A novel approach to solving ordinary differential equations: The $\star$-product framework

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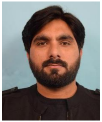

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How to solve an ODE

(Thanks to Fabio Durastante)

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today's fun math fact

Traduci post

We want to solve the differential equation

$$f' = f.$$

To do this rewrite it as an integral equation

$$f = \int f,$$

rearrange a bit

$$f - \int f = 0.$$

Collecting like terms

$$\left(1 - \int\right) f = 0,$$

then dividing on both sides

$$f = \left(1 - \int\right)^{-1} 0$$

Since we know that $(1-x)^{-1} = 1 + x + x^2 + \dots$ then

$$f = \left(1 + \int + \int\int + \dots\right) 0 = 0 + C + Cx + C\frac{x^2}{2} + C\frac{x^3}{6} + \dots,$$

which is just the Taylor series for e^x so

$$f(x) = Ce^x,$$

as required.

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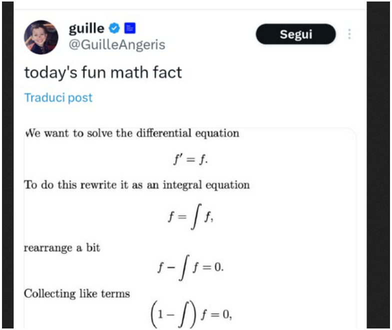
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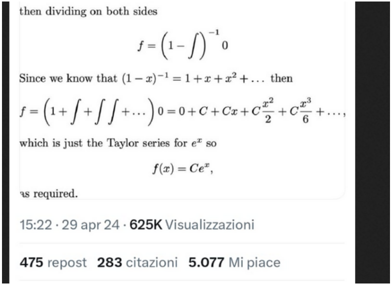
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- This makes sense once correctly formalized.
- It gives a new expression for the solution of DEs.

Motivation

Why a new approach?

- New explicit solutions for systems of non-autonomous ODEs (Bloch-Siegert Hamiltonian, Integral Series for Heun Functions, time-evolution of quantum spin systems). Works by Giscard, Bonhomme, Foroozandeh, and Tamar.
- Quasi-normal modes (black holes): find ω so that

$$\alpha(t,\omega)u''(t) + \beta(t,\omega)u'(t) + \gamma(t,\omega)u(t) = 0$$

  has a solution for some given boundary conditions. Work in progress by Mazza and P.
- Fractional differential equations. Where the derivative is fractional (Caputo). Work in progress by Durastante, Giscard, and P.

Numerical computations: Shrödinger equation

In Nuclear Magnetic Resonance (NMR) applications, the quantum dynamic of particles is described by the Schrödinger equation

$$\hbar \frac{\partial |\Psi\rangle}{\partial t} = -iH|\Psi\rangle,$$

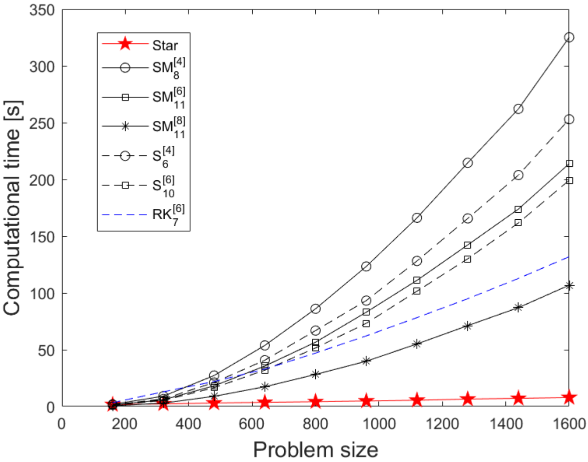
with H the (time-dependent) Hamiltonian and Ψ the wave function.

- Simulations are of great importance. They provide benchmarks for studies of new materials, and the development of new magnetic fields.
- H size increases exponentially with the number of particles.
- H is sparse and structured (Kronecker).

