# A $\star$-product approach to non-autonomous linear ordinary differential equations

Stefano Pozza, Niel Van Buggenhout

Charles university, Prague

Jablonec nad Nisou - PANM 2022
June 19–24, 2022

# Our teams

## Local team (Charles University)

S. Pozza
(PI)

N. Van Buggenhout
(Posdoc)

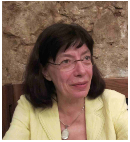
S. Zahid
(Ph.D.)

M. Faisal
(Ph.D.)

## External team

C. Bonhomme
(Sorbonne-Univ.)

P-L. Giscard
(ULCO)



M. Redivo-Zaglia
(Padova-Univ.)

S. Cipolla
(Edinburgh-Univ).

# Schrödinger equation

Nuclear Magnetic Resonance (NMR) spectroscopy analyses dynamics of nuclear spins in magnetic field:

$$\hbar \frac{d}{dt}\Psi(t) = -iH(t)\Psi(t),$$

with

wave function $\Psi(t)$

Hamiltonian $H(t)$

- $\ell$ spins $\rightarrow$ size $2^\ell \times 2^\ell$
- Sparse

# Schrödinger equation

Nuclear Magnetic Resonance (NMR) spectroscopy analyses dynamics of nuclear spins in magnetic field:

$$\hbar \frac{d}{dt}\Psi(t) = -iH(t)\Psi(t),$$

with

wave function $\Psi(t)$

Hamiltonian $H(t)$

- $\ell$ spins $\to$ size $2^\ell \times 2^\ell$
- Sparse

4 strongly coupled spins

$$\begin{bmatrix}
\times &&&&&&&&&&&&&&& \\
& \times & \times && \times &&&& \times &&&&&&& \\
& \times & \times && \times &&&& \times &&&&&&& \\
&&& \times && \times & \times &&& \times & \times &&&&& \\
& \times & \times && \times &&&& \times &&&&&&& \\
&&& \times && \times & \times &&& \times &&& \times &&& \\
&&& \times && \times & \times &&&& \times && \times &&& \\
&&&&&&& \times &&&& \times && \times & \times & \\
& \times & \times && \times &&&& \times &&&&&&& \\
&&& \times && \times &&&& \times & \times && \times &&& \\
&&& \times &&& \times &&& \times & \times && \times &&& \\
&&&&&&& \times &&&& \times && \times & \times & \\
&&&&& \times & \times &&& \times & \times && \times &&& \\
&&&&&&& \times &&&& \times && \times & \times & \\
&&&&&&& \times &&&& \times && \times & \times & \\
&&&&&&&&&&&&&&& \times
\end{bmatrix}$$

# Schrödinger equation

Nuclear Magnetic Resonance (NMR) spectroscopy analyses dynamics of nuclear spins in magnetic field:

$$\hbar \frac{d}{dt}\Psi(t) = -iH(t)\Psi(t),$$

with

wave function $\Psi(t)$

Hamiltonian $H(t)$

- $\ell$ spins $\rightarrow$ size $2^\ell \times 2^\ell$
- Sparse

4 uncoupled spins + pulse wave

$$\begin{bmatrix}
 & \times & \times & & \times & & & & \times & & & & & & & \\
\times & & & \times & & \times & & & & \times & & & & & & \\
\times & & & \times & & & \times & & & & \times & & & & & \\
 & \times & \times & & & & & \times & & & & \times & & & & \\
\times & & & & & \times & \times & & & & & & \times & & & \\
 & \times & & & \times & & & \times & & & & & & \times & & \\
 & & \times & & \times & & & \times & & & & & & & \times & \\
 & & & \times & & \times & \times & & & & & & & & & \times \\
\times & & & & & & & & & \times & \times & & \times & & & \\
 & \times & & & & & & & \times & & & \times & & \times & & \\
 & & \times & & & & & & \times & & & \times & & & \times & \\
 & & & \times & & & & & & \times & \times & & & & & \times \\
 & & & & \times & & & & \times & & & & & \times & \times & \\
 & & & & & \times & & & & \times & & & \times & & & \times \\
 & & & & & & \times & & & & \times & & \times & & & \times \\
 & & & & & & & \times & & & & \times & & \times & \times &
\end{bmatrix}$$

# Schrödinger equation

Nuclear Magnetic Resonance (NMR) spectroscopy analyses dynamics of nuclear spins in magnetic field:

$$\hbar \frac{d}{dt}\Psi(t) = -iH(t)\Psi(t),$$

with

wave function $\Psi(t)$

Hamiltonian $H(t)$

- $\ell$ spins $\to$ size $2^\ell \times 2^\ell$
- Sparse

Why? Computer simulation

improves design

improves analysis

of practical experiments

4 uncoupled spins + pulse wave

$$\begin{bmatrix}
 & \times & \times & & \times & & & & \times & & & & & & & \\
\times & & & \times & & \times & & & & \times & & & & & & \\
\times & & & \times & & & \times & & & & \times & & & & & \\
 & \times & \times & & & & & \times & & & & \times & & & & \\
\times & & & & & \times & \times & & & & & & \times & & & \\
 & \times & & & \times & & & \times & & & & & & \times & & \\
 & & \times & & \times & & & \times & & & & & & & \times & \\
 & & & \times & & \times & \times & & & & & & & & & \times \\
\times & & & & & & & & & \times & \times & & \times & & & \\
 & \times & & & & & & & \times & & & \times & & \times & & \\
 & & \times & & & & & & \times & & & \times & & & \times & \\
 & & & \times & & & & & & \times & \times & & & & & \times \\
 & & & & \times & & & & \times & & & & & \times & \times & \\
 & & & & & \times & & & & \times & & & \times & & & \times \\
 & & & & & & \times & & & & \times & & \times & & & \times \\
 & & & & & & & \times & & & & \times & & \times & \times &
\end{bmatrix}$$

