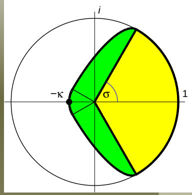

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Matrix exponentials and normalized numerical range

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Contents

Introduction

- Consider ODE system, constant coefficients

$$u' + Au = f, \qquad A \in \mathbb{C}^{n\times n}$$

. . . matrix exponential e^{-tA}

- Dissipative case: $-A$ dissipative, i.e., A accretive:

$$\text{Re}\,\langle Au, u\rangle \ge 0 \quad \forall\, u \in \mathbb{C}^n \qquad \Leftrightarrow \qquad \|e^{-tA}\| \le 1 \quad \forall\, t > 0$$

- . . . equivalent to resolvent condition

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

- ? What about

$$\|e^{-tA}\| \le C \quad \forall\, t > 0 \quad (C > 1) \quad \textbf{?}$$

Kreiss matrix theorem, exponential version

- Kreiss resolvent condition:

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

- 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 $\|A^\nu\| \leq C$).
- 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

$$\mathcal{R}(A) \subseteq \mathbb{C}^+ \; = \; \{ z : \; \text{Re}\, z \geq 0 \}$$

- 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

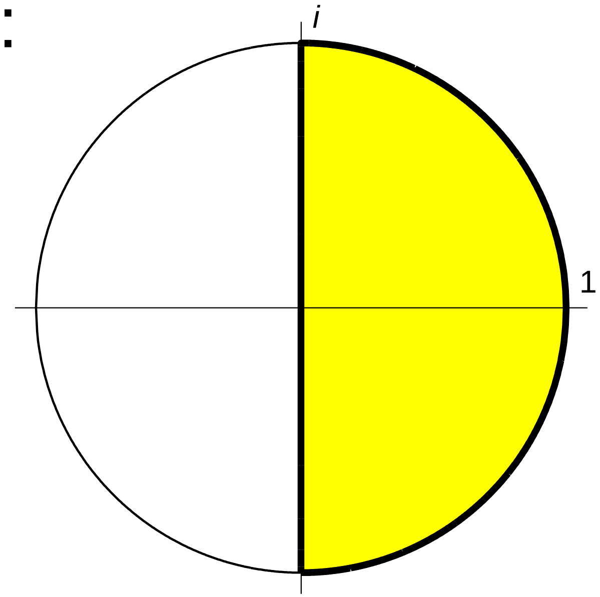
  (Cauchy-Schwarz inequality for u, Au)

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

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

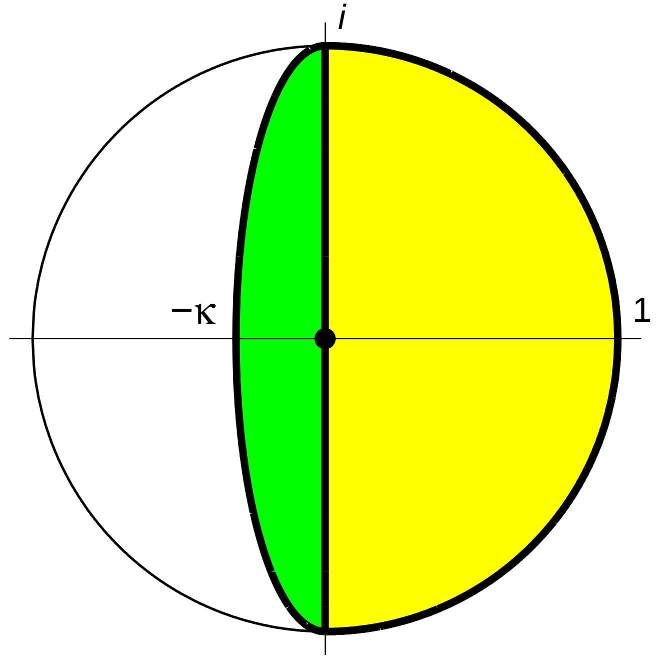
Kreiss resolvent condition expressed via $\mathcal{R}_N(A)$

