Functions of matrices with Kronecker sum structure: decay properties and computation

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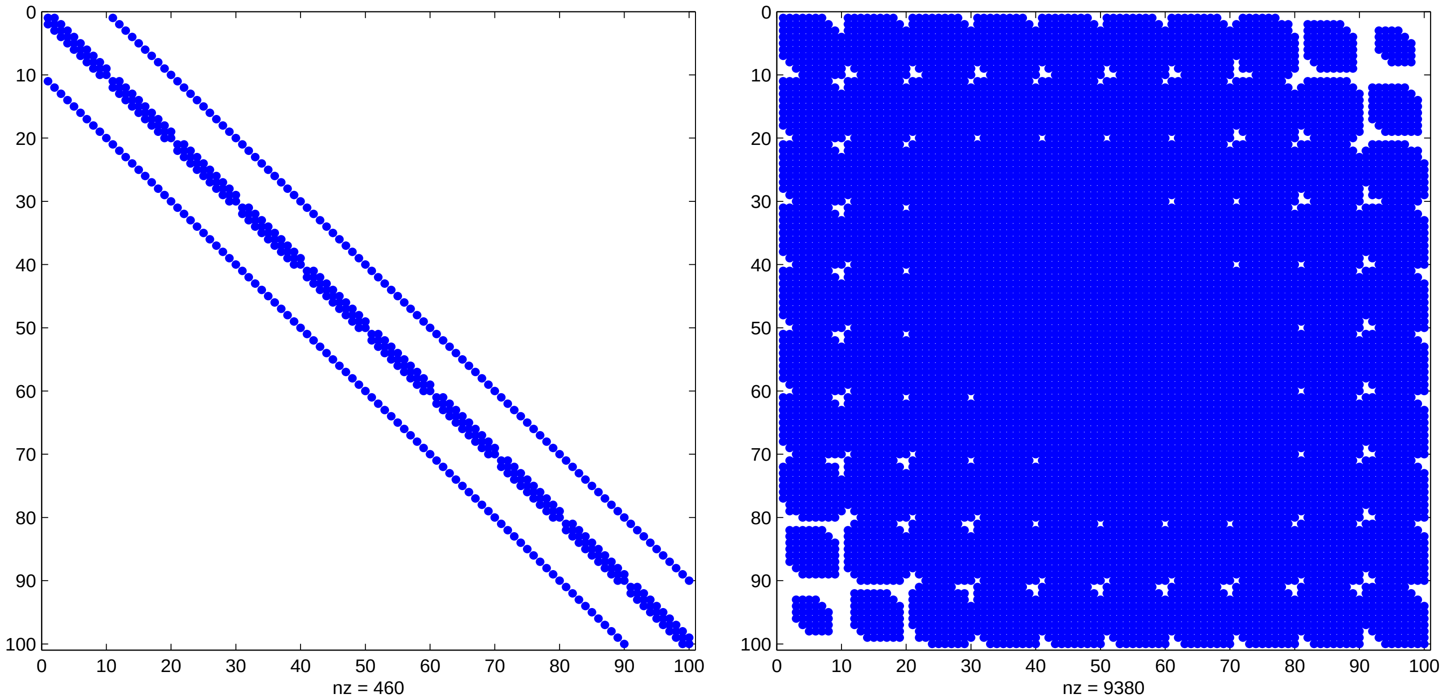
The inverse of the 2D Laplace matrix on the unit square

$$\mathcal{A} := M \otimes I_n + I_n \otimes M, \qquad M = \text{tridiag}(-1, 2, -1)$$

Sparsity pattern:



Matrix $\mathcal{A}$ $\qquad$ $\mathcal{A}^{-1}$

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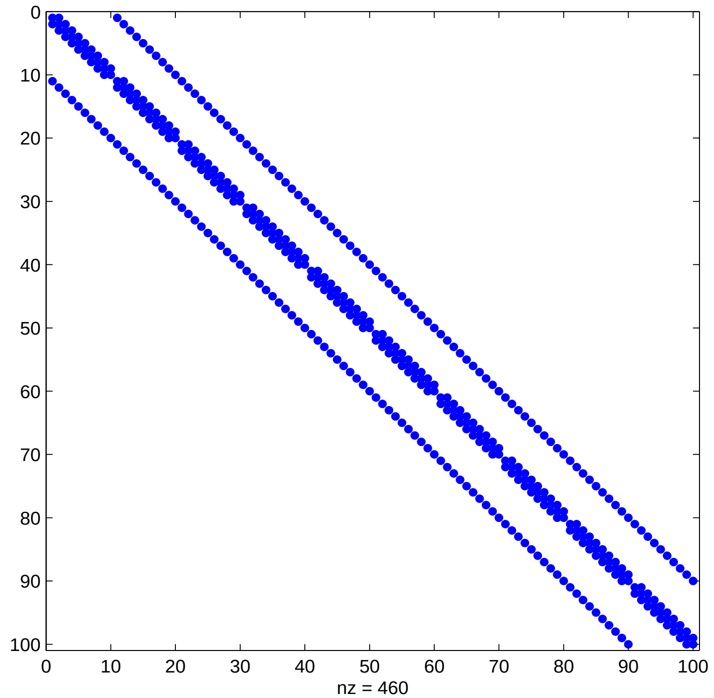
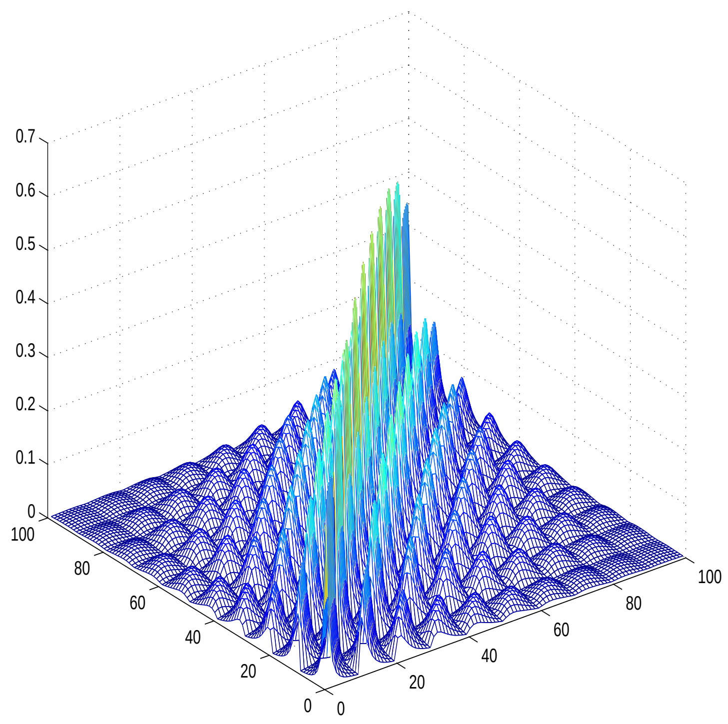


$\mathcal{A}$



$|(\mathcal{A}^{-1})_{ij}|$

The exponential decay

The classical bound (Demko, Moss & Smith):

If M spd is banded with bandwidth β, then

$$|(M^{-1})_{ij}| \leq \gamma q^{\frac{|i-j|}{\beta}}$$

where $q := \dfrac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} < 1$ (κ=cond(M)) $\qquad \gamma := \max\left\{\frac{1}{\lambda_{\min}(M)}, \frac{(1+\sqrt{\kappa})^2}{2\lambda_{\max}(M)}\right\}$

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If f analytic in region containing $\mathrm{spec}(M)$: $\qquad |f(M)_{ij}| \leq Cq^{\frac{i-j}{\beta}}$

with C, q depending on $\mathrm{spec}(M)$ and f (*Benzi & Golub, 1999*)

Many contributions: Bebendorf, Hackbusch, Benzi, Boito, Razouk, Golub, Tuma, Concus, Meurant, Mastronardi, Ng, Tyrtyshnikov, Nabben, ...

Decay bounds for Cauchy-Stieltjes (or Markov-type) functions

$$f(M) = \int_{-\infty}^{0} (M - \omega I)^{-1} \mathrm{d}\gamma(\omega), \quad x \in \mathbb{C} \setminus (-\infty, 0]$$

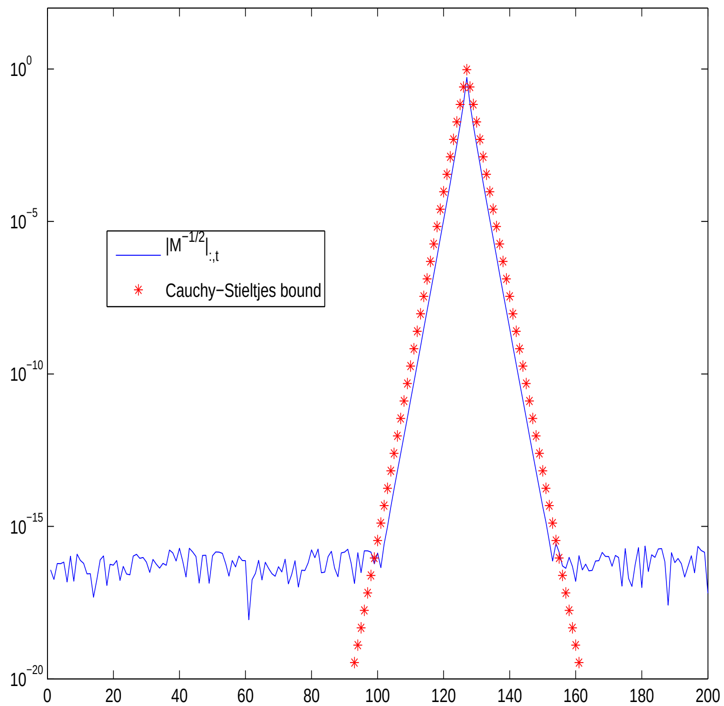
$f(x) = z^{-\frac{1}{2}}$, $f(x) = \frac{\mathrm{e}^{-t\sqrt{x}} - 1}{x}$, $f(x) = \frac{\log(1+x)}{x}$, ...

