Lanczos-like method for the time-ordered exponential

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MAT TRIAD
September 9, 2019
Let \( t' \geq t \in I \subseteq \mathbb{R} \), \( A(t') \) a time dependent matrix. The \textbf{time-ordered exponential} is the unique solution \( U(t', t) \) of the system of coupled linear differential equations

\[
A(t')U(t', t) = \frac{d}{dt'} U(t', t), \quad U(t, t) = \text{Id}.
\]

If \( A(\tau_1)A(\tau_2) = A(\tau_2)A(\tau_1) \) for all \( \tau_1, \tau_2 \in I \), then

\[
U(t', t) = \exp \left( \int_t^{t'} A(\tau) \, d\tau \right).
\]

Otherwise, \( U \) has \textbf{no known explicit form in terms of} \( A \). It can be denoted by the time-ordering operator \( \mathcal{T} \) as

\[
U(t', t) = \mathcal{T} \exp \left( \int_t^{t'} A(\tau) \, d\tau \right).
\]

[Dyson, 1952]
The time-ordering expression is more a notation than an explicit form as the action of the time-ordering operator is very difficult to evaluate.

- **Applications:** System dynamics (quantum physics); e.g., [Blanes & al., 2009]. Differential Riccati matrix equations (control theory, filter design); e.g., [Abou-Kandil et al., 2003].

- **Classical approaches** Magnus series [Magnus, 1954]: infinite series of increasing complexity (small convergence domain). Using Floquet theory: For A periodic, the solution is given in terms of a infinite system. See, e.g., [Blanes & al., 2009].

- **Path-sum approach:** Based on the *path-sum* decomposition of the graph whose A is the adjacency matrix [Giscard & al., 2015]. The expression has a finite number of terms, but it may be too complicate.
Outline

2. *-Lanczos algorithm for time-ordered exponentials.
3. Examples and outlook.

Warning 1:

*-Lanczos works on the space of complex generalized functions on \( I \times I \). We will not deal with approximations and finite-precision arithmetic. Our main goal is to give an exact expression for \( U \) in a finite number of steps.

Warning 2:

Rounding errors deeply effects (classical) Lanczos by loss of orthogonality. We expect a similar behavior in any numerical implementation of *-Lanczos. This must be investigated before confidently rely on the method in a computational setting.
Let $t' \geq t$ and let $A_1(t', t)$ and $A_2(t', t)$ be (doubly) time-dependent matrices. We define the convolution-like product

$$(A_2 \ast A_1)(t', t) := \int_t^{t'} A_2(t', \tau)A_1(\tau, t) \, d\tau.$$ 

Consider the $\ast$-resolvent

$$R_\ast(A) := (\text{Id}1_\ast - A)^{\ast-1} = \text{Id}1_\ast + \sum_{k \geq 1} A^{\ast k}$$

(it exists if every entry of $A$ is bounded for $t', t \in I$). Then

$$U(t', t) = \int_t^{t'} R_\ast(A)(\tau, t) \, d\tau,$$

with $1_\ast = \delta(t' - t)$ the Dirac delta function; [Giscard & al., 2015].
If we look at $A$ as the adjacency matrix of the graph $G$ with time-dependent weights, then the $(i,j)$ element of the $\ast$-resolvent, $(R_\ast)_{ij}$, can be rewritten in terms of the simple paths from $i$ to $j$ in $G$; [Giscard & al., 2015].

This approach provides exact solutions and it is convergent when $R_\ast$ exists. However, it suffers from drawbacks:

- It requires to find all the simple cycles and simple paths of the graph $G$ (computationally expensive);
- The expression for $U$ may be too complicated due to the structure of the graph $G$. 
We want to get a matrix $T$ so that

- $T$ is tridiagonal, i.e., it corresponds to a graph which is a path (with self-loops);
- $R_*(T)_{11} = R_*(A)_{ij}$, i.e., they have the same $*$-moments

\[(T^{*k})_{11} = (A^{*k})_{ij}, \quad k = 0, 1, 2, \ldots.\]

In the simple case in which $A$ is time-independent, a $T$ with analogous properties is given as the output of the last iteration of the Lanczos algorithm.