# Numerical methods - references (incomplete list)

- [Moro, Freed, 1981]
- [Tal-Ezer, Kosloff, 1984]
- [Park, Light, 1985]
- [Leforestier et al., 1991]
- [Chin, Chen, 2002]
- [Hochbruck, Lubich, 2003]
- [Veshtort, Griffin, 2006]
- [Lauvergnat, Blasco, Chapuisat, 2007]
- [Kormann, Holmgren, Karlsson, 2008]
- [Lubich, 2008]
- [Blanes, Casas, Oteo, Ros, 2009]
- [Tošner, Vosegaard, Kehlet, Khaneja, Glaser, Nielsen, 2009]
- [Mazzi, 2010]
- [Sánchez, Casas, Fernández, 2011]
- [Iserles, Munthe-Kaas, Nørsett, Zanna, 2015]
- [Blanes, Casas, Murua, 2015]
- [Bader, Iserles, Kropielnicka, Singh, 2016]
- [Blanes, Casas, 2016]
- . . .

Softwares: SIMPSON, SPINACH.

# Outline

- Solution of ODEs by $\star$-product.
- From the $\star$-product algebra to the matrix algebra.
- A new NLA approach for linear ODEs.

# Scalar ODE

For the sake of a simpler explanation, consider the scalar problem:

$$\frac{d}{dt}u(t) = \tilde{f}(t)u(t), \quad u(s) = 1, \quad t \geq s \in I \subset \mathbb{R}$$

with $\tilde{f}(t)$ a smooth and bounded function over $I$. Then

$$u(t) = \exp\left(\int_s^t \tilde{f}(\tau)\,\mathrm{d}\tau\right).$$

We are going to show an alternative expression for the solution.
Everything we are going to see can be easily extended to a system of ODEs.

# Volterra composition

Let $\tilde{f}_1(t,s), \tilde{f}_2(t,s)$ be bivariate matrices. The following operation

$$\big(\tilde{f}_2 \star_v \tilde{f}_1\big)(t,s) := \int_s^t \tilde{f}_2(t,\tau)\tilde{f}_1(\tau,s)\,\mathsf{d}\tau.$$

is known as Volterra composition. Picard iteration:

$$\frac{d}{dt'}u(t) = \tilde{f}(t)u(t), \quad u(s) = 1$$

$$\downarrow \ \text{integration}$$

$$u(t) = 1 + \int_s^t \tilde{f}(\tau)u(\tau)\mathrm{d}\tau$$

$$\downarrow \ \text{integration}$$

$$\begin{aligned} u(t) &= 1 + \int_s^t \tilde{f}(\tau)\left(1 + \int_s^\tau \tilde{f}(\rho)u(\rho)\mathrm{d}\rho\right)\mathrm{d}\tau \\ &= 1 + \int_s^t \tilde{f}(\tau) + \int_s^\tau \tilde{f}(\tau)\tilde{f}(\rho)u(\rho)\,\mathrm{d}\rho\,\mathrm{d}\tau \end{aligned}$$

$$\downarrow \ \text{after many iterations}$$

$$u(t) = 1 + \int_s^t \tilde{f}(\tau)\mathrm{d}\tau + \int_s^t \tilde{f}^{\star_v 2}(\tau)\mathrm{d}\tau + \cdots = 1 + \int_s^t \sum_{j=1}^{\infty} \tilde{f}^{\star_v j}(\tau)\mathrm{d}\tau.$$

# $\star$-product

We extend the Volterra composition defining the so-called $\star$-product

$$\big(f_2 \star f_1\big)(t, s) := \int_{-\infty}^{+\infty} f_2(t, \tau) f_1(\tau, s)\, \mathsf{d}\tau.$$

that is an actual product for a specific class of distributions [Giscard, P., Ryckebusch].
Let $\Theta(t - s)$ be the Heaviside function

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

Then

$$\tilde{f}_2(t-s)\Theta(t-s) \star \tilde{f}_1(t,s)\Theta(t-s) = \tilde{f}_2(t,s) \star_v \tilde{f}_1(t,s).$$

# Discontinuity

Definition: $\star$-product

- $f_1(t,s),\ f_2(t,s) \in$ specific class of distributions
- $(f_2 \star f_1)(t,s) := \int_{-1}^{1} f_2(t,\tau) f_1(\tau,s) d\tau$

# Discontinuity

Definition: $\star$-product

- $f_1(t,s),\ f_2(t,s) \in$ specific class of distributions
- $(f_2 \star f_1)(t,s) := \int_{-1}^{1} f_2(t,\tau) f_1(\tau,s) d\tau$

