Matrix exponential

Note Title 2023-03-28

$$\exp(A) = I + A + \frac{1}{2}A^2 + \frac{1}{3!}A^3 + \dots$$

⚠ expm in Matlab, ~~not~~ exp

The solution of the initial value problem

$$\frac{d}{dt} v(t) = A v(t) \qquad v(0) = v_0$$

is $\quad v(t) = \exp(tA) v_0$

Proof: differentiate term-by-term

$$\frac{d}{dt} v(t) = \frac{d}{dt}\left(v_0 + tAv_0 + \frac{t^2A^2}{2} v_0 + \frac{t^3A^3}{3!} v_0 + \dots \right)$$

$$= 0 + Av_0 + tA^2 v_0 + \frac{\cancel{3}t^2}{\cancel{3!}_{\,2}} A^3 v_0 + \dots = A v(t).$$

One can use methods to solve the differential equation to compute $\exp(A)$. For instance,
$$\begin{cases} X(0) = I \\ \frac{d}{dt} X(t) = AX(t) \end{cases} \qquad X(t) \in \mathbb{C}^{n\times n}$$

has solution $X(t) = \exp(At)$.

$$\frac{X_{m+1} - X_m}{h} = AX_m$$

$$X_{m+1} = X_m + hAX_m$$

This produces $\exp(A) \approx \left(I + \frac{1}{m}A\right)^m$.

Remark: $\exp(A+B) \neq \exp(A)\exp(B)$ in general!

It only holds if A, B commute with each other, $AB = BA$

How do we compute $\exp(A)$?

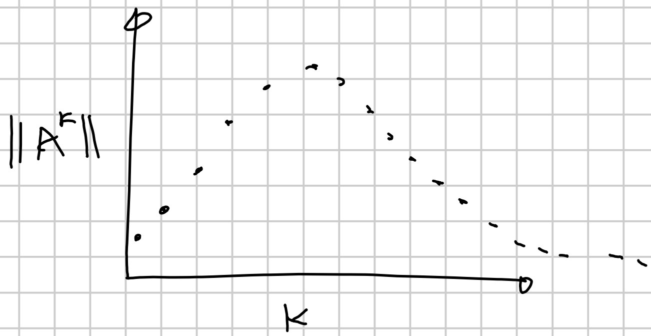
Problem for methods based on series such as $I + A + \frac{A^2}{2} + \dots$:

intermediate growth of terms. Even if $\lim_{k\to\infty} A^k = 0$,

the intermediate powers might grow. E.g.

$$A = \begin{bmatrix} 0 & M & 0 & 0 \\ 0 & 0 & M & 0 \\ 0 & 0 & 0 & M \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad A^2 = \begin{bmatrix} 0 & 0 & M^2 & 0 \\ & 0 & 0 & M^2 \\ & & 0 & 0 \\ & & & 0 \end{bmatrix} \qquad A^3 = \begin{bmatrix} 0 & 0 & 0 & M^3 \\ & 0 & 0 & 0 \\ & & 0 & 0 \\ & & & 0 \end{bmatrix} \qquad A^4 = 0$$

For many matrices, the plot of $\|A^k\|$ vs. k has a hump



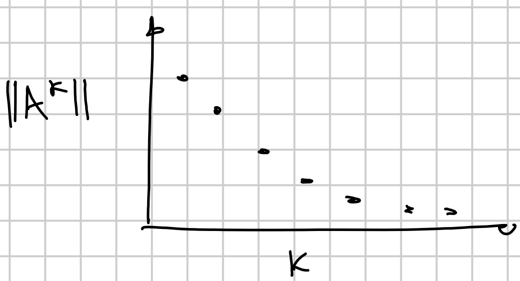
In general, we can bound

$$\|\exp(A)\| = \left\| I + A + \frac{A^2}{2} + \frac{A^3}{3!} + \dots \right\| \le \|I\| + \|A\| + \frac{\|A\|^2}{2} + \frac{\|A\|^3}{3!} + \dots = e^{\|A\|}$$

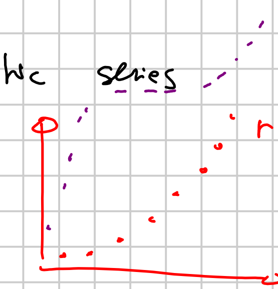
but the bound will be very loose, and there will be lots of cancellation if we sum the series term by term