Extended Rosen-Zener model

- The Rosen-Zener (RZ) model [Rosen, Zener, 1932] is of the highest importance as representative of two-level quantum systems.
- Important in Nuclear Magnetic Resonance (NMR) [Silver, Joseph, Hoult, 1984; Hioe, 1984] and Magnetic Resonance Imaging (MRI) [Zhang, Garwood et al., 2017].
- In [Koyseva et al., 2007; Vitanov, 2010] the RZ model was extended to multiple degenerate sets of states in the framework of quantum-state engineering $\rightarrow$ Large-size ODE.
- The extended RZ model has been used as a test model for numerical solvers of non-autonomous evolutions equations [Blanes, Casas, Thalhammer, 2017; Blanes, Casas, Murua, 2017; Auzinger et al., 2019; Bader et al., 2022]

A new (linear scaling) algorithm



Approach outline

Problem	Linear ODE
↓	
New solution expression	$\star$-product
↓	
Discretization	Legendre polynomials
↓	
Matrix problem	Kronecker, low rank
↓	
Numerical solution	Iterative methods

The $\star$-product

Given convenient bivariate functions $f_1(t,s), f_2(t,s)$ on an interval I, the $\star$-product is defined as [Giscard, P., Ryckebusch]

$$(f_2 \star f_1)(t,s) := \int_I f_2(t,\tau) f_1(\tau,s) \, \mathrm{d}\tau.$$

It generalizes

- Convolution
- Volterra compositions
- the matrix product
- ...

The Heaviside function

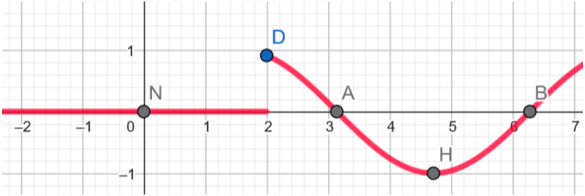
Consider the set $\mathcal{A}_\Theta(I)$ of the functions of the kind

$$f(t,s) = \tilde{f}(t,s)\Theta(t-s),$$

where

$$\Theta(t-s) = \begin{cases} 1, & t \geq s, \\ 0, & t < s \end{cases}$$

is the Heaviside function and $\tilde{f}$ is analytic in $t, s \in I$.



$$f(t,s) = \sin(t)\Theta(t-s), \; s = 2$$

An example

Let's $\star$-multiply the following functions:

$$ts\Theta(t-s) \text{ and } ts^2\Theta(t-s)$$

An example

Let's $\star$-multiply the following functions:

$$ts\Theta(t-s) \text{ and } ts^2\Theta(t-s)$$

$$\begin{aligned}
ts\Theta(t-s) \star ts^2\Theta(t-s) &= \int_I t\tau\Theta(t-\tau)s^2\tau\Theta(\tau-s)\mathrm{d}\tau \\
&= ts^2 \int_I \tau^2\Theta(t-\tau)\Theta(\tau-s)\mathrm{d}\tau \\
&= ts^2\Theta(t-s)\int_s^t \tau^2\mathrm{d}\tau \\
&= \frac{1}{3}ts^2(t^3-s^3)\Theta(t-s).
\end{aligned}$$

The set $\mathcal{A}_\Theta(I)$ is closed under $\star$-multiplication.

Let's compute

$$\Theta^{\star 2} := \Theta(t-s) \star \Theta(t-s)$$

$\star$-powers

Let's compute

$$\Theta^{\star 2} := \Theta(t-s) \star \Theta(t-s)$$

$$\begin{aligned}\Theta^{\star 2} &= \int_I \Theta(t-\tau)\Theta(\tau-s)\mathrm{d}\tau \\ &= \Theta(t-s)\int_s^t \mathrm{d}\tau \\ &= (t-s)\Theta(t-s)\end{aligned}$$

$$
\begin{aligned}
\Theta^{\star 3} &= \int_I (t-\tau)\Theta(t-\tau)\Theta(\tau-s)\mathrm{d}\tau \\
&= \Theta(t-s)\int_s^t t-\tau \mathrm{d}\tau \\
&= \left[t(t-s)-\frac{1}{2}(t^2-s^2)\right]\Theta(t-s) \\
&= \frac{1}{2}\left[t^2-2ts+s^2\right]\Theta(t-s) \\
&= \frac{1}{2}(t-s)^2\Theta(t-s)
\end{aligned}
$$

Lemma

$$
\Theta^{\star(k+1)} = \frac{1}{k!}(t-s)^k\Theta(t-s)
$$

$\star$-Identity: Schwartz distributions

To define an identity for this product, we need to move from functions to distributions in the Schwartz sense.