The class consists of $f(t,s) = \tilde{f}(t)\Theta(t-s)$

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

# Discontinuity

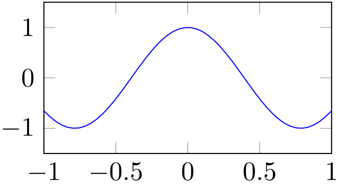
Definition: $\star$-product

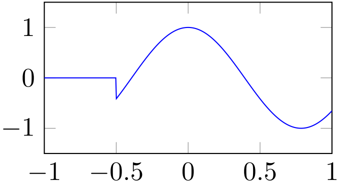
- $f_1(t,s),\ f_2(t,s) \in$ specific class of distributions
- $(f_2 \star f_1)(t,s) := \int_{-1}^{1} f_2(t,\tau) f_1(\tau,s) d\tau$

The class consists of $f(t,s) = \tilde{f}(t)\Theta(t-s)$

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

Example: $\tilde{f}(t) = \cos(4t)$ $\qquad$ $f(t,s) = \cos(4t)\Theta(t-s)|_{s=-0.5}$



# Discontinuity

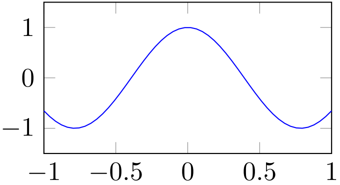
Definition: $\star$-product

- $f_1(t,s),\ f_2(t,s) \in$ specific class of distributions
- $(f_2 \star f_1)(t,s) := \int_{-1}^{1} f_2(t,\tau) f_1(\tau,s) d\tau$

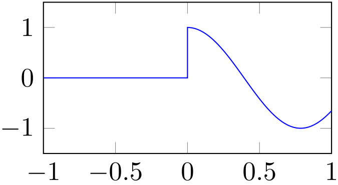
The class consists of $f(t,s) = \tilde{f}(t)\Theta(t-s)$

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

Example: $\tilde{f}(t) = \cos(4t)$



$f(t,s) = \cos(4t)\Theta(t-s)|_{s=0}$



# The $\star$-product algebra

| | |
|---|---|
| $r(t,s) = f(t,s) \star g(t,s)$ | $\tilde{f}\Theta \star \tilde{g}\Theta \to \tilde{r}\Theta$, closed |
| $f + g$ | closed |
| $1_\star = \delta(t-s)$ | Dirac delta |
| $f^{\star -1}(t,s)$ | Dirac delta derivatives $\delta', \delta'', \ldots$ |
| $R_\star(f)(t,s) := (1_\star - f)^{\star -1}(t,s)$ | $\star$-resolvent |

# Solution by $\star$-resolvent

Let us define $f(t,s) = \tilde{f}(t)\Theta(t-s)$. The $\star$-resolvent is defined as

$$\mathsf{R}_\star(f) := (1_\star - f)^{\star-1} = 1_\star + \sum_{k\geq 1} f^{\star k}$$

with $1_\star = \delta(t-s)$ the Dirac delta function. The $\star$-resolvent exists if $f$ is bounded for $t, s \in I$. Then the Time-ordered exponential can be given as

$$\mathsf{U}(t,s) = \int_s^t \mathsf{R}_\star(f)(\tau, s)\, d\tau = \Theta(t-s) \star \mathsf{R}_\star(f)(t,s),$$

where for a fixed $s$, $\mathsf{U}(t,s)$ solves the ODE with starting time $s$; [Giscard & al., 2015].

# Example

Consider the simple case $\widetilde{f}(t) = 1$,

$$\frac{d}{dt}u(t) = u(t), \quad u(s) = 1.$$

Then $f(t,s) = \Theta(t-s)$ and

$$R_\star(f)(t,s) = \sum_{k=0}^{\infty} \Theta(t-s)^{\star k}.$$

Hence

$$U(t,s) = \Theta(t-s) \star R_\star(f)(t,s) = \sum_{k=0}^{\infty} (\Theta(t-s))^{*(k+1)} = \sum_{k=0}^{\infty} \frac{(t-s)^k}{(k)!}\Theta(t-s).$$

As expected, for a fixed $s$, the solution is

$$u(t) = U(t,s) = \exp(t-s)\Theta(t-s).$$

# Vito Volterra

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

9. Abbiasi una funzione analitica del tipo (1)

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

Scriviamo l'equazione

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

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

ove

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

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

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

[Volterra, Rend Lincei, 1910]

# Vito Volterra - 91 years from "fascism oath" rejection

- In 1931, the Italian fascist regime imposed an oath of allegiance to the fascist government to 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 '38, also because of the racial laws).
- First helped by the Vatican Science Academy, he then lived in Spain and France.

# Systems of ODEs

Let $t \geq s \in I \subseteq \mathbb{R}$, $\mathsf{A}(t)$ a time dependent matrix. The time-ordered exponential is the unique solution $\mathsf{U}(t,s)$ of

$$\widetilde{\mathsf{A}}(t)\mathsf{U}(t,s) = \frac{d}{dt}\mathsf{U}(t,s), \quad \mathsf{U}(s,s) = \mathsf{I}_N.$$

If $\widetilde{\mathsf{A}}(\tau_1)\widetilde{\mathsf{A}}(\tau_2) = \widetilde{\mathsf{A}}(\tau_2)\widetilde{\mathsf{A}}(\tau_1)$ for all $\tau_1, \tau_2 \in I$, then

$$\mathsf{U}(t,s) = \exp\left(\int_s^t \widetilde{\mathsf{A}}(\tau)\, d\tau\right).$$

U has generally no explicit form. Expression by ([Dyson, 1948])

$$\mathsf{U}(t,s) = \mathcal{T}\exp\left(\int_s^t \widetilde{\mathsf{A}}(\tau)\, d\tau\right).$$

with $\mathcal{T}$ the time-ordering operator.