We will derive a Lanczos-like method based on an $*$-orthogonalization process.
Recall: Non-Hermitian Lanczos algorithm

Let $A$ be a time-independent matrix and $v, w$ time-independent vectors. Our goal is to approximate

$$w^H \exp(A) v.$$

Consider the Krylov subspaces

$$\text{span}\{v, Av, \ldots, A^{n-1}v\}, \quad \text{span}\{w, A^Hw, \ldots, (A^H)^{n-1}w\}.$$ 

Assuming not breakdowns, the non-Hermitian Lanczos computes the matrices

$$V_n = [v_0, \ldots, v_{n-1}], \quad W_n = [w_0, \ldots, w_{n-1}]$$

respectively basis of the Krylov subspaces, so that $W_n^H V_n = \text{Id}$. 
The tridiagonal matrix defined as

$$T_n = W_n^H A V_n,$$

satisfies the matching moment property

$$w^H A^k v = e_1^H T_n^k e_1, \quad k = 0, \ldots, 2n - 1.$$

Hence we get the approximation (model reduction)

$$w^H \exp(A) v \approx e_1^H \exp(T_n) e_1;$$

e.g., [Golub, Meurant, 2010].

In particular, for $n$ equal to the size of $A$ minus 1 (or for lucky or incurable breakdowns) we get exactness.
Now, $A(t')$ is time-dependent and we want to approximate the $i,j$ element of the time-ordered exponential of $A$, i.e.,

$$U(t', t)_{i,j} = e^{H} T \exp \left( \int_{t}^{t'} A(\tau) d\tau \right) e_j = \int_{t}^{t'} e^{H} R_{*}(A)(\tau, t) e_j d\tau.$$  

Hence we want to approximate the value

$$w^{H} R_{*}(A)(t', t) v,$$

with $v, w$ time-independent vectors.
Given the distributions $\alpha_0(t', t), \ldots, \alpha_k(t', t)$ (coefficients),

\[
\text{matrix } *\text{-polynomial: } p(A)(t', t) := \sum_{j=0}^{k} (A^* j * \alpha_j)(t', t),
\]

\[
\text{dual } *\text{-polynomial: } p^D(A)(t', t) := \sum_{j=0}^{k} (\overline{\alpha}_j * (A^* j)^H)(t', t),
\]

and hence the time-dependent Krylov subspaces as

\[
\mathcal{K}_n(A, v)(t', t) := \{ (p(A)v) \mid p \text{ of degree } \leq n - 1 \},
\]

\[
\mathcal{K}_n^D(A^H, w)(t', t) := \left\{ \left( w^H p^D(A^H) \right) \mid p \text{ of degree } \leq n - 1 \right\}.
\]

Note: To work with distribution we need to set $A(t', t) = \tilde{A}(t') \Theta(t' - t)$ and generalize the definition of $*$. 
Building up the $\ast$-Lanczos process

We aim to build basis for $\mathcal{K}_n(A, \mathbf{v})$ and $\mathcal{K}^D_n(A^H, \mathbf{w})$

$$V_n = [\mathbf{v}_0, \ldots, \mathbf{v}_{n-1}], \quad W_n^H = [\mathbf{w}_0, \ldots, \mathbf{w}_{n-1}]^H$$

which are $\ast$-biorthonormal, i.e.,

$$W_n^H \ast V_n = I_1\ast.$$ 

Assuming $\mathbf{w}^H \mathbf{v} = 1$, the first vectors are

$$\mathbf{v}_0 = \mathbf{v} 1_\ast, \quad \mathbf{w}_0^H = \mathbf{w}^H 1_\ast.$$
Building up the $\ast$-Lanczos process

Consider a vector $\hat{\mathbf{v}}_1 \in \mathcal{K}_2(A, \mathbf{v})$

$$\hat{\mathbf{v}}_1 = A \ast \mathbf{v}_0 - \mathbf{v}_0 \ast \alpha_0 = A\mathbf{v} - \mathbf{v}\alpha_0.$$

