CTAC2010, Uni. of NSW, 28th Nov – 1st Dec 2010

Some results relating to Krylov subspace approximation of the matrix function $\varphi(\mathbf{A})\mathbf{b} = \mathbf{A}^{-1}(e^{\mathbf{A}} - \mathbf{I})\mathbf{b}$.

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Motivation

Initial value problem

- System of nonlinear differential equations

$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{g}(\boldsymbol{u}); \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0 \in \mathbb{R}^N$$

  where $\boldsymbol{g} : \mathbb{R}^N \to \mathbb{R}^N$.

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- For stiff problems, the Backward Differentiation Formulae (BDF) are currently the state-of-the-art techniques.

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  exactly to obtain

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \tau\varphi(\tau\boldsymbol{J}_n)\boldsymbol{g}_n.$$

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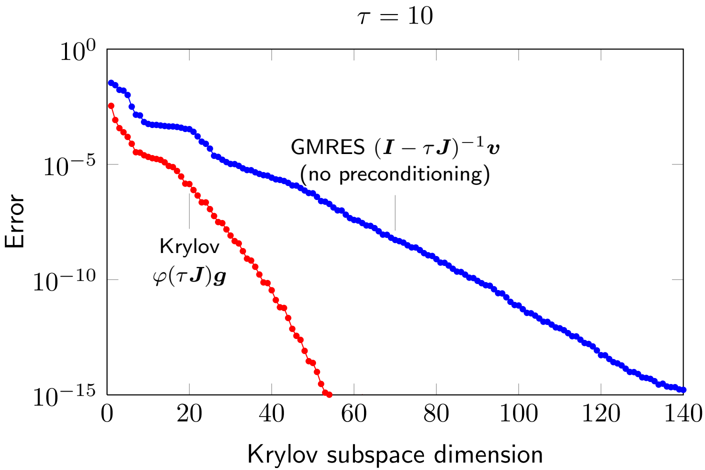
- Allow for a large integration stepsize (comparable to BDF)
- Krylov subspace methods to $\varphi(\tau\boldsymbol{J})\boldsymbol{g}$ converge substantially faster than those for shifted linear systems of the form $(\boldsymbol{I} - \tau\boldsymbol{J})^{-1}\boldsymbol{v}$.

Motivation



$\tau = 10$
10^{0}
10^{-5}
10^{-10}
10^{-15}
Error
0
20
40
60
80
100
120
140
Krylov subspace dimension
GMRES $(\boldsymbol{I} - \tau\boldsymbol{J})^{-1}\boldsymbol{v}$
(no preconditioning)
Krylov
$\varphi(\tau\boldsymbol{J})\boldsymbol{g}$

Krylov approximation of $\varphi(t\boldsymbol{A})\boldsymbol{b}$

To extract an approximation from

$$\mathcal{K}_m(\boldsymbol{A}, \boldsymbol{b}) = \text{span}\left\{\boldsymbol{b}, \boldsymbol{A}\boldsymbol{b}, \ldots, \boldsymbol{A}^{m-1}\boldsymbol{b}\right\} \subseteq \mathbb{R}^N,$$

Arnoldi's method is used to construct an orthonormal basis $\boldsymbol{V}_m = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m]$, which satisfies

$$\boldsymbol{A}\boldsymbol{V}_m = \boldsymbol{V}_m\boldsymbol{H}_m + \beta_m \boldsymbol{v}_{m+1}\boldsymbol{e}_m^T.$$

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The Krylov approximant takes the form

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$$\varphi(t\boldsymbol{A})\boldsymbol{b} = \beta_0 \varphi(t\boldsymbol{A})\boldsymbol{V}_m\boldsymbol{e}_1 \approx \beta_0 \boldsymbol{V}_m \varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1.$$

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The Krylov approximant takes the form

$$\varphi(t\boldsymbol{A})\boldsymbol{b} = \beta_0\varphi(t\boldsymbol{A})\boldsymbol{V}_m\boldsymbol{e}_1 \approx \beta_0\boldsymbol{V}_m\varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1.$$

Problem statement: How do we know when $\beta_0\boldsymbol{V}_m\varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1$ is a sufficiently accurate approximation to $\varphi(t\boldsymbol{A})\boldsymbol{b}$?