# Time-ordered exponential

The time-ordering expression is more a notation as the action of the time-ordering operator is very difficult to evaluate.

- Classical approaches Perturbative methods (Floquet-based and Magnus series techniques), often prohibitively involved, e.g., [Blanes & al., 2009];
- Path-sum approach: The expression has a finite number of scalar integro-differential equations, but its complexity can be too large; [Giscard & al., 2015].
- $\star$-Lanczos $+$ Path-sum: [Giscard, P., 2020-2022]

# Solution by $\star$-product

Nevertheless, the $\star$-resolvent expression for the solution remains:

$$U(t,s) = \Theta(t-s) \star R_\star(A),$$

with

$$R_\star(A)(t,s) = \sum_{k=0}^{\infty} \left(\widetilde{A}(t)\Theta(t-s)\right)^{\star k},$$

where the $\star$-product here is extended in the matrix-product sense.

The probelm is: How do we compute $R_\star(A)$?

Symbolic expression: Path-sum method [Giscard & al., 2015] and $\star$-Lanczos symbolic method [Giscard, P., 2020-2022].

# Compute $u(t, s)$

Compute $u(t, s)$

- Symbolically: slow
- Numerically: rest of the presentation

Numerical procedure:

1. Discretize $f(t, s)$
2. Discrete analogue of $\star$-operations
3. Compute discretized resolvent
4. Express $u(t, s)$ in terms of resolvent

# Discretize input $f(t, s)$

Function of interest

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

Use Legendre polynomials $\{p_k\}$

$$\int_{-1}^{1} p_k(\tau)p_l(\tau)d\tau = \begin{cases} 0, & \text{if } k \neq l \\ 1, & \text{if } k = l \end{cases}$$

Legendre series

$$f(t,s) \approx \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} f_{i,j}p_i(t)p_j(s)$$

# Discretize input $f(t, s)$

Function of interest

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

Use Legendre polynomials $\{p_k\}_{k=0}^{M}$

$$\int_{-1}^{1} p_k(\tau)p_l(\tau)d\tau = \begin{cases} 0, & \text{if } k \neq l \\ 1, & \text{if } k = l \end{cases}$$

Legendre series

$$f(t, s) \approx \sum_{i=0}^{M} \sum_{j=0}^{M} f_{i,j} p_i(t) p_j(s) =: f_M(t, s)$$

# Discretize input $f(t, s)$

Function of interest

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

Use Legendre polynomials $\{p_k\}_{k=0}^{M}$

$$\int_{-1}^{1} p_k(\tau)p_l(\tau)d\tau = \begin{cases} 0, & \text{if } k \neq l \\ 1, & \text{if } k = l \end{cases}$$

Legendre series

$$f(t,s) \approx \sum_{i=0}^{M}\sum_{j=0}^{M} f_{i,j}p_i(t)p_j(s) =: f_M(t,s)$$

$$f_M(t,s) = \begin{bmatrix} p_0(t) & p_1(t) & \dots & p_M(t) \end{bmatrix} \begin{bmatrix} f_{0,0} & f_{0,1} & \dots & f_{0,M} \\ f_{1,0} & f_{1,1} & \dots & f_{1,M} \\ \vdots & \vdots & & \vdots \\ f_{M,0} & f_{M,1} & \dots & f_{M,M} \end{bmatrix} \begin{bmatrix} p_0(s) \\ p_1(s) \\ \vdots \\ p_M(s) \end{bmatrix}$$

# Discretize input $f(t, s)$

Function of interest

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

Use Legendre polynomials $\{p_k\}_{k=0}^{M}$

$$\int_{-1}^{1} p_k(\tau)p_l(\tau)d\tau = \begin{cases} 0, & \text{if } k \neq l \\ 1, & \text{if } k = l \end{cases}$$

Legendre series

$$f(t, s) \approx \sum_{i=0}^{M} \sum_{j=0}^{M} f_{i,j} p_i(t) p_j(s) =: f_M(t, s)$$

$$f_M(t, s) = \begin{bmatrix} p_0(t) & p_1(t) & \dots & p_M(t) \end{bmatrix} F_M \begin{bmatrix} p_0(s) \\ p_1(s) \\ \vdots \\ p_M(s) \end{bmatrix}$$

# The matrix algebra

In Legendre basis:

$$f(t,s) \approx \begin{bmatrix} p_0(t) & p_1(t) & \dots & p_M(t) \end{bmatrix} F_M \begin{bmatrix} p_0(s) \\ p_1(s) \\ \vdots \\ p_n(s) \end{bmatrix}$$

| | |
|---|---|
| $f(t,s)$ | $F_M$ |
| $\star$-operation | matrix operation |
| $s(t,s) = f(t,s) \star g(t,s)$ | $S_M = F_M G_M$ |
| $f + g$ | $F_M + G_M$ |
| $1_\star = \delta(t-s)$ | $I_M$, identity matrix |
| $f^{\star-1}(t,s)$ | $F_M^{-1}$ |
| $R_\star(f)(t,s) := (1_\star - f)^{\star-1}(t,s)$ | $R(F_M) := (I_M - F_M)^{-1}$ |