Under the condition $\mathbf{w}_0^H \ast \hat{\mathbf{v}}_1 = 0$, we get

$$\alpha_0 = \mathbf{w}_0^H \ast A \ast \mathbf{v}_0 = \mathbf{w}^H A \mathbf{v} \quad (1)$$

Similarly,

$$\hat{\mathbf{w}}_1^H = \mathbf{w}_0^H \ast A - \alpha_0 \ast \mathbf{w}_0^H = \mathbf{w}^H A - \alpha_0 \mathbf{w}^H,$$

with $\alpha_0$ given by (1).
Building up the $\ast$-Lanczos process

The condition

$$w_1^H \ast v_1 = 1_\ast,$$

is satisfied defining

$$v_1 = \hat{v}_1 \ast (\beta_1)^{-1}, \quad w_1 = \hat{w}_1,$$

with

$$\beta_1 = \hat{w}_1^H \ast \hat{v}_1 = w^H A^2 v - \alpha_0^2.$$

- We assume $\beta_1 \ast$-invertible;
- We proved that every non-identically null holonomic (D-finite) function is invertible.
By induction, consider the vector

$$\hat{v}_n = A \ast v_{n-1} - \sum_{i=0}^{n-1} v_i \ast \gamma_i.$$ 

The condition $$w_j^H \ast \hat{v}_n = 0$$ for $$j = 0, \ldots, n-1$$ gives

$$\gamma_j = w_j^H \ast A \ast v_{n-1}, \quad j = 0, \ldots, n-1.$$ 

Since $$w_j^H \ast A \in K_{j+1}^D(A^H, w)$$ we get

$$\gamma_j = 0, \quad j = 0, \ldots, n-3.$$
Building up the $*$-Lanczos process

Assuming $v_{-1} = w_{-1} = 0$, we get the three-term recurrences

\[
\begin{align*}
  w_n^H &= w_{n-1}^H * A - \alpha_{n-1} * w_{n-1}^H - \beta_{n-1} * w_{n-2}^H, \\
  v_n * \beta_n &= A * v_{n-1} - v_{n-1} * \alpha_{n-1} - v_{n-2},
\end{align*}
\]

with the coefficients given by

\[
\alpha_{n-1} = w_{n-1}^H * A * v_{n-1}, \quad \beta_n = w_n^H * A * v_{n-1}.
\]

- If $\beta_n$ is not $*$-invertible we have a breakdown;
- We assume no breakdowns in this first study;
- The algorithm converges whenever $v_n = 0$ or $w_n = 0$ (lucky breakdown).
**Lanczos Algorithm**

Initialize: \( \mathbf{v}_{-1} = \mathbf{w}_{-1} = 0, \mathbf{v}_0 = \mathbf{v}_1^* \), \( \mathbf{w}_0^H = \mathbf{w}_1^H \).

\[ \alpha_0 = \mathbf{w}^H A \mathbf{v}, \]
\[ \mathbf{w}_1^H = \mathbf{w}^H A - \alpha_0 \mathbf{w}^H, \]
\[ \hat{\mathbf{v}}_1 = A \mathbf{v} - \mathbf{v} \alpha_0, \]
\[ \beta_1 = \mathbf{w}^H A^2 \mathbf{v} - \alpha_0^2, \]

If \( \beta_1 \) is not \( * \)-invertible, then stop, otherwise,
\[ \mathbf{v}_1 = \hat{\mathbf{v}}_1 * \beta_1^{-1}. \]

For \( n = 2, \ldots \)

\[ \alpha_{n-1} = \mathbf{w}_{n-1}^H * A * \mathbf{v}_{n-1}, \]
\[ \mathbf{w}_n^H = \mathbf{w}_{n-1}^H * A - \alpha_{n-1} * \mathbf{w}_{n-1}^H - \beta_{n-1} * \mathbf{w}_{n-2}^H, \]
\[ \hat{\mathbf{v}}_n = A * \mathbf{v}_{n-1} - \mathbf{v}_{n-1} * \alpha_{n-1} - \mathbf{v}_{n-2}, \]
\[ \beta_n = \mathbf{w}_n^H * A * \mathbf{v}_{n-1}, \]