To keep it simple, consider a bounded interval I and define as the test functions the set of analytic functions $\varphi(\tau)$ over I. Then, a distribution d is a continuous linear functional

$$d : \varphi(\cdot) \to \alpha \in \mathbb{C}$$

For instance, the Dirac distribution δ is the distribution

$$\delta : \varphi(\cdot) \to \varphi(0)$$

For $s \in I$ this can be denoted in the integral form:

$$\int_I \varphi(\tau)\delta(\tau - s)\mathrm{d}\tau = \varphi(s)$$

$\star$-Identity

Allow us to play with these definitions. Given $t, s \in I$,

$$\begin{aligned}\tilde{f}(t,s)\Theta(t-s) \star \delta(t-s) &= \int_I \tilde{f}(t,\tau)\Theta(t-\tau)\delta(\tau-s)\mathrm{d}\tau \\ &= \tilde{f}(t,s)\Theta(t-s)\end{aligned}$$

With a change of variable (allowed by Schwartz theory) it is easy to show that also

$$\delta(t-s) \star \tilde{f}(t,s)\Theta(t-s) = \tilde{f}(t,s)\Theta(t-s)$$

The Dirac delta $\delta(t-s)$ acts as the identity of the $\star$-product.

$\star$-Identity

What happens if we follow the rules explained above . . .

$$\delta(t-s) \star \delta(t-s) = \int_I \delta(t-\tau)\delta(\tau-s)\mathrm{d}\tau$$
$$= \delta(t-s)???$$

$\delta(t-s)$ is not a function!

What we mean is:

$$\int_I [\delta \star \delta](\tau, s)\varphi(\tau)\mathrm{d}\tau = \int_I \delta(\tau - s)\varphi(\tau)\mathrm{d}\tau = \varphi(s).$$

for every test function φ.

The $\star$-product is well-defined

The $\star$-product is, in fact, a product of distributions:

$$\star : \mathcal{D}_0(I) \times \mathcal{D}_0(I) \to \mathcal{D}_0(I)$$

with $\mathcal{D}_0(I)$ the set of distributions in the form

$$\tilde{f}_{-1}(t,s)\Theta(t-s) + \tilde{f}_0(t,s)\delta(t-s)$$

See: Ryckebusch, Bouhamidi, Giscard, *A Fréchet Lie group on distributions*, JMAA, 2025

$\star$-inverse

Now that we have defined the $\star$-product and its identity, we can wonder if $\star$-inverses exist. Given, $f(t,s) \in \mathcal{D}_0(I)$, does an x exist such that

$$f(t,s) \star x(t,s) = \delta(t-s)$$

Consider the distribution $\delta'(t-s)$, the Dirac delta derivative:

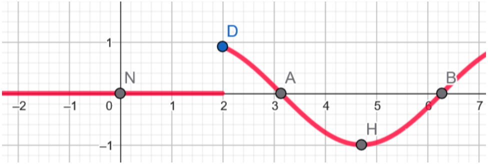
$$\int_I \delta'(\tau - s)\varphi(\tau)\mathrm{d}\tau = \varphi'(s)$$

What about discontinuous functions?

$\star$-inverse if $\Theta(t-s)$

By Schwartz's theory, we get

$$\int_I \delta'(t-\tau)\tilde{f}(\tau,s)\Theta(\tau-s)\mathrm{d}\tau = \frac{\partial}{\partial t}\tilde{f}(t,s)\Theta(t-s) + \tilde{f}(s,s)\delta(t-s)$$



$$f(t,s) = \sin(t)\Theta(t-s), \;\; s=2$$

As a consequence, $\delta'(t-s)$ is the $\star$-inverse of $\Theta(t-s)$

$$\delta'(t-s) \star \Theta(t-s) = 0 \times \Theta(t-s) + \delta(t-s) = \delta(t-s)$$