⋆ Demko etal bound to estimate $|f(M)|_{kt}$ for M spd and $\beta-$banded:

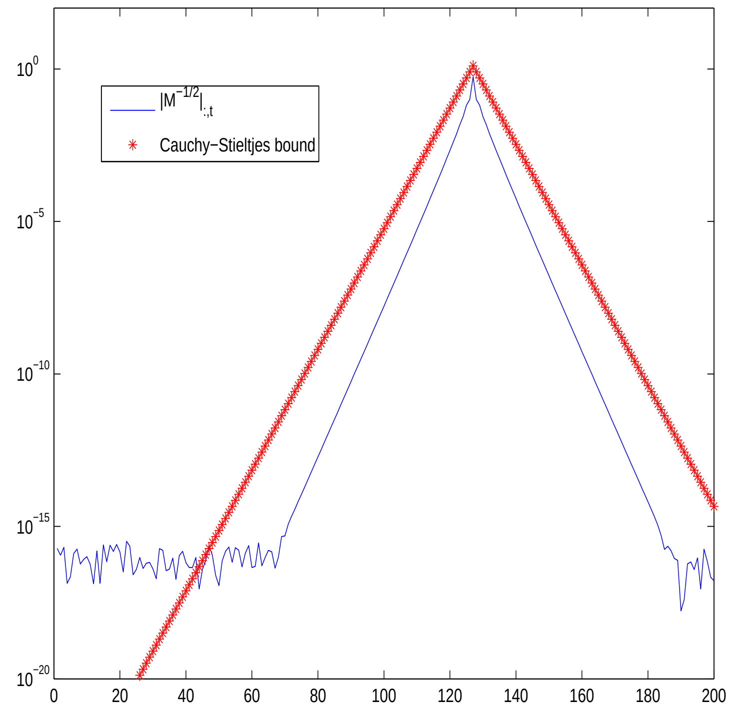
$$|M_{kt}^{-\frac{1}{2}}| \le C \left(\frac{\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}}} \right)^{\frac{|k-t|}{\beta}}$$

(C depends on spec(M))

Estimates for $|M^{-1/2}|_{:,t}$, $t = 127$, $n = 200$ (log-scale)



