Matrix exponentials and normalized numerical range

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Consider ODE system, constant coefficients

\[ u' + Au = f, \quad A \in \mathbb{C}^{n \times n} \]

\[ \ldots \text{ matrix exponential } e^{-tA} \]

Dissipative case: \(-A\) dissipative, i.e., \(A\) accretive:

\[ \Re \langle Au, u \rangle \geq 0 \quad \forall u \in \mathbb{C}^n \quad \Leftrightarrow \quad \|e^{-tA}\| \leq 1 \quad \forall t > 0 \]

\[ \ldots \text{ equivalent to resolvent condition} \]

\[ \| (zI - A)^{-1} \| \leq \frac{1}{\Re z} \quad \forall z : \Re z < 0 \]

? What about

\[ \|e^{-tA}\| \leq C \quad \forall t > 0 \quad (C > 1) \quad ? \]
Kreiss matrix theorem, exponential version

Kreiss resolvent condition:

\[ \|(zI - A)^{-1}\| \leq \frac{K}{\text{Re} \, z} \quad \forall \, z : \text{Re} \, z < 0, \]

with \( K > 1 \), is equivalent to uniformly bounded matrix exponential,

\[ \|e^{-tA}\| \leq enK \quad \forall \, t > 0 \]

= quantitative criterion, similar as in classical KMT (characterization of \( \|A^n\| \leq C \)).

Our concern: What is the natural generalization of the notion of accretivity (special case \( K = 1 \)) in the general case \( K > 1 \) ?
Accretivity and [normalized] numerical range $\mathcal{R}_{[N]}(A)$

- **Numerical range** $\mathcal{R}(A)$:
  $$\mathcal{R}(A) := \left\{ \frac{\langle Au, u \rangle}{\langle u, u \rangle} : 0 \neq u \in \mathbb{C}^n \right\}$$

- **Accretivity of** $A$ **is equivalent to**
  $$\mathcal{R}(A) \subseteq \mathbb{C}^+ = \{ z : \Re z \geq 0 \}$$

- **Now consider** normalized numerical range $\mathcal{R}_{N}(A)$:
  $$\mathcal{R}_{N}(A) := \left\{ \frac{\langle Au, u \rangle}{\|Au\| \|u\|} : u \in \mathbb{C}^n, Au \neq 0 \right\}$$

  ... subset of the complex unit circle
  (Cauchy-Schwarz inequality for $u, Au$)
Accretivity and normalized numerical range $\mathcal{R}_N(A)$

- Accretivity of $A$ is equivalent to
  \[ \mathcal{R}_N(A) \subseteq \mathcal{M}_1 := \{ z : |z| \leq 1, \, \text{Re} z \geq 0 \} \]

- The set $\mathcal{M}_1$ (half moon):

- ... equivalent to resolvent condition
  \[ \| (zI - A)^{-1} \| \leq \frac{1}{\text{Re} z} \quad \forall z : \text{Re} z < 0 \]
Kreiss resolvent condition expressed via $\mathcal{R}_N(A)$

- Proposition ‘M’: Resolvent estimate in exponential KMT,

$$\|(zI - A)^{-1}\| \leq \frac{K}{\text{Re} \, z} \quad \forall \, z : \text{Re} \, z < 0,$$

with $K > 1$, is equivalent to $\mathcal{R}_N(A) \subseteq \mathcal{M}_K$

- The moon-shaped set $\mathcal{M}_K$:

- Note: $\kappa = \kappa(K) = \sqrt{1 - K^{-2}}$

Idea of proof:

- Rewrite resolvent condition as

\[ \|zu - Au\|^2 \geq \frac{(\text{Re } z)^2}{K^2} \quad \forall z : \text{Re } z < 0, \quad \forall u \in \mathbb{C}^n \]

- For arbitrary (fixed) \( u \in \mathbb{C}^n \): Determine

\[ z^* := \text{arg min}_{\text{Re } z < 0} \phi(z; u) \]

where

\[ \phi(z; u) := \|zu - Au\|^2 - \frac{(\text{Re } z)^2}{K^2} \]

- Evaluate the inequality \( \phi(z^*; u) \geq 0 \)

\( \Rightarrow \) ‘moon condition’ involving \( \mathcal{R}_N(A) \) \( \square \)
Sectorial operators

Classical definition (Hilbert space setting):

\[ A \text{ sectorial} \iff \mathcal{R}(A) \subseteq S_\sigma \]

where \( S_\sigma \) = sector in \( \mathbb{C}^+ \):

Typical example:

[Spatial discretization of] parabolic PDE
Sectorial property and $\mathcal{R}_N(A)$

- Sectorial property of $A$ is equivalent to
  $$\mathcal{R}_N(A) \subseteq A_{\sigma,1} := \{ z : |z| \leq 1, |\text{Arg } z| \leq \sigma \}$$

- The set $A_{\sigma,1}$:

- ... equivalent to resolvent condition
  $$\|(zI - A)^{-1}\| \leq \frac{1}{\text{dist}(z, \mathcal{S}_\sigma)} \quad \forall \; z \notin \mathcal{S}_\sigma,$$
Sectorial operators (2)

Consider linear operators $A$ satisfying resolvent estimate

$$
\|(zI - A)^{-1}\| \leq \frac{K}{\text{dist}(z, S_\sigma)} \quad \forall z \notin S_\sigma,
$$

with $K > 1$

- ... = general sector condition
- ... $A$ not accretive in general, but shares most properties of conventional sectorial operators (smoothing behavior)

Numerical analysis of time integration methods for $u' + Au = f$ is strongly based on resolvent estimate

... value of $K$ not essential
Proposition ‘A’: Resolvent estimate in general sectorial property,

\[ \| (zI - A)^{-1} \| \leq \frac{K}{\text{dist}(z, S_{\sigma})} \quad \forall \ z \notin S_{\sigma}, \]

with \( K > 1 \), is equivalent to \( \mathcal{R}_N(A) \subseteq \mathcal{A}_{\sigma,K} \).

The axe-shaped set \( \mathcal{A}_{\sigma,K} \):

Note: \( \kappa = \kappa(K) = \sqrt{1 - K^{-2}} \)
Proof of Proposition ‘A’ (Auzinger (2003)) : extension of above proof for Proposition ‘M’

... strengthened Cauchy-Schwarz inequality valid for all pairs \( u, Au \) \( u \in \mathbb{C}^n \)

Numerical calculation of \( R_N(A) \) (Auzinger (2003)) : generalization of the procedure given in Gustafson & Rao (1991) for \( R(A) \) (scan boundary); more expensive in general

Results extend to general Hilbert space context

Example to follow: Spatial discretization of convection/diffusion operator

\[-u'' - \beta u'\]

with downstream BDF2 formula for first derivative
Example 1: $\beta = 1.0$

$$A_1 = \begin{pmatrix} 1.00 & -1.00 \\ 1.00 & 0.50 & -1.00 \\ -0.50 & 1.00 & 0.50 & -1.00 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -0.50 & 1.00 & 0.50 & \end{pmatrix}$$

$\mathcal{R}(A_1)$, eigenvalues:

$(A_1$ is sectorial in conventional sense, $K = 1$)
Example 2: $\beta = 1.1$

$$A_2 = \begin{pmatrix}
0.90 & -1.00 \\
1.20 & 0.35 & -1.00 \\
-0.55 & 1.20 & 0.35 & -1.00 \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & -1.00 \\
-0.55 & 1.20 & 0.35 \\
\end{pmatrix}$$

$\mathcal{R}(A_2)$, eigenvalues:

$(A_2$ is $not$ sectorial in conventional sense)
Example 2 (continued)

Inclusion for $\mathcal{R}_N(A_2)$:

$\Rightarrow A_2$ is sectorial, $K > 1$
Numerical range $\mathcal{R}(A)$:
Important object in stability theory for matrix exponentials, matrix powers, . . .

Criteria involving $\mathcal{R}(A)$ are usually equivalent to certain resolvent estimates valid outside $\mathcal{R}(A)$

(Generalized) resolvent estimates can be rewritten as certain strengthened Cauchy-Schwarz inequalities valid for all pairs $u, Au$ ($u \in \mathbb{C}^n$)

These involve $\langle Au, u \rangle / \langle u, u \rangle$ as well as $\|Au\|/\|u\|$

This talk: Consider $\mathcal{R}_N(A)$ instead of $\mathcal{R}(A)$
Other example: Classical **Kreiss Matrix Theorem** characterizing bounded matrix powers, $\|A^\nu\| \leq C$:

Kreiss resolvent condition is again equivalent to a strengthened Cauchy-Schwarz inequality (Auzinger & Kirlinger (1995))

- ... useful for numerical investigations
- ? useful ? for theoretical investigations (?)
- Questions worth studying:
  - Other resolvent conditions
  - Connection with pseudospectra
References

[1] W. Auzinger, G. Kirlinger,
Kreiss resolvent conditions and strengthened Cauchy-Schwarz inequalities,

[2] W. Auzinger,
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