$\star$-inverses

In general, under some regularity assumption, the $\star$-inverses of elements from $\mathcal{D}_0(I)$ can be found in the set $\mathcal{D}(I)$ of the distributions $f(t,s)$ that can be written in the form

$$f(t,s) = \tilde{f}_{-1}(t,s)\Theta(t-s) + \tilde{f}_0(t,s)\delta(t-s) + \cdots + \tilde{f}_k(t,s)\delta^{(k)}(t-s).$$

See: [Giscard, P., 2020]

Derivatives and integrals

Roughly speaking, Θ represents integration:

$$\Theta(t-s)\star\tilde{f}(t)\Theta(t-s)=\Theta(t-s)\int_s^t\tilde{f}(\tau)\mathrm{d}\tau$$

δ' represents differentiation:

$$\delta'(t-s)\star\tilde{f}(t)\Theta(t-s)=\frac{\partial}{\partial t}\tilde{f}(t)\Theta(t-s)+\tilde{f}(s)\delta(t-s)$$

In the $\star$-algebra, "integration" is the unique inverse of "differentiation":

$$\Theta(t-s)\star\delta'(t-s)\star\tilde{f}(t)\Theta(t-s)=\delta(t-s)\star\tilde{f}(t)\Theta(t-s)=\tilde{f}(t)\Theta(t-s)$$

In summary

Table: Main properties of the $\star$-product and related definitions ($f, g, x \in \mathcal{A}_\Theta(I)$).

Name	Symbol	Definition	Comments
$\star$-identity	δ	$f \star \delta = \delta \star f = f$	
$\star$-inverse	$f^{-\star}$	$f \star f^{-\star} = f^{-\star} \star f = \delta$	
Dirac 1st derivative	δ'	$\delta'(t-s)$	$\delta' \star \Theta = \Theta \star \delta' = \delta$
Dirac derivatives	$\delta^{(j)}$	$\delta^{(j)}(t-s)$	$\delta^{(j)} \star \delta^{(i)} = \delta^{(i+j)}$
$\star$-powers	$f^{\star j}$	$f \star f \star \cdots \star f$, j times	$f^{\star 0} := \delta$
$\star$-resolvent	$R^\star(x)$	$\sum_{j=0}^{\infty} x^{\star j}$, $x \in \mathcal{A}_\Theta(\mathcal{I})$	$R^\star(x) = (\delta - x)^{-\star}$

We can exploit the $\star$-product to solve differential equations.

Solving linear ODEs by the $\star$-approach

Consider the simplest example of a linear ODE

$$\frac{\partial}{\partial t}\tilde{u}(t) = \tilde{u}(t), \quad \tilde{u}(0) = 1, \quad t \geq 0$$

whose solution is

$$\tilde{u}(t) = \exp(t)$$

Generalize the problem introducing the family of ODEs

$$\frac{\partial}{\partial t}\tilde{u}(t,s) = \tilde{u}(t,s), \quad \tilde{u}(s,s) = 1, \quad t \geq s$$

with solution $\tilde{u}(t,s) = \exp(t-s)$. Equivalently $(t \geq s)$,

$$\left[\frac{\partial}{\partial t}\tilde{u}(t,s)\right]\Theta(t-s) = \tilde{u}(t,s)\Theta(t-s), \quad \tilde{u}(s,s) = 1, \quad t,s \in I$$

Solving linear ODEs by the $\star$-approach

$$\left[\frac{\partial}{\partial t}\tilde{u}(t,s)\right]\Theta(t-s) = \tilde{u}(t,s)\Theta(t-s), \quad \tilde{u}(s,s) = 1, \quad t,s \in I$$

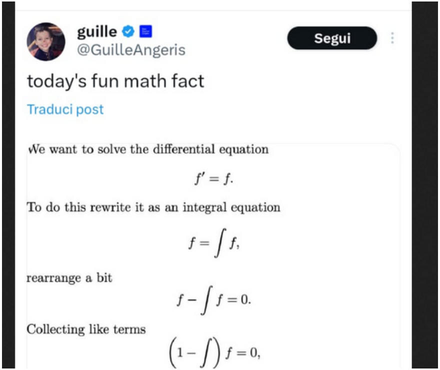
By defining the distributions:

$$u(t,s) := \tilde{u}(t,s)\Theta(t-s) \in \mathcal{A}_\Theta(I)$$
$$u'(t,s) := \left[\frac{\partial}{\partial t}\tilde{u}(t,s)\right]\Theta(t-s) = u(t,s)$$