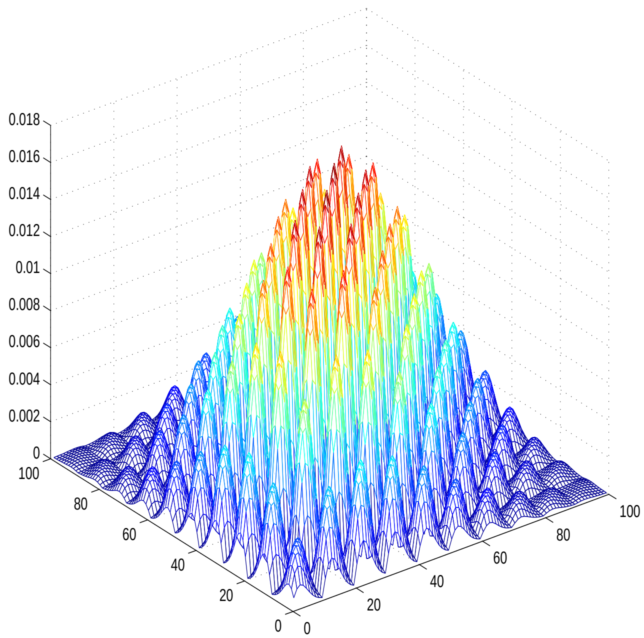
$M = \text{tridiag}(-1, 4, -1)$

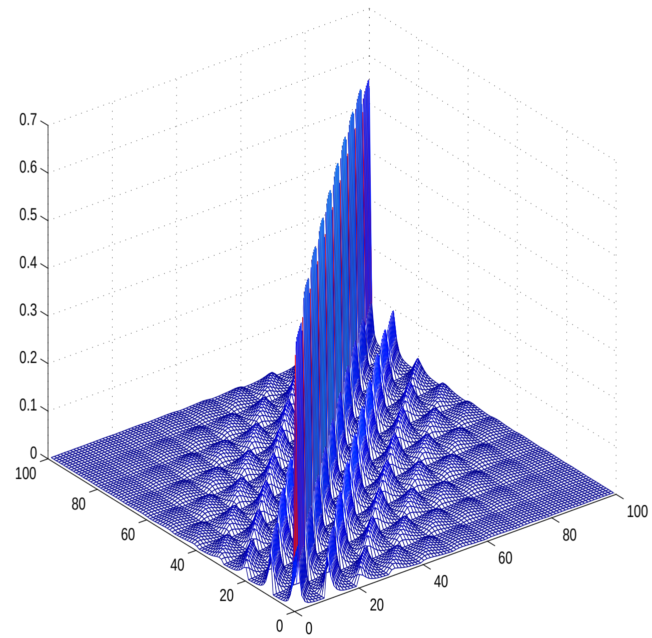


$M = \text{pentadiag}(-0.5, -1, 4, -1, -0.5)$

Typical decay plot for $f(\mathcal{A})$

$\mathcal{A}$: Laplace operator as before





$$f(\mathcal{A}) = \exp(-5\mathcal{A}) \qquad\qquad f(\mathcal{A}) = \mathcal{A}^{-1/2}$$

Much richer structure

In general, $\mathcal{A} = M_1 \oplus M_2 := M_1 \otimes I + I \otimes M_2$, M_1, M_2 banded spd

Decay bounds for the exponential function

$$\text{Keynote formula :} \qquad \exp(M_1 \oplus M_2) = \exp(M_1) \otimes \exp(M_2)$$

Let M be spsd, β-banded; $\mathrm{spec}(M) \subset [0, 4\rho]$, $\mathcal{A} = I \otimes M + M \otimes I$. Then

$$(\exp(-\tau\mathcal{A}))_{kt} = (\exp(-\tau M))_{k_1 t_1} (\exp(-\tau M))_{k_2 t_2}$$

for all $t = (t_1, t_2)$ and $k = (k_1, k_2)$

For $\min\{|t_1 - k_1|, |t_2 - k_2|\} \geq \sqrt{4\rho\tau}\beta$

i) For $\rho\tau \geq 1$ and $\sqrt{4\rho\tau} \leq |k_j - t_j|/\beta \leq 2\rho\tau$,

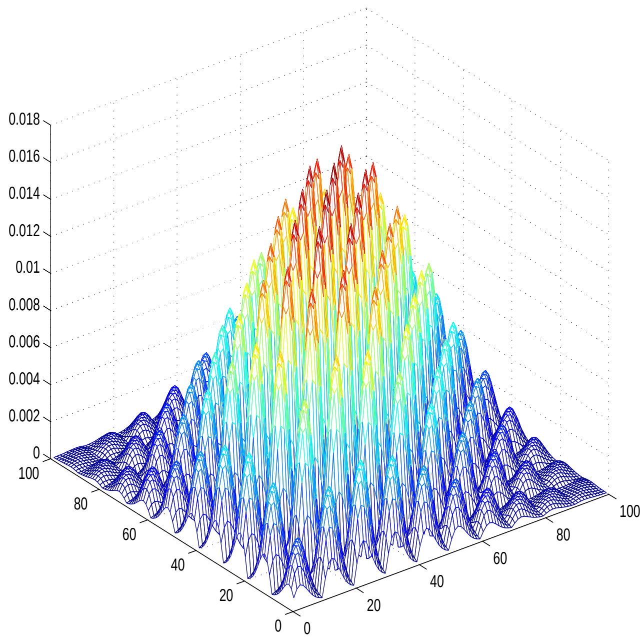
$$|(\exp(-\tau M))_{k_j t_j}| \leq 10 \exp\left(-\frac{(|k_j - t_j|/\beta)^2}{5\rho\tau}\right);$$

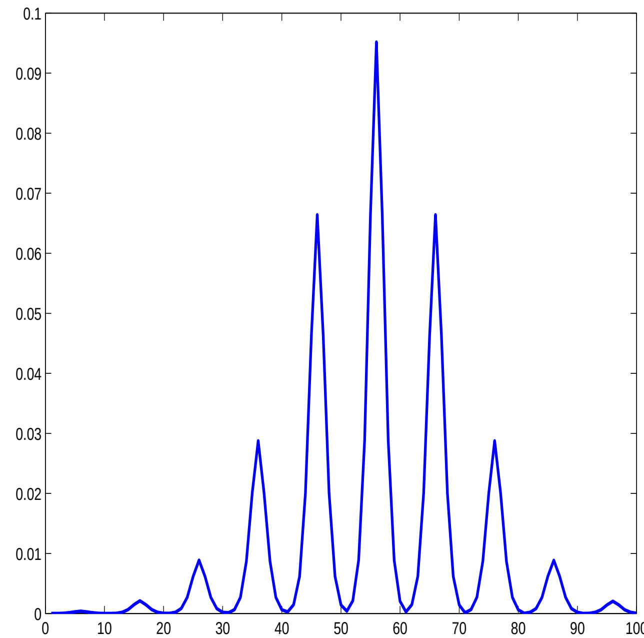
ii) For $|k_j - t_j|/\beta \geq 2\rho\tau$,

