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Approximation of the matrix exponential on the negative line

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INSTITUT FÜR ANGEWANDTE UND NUMERISCHE MATHEMATIK

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Wave phenomena

Outline

Approximation of the matrix exponential

Faber transform

Approximation on unit disk

An extremal curve

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Approximation of the matrix exponential

Shift-and-invert Krylov subspace

$$\mathcal{K}_n((\gamma I - A)^{-1}, b) = \text{span}\{b, (\gamma - A)^{-1} b, \cdots, (\gamma - A)^{-n+1} b\}$$

Approximation of matrix exponential

Let $A \in \mathbb{C}^{N,N}$ with $W(A) \subset (-\infty, 0]$, $b \in \mathbb{C}^N$, and P_n an orthogonal projection to the shift-and-invert Krylov subspace with shift γ_n. Let $A_n = P_n A P_n$. Then we have

$$\|e^A b - e^{A_n} b\| \leq 2\|b\| \inf_{p \in \mathcal{P}_{n-1}} \left\| e^{-x} - \frac{p(x)}{(\gamma_n + x)^{n-1}} \right\|_{[0,\infty)}$$

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Approximation problem

Approximate e^{-x} on $[0,\infty)$ by rational functions of type

$$R_n(q) = \left\{ \frac{p_n(x)}{(x+nq)^n} \,\middle|\, p_n \in \mathcal{P}_n \right\}$$

Rate on best approximation

$$\rho_n(q) := \inf\{\sup_{x\geq 0} |e^{-x} - r(x)| \ : \ r \in R_n(q)\}$$

Transform

$$t = (nq - x)/(nq + x)$$

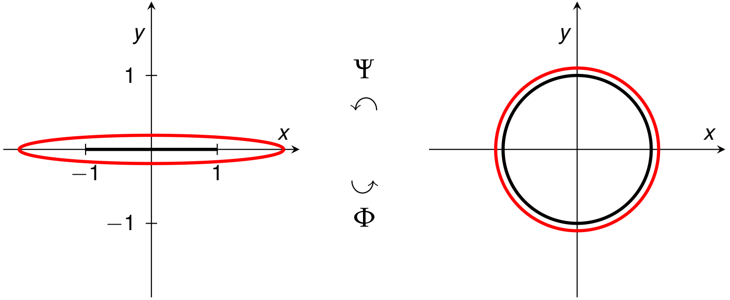
leads to

$$\rho_n(q) := \inf\{\|f_n - p\|_{[-1,1]} \ : \ p \in \mathcal{P}_n\}$$

where

$$f_n(t) = e^{nq\frac{t-1}{t+1}}$$

Mapping of curves



$$C_R = \{z \ : \ |\Phi(x)| = R > 1\} \qquad \mathbb{D} = \{w \ : \ |w| \leq 1\}$$

$$\Psi(w) = \frac{1}{2}\left(w + \frac{1}{w}\right)$$

Faber transform for polynomials

$$T \ : \ w^n \to F_n(z), \qquad n = 0, 1, 2, \ldots$$

$$F_n(z) = \frac{1}{2\pi i}\int_{C_R} \frac{\big(\Phi(\zeta)\big)^n}{\zeta - z}\, d\zeta = \frac{1}{2\pi i}\int_{|w|=R} \frac{w^n\,\Psi'(w)}{\Psi(w) - z}\, dw$$

$$\frac{1}{2\pi i}\int_{|w|=R} \frac{w^n\,\Psi'(w)}{\Psi(w) - z}\, dw = \frac{1}{2\pi i}\int_{|w|=\frac{1}{R}} \frac{\frac{1}{w}\,\Psi'\big(\frac{1}{w}\big)}{\Psi\big(\frac{1}{w}\big) - z} \cdot w^{-n-1}\, dw$$

$$\frac{\frac{1}{w}\,\Psi'\big(\frac{1}{w}\big)}{\Psi\big(\frac{1}{w}\big) - z} = \frac{1 - w^2}{1 + w^2 - 2zw} = F_0(z) + F_1(z)w + F_2(z)w^2 + \cdots$$

Comparing coefficients gives...