We get the $\star$-algebra formulation:

$$\begin{aligned}\delta'(t-s) \star u(t,s) &= u'(t,s) + \tilde{u}(s,s)\delta(t-s), \quad t,s \in I \\ &= u(t,s) + 1 \times \delta(t-s), \quad t,s \in I\end{aligned}$$

Solving linear ODEs by the $\star$-approach

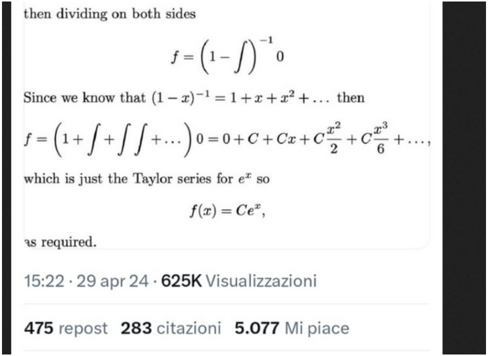


$$\delta' \star u = u + \delta$$

$$\Theta \star \delta' \star u = \Theta \star u + \Theta$$
$$\delta \star u - \Theta \star u = \Theta$$

$$(\delta - \Theta) \star u = \Theta$$

Solving linear ODEs by the $\star$-approach



then dividing on both sides

$$f = \left(1 - \int\right)^{-1} 0$$

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$$\begin{aligned} u &= (\delta - \Theta)^{-\star} \star \Theta \\ &= \sum_{k=0}^{\infty} \Theta^{\star k} \star \Theta \\ &= \sum_{k=0}^{\infty} \Theta^{\star k+1} \\ &= \Theta \sum_{k=0}^{\infty} \frac{(t-s)^k}{k!} \end{aligned}$$

$$u = \exp(t-s)\Theta(t-s)$$

Solving linear ODEs by the $\star$-approach

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As required ;)

So much work for what?

Non-autonomous equations:

$$\frac{\partial}{\partial t}\tilde{u}(t) = \tilde{f}(t)\tilde{u}(t), \quad \tilde{u}(0) = 1, \quad t \geq 0$$

$$u(t,s) = \Theta \star \left(\delta - \tilde{f}(t)\Theta\right)^{-\star} = \exp\left(\int_s^t \tilde{f}(\tau)\mathrm{d}\tau\right), \quad \tilde{u}(t) = u(t,0)$$

Systems of autonomous equations, $\tilde{A}$ is a square matrix:

$$\frac{\partial}{\partial t}\tilde{u}(t) = \tilde{A}\tilde{u}(t), \quad \tilde{u}(0) = v, \quad t \geq 0$$

$$u(t,s) = \Theta \star \left(\delta Id - \tilde{A}\Theta\right)^{-\star} v = \exp(\tilde{A}(t-s))v, \quad \tilde{u}(t) = u(t,0)$$

Systems of non-autonomous ODEs

$$\frac{\partial}{\partial t}\tilde{u}(t) = \tilde{A}(t)\tilde{u}(t), \quad \tilde{u}(0) = v, \quad t \geq 0$$

However,

$$u(t,s) = \Theta \star (\delta Id - \tilde{A}(t)\Theta)^{-\star} v \sout{= \exp\left(\int_s^t \tilde{A}(\tau)\mathrm{d}\tau\right) v},$$

$\tilde{u}(t) = u(t, 0)$

While the $\star$-product expression for the solution of a scalar non-autonomous ODE generalizes straightforwardly to systems of non-autonomous ODEs, this is not true for the exponential expression.

Vito Volterra

§ 4. — **Risoluzione generale di equazioni integrali.**

9. Abbiasi una funzione analitica del tipo (1)

$$\mathbf{F}(z_1, z_2, \ldots, z_n). \tag{1'}$$

Scriviamo l'equazione

$$\mathbf{F}(z_1, z_2, \ldots, z_n) = 0. \tag{4}$$

$$S(x, y) = R(x \,.\, y) - \frac{1}{2} R^2(x, y) + \frac{1}{3} R^3(x, y) - \cdots + \frac{(-1)^n}{n} R^n(x, y) + \cdots$$

ove

$$R^n(x, y) = \int_x^y R^{n-1}(x, \xi)\, R(\xi, y)\, d\xi \,.$$

e non dovremo porre alcuna limitazione per i valori assoluti di $S(x, y)$, $R(x, y)$, purchè siano finiti.