$$|(\exp(-\tau M))_{k_j t_j}| \leq 10 \frac{\exp(-\rho\tau)}{\rho\tau} \left(\frac{\mathrm{e}\rho\tau}{\frac{|k_j - t_j|}{\beta}}\right)^{\frac{|k_j - t_j|}{\beta}}$$

(generalization to $\mathcal{A} = I \otimes M_1 + M_2 \otimes I$)

Decay bounds for the exponential function





Left: whole pattern of $\exp(-\mathcal{A})$ Right: Row 56 of $\exp(-\mathcal{A})$

$|\exp(-\mathcal{A})|_{kt}$ with $k = 56 \Rightarrow k = (k_1, k_2) = (6, 5)$

For $t = 50 \Rightarrow t = (t_1, t_2) = (10, 4)$ so that $|k_1 - t_1| \gg 0$

For $t = 45 \Rightarrow t = (t_1, t_2) = (5, 4)$ so that $|k_1 - t_1| \not\gg 0$

Decay bounds for Laplace-Stieltjes function

$$f(M) = \int_0^\infty e^{-\tau M} \mathrm{d}\alpha(\tau)$$

e.g., $f(x) = x^{-\sigma}$ ($\sigma > 0$), $f(x) = e^{-x}$, $f(x) = e^{1/x}$, $f(x) = (1 - e^{-x})/x$, $f(x) = \log(1 + 1/x)$, ...

- For M spd and β-banded, $\widehat{M} = M - \lambda_{\min} I$

$$|f(M)|_{k,t} \le \int_0^\infty \exp(-\lambda_{\min}\tau) |(\exp(-\tau \widehat{M}))_{k,t}| \mathrm{d}\alpha(\tau)$$

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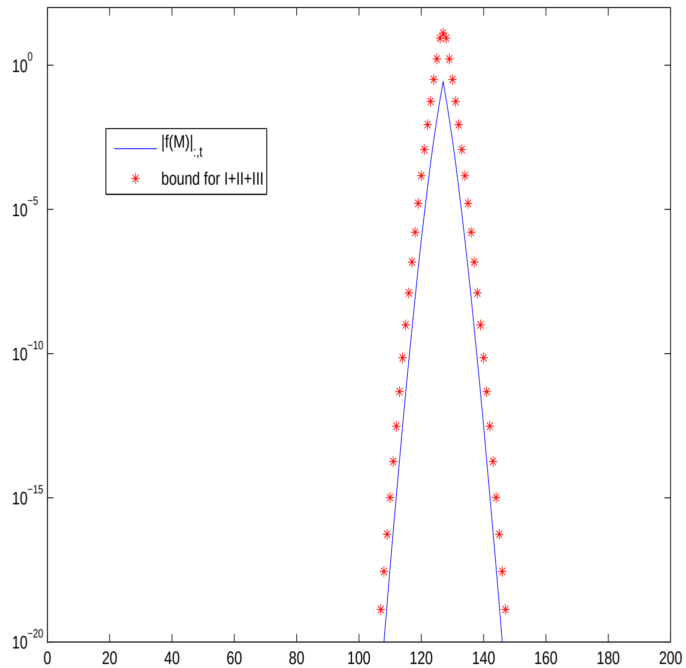
- For $\mathcal{A} = M \otimes I + I \otimes M$

$$(f(\mathcal{A}))_{kt} = \int_0^\infty (\exp(-\tau M))_{k_1 t_1} (\exp(-\tau M))_{t_2 k_2} \mathrm{d}\alpha(\tau)$$

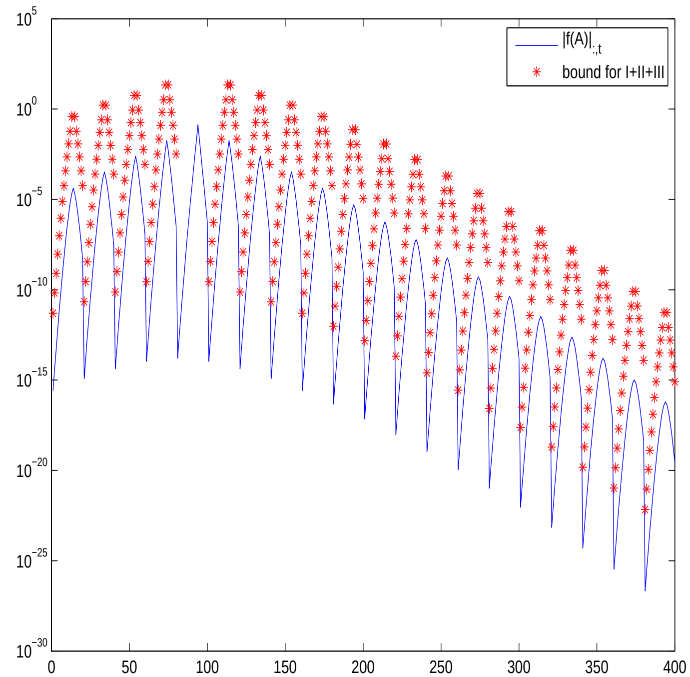
then, more precise bounds for specific choices of $\mathrm{d}\alpha(\tau)$