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$$
\begin{aligned}
(1-w^2) &= \left(\sum_{k=0}^{\infty} F_k(z) w\right)\left(w^2 - 2zw + 1\right) \\
&= F_0(z) + (F_1(z) - 2zF_0(z))w + (F_2(z) - 2zF_1(z) + F_0(z))w^2 \\
&+ \sum_{k=3}^{\infty} (F_k(z) - 2zF_{k-1}(z) + F_{k-2}(z))w^k
\end{aligned}
$$

hence $F_0(z) = 1$, $F_1(z) = 2z$, $F_2(z) = 2(2z^2 - 1)$, and

$$
F_{k+1}(z) = 2zF_k(z) - F_{k-1}(z), \qquad n = 2, 3, \ldots
$$

Finally

$$
F_0(z) = T_0(z) = 1, \qquad F_k(z) = 2T_k(z), \quad k = 1, 2, 3, \ldots
$$

Bound on Faber polynomials

Lemma

$$\|F_k\|_{[-1,1]} \leq 2\|w^k\|_{\mathbb{D}} = 2$$

Proof

$$F_n(z) = \frac{1}{2\pi i} \int_{|w|=R} \frac{w^n \Psi'(w)}{\Psi(w) - z}\, dw$$

Idea: we add

$$\frac{1}{2\pi i} \int_{|w|=R} \frac{\overline{w}^n \Psi'(w)}{\Psi(w) - z}\, dw = 0, \qquad n \geq 1\,.$$

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This holds true due to...

$$\frac{1}{2\pi i}\int_{|w|=R}\frac{w^{-n}\Psi'(w)}{\Psi(w)-z}\,dw = 0, \qquad n \geq 1\,,$$

since

$$w^{-n}\cdot\frac{\frac{1}{2}(1-\frac{1}{w^2})}{\frac{1}{2}(w+\frac{1}{w})-z} = w^{-(n+1)}\frac{\frac{1}{2}(1-\frac{1}{w^2})}{\frac{1}{2}(1+\frac{1}{w^2})-\frac{z}{w}} = \mathcal{O}(\frac{1}{|w|^2}),$$

for $|w| = R \to \infty$ and

$$\frac{1}{2\pi i}\int_{|w|=R}\frac{\overline{w}^n\Psi'(w)}{\Psi(w)-z}\,dw = R^{2n}\frac{1}{2\pi i}\int_{|w|=R}\frac{w^{-n}\Psi'(w)}{\Psi(w)-z}\,dw = 0\,.$$

New representation of Faber polynomials

Subtracting

$$F_n(z) = \frac{1}{2\pi i} \int_{|w|=R} \frac{w^n \Psi'(w)}{\Psi(w) - z}\, dw = \frac{1}{2\pi i} \int_{|w|=R} w^n d_w \log(\Psi(w) - z)$$

and

$$0 = \frac{1}{2\pi i} \int_{|w|=R} \overline{w}^n d_w \log(\Psi(w) - z) = \frac{1}{2\pi i} \int_{|w|=R} w^n d_w \overline{\log(\Psi(w) - z)}$$

we obtain

$$\begin{aligned} F_n(z) &= \frac{1}{\pi} \int_{|w|=R} w^n d_w \arg(\Psi(w) - z) \\ &= \frac{R^n}{\pi} \int_0^{2\pi} e^{int} d_t \arg(\Psi(Re^{it}) - z)\,. \end{aligned}$$

End of proof

Since

$$V = \int_0^{2\pi} |d_t \arg(\Psi(Re^{it}) - z)| = 2\pi\,,$$

we obtain (for $z \in [-1, 1]$, $k \geq 1$) the bound

$$|F_k(z)| = \left| \frac{R^n}{\pi} \int_0^{2\pi} e^{int} d_t \arg(\Psi(Re^{it}) - z) \right| \leq R^n \cdot \frac{2\pi}{\pi} = 2R^n \to 2\,,$$

for $R \to 1$ and

$$\|F_k(z)\|_{[-1,1]} \leq 2 = 2\|w^k\|_{\mathbb{D}}\,.$$

The Faber transform as bounded map

Theorem

The *Faber transform*

$$T : \begin{cases} \mathcal{P} & \to & \mathcal{P} \\ p & \mapsto & T(z) = \frac{1}{2\pi i} \int_{C_R} \frac{p(\Phi(\zeta))}{\zeta - z} \, d\zeta \end{cases}$$

is bounded by

$$\| Tp \|_{[-1,1]} \leq \underbrace{\left(1 + \frac{2V}{\pi}\right)}_{\leq 5} \| p \|_{\mathbb{D}} , \qquad p \in \mathcal{P}$$

.