10. Supponiamo in particolare che la (4') sia un polinomio razionale e

[Volterra, Rend Lincei, 1910]

Remark: Volterra and Pérès did not have the distribution theory by Schwartz at their time!

Vito Volterra - 80 years from the end of Nazi-Fascism

- In 1931, the fascist regime imposed an oath of allegiance to the fascist government on all university professors.
- Only 12 professors refused to sign it. They lost their position.
- Vito Volterra was one of them. He was marginalized from the Italian scientific community (from 1938, also because of the racial laws).
- First helped by the Vatican Science Academy, he lived in Spain and France until he died in 1940.

Discretization: Legendre polynomial expansion

If $I = [-1, 1]$, $f(t,s)$ can be expanded in a 2D series:

$$f(t,s) = \tilde{f}(t)\Theta(t-s) \approx \sum_{k=0}^{m-1} \sum_{\ell=0}^{m-1} \alpha_{k,\ell} p_k(t) p_\ell(s),$$

with p_k the orthonormal Legendre polynomials:

$$\int_{-1}^{1} p_k(\tau) p_\ell(\tau) d\tau = \delta_{k\ell},$$

and

$$\alpha_{k,l} = \int_{-1}^{1} p_k(\rho) \left(\int_{-1}^{1} f(\tau,\rho) p_\ell(\tau) d\tau \right) d\rho.$$

Discretization: Legendre polynomial coefficients

The function is then represented by the matrix:

$$f(t,s) \to \begin{bmatrix} \alpha_{0,0} & \alpha_{0,1} & \dots & \alpha_{0,m-1} \\ \alpha_{1,0} & \alpha_{1,1} & \dots & \alpha_{1,m-1} \\ \vdots & \vdots & & \vdots \\ \alpha_{m-1,0} & \alpha_{m-1,1} & \dots & \alpha_{m-1,m-1} \end{bmatrix} =: F$$

Note that

$$f(t,s) \approx \sum_{k=0}^{m-1} \sum_{\ell=0}^{m-1} \alpha_{k,\ell} p_k(t) p_\ell(s) = \varphi_m(t)^T F \varphi_m(s)$$

$$\approx \begin{bmatrix} p_0(t) & \dots & p_{m-1}(t) \end{bmatrix} F \begin{bmatrix} p_0(s) \\ \vdots \\ p_{m-1}(s) \end{bmatrix}.$$

Matrix problem: the resolvent

The discretized $\star$-product translates into the usual matrix algebra.

$f(t,s)$	F_m
$1_\star = \delta(t-s)$	I_m
$f^{\star -1}$	F_m^{-1}
$g(t,s)$	G_m
$f \star g$	$F_m G_m$
$f + g$	$F_m + G_m$
$\Theta(t-s)$	T_m
$R_\star(f)$	$(I_m - F_m)^{-1}$
$\hat{U}(t,s)$	$T_m(I_m - F_m)^{-1}$

Go to MatLab

Kronecker structure and low-rank

In many applications, $H(t)$ is given as a sum of products:

$$H(t) = \sum_{j=0}^{s} H_j \times \tilde{f}_j(t),$$

with H_j sparse matrices, and $\tilde{f}_j(t)$ analytic scalar functions. Our approach reformulates the problem as the linear system

$$\left(I_{Nm} + i \sum_{j=0}^{s} H_j \otimes F_j \right) \text{vec}(X) = \psi_0 \otimes \varphi_m(-1),$$

with vec the vectorization transformation and F_j the Legendre discretization matrices. Equivelently, we have the matrix equation with a low-rank rhs (state vector case)

$$X + i \sum_{j=0}^{s} F_j X H_j^T = \varphi_m(-1)\psi_0^T.$$

The problem: two systems of linear ODEs

We will solve two related problems.
First, the quantum state vector case. Compute the N-size vector $\psi(t)$ solving:

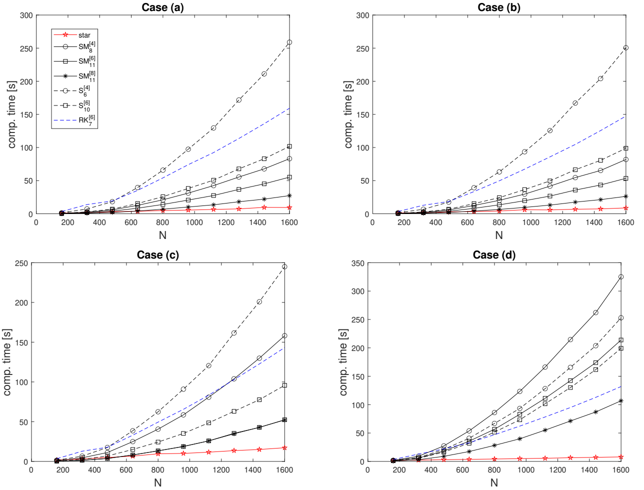
$$\frac{\partial}{\partial t}\psi(t) = -H(t)\psi(t), \quad \psi(t_0) = \psi_0 \in \mathbb{C}^N, \quad t \in I = [t_0, t_f].$$

Second, the operator case. Compute the $N \times N$ matrix-valued function $U(t)$ solving

$$\frac{\partial}{\partial t}U(t) = -H(t)U(t), \quad U(t_0) = I_N, \quad t \in I = [t_0, t_f].$$

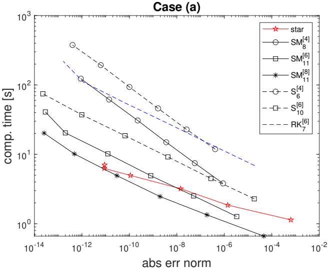
Note that $\psi(t) = U(t)\psi_0$.

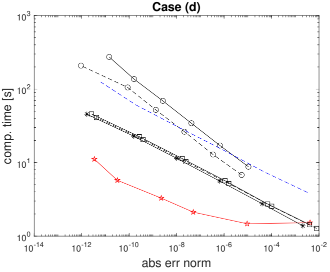
Comparison: size



Error order $1e-7$. Examples and methods for the comparison from: [Blanes, Casas, Murua, The Journal of Chemical Physics, 2017]

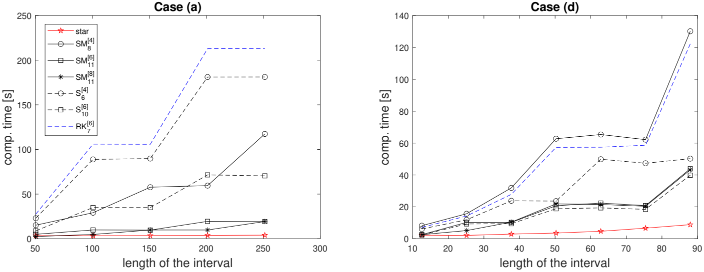
Comparison: accuracy





$N = 400$

Comparison: interval length



$N = 400$, Error order $1e-7$.

Future

The work of Y. N. Kosovtsov [arXiv:math-ph/0202040, arXiv:0409035v1, arXiv:0910.3923v1] shows that it is possible to formally express also PDEs and nonlinear DE by a time-ordered exponential. This opens the way to extend our approach to a larger category of DEs.
This and other considerations mean that the presented approach can be extended to:

- PDEs
- nonlinear DEs
- Fractional DEs
- modes and eigenfunction problems

References

- P. L. Giscard and S. Pozza, Appl. Math. **65**(6), 807–827 (2020).
- P. L. Giscard and S. Pozza, Boll. Unione Mat. Ital. **16**(1), 81–102 (2023).
- S. Pozza, Linear and Multilinear Algebra (2024).
- S. Pozza and N. V. Buggenhout, ETNA pp. 292–326 (2024).

Projects

- Charles University PRIMUS research poject: *A Lanczos-like Method for the Time-Ordered Exponential, www.starlanczos.cz*.
- French ANR research project: *MAGICA (MAGnetic resonance techniques and Innovative Combinatorial Algebra)*.