Interval Matrix Exponentiation

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Simulation of Linear ODE

From Linear ODE to Matrix Exponentiation

- $x'(t) = Ax(t)$

$\Rightarrow$ $x''(t) = (Ax(t))' = A^2x(t)$, and by induction $x^{(n)}(t) = A^n x(t)$

- Taylor expansion:

$$x(t) = x_0 + (tA)x_0 + \frac{(tA)^2 x_0}{2} + \frac{(tA)^3 x_0}{3!} + \cdots = (\exp tA)x_0$$

Matrix Exponentiation

- Truncated Taylor or Padé expansion computed in double precision
  - $||A||$ too large $\Rightarrow$ high expansion order
  - Idea: $\exp(A) = \exp(A/2^s)^{2^s}$
  - Scaling and Squaring: $\exp(A) = \left(\cdots\left(\left(r_m(A/2^s)\right)^2\right)^2\cdots\right)^2$
- Issue: Find s and m
  - Lower computational cost
  - Improve precision

Simulation of Uncertain Linear ODE

Uncertain Linear ODE

- $x'(t) = Ax(t)$ with $A \in \mathbf{A}$

$\Rightarrow$ $x(t) \in \{(\exp A)\, x_0 : A \in \mathbf{A}\}$

Interval Matrix Exponentiation

- $\exp \mathbf{A} := \square\{\exp A : A \in \mathbf{A}\} \in \mathbb{IR}^{n\times n}$

$\Rightarrow$ $x(t) \in (\exp \mathbf{A})\, x_0$

- Issue: sharp enclosure of $\exp \mathbf{A}$

Pessimism in Taylor Series Interval Evaluation

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 0 & [-3,-2] \end{pmatrix} \quad \exp \mathbf{A} \approx \begin{pmatrix} 1 & [0.31, 0.44] \\ 0 & [0.04, 0.14] \end{pmatrix} \quad \mathbf{T}_{10} \approx \begin{pmatrix} 1 & [-1.21, 1.96] \\ 0 & [-6.26, 6.45] \end{pmatrix}$$

Interval Matrix Exponentiation

Issue

- Sharp enclosure of $\exp \mathbf{A}$
- Taylor expansion of $\exp A \rightarrow$ heavy multi-occurrences of variables a_{ij}

$\neq$ Issue wrt matrix exponentiation in numerical analysis

Outline

1. NP-hardness
2. Polynomial Algorithms
3. Experiments
4. Experiments

Outline

ϵ-Accurate Enclosures

Definition

- Let $\mathbb{A} \subseteq \mathbb{R}^{n \times m}$ and $\mathbf{A} = \Box\mathbb{A} \in \mathbb{IR}^{n \times m}$
- $\mathbf{B} \in \mathbb{IR}^{n \times m}$ is an ϵ-enclosure of $\mathbb{A}$ iff $\mathbf{B} \supseteq \mathbb{A}$ and

$$\max\{ \max_{ij} |\underline{a}_{ij} - \underline{b}_{ij}| \ , \ \max_{ij} |\overline{a}_{ij} - \overline{b}_{ij}| \ \} \ \leq \ \epsilon$$

- Idem for sets of reals, sets of vectors

Central Result

- Computing ϵ-accurate enclosure of the range over a box of a bilinear function is NP-hard
  (nonconvex quadratic programming is NP-hard)

ϵ-Accurate Interval Matrix Exponential Enclosure

Theorem

Computing an ϵ-accurate enclosure of the interval matrix exponential is NP-hard

Proof

- Consider $x'By$ and $\mathbf{x}, \mathbf{y} \in \mathbb{IR}^n$ and

$$A := \left(\begin{array}{c|c|c|c} 0 & x' & 0 & 0 \\ \hline 0 & 0 & B & 0 \\ \hline 0 & 0 & 0 & y \\ \hline 0 & 0 & 0 & 0 \end{array}\right) \quad A^2 = \left(\begin{array}{c|c|c|c} 0 & 0 & x'B & 0 \\ \hline 0 & 0 & 0 & By \\ \hline 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right) \quad A^3 = \left(\begin{array}{c|c|c|c} 0 & 0 & 0 & x'By \\ \hline 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right) \quad A^4 = 0$$

- A is nilpotent $\Rightarrow (\exp A)_{1,2n+2} = \frac{1}{6} x'By$
- ϵ-accurate enclosure of exp $\mathbf{A}$ gives rise to ϵ-accurate enclosure of $\{x'By : x \in \mathbf{x}, y \in \mathbf{y}\}$