Error representation

Since $\varphi(\zeta) = (e^{\zeta} - 1)/\zeta$, $\zeta \in \mathbb{C}$ is analytic everywhere

$$\varphi(t\boldsymbol{A}) = \frac{1}{2\pi i} \oint_{\Gamma} \varphi(\zeta)(\zeta \boldsymbol{I} - t\boldsymbol{A})^{-1} \, d\zeta,$$

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where Γ encloses $\sigma(t\boldsymbol{A})$. Hence,

$$\begin{aligned}
\boldsymbol{\varepsilon}_m &= \varphi(t\boldsymbol{A})\boldsymbol{b} - \beta_0 \boldsymbol{V}_m \varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1 \\
&= \frac{1}{2\pi i} \oint_{\Gamma} \varphi(\zeta) \Big\{ (\zeta \boldsymbol{I} - t\boldsymbol{A})^{-1}\boldsymbol{b} - \beta_0 \boldsymbol{V}_m (\zeta \boldsymbol{I} - t\boldsymbol{H}_m)^{-1} \boldsymbol{e}_1 \Big\} \, d\zeta \\
&= \frac{1}{2\pi i} \oint_{\Gamma} \varphi(\zeta) \boldsymbol{\varepsilon}_m(\zeta) \, d\zeta,
\end{aligned}$$

where Γ encloses both $\sigma(t\boldsymbol{A})$ and $\sigma(t\boldsymbol{H}_m)$ and $\boldsymbol{\varepsilon}_m(\zeta)$ is the exact error associated with the FOM approximation to $(\zeta \boldsymbol{I} - t\boldsymbol{A})^{-1}\boldsymbol{b}$.

Error estimate

[Hochbruck *et al.*, 1998] Using the integral representation

$$\boldsymbol{\varepsilon}_m = \frac{1}{2\pi i}\int_\Gamma \varphi(\zeta)\boldsymbol{\varepsilon}_m(\zeta)\,d\zeta,$$

approximate $\boldsymbol{\varepsilon}_m(\zeta)$ by $\boldsymbol{r}_m(\zeta) = \beta_0\beta_m \boldsymbol{e}_m^T(\zeta\boldsymbol{I} - t\boldsymbol{H}_m)^{-1}\boldsymbol{e}_1\boldsymbol{v}_{m+1}$

$$\boldsymbol{\varepsilon}_m \approx \frac{1}{2\pi i}\int_\Gamma \varphi(\zeta)\boldsymbol{r}_m(\zeta)\,d\zeta$$

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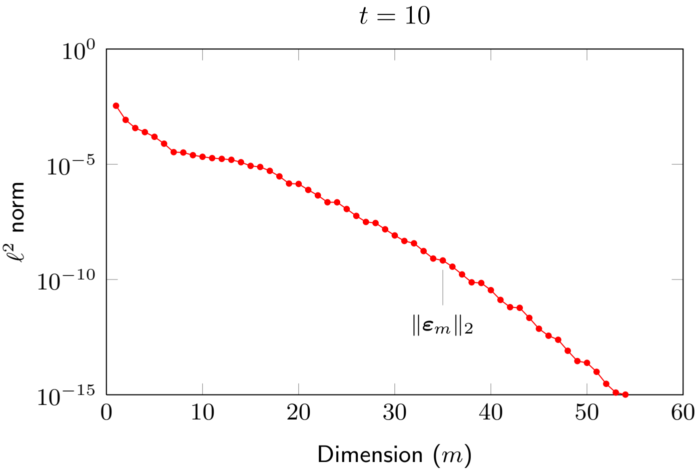
Taking norms:

$$\left\|\boldsymbol{\varepsilon}_m\right\|_2 \approx t\beta_0\beta_m\left|\boldsymbol{e}_m^T\varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1\right|.$$

