace dimension of size $k = 20$ and $n_{quad} = 30$.

Thank You!