# The matrix algebra

In Legendre basis:

$$f(t,s) \approx \begin{bmatrix} p_0(t) & p_1(t) & \dots & p_M(t) \end{bmatrix} F_M \begin{bmatrix} p_0(s) \\ p_1(s) \\ \vdots \\ p_n(s) \end{bmatrix}$$

| | |
|---|---|
| $f(t,s)$ | $F_M$ |
| $\star$-operation | matrix operation |
| $s(t,s) = f(t,s) \star g(t,s)$ | $S_M = F_M G_M$ |
| $f + g$ | $F_M + G_M$ |
| $1_\star = \delta(t-s)$ | $I_M$, identity matrix |
| $f^{\star-1}(t,s)$ | $F_M^{-1}$ |
| $R_\star(f)(t,s) := (1_\star - f)^{\star-1}(t,s)$ | $R(F_M) := (I_M - F_M)^{-1}$ |

Solution to $\star$-ODE:

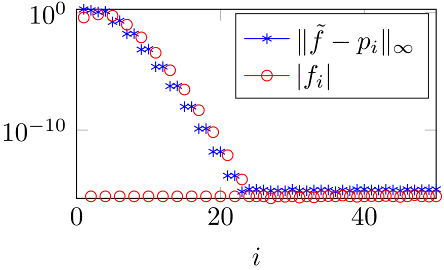
| | |
|---|---|
| $U(t,s)$ | $U_M$ |
| $\Theta(t-s) \star (1_\star - f)^{\star-1}(t,s)$ | $H_M(I_M - F_M)^{-1}$ |

# Legendre approximation

Analytic $\rightarrow$ geometric convergence

$$\tilde{f}(t) = \cos(4t) \approx \sum_{i=0}^{M} \tilde{f}_i p_i(t)$$

$$M = 23$$

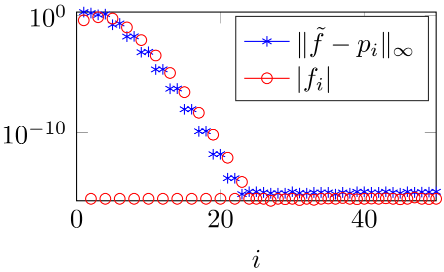


# Legendre approximation

Analytic → geometric convergence

$$\tilde{f}(t) = \cos(4t) \approx \sum_{i=0}^{M} \tilde{f}_i p_i(t)$$

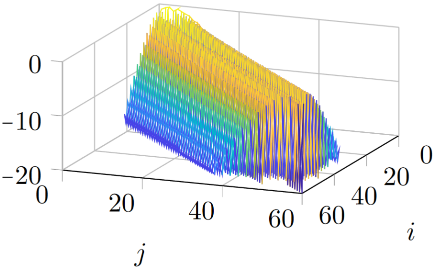
$$M = 23$$




$\star$-framework ⇒ discontinuous

$$f(t,s) = \cos(4t)\Theta(t-s)$$

$$\approx \sum_{i=0}^{M} \sum_{j=0}^{M} f_{i,j} p_i(t) p_j(s)$$

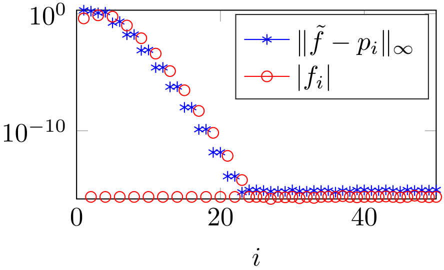


# Legendre approximation

Analytic $\rightarrow$ geometric convergence

$$\tilde{f}(t) = \cos(4t) \approx \sum_{i=0}^{M} \tilde{f}_i p_i(t)$$

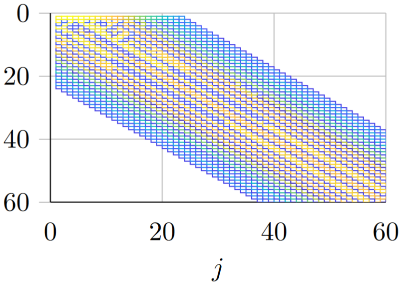
$$M = 23$$




$\star$-framework $\Rightarrow$ discontinuous

$$f(t,s) = \cos(4t)\Theta(t-s)$$

$$\approx \sum_{i=0}^{M} \sum_{j=0}^{M} f_{i,j} p_i(t) p_j(s)$$




$F_M$ is (numerically) banded!
Note: $f(t,-1) = \tilde{f}(t)$

# Reconstruction and Gibbs phenomenon

Even if $\tilde{f}(t)$ is analytic, $f(t,s) = \tilde{f}(t)\Theta(t-s)$ is discontinuos. Therefore, the expansion

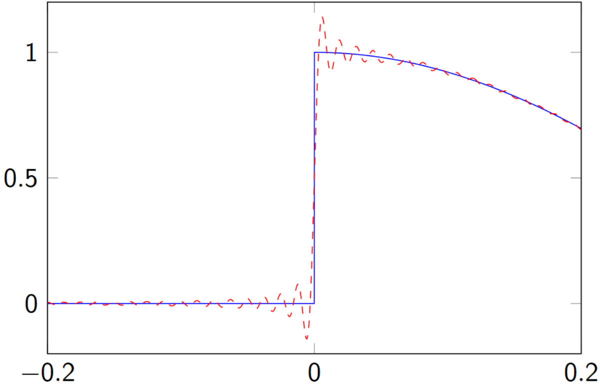
$$f(t,s) = \tilde{f}(t)\Theta(t-s) \approx \sum_{k=0}^{m-1}\sum_{\ell=0}^{m-1} \alpha_{k,\ell} p_k(t) p_\ell(s),$$

is affected by the so-called Gibbs phenomenon. Assuming to only know a matrix $F$, we may not be able to accurately reconstruct $f(t,s)$.