Performance of Error estimate



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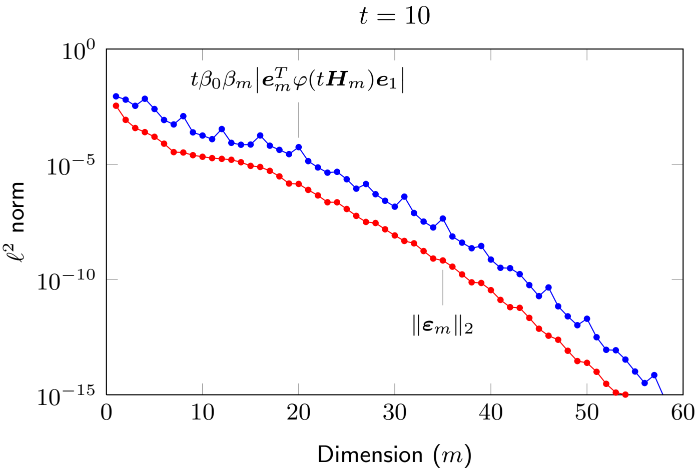
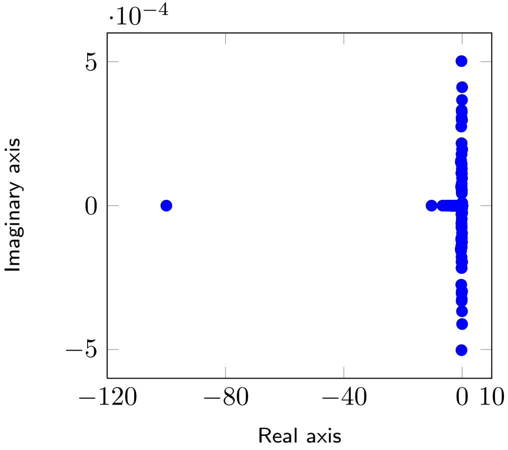


Spectrum of A



Error bound

Suppose $\boldsymbol{A}$ and $\boldsymbol{H}_m$ are diagonalisable such that:

$$\begin{aligned} \boldsymbol{A}\boldsymbol{P} &= \boldsymbol{P}\boldsymbol{D}; & \boldsymbol{D} &= \mathsf{diag}\{\lambda_j, j = 1, \ldots, N\} \\ \boldsymbol{H}_m\boldsymbol{Y}_m &= \boldsymbol{Y}_m\boldsymbol{\Lambda}_m; & \boldsymbol{\Lambda}_m &= \mathsf{diag}\{\mu_i, i = 1, \ldots, m\}, \end{aligned}$$

and $\lambda_{\max} = \mathsf{max}\,\{\mathrm{Re}(\lambda_j)\}$.

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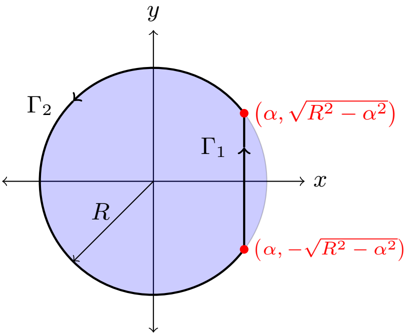
and $\lambda_{\max} = \max\{\mathrm{Re}(\lambda_j)\}$. For α positive and $\alpha > t\lambda_{\max}$

$$\left\|\boldsymbol{\varepsilon}_m\right\|_2 \le \mathcal{C}_\alpha(m)\left\|\boldsymbol{r}_m(\alpha)\right\|_2,$$