- Proposition 'M' :
  Resolvent estimate in exponential KMT,

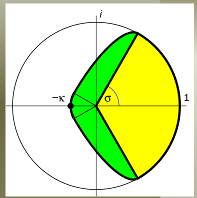
$$\|(zI - A)^{-1}\| \le \frac{K}{\mathrm{Re}\, z} \qquad \forall\, z : \ \mathrm{Re}\, z < 0,$$

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

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



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



Proof of Proposition ‘M’: Auzinger & Kirlinger (1995)

Idea of proof:

- Rewrite resolvent condition as

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

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

$$z^* := \operatorname{arg\,min}_{\mathrm{Re}\, z<0} \phi(z;u)$$

  where

$$\phi(z;u) := \|zu - Au\|^2 - \frac{(\mathrm{Re}\, z)^2}{K^2}$$

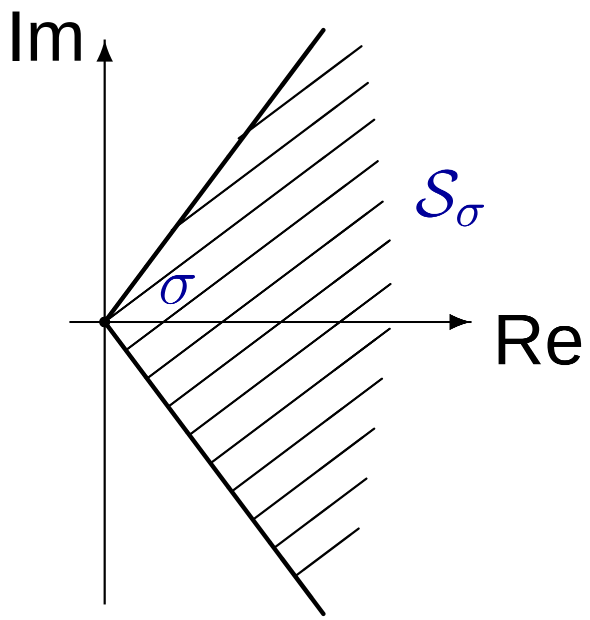
- Evaluate the inequality $\phi(z^*;u) \geq 0$
- $\Rightarrow$ ‘moon condition’ involving $\mathcal{R}_N(A)$ $\square$

Sectorial operators

- Classical definition (Hilbert space setting):

$$A \text{ sectorial } :\Longleftrightarrow \mathcal{R}(A) \subseteq \mathcal{S}_\sigma$$

where $\mathcal{S}_\sigma$ = sector in $\mathbb{C}^+$:



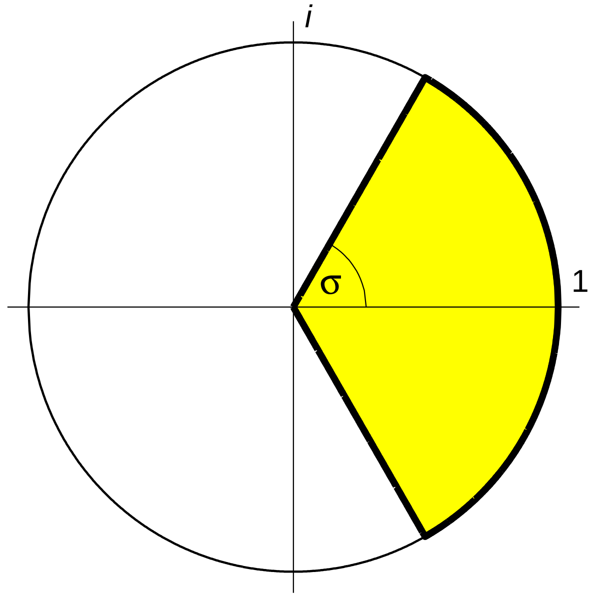
- Typical example:
  [Spatial discretization of] parabolic PDE