If \( \beta_n \) is not \( * \)-invertible, then stop, otherwise,
\[ \mathbf{v}_n = \hat{\mathbf{v}}_n * \beta_n^{-1}. \]

end.
Tridiagonal matrix

\[ T_n := \begin{bmatrix}
\alpha_0 & 1_* \\
\beta_1 & \alpha_1 & \ddots \\
\vdots & \ddots & \ddots & 1_* \\
\beta_{n-1} & \alpha_{n-1}
\end{bmatrix}, \]

and \( V_n := [v_0, \ldots, v_{n-1}] \) and \( W_n := [w_0, \ldots, w_{n-1}] \). Then

\[ A \ast V_n = V_n \ast T_n + (v_n \ast \beta_n)e_n^H 
\]

\[ W_n^H \ast A = T_n \ast W_n^H + e_n w_n^H. \]

Hence \( T_n \) is the \( \ast \)-projection of \( A \) onto \( \mathcal{K}_n(A, v) \) along the direction of \( \mathcal{K}_n^D(A^H, w) \), i.e.,

\[ T_n = W_n^H \ast A \ast V_n. \]
Matching moment

Matching moment property

Let $A, \mathbf{w}, \mathbf{v}$ and $T_n$ be as described above, then

$$
\mathbf{w}^H (A^* k) \mathbf{v} = e_1^H (T_n^* k) e_1, \quad \text{for} \quad k = 0, \ldots, 2n - 1.
$$

In particular, for $n$ equal to the size of $A$ minus 1 we get

$$
\mathbf{w}^H (A^* k) \mathbf{v} = e_1^H (T_n^* k) e_1, \quad \text{for} \quad k = 0, 2, \ldots,
$$

and, hence,

$$
\mathbf{w}^H R_*(A) \mathbf{v} = e_1^H R_*(T_n) e_1.
$$
Consider the time-ordered exponential $U_n$ given by

$$T_n(t', t)U_n(t', t) = \frac{d}{dt'} U_n(t', t).$$

The matching moment property justify the use of the approximation

$$w^H U(t', t)v \approx e_1^H U_n(t', t) e_1 = e_1^H \int_t^{t'} R_*(T_n)(\tau, t) d\tau e_1.$$

The path-sum method gives the finite $*$-continued fraction

$$R_*(T_n)_{11} = \left(1_* - \alpha_0 - (1_* - \alpha_1 - (\cdots * \beta_{n-1})^{*-1} \cdots * \beta_2)^{*-1} * \beta_1 \right)^{*-1},$$

Error bound?

Conjecture

If the entries of $A(t')$ are smooth, then the $*$-Lanczos coefficients $\alpha_j$ and $\beta_j$ are (usual) functions.

Proposition

Under the previous conjecture, the approximation error of the $n$th $*$-Lanczos can be bound by

$$
\left| w^H U(t', t) v - \int_t^{t'} R_*(T_n)_{1,1}(\tau, t) d\tau \right| \leq (C^{2n} + D_n^{2n}) \frac{(t' - t)^{2n}}{(2n)!},
$$

with the finite coefficients

$$
C := \sup_{t' \in I} \| \tilde{A}(t') \|_\infty, \quad D_n := \sup_{t', t \in I} \max_{0 \leq j \leq n-1} \{ |\tilde{\alpha}_j(t', t)|, |\tilde{\beta}_j(t', t)| \}.
$$
Consider the matrix

\[
A = \begin{pmatrix}
\cos(t') & 0 & 1 & 2 & 1 \\
0 & \cos(t') - t' & 1 - 3t' & t' & 0 \\
0 & t' & 2t' + \cos(t') & 0 & 0 \\
0 & 1 & 2t' + 1 & t' + \cos(t') & t' \\
t' & -t' - 1 & -6t' - 1 & 1 - 2t' & \cos(t') - 2t'
\end{pmatrix}
\]