where $\boldsymbol{r}_m(\alpha)$ is the residual error associated with the FOM approximation to $(\alpha\boldsymbol{I} - t\boldsymbol{A})^{-1}\boldsymbol{b}$ and

$$\mathcal{C}_\alpha(m) = \frac{k_2(\boldsymbol{P})(e^\alpha + 1)}{2\sqrt{\alpha(\alpha - t\lambda_{\max})}}\sqrt{\prod_{i=1}^{m}\left[1 + \left(\frac{t\mathrm{Im}(\mu_i)}{\alpha - t\mathrm{Re}(\mu_i)}\right)^2\right]}.$$

Sketch of proof



$$\Gamma_1: \quad \zeta = \alpha + iy; \quad -\sqrt{R^2 - \alpha^2} \leq y \leq \sqrt{R^2 - \alpha^2}$$

$$\Gamma_2: \quad \zeta = Re^{i\theta}; \quad \arccos\left(\frac{\alpha}{R}\right) \leq \theta \leq 2\pi - \arccos\left(\frac{\alpha}{R}\right)$$

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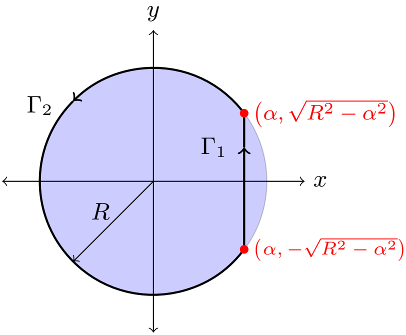

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Taking the limit as $R \to \infty$

$$\boldsymbol{\varepsilon}_m = \frac{1}{2\pi} \int_{-\infty}^{\infty} \varphi(\alpha + iy)((\alpha + iy)\boldsymbol{I} - t\boldsymbol{A})^{-1} \boldsymbol{r}_m(\alpha + iy)\, dy$$

Sketch of proof

Taking norms:

$$\left\|\boldsymbol{\varepsilon}_m\right\|_2 \leq \frac{1}{2\pi}\int_{-\infty}^{\infty}\left|\varphi(\alpha+iy)\right|\left\|((\alpha+iy)\boldsymbol{I}-t\boldsymbol{A})^{-1}\right\|_2\left\|\boldsymbol{r}_m(\alpha+iy)\right\|_2 dy$$

and using the results:

$$\left\|((\alpha+iy)\boldsymbol{I}-t\boldsymbol{A})^{-1}\right\|_2 \leq k_2(\boldsymbol{P}) \max_{1\leq j\leq N} \frac{1}{\sqrt{(\alpha-t\mathrm{Re}(\lambda_j))^2+(y-t\mathrm{Im}(\lambda_j))^2}}$$

$$\begin{aligned}\left\|\boldsymbol{r}_m(\alpha+iy)\right\|_2^2 &= \prod_{i=1}^{m}\frac{\left|\alpha-t\mu_i\right|}{\left|\alpha+iy-t\mu_i\right|}\left\|\boldsymbol{r}_m(\alpha)\right\|_2^2 \\ &\leq \prod_{i=1}^{m}\left[1+\left(\frac{t\mathrm{Im}(\mu_i)}{\alpha-t\mathrm{Re}(\mu_i)}\right)^2\right]\left\|\boldsymbol{r}_m(\alpha)\right\|_2^2\end{aligned}$$

Sketch of Proof

End up with an integral of the form

$$I = \int_{-\infty}^{\infty} \frac{\left|\varphi(\alpha + iy)\right|}{\sqrt{(\alpha - t\mathrm{Re}(\lambda_j))^2 + (y - t\mathrm{Im}(\lambda_j))^2}}\, dy.$$