Sectorial property and $\mathcal{R}_N(A)$

- Sectorial property of of A is equivalent to

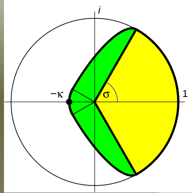
$$\mathcal{R}_N(A) \subseteq \mathcal{A}_{\sigma,1} := \{z : \ |z| \leq 1, \ |\text{Arg}\, z| \leq \sigma\}$$

- The set $\mathcal{A}_{\sigma,1}$:



- . . . equivalent to resolvent condition

$$\|(zI - A)^{-1}\| \leq \frac{1}{\text{dist}(z, \mathcal{S}_\sigma)} \qquad \forall\ z \notin \mathcal{S}_\sigma,$$



Sectorial operators (2)

- Consider linear operators A satisfying resolvent estimate

$$\|(zI - A)^{-1}\| \leq \frac{K}{\text{dist}(z, \mathcal{S}_\sigma)} \qquad \forall\, z \notin \mathcal{S}_\sigma,$$

  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

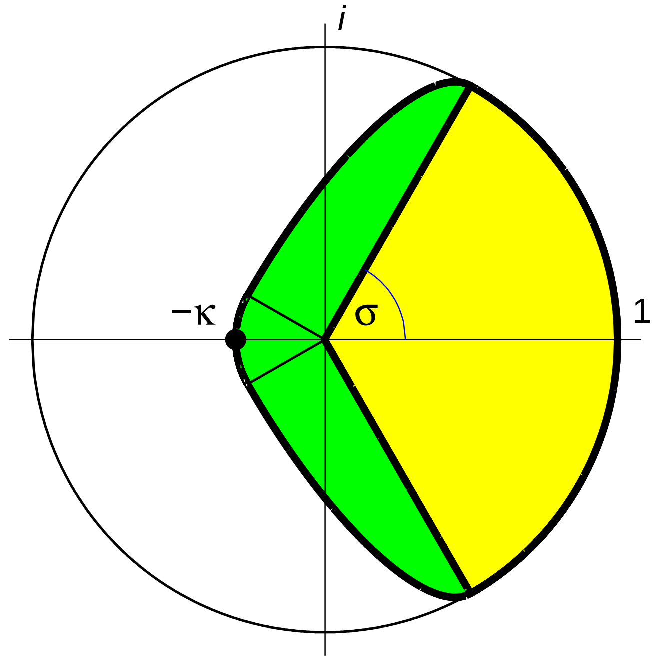
General sector condition expressed via $\mathcal{R}_N(A)$

- Proposition 'A':
  Resolvent estimate in general sectorial property,

$$\|(zI - A)^{-1}\| \leq \frac{K}{\mathrm{dist}(z, \mathcal{S}_\sigma)} \qquad \forall\, z \notin \mathcal{S}_\sigma,$$

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

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



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

Remarks

- 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 $\mathcal{R}_N(A)$ (Auzinger (2003)) : generalization of the procedure given in Gustafson & Rao (1991) for $\mathcal{R}(A)$ (scan boundary); more expensive in general
- Results extend to general Hilbert space context
- Example to follow: Spatial discretization of convection/diffusion operator

$$-u'' - \beta\, u'$$

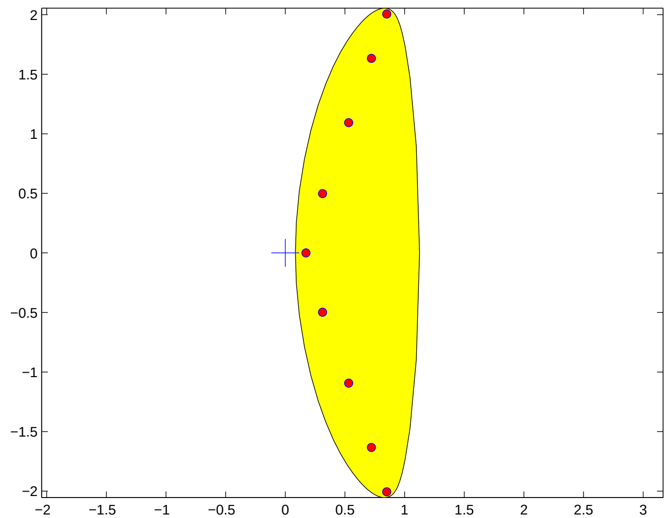
with downstream BDF2 formula for first derivative