# Gibbs phenomenon

Gibbs phenomenon:

- Overshoot near discontinuity
- Spurious oscillations in whole domain



# Is it really a problem?

For $s = -1$ the function $f(t, -1) = \tilde{f}(t)$, for $t \in [-1, 1]$. Therefore,

$$\tilde{f}(t) \approx f(t, -1) = \begin{bmatrix} p_0(t) & p_1(t) & \dots & p_M(t) \end{bmatrix} F_M \begin{bmatrix} p_0(-1) \\ p_1(-1) \\ \vdots \\ p_M(-1) \end{bmatrix}.$$

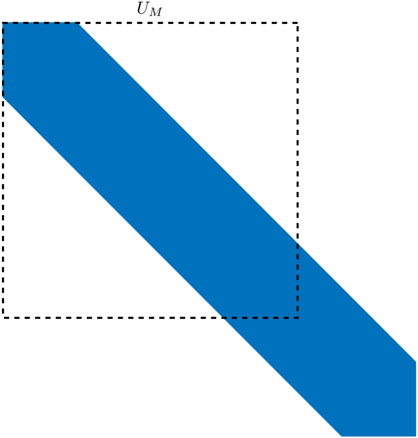
Therefore $F_M \begin{bmatrix} p_0(-1) & p_1(-1) & \dots & p_M(-1) \end{bmatrix}^T$ is a vector containing the Legendre coefficients of the $1D$ expansion

$$\widetilde{f}(t) = \sum_{k=0}^{m-1} \tilde{\alpha}_k p_k(t).$$

However, we still need to analyze the truncation error.

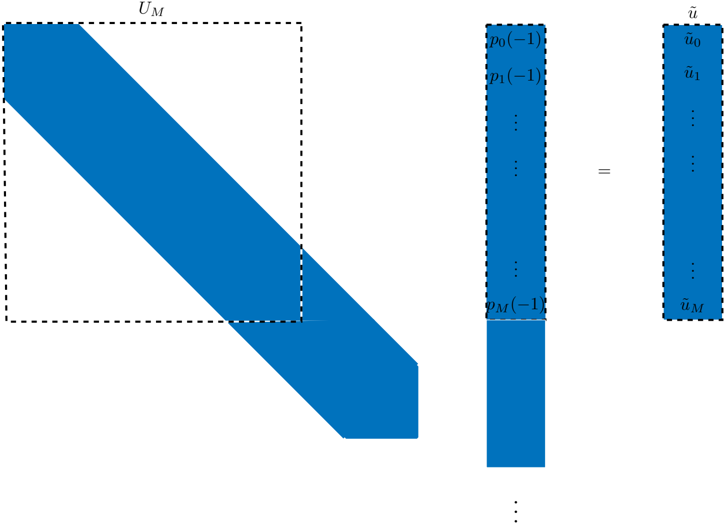
# Solution

$$u(t,s) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} u_{i,j} p_i(t) p_j(s) \approx \sum_{i=0}^{M} \sum_{j=0}^{M} u_{i,j} p_i(t) p_j(s)$$



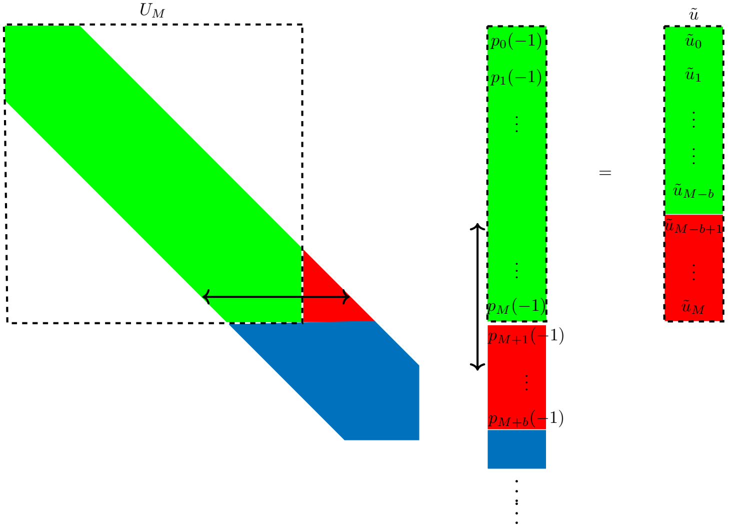
# Solution

$$\tilde{u}(t) = u(t,-1) \approx \sum_{i=0}^{M}\sum_{j=0}^{M} u_{i,j} p_i(t) p_j(-1) = \sum_{i=0}^{M} \tilde{u}_i p_i(t)$$



# Solution

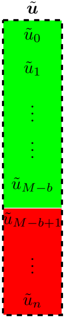
$$\tilde{u}(t) = u(t,-1) \approx \sum_{i=0}^{M} \sum_{j=0}^{M} u_{i,j} p_i(t) p_j(-1) = \sum_{i=0}^{M-b} \tilde{u}_i p_i(t)$$