Outline

Outline

Taylor Series Interval Evaluation

Definition

$$\begin{aligned} \tilde{\mathcal{T}}_K(\mathbf{A}) &:= I + \mathbf{A} + \tfrac{1}{2}\mathbf{A}^2 + \ldots + \tfrac{1}{K!}\mathbf{A}^K \\ \mathcal{T}_K(\mathbf{A}) &:= \tilde{\mathcal{T}}_K(\mathbf{A}) + \mathcal{R}_K(\mathbf{A}) \end{aligned}$$

where the interval remainder $[\mathcal{R}]([A], K)$ is

$$\mathcal{R}_K(\mathbf{A}) := \rho(||\mathbf{A}||, K)\,[-E, E] \text{ with } \rho(\alpha, K) = \frac{\alpha^{K+1}}{(K+1)!\,\left(1 - \frac{\alpha}{K+2}\right)}$$

$\rho(\alpha, K)$: well known upper bound truncation error valid for $||A|| \leq K + 2$

Example

$$\mathcal{T}_{16}(\mathbf{A}) \approx \begin{pmatrix} 1 \pm 9 \times 10^{-7} & [-1.21, 1.96] \\ \pm 9 \times 10^{-7} & [-6.26, 6.45] \end{pmatrix} \supseteq \begin{pmatrix} 1 & [0.31, 0.44] \\ 0 & [0.04, 0.14] \end{pmatrix}$$

Higher order for the expansion do not improve the entries $(1, 2)$ and $(2, 2)$ anymore

Outline

Taylor Series Horner Interval Evaluation

Definition

$$\begin{aligned} \tilde{\mathcal{H}}_K(\mathbf{A}) &:= \quad I + \mathbf{A}\Big(I + \tfrac{\mathbf{A}}{2}\Big(I + \tfrac{\mathbf{A}}{3}\Big(\quad \cdots \quad \Big(I + \tfrac{\mathbf{A}}{K}\Big)\cdots\Big)\Big)\Big) \\ \mathcal{H}_K(\mathbf{A}) &:= \quad \tilde{\mathcal{H}}_K(\mathbf{A}) + \mathcal{R}_K(\mathbf{A}) \end{aligned}$$

Remark: Multi-occurrences decreased by Horner scheme

Example

$$\mathcal{H}_{16}(\mathbf{A}) \approx \begin{pmatrix} 1 \pm 1.1 \times 10^{-6} & [-0.08, 0.74] \\ \pm 1.1 \times 10^{-6} & [-1.21, 1.22] \end{pmatrix} \supseteq \begin{pmatrix} 1 & [0.31, 0.44] \\ 0 & [0.04, 0.14] \end{pmatrix}$$

Horner scheme reduces the pessimism (well known for real polynomials, e.g. Ceberio & Granvilliers 2002)

Outline

Interval Scaling and Squaring

Definition

$$\mathcal{S}_{L,K}(\mathbf{A}) := \left(\mathcal{H}_K(\mathbf{A}/2^L)\right)^{2^L}$$

Theorem

$\mathcal{S}_{L,K}(\mathbf{A})$ contains $\exp A$ for every $A \in \mathbf{A}$

Proof:

- $\mathcal{H}_K(\mathbf{A}/2^L)$ contains $\exp A/2^L$

$\Rightarrow$ $\mathcal{S}_{L,K}(\mathbf{A})$ contains $(\exp A/2^L)^{2^L} = \exp A$

Example

$$\mathcal{S}_{10,6}(\mathbf{A}) \approx \begin{pmatrix} 1 \pm 1. \times 10^{-11} & [0.31, 0.44] \\ \pm 2.4 \times 10^{-19} & [0.04, 0.14] \end{pmatrix} \supseteq \begin{pmatrix} 1 & [0.31, 0.44] \\ 0 & [0.04, 0.14] \end{pmatrix}$$

Much sharper than Taylor and Horner Taylor

Outline

State of the Art

Michel and Oppenheimer (IEEE Trans. Circuits and Systems 1988)

- Specific centered form: $\exp \mathbf{A} \subseteq \mathcal{H}_K(\hat{\mathbf{A}}) + [\underline{\Delta}, \overline{\Delta}]$
- – Tedious proofs with gaps, very complex computation of $[\underline{\Delta}, \overline{\Delta}]$
- – Horner not sharp even for a thin matrix (cf. Experiments)

Gambill and Skeel (SINUM 1988)