Proof of theorem

We have the representation

$$Tp(z) = \sum_{k=0}^{n} a_k F_k(z) = a_0 + \frac{1}{\pi} \int_0^{2\pi} \left(\sum_{k=1}^{n} a_k (Re^{it})^k \right) d_t \arg(\Psi(Re^{it}) - z)$$

and therefore, with $R \to 1$,

$$\left\| \sum_{k=0}^{n} a_k F_k(z) \right\|_{[-1,1]} \leq |a_0| + \left(|a_0| + \left\| \sum_{k=0}^{n} a_k w^k \right\|_{\mathbb{D}} \right) \cdot \frac{V}{\pi}$$

Due to

$$|a_0| \leq |p(0)| \leq \|p\|_{\mathbb{D}}$$

our theorem is proved.

Extension of Faber map

- let $A(\mathbb{D})$ be set of functions continuous on $\mathbb{D}$ and holomorphic in $\operatorname{int}\mathbb{D}$
- $(A(\mathbb{D}), \|\cdot\|_{\mathbb{D}})$ is a Banach space
- Set of polynomials $\mathcal{P}$ is dense in $(A(\mathbb{D}), \|\cdot\|_{\mathbb{D}})$

Since T is bounded, extend to map

$$T : (A(\mathbb{D}), \|\cdot\|_{\mathbb{D}}) \to (C([-1,1]), \|\cdot\|_{[-1,1]})$$

it obviously holds

$$\|Tf\|_{[-1,1]} \leq \underbrace{\left(1 + \frac{2V}{\pi}\right)}_{\leq 5} \|f\|_{\mathbb{D}}, \qquad f \in A(\mathbb{D})$$

‘Inverse’ of Faber map

For $f \in C([-1,1])$ define

$$\widetilde{f}(w) := \frac{1}{2\pi i} \int_{\partial\mathbb{D}} \frac{f(\Psi(u))}{u-w}\, du, \qquad |w| < 1\,.$$

If $\widetilde{f} \in A(\mathbb{D})$, then $T\widetilde{f} = f$.

For our function of interest

$$f_n(t) = e^{nq\frac{t-1}{t+1}}, \qquad f(\Psi(u)) = F_n(u) = e^{nq\left(\frac{u-1}{u+1}\right)^2}$$

We have $\widetilde{f} \in A(\mathbb{D})$ with

$$\widetilde{f}_n(w) = \frac{1}{2\pi i} \int_{\partial\mathbb{D}} \frac{F_n(u)}{u-w}\, du\,, \qquad |w| < 1\,.$$

Approximation on unit disk

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Lemma

Let p be the Taylor polynomial of order $n-1$ at the origin for $\widetilde{f}$. Then,

$$\widetilde{f}_n(w) - p(w) = w^n \int_{\partial\mathbb{D}} F_n(u) u^{-n} (u-w)^{-1} \, du \,, \qquad |w| < 1$$

Proof Direct conclusion of

$$\begin{aligned}\int_{\partial\mathbb{D}} F_n(u) \left(\frac{w}{u}\right)^n \frac{1}{u-w} \, du &= \widetilde{f}_n(w) - \int_{\partial\mathbb{D}} F_n(u) \left(\frac{u^n - w^n}{u-w}\right) \frac{1}{u^n} \, du \\ &= \widetilde{f}_n(w) - \sum_{k=0}^{n-1} w^k \int_{\partial\mathbb{D}} F_n(u) \frac{1}{u^{k+1}} \, du\end{aligned}$$

Transfer complete

We have the estimate

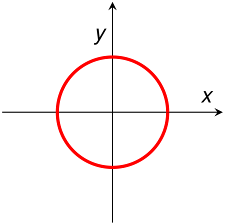
$$\inf_{p\in\mathcal{P}_n} \|f_n(t) - p(t)\|_{[-1,1]} \leq 5 \inf_{p\in\mathcal{P}_n} \|\widetilde{f}_n - p\|_{\mathbb{D}} =: E_n(\widetilde{f})$$