Example 1: $\beta = 1.0$

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

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

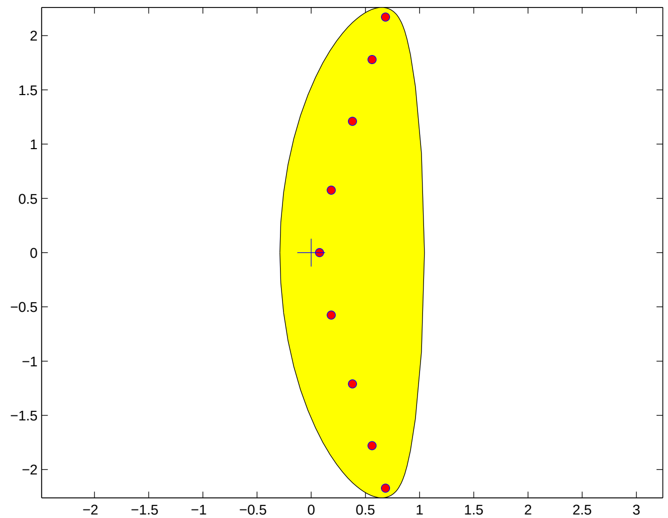
(A_1 is sectorial in conventional sense, $K = 1$)



Example 2: $\beta = 1.1$

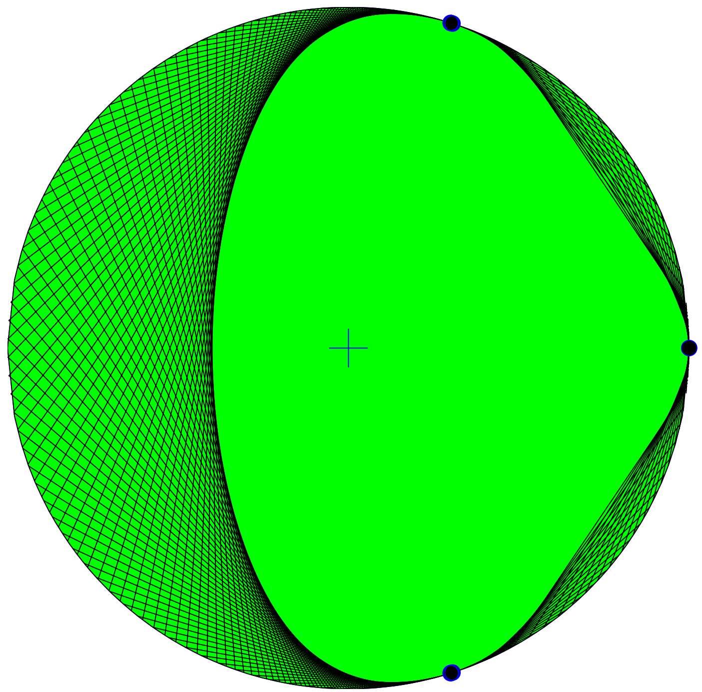
$$A_2 = \begin{pmatrix} 0.90 & -1.00 & & & & \\ 1.20 & 0.35 & -1.00 & & & \\ -0.55 & 1.20 & 0.35 & -1.00 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & -1.00 \\ & & & -0.55 & 1.20 & 0.35 \end{pmatrix}$$

$\mathcal{R}(A_2)$, eigenvalues:
(A_2 is *not* sectorial in conventional sense)



Example 2 (continued)

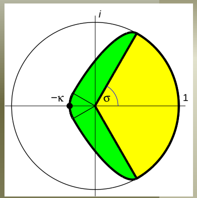
Inclusion for $\mathcal{R}_{\mathcal{N}}(A_2)$:



$\Rightarrow \quad A_2$ is sectorial, $K > 1$

Conclusion (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 $\mathcal{R}_{\mathcal{N}}(A)$ instead of $\mathcal{R}(A)$



Conclusion (2)

- 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

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