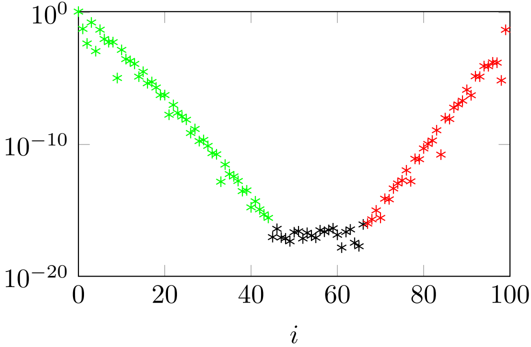


# Coefficient vector $\tilde{\boldsymbol{u}}$

Approximate solution

$$U(t,-1) \approx \sum_{i=0}^{M-b} \tilde{u}_i p_i(t), \quad \tilde{\boldsymbol{u}} = U_M p, \qquad \text{with } b \approx 40$$

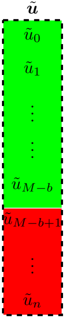


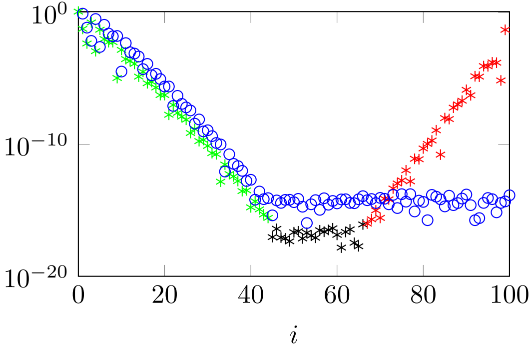



# Coefficient vector $\tilde{\boldsymbol{u}}$

Approximate solution

$$U(t,-1) \approx \sum_{i=0}^{M-b} \tilde{u}_i p_i(t), \quad \tilde{\boldsymbol{u}} = U_M p, \qquad \text{with } b \approx 40$$



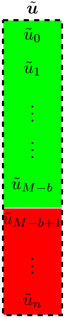



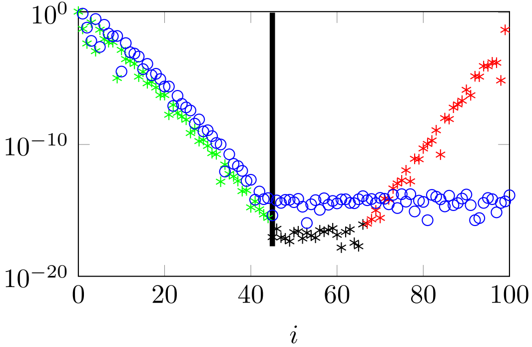

Analytic solution:
$u(t) = \exp\left(\frac{1}{4}\sin(4t)\right) = \sum_{i=0}^{\infty} \alpha_i p_i(t)$

# Coefficient vector $\tilde{\boldsymbol{u}}$

Approximate solution

$$U(t,-1) \approx \sum_{i=0}^{M-b} \tilde{u}_i p_i(t), \quad \tilde{\boldsymbol{u}} = U_M p, \qquad \text{with } b \approx 40$$




Analytic solution:
$u(t) = \exp\left(\frac{1}{4}\sin(4t)\right) = \sum_{i=0}^{\infty} \alpha_i p_i(t)$

Error:
$\|\hat{u}(t) - u(t)\|_\infty = 8e-16$

# Proposed procedure

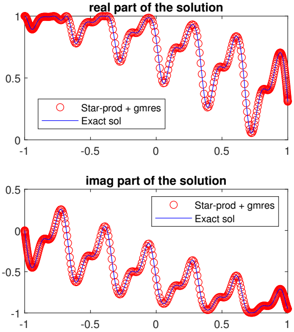
Solve $\frac{d}{dt}\tilde{u}(t) = \tilde{f}(t)\tilde{u}(t)$:

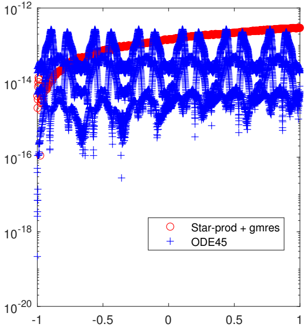
1. Represent $\tilde{f}(t)\Theta(t-s)$ as Legendre series $\Rightarrow F_M$
2. Compute $\tilde{\boldsymbol{u}}_M = H_M(I_M - F_M)^{-1}p$ (GMRES!)
3. Choose right amount of coefficients to keep $\tilde{\boldsymbol{u}}_{M-b}$
4. Solution is $\tilde{u}(t) \approx \sum_{i=0}^{M-b} \tilde{u}_i p_i(t)$

# Example

$$\frac{d}{dt}u(t) = \tilde{f}(t)u(t), \quad u(-1) = 1, \quad t \in [-1, 1]$$

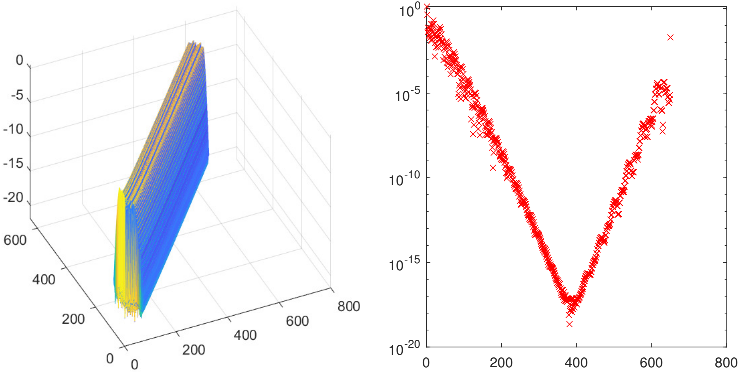
$$\tilde{f}(t) = -2\pi i(0.1 + \cos(6\pi(t+1)) + \cos(12\pi(t+1)))$$




GMRES: $13$ iterations for a $800 \times 800$ matrix.