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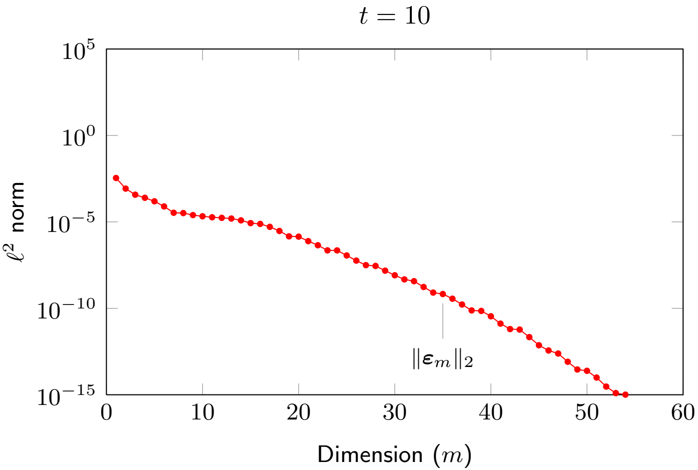
which can be bounded above using the Cauchy-Schwarz Inequality. ■

Performance of Error bound



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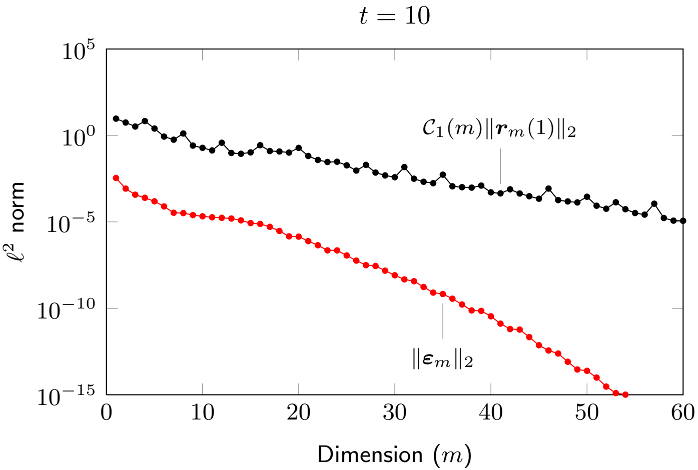

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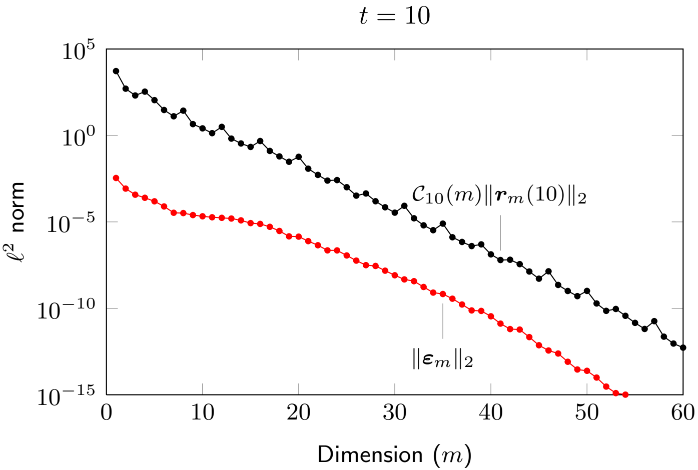

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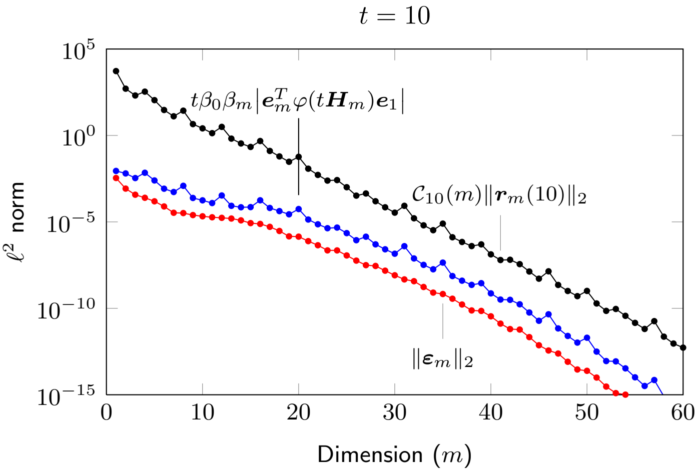