The matrix does not commute with itself at different times and the corresponding differential system has no known analytical solution.
Example: time-dependent matrix

We get

\[ T_5 = \begin{pmatrix}
\cos(t')\Theta & \delta & 0 & 0 \\
\frac{1}{2}(t'^2 - t^2)\Theta & \cos(t)\Theta & \delta & 0 \\
0 & t(t' - t)\Theta & \tilde{\alpha}_2(t', t)\Theta & \delta \\
0 & 0 & -\frac{1}{2}(3t^2 - 4tt' + t'^2)\Theta & \tilde{\alpha}_3(t', t)\Theta \\
0 & 0 & 0 & (-2t^2 + 3tt' - t'^2)\Theta & \tilde{\alpha}_4(t', t)\Theta \\
\end{pmatrix}, \]

with

\[
\tilde{\alpha}_2(t', t) = (t' - t)\sin(t) + \cos(t), \\
\tilde{\alpha}_3(t', t) = \frac{1}{2} \left( 4(t' - t)\sin(t) - \left( (t - t')^2 - 2 \right) \right) \cos(t), \\
\tilde{\alpha}_4(t', t) = \frac{1}{6} \left( (t - t')^2 - 18 \right) (t - t')\sin(t) + \left( 6 - 9(t - t')^2 \right) \cos(t),
\]

Here \( \Theta = \Theta(t' - t) \) (Heaviside function) and \( \delta = \delta(t' - t) \) (Dirac delta function).
With the $*$-biorthonormal basis

$$V_5 = \begin{pmatrix}
\delta & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \delta^{(3)} & -2\delta^{(4)} \\
0 & 0 & \delta'' & -\delta^{(3)} & \delta^{(4)} \\
0 & \delta' & -2\delta'' & 2\delta^{(3)} & -3\delta^{(4)} \\
0 & 0 & 0 & 0 & \delta^{(4)}
\end{pmatrix},$$

and

$$W_5^H = \begin{pmatrix}
\delta & 0 & 0 & 0 & 0 \\
0 & 0 & \Theta & 2\Theta & \Theta \\
0 & (t' - t)\Theta & (t' - t)\Theta & (t' - t)\Theta & 0 \\
0 & \frac{1}{2}(t - t')^2\Theta & (t - t')^2\Theta & 0 & 0 \\
0 & 0 & -\frac{1}{6}(t - t')^3\Theta & 0 & 0
\end{pmatrix}.$$
Summarizing

-Lanczos is able to express the solution of a coupled linear differential equations with non-constant coefficients. It presents several difficulties (*-inverses, integral solutions, ...). Nevertheless,

- It is convergent in a finite number of steps;
- It express the solution with a finite formulation (as the path-sum method);
- It admits an expression in terms of a simple finite continued fraction.

Such a general approach has been so far out of reach.
There exists an isometry $\Phi$ between the algebra of generalized functions depending on two time variables and the algebra of “time continuous” operators (for which the time variables $t'$ and $t$ serve as line and row indices).

Once time is discretized, $\Phi$ sends the $\ast$-product to the ordinary matrix product. Most importantly, $\Phi$ sends usual functions of two times ($f(t', t) = \tilde{f}(t', t)\Theta(t', t)$) to lower triangular matrices, the matrix inverse of which is the image under $\Phi$ of the $\ast$-inverse of $f(t', t)$.

This is a natural time-discretization strategy that we will investigate in a future work.
Other open issues

- Convergence properties of the approximation (conjecture);
- Breakdown and near-breakdown issues;
- Computational approach: loss of orthogonality, reorthogonalization, stability, inexact approaches, better error estimates, . . . ;
- Numerical tests;
- Application of this *-strategy to other analogous problems.

More information:
Other open issues

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- Computational approach: loss of orthogonality, reorthogonalization, stability, inexact approaches, better error estimates, . . . ;
- Numerical tests;
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More information:

Thank you for your attention!