Exception: normal matrices: if $A = QDQ^*$ with Q orthogonal,

$$\|A^k\|_2 = \|QD^kQ^*\|_2 = \|D^k\|_2 = \max_\lambda |\lambda^k| = \|A\|_2^k$$



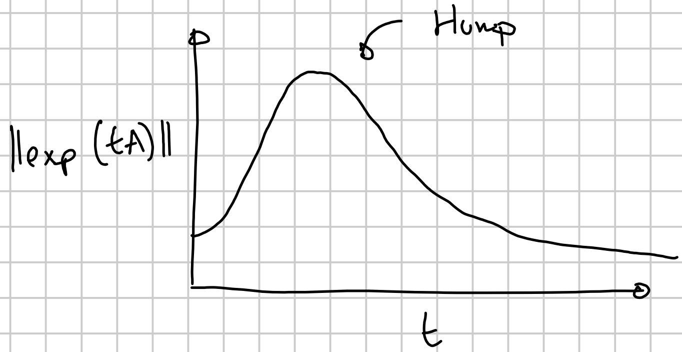
& geometric series r^k



This "hump phenomenon" is present also for $\exp(tA)$ vs. t

Even when $\Lambda(A) \subset LHP$ and $\lim_{t\to\infty} \exp(tA) = 0$,

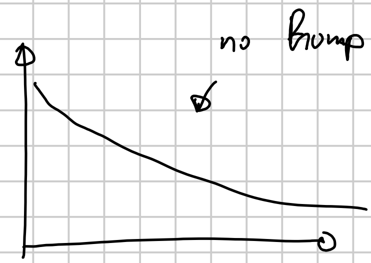
there might be intermediate growth:



For a normal matrix, $A = QDQ^*$

$$\|\exp(tA)\|_2 = \|Q\exp(tD)Q^*\|_2 = \|\exp(tD)\|_2 = \max_{\lambda} |e^{t\lambda}|$$

$$= e^{\max_{\lambda} \mathrm{Re}(t\lambda)} \underset{\text{if } t>0}{=} \left(e^{\max_{\lambda} \mathrm{Re}(\lambda)}\right)^t = \|\exp(A)\|^t$$



Fréchet derivative and conditioning

$$\exp(A+E) = I + (A+E) + \frac{1}{2}(A^2 + AE + EA + E^2) + \frac{1}{3!}(A^3 + A^2E + AEA + EA^2 + \dots) + \dots$$

$$= \exp(A) + \underbrace{\sum_{k=1}^{\infty} \frac{1}{k!}\left(A^{k-1}E + A^{k-2}EA + A^{k-3}EA^2 + \dots + EA^{k-1}\right)}_{L_{\exp,A}[E]} + o(\|E\|)$$

$$L_{\exp,A}[E] = \sum_{i,j=0}^{\infty} \frac{1}{(i+j+1)!} A^i E A^j$$

Integral version:

Lemma:

$$L_{\exp,A}[E] = \int_0^1 \exp(A(1-t))\, E\, \exp(A t)\, dt$$

Proof:

$$\text{RHS} = \int_0^1 \left(\sum_{i=0}^{\infty} \frac{1}{i!} A^i (1-t)^i\right) \cdot E \left(\sum_{j=0}^{\infty} \frac{1}{j!} A^j t^j\right) dt$$

$$= \sum_{i,j=0}^{\infty} A^i E A^j \cdot \underbrace{\boxed{\frac{1}{i!\,j!}\int_0^1 (1-t)^i t^j \, dt}}_{= \frac{1}{(i+j+1)!}} = L_{\exp,A}[E]$$

classical, related to Beta functions

$\square$

In particular,

$$\|L_{\exp,A}[E]\| = \left\| \int_0^1 \exp(A(1-t))\, E \exp(At)\, dt \right\|$$

$$\leq \int_0^1 \|\exp(A(1-t))\| \cdot \|E\| \cdot \|\exp(At)\| \, dt$$

$$\leq \int_0^1 e^{\|A(1-t)\|} \cdot \|E\| \cdot e^{\|At\|} \, dt$$

$$= \|E\| \int_0^1 e^{\|A\|(1-t)} \cdot e^{\|A\| t} \, dt = \|E\| \int_0^1 e^{\|A\|} dt = \|E\| \cdot e^{\|A\|}$$