An example: $f(x) = \frac{1-e^{-x}}{x}$

$M = \text{tridiag}(-1, 4, -1)$, $n = 200$



Typical row of $f(M)$



Typical row of $f(\mathcal{A})$

Cauchy-Stieltjes functions of Kronecker sum: $f(\mathcal{A}) = \int_\Gamma (\mathcal{A} - \omega I)^{-1} \mathrm{d}\gamma(\omega)$

$$e_k^T f(\mathcal{A}) e_t = \int_\Gamma e_k^T (\mathcal{A} - \omega I)^{-1} e_t \mathrm{d}\gamma(\omega),$$

where we can write $\mathcal{A} - \omega I = M \otimes I + I \otimes (M - \omega I)$

- For each t, $x_t := (\mathcal{A} - \omega I)^{-1} e_t$, so that $X_t = X_t(\omega) \in \mathbb{C}^{n \times n}$ solution to

$$MX_t + X_t(M - \omega I) = E_t, \qquad x_t = \mathrm{vec}(X_t), \quad e_t = \mathrm{vec}(E_t)$$

Then (e.g., Lancaster 1970)

$$X_t = -\int_0^\infty \exp(-\tau M) E_t \exp(-\tau(M - \omega I)) \mathrm{d}\tau$$

so that (with $k = (k_1, k_2), t = (t_, t_2)$)

$$e_k^T (\omega I - \mathcal{A})^{-1} e_t = e_{k_1}^T X_t e_{k_2} = -\int_0^\infty |\exp(-\tau M)|_{k_1, t_1} |\exp(-\tau(M - \omega I))|_{t_2, k_2} \mathrm{d}\tau$$

then, more precise bounds for specific choices of f...

Computational strategies

$$f(\mathcal{A})b, \qquad \mathcal{A} = M_1 \otimes I + I \otimes M_2$$

Projection strategy for large $\mathcal{A}$: given approximation space range($\mathcal{V}$),

$$f(\mathcal{A})b \approx \mathcal{V} f(H)(\mathcal{V}^T b), \qquad H = \mathcal{V}^T \mathcal{A} \mathcal{V}$$

- Typical choices: $K_m(\mathcal{A}, b)$, $EK_m(\mathcal{A}, b)$, $RK_m(\mathcal{A}, b)$

(standard, extended, rational Krylov subspaces, and their variants)

Structure not exploited!

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Structure not exploited!

• If $B = b_1 b_2^T$, then structure-aware choice:

$$\text{range}(\mathcal{V}) = K_m(M_1, b_2) \otimes K_m(M_2, b_2) \qquad \text{(or their variants)}$$

that is, $\mathcal{V} = P_m \otimes Q_m$, so that

$$f(\mathcal{A})b \;\approx\; x_m^{\otimes} := (P_m \otimes Q_m)z, \qquad z = f(\mathcal{T}_m)(P_m \otimes Q_m)^T b$$

with $\mathcal{T}_m = T_2 \otimes I_m + I_m \otimes T_1$, $\quad T_1 = Q_m^T M_1 Q_m$, $\; T_2 = P_m^T M_2 P_m$

Advantages of the structured approximation

$$f(\mathcal{A})b \;\approx\; x_m^{\otimes} := (P_m \otimes Q_m)z, \quad z = f(\mathcal{T}_m)(P_m \otimes Q_m)^T b$$

- No need to explicitly compute $P_m \otimes Q_m$, as

$$(P_m \otimes Q_m)z = \mathrm{vec}(Q_m Z P_m^T)$$

- No need to explicitly compute $\mathcal{T}_m$ if eigencomposition of T_1, T_2 is reliable
- Memory requirements drastically reduced from mn^2 to $2mn$
- Accurate approximate solution obtained with much smaller space dimension