Concept of a Differential Equation Residual

Relies on the fact that $\boldsymbol{x}(t) = \boldsymbol{A}^{-1}(e^{t\boldsymbol{A}} - \boldsymbol{I})\boldsymbol{b} = t\varphi(t\boldsymbol{A})\boldsymbol{b}$ exactly satisfies

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}.$$

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Let $\boldsymbol{x}_m(t) = t\beta_0 \boldsymbol{V}_m \varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1$ and define the "residual"

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&= \boldsymbol{b} + t\boldsymbol{A}\beta_0 \boldsymbol{V}_m \varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1 - \beta_0 \boldsymbol{V}_m e^{t\boldsymbol{H}_m}\boldsymbol{e}_1 \\
&= t\beta_0(\boldsymbol{A}\boldsymbol{V}_m - \boldsymbol{V}_m\boldsymbol{H}_m)\varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1 \\
&= t\beta_0\beta_m \boldsymbol{e}_m^T \varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1 \boldsymbol{v}_{m+1}.
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&= t\beta_0(\boldsymbol{A}\boldsymbol{V}_m - \boldsymbol{V}_m\boldsymbol{H}_m)\varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1 \\
&= t\beta_0\beta_m \boldsymbol{e}_m^T \varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1 \boldsymbol{v}_{m+1}.
\end{aligned}$$

which reproduces the result of Hochbruck *et al.* (1998).

Minimal residual approach

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&= \boldsymbol{b} + \boldsymbol{A}\boldsymbol{V}_m\boldsymbol{y}_m - \boldsymbol{V}_m\frac{d\boldsymbol{y}_m}{dt} \\
&= \boldsymbol{V}_{m+1}\left[\beta_0\boldsymbol{e}_1 + \overline{\boldsymbol{H}}_m\boldsymbol{y}_m - \begin{pmatrix}\boldsymbol{I}_m \\ \mathbf{0}^T\end{pmatrix}\frac{d\boldsymbol{y}_m}{dt}\right]
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\end{aligned}$$

Hence, minimiser:

$$\boldsymbol{y}_m = \arg\min_{\boldsymbol{y}\in\mathbb{R}^m}\left\|\beta_0\boldsymbol{e}_1 + \overline{\boldsymbol{H}}_m\boldsymbol{y} - \begin{pmatrix}\boldsymbol{I}_m \\ \boldsymbol{0}^T\end{pmatrix}\frac{d\boldsymbol{y}}{dt}\right\|_2.$$

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Assume $\boldsymbol{x}_m = \boldsymbol{V}_m \boldsymbol{y}_m(t)$

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&= \boldsymbol{b} + \boldsymbol{A}\boldsymbol{V}_m \boldsymbol{y}_m - \boldsymbol{V}_m \frac{d\boldsymbol{y}_m}{dt} \\
&= \boldsymbol{V}_{m+1} \left[\beta_0 \boldsymbol{e}_1 + \overline{\boldsymbol{H}}_m \boldsymbol{y}_m - \begin{pmatrix} \boldsymbol{I}_m \\ \boldsymbol{0}^T \end{pmatrix} \frac{d\boldsymbol{y}_m}{dt} \right]
\end{aligned}$$

Hence, minimiser:

$$\boldsymbol{y}_m = \arg \min_{\boldsymbol{y} \in \mathbb{R}^m} \left\| \beta_0 \boldsymbol{e}_1 + \overline{\boldsymbol{H}}_m \boldsymbol{y} - \begin{pmatrix} \boldsymbol{I}_m \\ \boldsymbol{0}^T \end{pmatrix} \frac{d\boldsymbol{y}}{dt} \right\|_2 .$$

But how do we minimise such an expression?