$$K_{rel}(\exp, A) = \frac{\|L_{\exp,A}\| \cdot \|A\|}{\|\exp(A)\|} \leq \boxed{\frac{e^{\|A\|}}{\|\exp(A)\|}} \cdot \|A\|$$

this can be $\gg 1$, leading to ill-conditioning

Ex. $\quad A = \begin{bmatrix} 0 & 30 \\ -30 & 0 \end{bmatrix} \qquad K_{rel}(\exp, A) \approx 10^{14}$

For normal matrices, we can replace $\|\exp(At)\| \leq e^{\|A\| t}$

with $\|\exp(At)\| = \|\exp(A)\|^t$,

and we obtain $\|L_{\exp,A}[E]\| \leq \|\exp(A)\| \cdot \|E\|$

and $K_{rel}(\exp, A) \leq \|A\|$.

Towards Matlab's expm.

<u>Padé approximants</u>

The <u>Padé approximant</u> to a function $f(x)$ (in 0) of degrees (p,q) is a rational function

$r(x) \doteq \dfrac{n(x)}{d(x)}$, with $\deg n = p$, $\deg d = q$, such that

$$f(x) - \frac{n(x)}{d(x)} = O\left(x^{p+q+1}\right) \quad \text{when } x \to 0.$$

In other words, the Maclaurin expansion of $r(x) = \dfrac{n(x)}{d(x)}$

$$= \underline{a_0} + \underline{a_1} x + \underline{a_2} x^2 + \dots + \underline{a_{p+q}} x^{p+q} + a_{p+q+1} x^{p+q+1} + \dots$$

has the first $p+q+1$ coefficients that match those of the Maclaurin expansion of $f(x)$

Note that a rational function $\dfrac{n(x)}{d(x)}$ has $(p+1)+(q+1)$ coefficients, minus 1 degree of freedom for common scaling (e.g., we can assume that $d(x)$ is monic); so the degrees of freedom are those that I would need to "match" $p+q+1$ coefficients.

<u>Matlab example</u>: compute the $p=q=2$ Padé approximant, by solving the system obtained imposing that the first 5 coefficients of $\exp(x) \cdot d(x) - n(x)$ are 0,

i.e., $\quad e^x n(x) - d(x) = O(x^5)$

$$n(x) = x^2 + 6x + 12$$
$$d(x) = x^2 - 6x + 12$$

Padé approximants for $\exp(x)$ are known in closed form

For $p=q$:

$$N_{pq}(x) = \sum_{j=0}^{p} \frac{(2p-j)!\,p!}{(2p)!\,j!\,(p-j)!} x^j$$

$$D_{pq}(x) = N(-x)$$

Rational approximants often work better in approximation theory because they match the behavior of $f(x)$ in a larger region.

Next lecture: we are interested in finding a sort of "backward error" of these Padé approximants: write

$$[d(A)]^{-1} n(A) = \exp(A+H),$$

and bound the norm of $\mathbf{H}$.

If we manage to bound $\|H\|/\|A\| \leq u = 2.2 \cdot 10^{-16}$,

then the error $\exp(A) - [d(A)]^{-1} n(A)$ is of the same order of magnitude as the one induced by machine-number approximation $\tilde{A} = fl(A)$

We will see that this inequality holds for $\|A\| \leq 5.4$, when one takes Padé approximants with $p = q = 13$.

13 is chosen because of convenience with the number of products required for polynomials

$$N(x) = A(x^2)x + B(x^2)$$

$$D(x) = -A(x^2)x + B(x^2)$$

with A, B of degree 6

For a matrix A one can compute $\overset{①}{A^2}, \overset{②}{A^3},$

$$a_0 + a_1 A + \dots + a_6 A^6 = \underbrace{a_0 + a_1 A + a_2 A^2 + a_3 A^3} + \overset{③}{A^3} \underbrace{(a_4 A + a_5 A^2 + a_6 A^3)}$$

$$b_0 + \dots + b_6 A^6 = \underbrace{b_0 + \dots + b_3 A^3}_{} + \underset{4}{A^3}\left(b_4 A + \dots + b_6 A^3\right)$$