- Specific method for non autonomous non homogeneous linear ODE:

$$((\mathbf{G}_8\mathbf{G}_7)(\mathbf{G}_6\mathbf{G}_5))((\mathbf{G}_4\mathbf{G}_3)(\mathbf{G}_2\mathbf{G}_1)) \text{ instead of } \mathbf{G}_8(\mathbf{G}_7(\cdots(\mathbf{G}_1)\ldots))$$

- Similar to scaling and squaring when applied to autonomous homogeneous linear ODE
- \+ Applies to more general systems
- – Use $(\mathcal{T}_K(\mathbf{A}/2^L))^{2^L}$ which is less sharp than $(\mathcal{H}_K(\mathbf{A}/2^L))^{2^L}$ (necessary in the general case)
- – Repeated computations (necessary in the general case)

Outline

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1. NP-hardness
2. Polynomial Algorithms
3. Experiments
   - Exponentiation of a Thin Matrix
   - Exponentiation of an Interval Matrix
   - Tridiagonal Matrices
4. Experiments

Exponentiation of a Thin Matrix

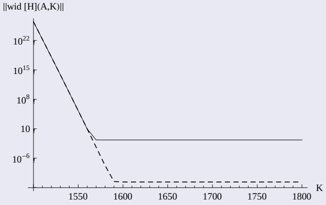
Matrix from Bochev and Markov (Computing 1999)

$$A := \begin{pmatrix} -131 & 19 & 18 \\ -390 & 56 & 54 \\ -387 & 57 & 52 \end{pmatrix}$$

Difficult to exponentiate:

- Significant eigenvalue separation
- Poorly conditioned eigenvector set

Horner Evaluation



- $||A|| = 500$ implies $K \geq 502$
- 110 and 120 digits interval arithmetic (Mathematica)

Scaling and Squaring

$$||\mathrm{wid}\, \mathcal{S}_{12,12}(A)|| \approx 10^{-6}$$

- Standard double precision interval arithmetic

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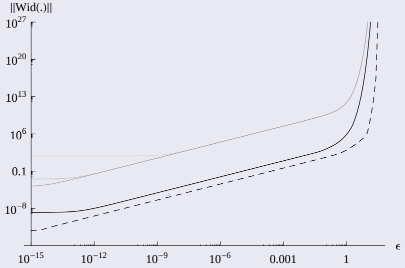
Exponentiation of an Interval Matrix

Matrix from Bochev and Markov (Computing 1999)

$$\mathbf{A}_\epsilon := 0.1A + [-\epsilon, \epsilon]$$



- Gray: Horner evaluation
- Black: Scaling and squaring
- Dashed: Inner approximation

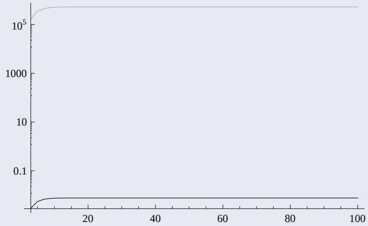
Outline

Tridiagonal Matrices (1/2)

Exponentiation of an Interval Matrix

- $\mathbf{T}_n$ defined by $t_{ii} = [-11, -9]$ and $t_{i+1,i} = t_{i,i+1} = [0, 2]$

$$[\mathbf{T}_3] = \begin{pmatrix} [-11,-9] & [0,2] & 0 \\ [0,2] & [-11,-9] & [0,2] \\ 0 & [0,2] & [-11,-9] \end{pmatrix}$$

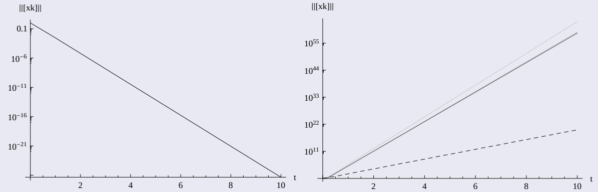


- n varies from 3 to 100
  - Gray: Horner evaluation
  - Black: Scaling and squaring

Tridiagonal Matrices (2/2)

Simulation of Linear ODE

- Simulation of $x'(t) = Ax(t)$ with $A \in \mathbf{T}_3$



- Left: Scaling and squaring
- Right: Basic method (full lines), and VNODE-LP (dashed line)

Conclusion

Originality vs State of the Art

- Most is known to the experts
- Gambill and Skeel:
  - Experiments with thin matrices
  - In this case, parallelotope methods better
  - Our experiments: Better than parallelotope methods for uncertain linear ODE
- Michel and Oppenheimer: Scaling and squaring simpler and sharper

Future Work

- Use parallelotope and interval matrix exponential
- Generalize Gambill and Skeel to nonlinear ODE