M_1, M_2 not necessarily symmetric

An example from Frommer, Güttel, Schweitzer, 2014

$f(z) = (e^{10^{-3}\sqrt{z}} - 1)/z, \;\; M = \text{tridiag}(-1, 2, -1), \; b = \mathbf{1}, \; n = 50$

m	$\|f(\mathcal{A})b - x_m\|$	$\|f(\mathcal{A})b - x_m^{\otimes}\|$	$\frac{\|x_m - x_{m,old}\|}{\|x_m\|}$	$\frac{\|x_m^{\otimes} - x_{m,old}^{\otimes}\|}{\|x_m^{\otimes}\|}$
4	4.2422e-01	3.9723e-01	1.0000e+00	1.0000e+00
8	2.6959e-01	2.1025e-01	2.2710e-01	2.5313e-01
12	1.7072e-01	1.0365e-01	1.3066e-01	1.2971e-01
16	1.0324e-01	4.2407e-02	8.3444e-02	6.9960e-02
20	5.7342e-02	1.1176e-02	5.4224e-02	3.3969e-02
24	2.7550e-02	4.8230e-04	3.4054e-02	1.0935e-02
28	1.0351e-02	2.8883e-12	1.9296e-02	4.8230e-04
32	3.4273e-03	2.8496e-12	8.3585e-03	1.1366e-13
36	2.2906e-03	2.9006e-12	1.7514e-03	1.4799e-13
⋮	⋮			
48	1.8744e-04	2.8235e-12	3.0332e-04	2.5965e-13

An example from Frommer, Güttel, Schweitzer, 2014

$f(z) = (e^{10^{-3}\sqrt{z}} - 1)/z$, $M = \text{tridiag}(-1, 2, -1)$, $b = \mathbf{1}$, $n = 100$

m	$\frac{\|x_m - x_{m,old}\|}{\|x_m\|}$	$\frac{\|x_m^{\otimes} - x_{m,old}^{\otimes}\|}{\|x_m^{\otimes}\|}$
4	1.0000e+00	1.0000e+00
8	2.3942e-01	2.7720e-01
12	1.5010e-01	1.6289e-01
16	1.0716e-01	1.0966e-01
20	8.1062e-02	7.8150e-02
28	5.0347e-02	4.1674e-02
36	3.2507e-02	2.0802e-02
44	2.0667e-02	7.5529e-03
52	1.2194e-02	3.1470e-04
56	8.8234e-03	1.1354e-12
60	5.9194e-03	3.4639e-13

The matrix exponential: $\exp(\mathcal{A})b$

$$\begin{aligned}
x_m^{\otimes} &= (P_m \otimes Q_m)\exp(T_2 \otimes I_m + I_m \otimes T_1)(P_m \otimes Q_m)^T b \\
&= (P_m \otimes Q_m)(\exp(T_2) \otimes \exp(T_1))(P_m \otimes Q_m)^T b \\
&= \mathrm{vec}(\left(Q_m \exp(T_1) Q_m^T b_1\right) \left(b_2^T P_m \exp(T_2)^T P_m^T\right)) \\
&=: \mathrm{vec}(x_m^{(1)} (x_m^{(2)})^T)
\end{aligned}$$

Convergence driven by the most slowly converging between $x_m^{(1)}$, $x_m^{(2)}$

An example from graph and network analysis

Graphs: $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ Cartesian product[a]: $\mathcal{G} = G_1 \square G_2$

$\Rightarrow$ Adjacency matrix $\mathcal{A}$ of $\mathcal{G}$ is Kronecker sum of adjacency matrices of G_1 and G_2

Of interest, Total Communicability of $\mathcal{G}$: $e^{\mathcal{A}}\mathbf{1}$

---

[a] *The vertex set of $\mathcal{G}$ is $V_1 \times V_2$; there is an edge between vertices (u_1, u_2) and (v_1, v_2) of $\mathcal{G}$ if either $u_1 = v_1$ and $(u_2, v_2) \in E_2$, or $u_2 = v_2$ and $(u_1, v_1) \in E_1$*

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EXAMPLE: Consider $\mathcal{G}_i = G_i \square G_i$, with each G_i being a Barabasi–Albert graph constructed using the preferential attachment model
(`pref` in Matlab toolbox CONTEST)

number of nodes: $n = 1000, 2000, \ldots, 5000$

$\Rightarrow$ the adjacency matrices of the corresponding Cartesian product graphs $\mathcal{G}_i$ have dimension ranging between one and twenty-five millions