Petrov-Galerkin approach

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and the approximation

$$\varphi(t\boldsymbol{A})\boldsymbol{b} \approx \beta_0 \boldsymbol{V}_m \varphi(t\boldsymbol{\mathcal{H}}_m)\boldsymbol{e}_1; \quad \boldsymbol{\mathcal{H}}_m = \boldsymbol{H}_m + \beta_m^2 \boldsymbol{H}_m^{-T} \boldsymbol{e}_m \boldsymbol{e}_m^T.$$

Ritz-Galerkin approach

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$$\boldsymbol{V}_m^T \left(\boldsymbol{b} + \boldsymbol{A}\boldsymbol{x}_m - \frac{d\boldsymbol{x}_m}{dt} \right) = \boldsymbol{0}$$

$$\boldsymbol{V}_m^T \left(\boldsymbol{b} + \boldsymbol{A}\boldsymbol{V}_m \boldsymbol{y}_m - \boldsymbol{V}_m \frac{d\boldsymbol{y}_m}{dt} \right) = \boldsymbol{0},$$

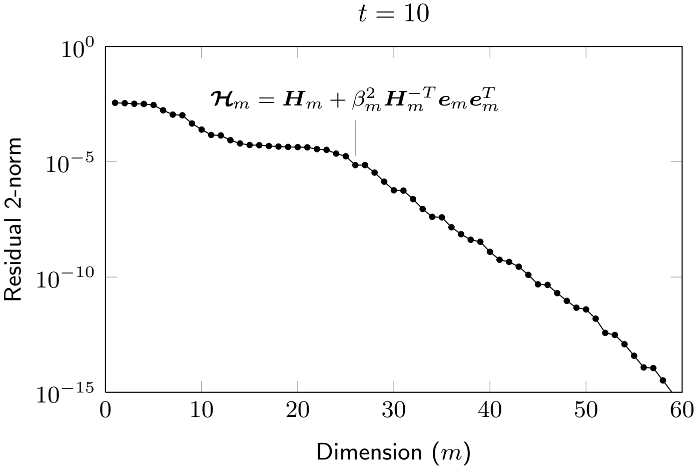
which leads to

$$\frac{d\boldsymbol{y}_m}{dt} = \boldsymbol{H}_m \boldsymbol{y}_m + \beta_0 \boldsymbol{e}_1,$$

and the standard Krylov approximation

$$\varphi(t\boldsymbol{A})\boldsymbol{b} \approx \beta_0 \boldsymbol{V}_m \varphi(t\boldsymbol{H}_m)\boldsymbol{e}_1.$$

Comparison of Residuals



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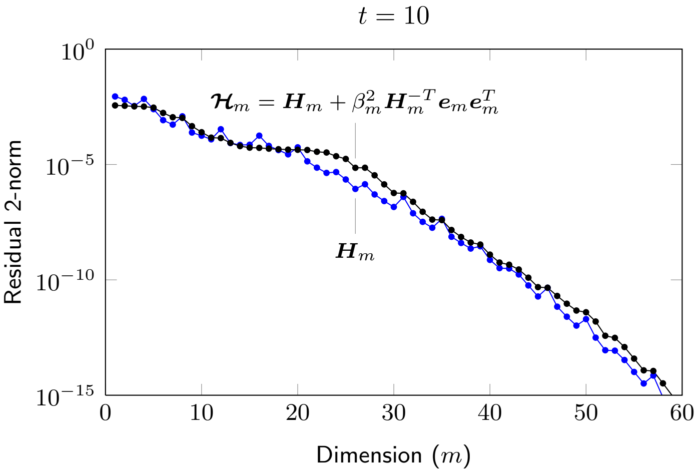

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Thank you for listening!