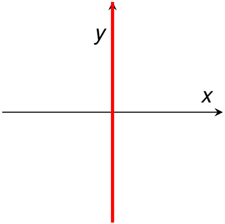
With the representation of $\widetilde{f}$:

$$E_n(\widetilde{f}) \leq \frac{1}{2\pi} \sup_{|w|<1} \left| \int_{\partial\mathbb{D}} F_n(u) u^{-n} \frac{1}{u-w}\, du \right|$$

- $F_n(u)$ holomorphic in whole extended plane except for $u = -1$
- $\partial\mathbb{D}$ can be replaced by any curve γ as long as it behaves adequately at $u = -1$

A final mapping





With the transform

$$z = \frac{u-1}{u+1}, \qquad u = u(z) = \frac{1+z}{1-z}$$

we obtain

$$\left| F_n(u) u^{-n} \right| = exp(nG(z,q))$$

where

$$G(z,q) = \mathrm{Re}\, H(z), \qquad H(z) = \log\left(\frac{1-z}{1+z}\right) + qz^2$$

An extremal curve

Let Σ be the class of all closed curves σ in the extended right half-plane symmetric with respect to the real axis that passes through ∞

For $\sigma \in \Sigma$ define

$$g(\sigma) = \max\{G(z, q) \ : \ z \text{ on } \sigma\}$$

and

$$\widehat{g} = \inf\{g(\sigma) \ : \ \sigma \in \Sigma\}$$

- for R large, the set $\sigma \cap \{|z| \geq R\}$ consists of two rays $z = t(1 \pm i\sqrt{3})$, $t \geq R/2$.
- in $\{z \ : \ |z| \leq R, \mathrm{Re}\, z \geq 0\}$ only singular point $z = 1$
- $G(z, q) \to -\infty$, for $z \to 1$
- σ does not pass $[1, \infty)$ (but ∞!)
- $G'_x < 0$, for $z = x + iy$ and x close to zero

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An extremal curve

Curve can be chosen such that maximum is attained at grad $G = 0$.

Cauchy-Riemann equations give at $H'(z) = 0$

$$H'(z) = 1 + q(z^3 - z) = 0, \qquad q > 0\,.$$

One negative root, for the other two:

- complex conjugated if $q < \frac{3\sqrt{3}}{2}$
- both equal $z = \frac{1}{\sqrt{3}}$ if $q = \frac{3\sqrt{3}}{2}$
- real distinct, both between 0 and 1, if $q > \frac{3\sqrt{3}}{2}$

Lower bound for minimum

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- Optimal curves pass rays $z = t(1+i)$, $t > 0$

$$G^*(q) = \widehat{g}(\sigma) \geq \min\{G(z,q)\ :\ z = t(1+i),\ t \geq 0\} = \log(\sqrt{2}-1)$$

- Minimum attained for $z_0 = \frac{1+i}{\sqrt{2}}$

- Only chance for $G^*(q) = \log(\sqrt{2}-1)$ is for $H'(z_0) = 0$, hence

$$q = \frac{1}{\sqrt{2}}$$

Final estimate

For n large enough and $|w| < 1$, along optimal curve γ,

$$|F_n(u)u^{-n}|\frac{1}{|u-w|} \leq \left(-\frac{G^*(q)}{K}\right)^{\frac{1}{2}} \exp(nG^*(q))$$

Hence

$$\left|\frac{1}{2\pi i}\int_\gamma F_n(u)u^{-n}\frac{1}{u-w}\,dw\right| \leq \frac{1}{2\pi}\ell(\gamma)\left(-\frac{G^*(q)}{K}\right)^{\frac{1}{2}} \exp(nG^*(q))$$

and for $q = 1/\sqrt{2}$

$$E_n(\widetilde{f}) \leq \frac{K}{2\pi}(\sqrt{2}-1)^n,$$

or

$$\rho_n(f) \leq \frac{5K}{2\pi}(\sqrt{2}-1)^n$$

respectively.

Summary

- fast convergence of approximation to matrix exponential in shift-and-invert Krylov subspace
- Faber transform works for more general sets
- steepest descent analysis
- complex approximation