$\Rightarrow$ All the resulting matrices are symmetric indefinite

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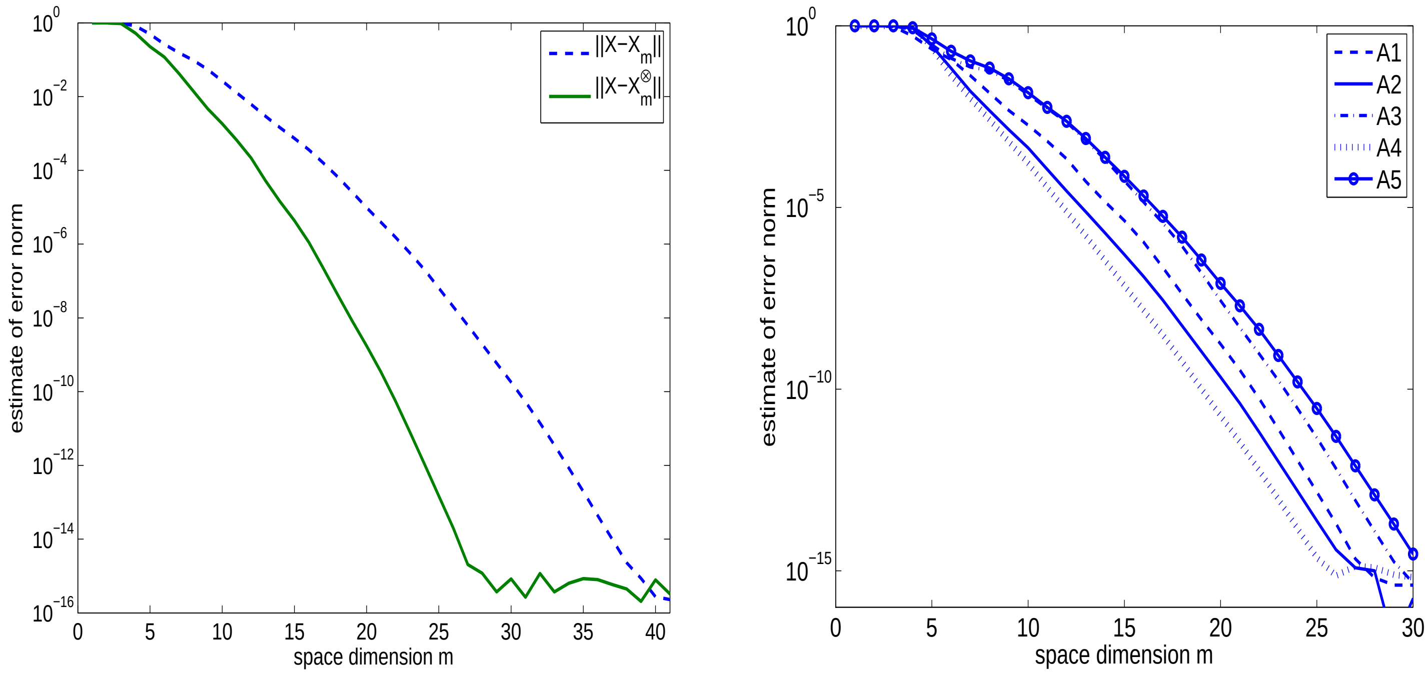
An example from graph and network analysis. Cont'd

CPU time to construct an approximation space of dimension $m = 30$:

n	CPU Time $K_m(M_1, b_1)$	CPU Time $K_m(\mathcal{A}, b)$
1000	0.02662	29.996
2000	0.04480	189.991
3000	0.06545	–
4000	0.90677	–
5000	0.99206	–

An example from graph and network analysis. Cont'd

Convergence history to $\exp(\mathcal{A})b$



Left: case $n = 1000$

Right: convergence history for all five cases

Convergence for standard Krylov approximation. $\mathcal{A} = M \otimes I + I \otimes M$

$\lambda_{\min}$, $\lambda_{\max}$ extreme eigenvalues of M, and $\widehat{\kappa} = \frac{\lambda_{\max}+\lambda_{\min}}{\lambda_{\min}+\lambda_{\min}}$

- ⋆ For Cauchy-Stieltjes functions

$$\|f(\mathcal{A})v - x_m^{\otimes}\| = \mathcal{O}\left(\exp\left(-\frac{2m}{\sqrt{\widehat{\kappa}}}\right)\right)$$

for m and $\widehat{\kappa}$ large enough

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$$\|f(\mathcal{A})v - x_m^{\otimes}\| \le C\left(\frac{\sqrt{\widehat{\kappa}}-1}{\sqrt{\widehat{\kappa}}+1}\right)^m$$

with C computable and depending on f and M.

(for $\widehat{\kappa}$ large the two bounds are equivalent)

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Faster rate of convergence than for $f(\mathcal{A})b$ *and* $f(M)b_1$

More bounds for extended and rational Krylov approximation spaces

Conclusions and outlook

- Exploring/Exploiting structure is beneficial
- Generalization to d-Kronecker sum is possible, e.g.,

$$\mathcal{A} = M \otimes I \otimes I + I \otimes M \otimes I + I \otimes I \otimes M$$

- Possibility of using quasi-sparsity information in applications ?
  (already done for $f(x) = x^{-1}$)

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