# Example




Left: Element magnitude of the Legendre coefficient matrix $F$.
Right: Element magnitude of the computed Legendre coefficients $c$.

# Proposed procedure

Compute $w^H \tilde{U}(t) v$, with $\frac{d}{dt}\tilde{U}(t) = \tilde{A}(t)\tilde{U}(t)$:

1. Represent $\tilde{A}(t)\Theta(t-s)$ as Legendre series $\Rightarrow \mathcal{F}_n$ block matrix $[F_{i,j}]_{i,j=1}^m$

$$\begin{bmatrix} \tilde{a}_{1,1}(t) & \dots & \tilde{a}_{1,m}(t) \\ \vdots & & \vdots \\ \tilde{a}_{m,1}(t) & \dots & \tilde{a}_{m,m}(t) \end{bmatrix} \Theta(t-s) \underset{\text{discretize}}{\rightarrow} \begin{bmatrix} \boxed{F_{1,1}} & \dots & \boxed{F_{1,m}} \\ \vdots & & \vdots \\ \boxed{F_{m,1}} & \dots & \boxed{F_{m,n}} \end{bmatrix}$$

2. Compute $w^H \tilde{\boldsymbol{U}}_M v = (w \otimes I_M)^H \mathcal{H}_M (\mathcal{I}_M - \mathcal{F}_M)^{-1} (v \otimes I_n) p$ (GMRES!)
3. Choose right amount of coefficients to keep $\tilde{\boldsymbol{u}}_{M-b}$
4. Solution is $w^H \tilde{U}(t) v \approx \sum_{i=0}^{M-b} \tilde{u}_i p_i(t)$

# Kronecker structure

In many applications, the function $\tilde{A}(t)$ is given as a sum of Kronecker products:

$$\tilde{A}(t) = \sum_{j=0}^{s} A_j \otimes \tilde{f}_j(t),$$

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

$$(Id - \sum_{j=0}^{s} A_j \otimes F_j)\mathrm{vec}(X) = v \otimes \boldsymbol{\varphi}_m(-1),$$

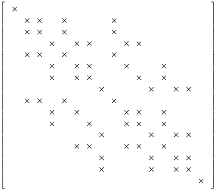
with $F_j$ the Legendre discretization matrices, or, equivelently, as the matrix equation with a low-rank rhs

$$X - \sum_{j=0}^{s} F_j X A_j^T = \boldsymbol{\varphi}_m(-1) v^T.$$

# Experiment 1 [Baligács, Bonhomme]

Setup:

- $\ell = 4$ spins $\rightarrow 16 \times 16$
- homonuclear dipolar coupling
- Magic angle spinning $\nu \in [5e3, 120e3]$
- $H(t) = D + B\cos(2\pi\nu t) + C\cos(4\pi\nu t)$
- time $t \in [0, 1e{-}4]$ (practical: $\mathcal{O}(e-2)$)
- Structure $B$ and $C$



Compute:

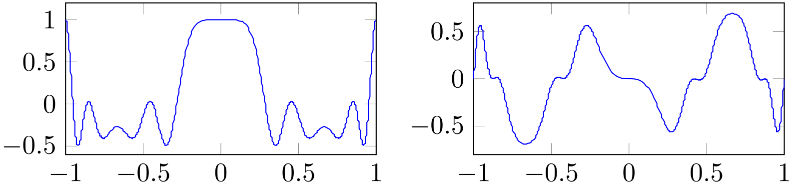
- bilinear form $w^H \tilde{U}(t) v$
- Initial state $v = \begin{bmatrix} 1 & \dots & 1 \end{bmatrix}^\top \in \mathbb{C}^m$
- Measurement $w = \begin{bmatrix} 1 & \dots & 1 \end{bmatrix}^\top \in \mathbb{C}^m$

# Experiment 1: numerical

Numerical:

- $\tilde{\boldsymbol{u}} := U_n p = H_n(I_n - F_n)^{-1} p \rightarrow$ GMRES
- Reference solution $\hat{u}$: `ode45` in Matlab
- Error: $\text{err} := \|\hat{u}(t) - \sum_{i=0}^{n} \tilde{u} p_i(t)\|_\infty$

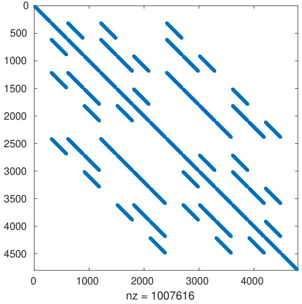
Solution $\hat{u}(t)$



# Result $M = 300$ & cutoff at $k = 137$

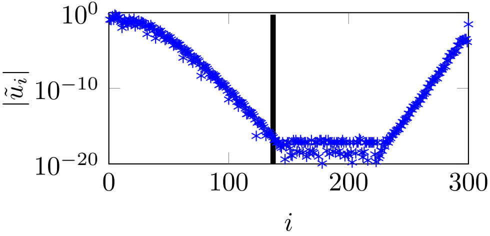
Approximation for $\tilde{u}(t) \approx \sum_{i=0}^{k} \tilde{u}_i p_i(t)$

- Solve system $(I_M - F_M)y = p$
- Multiplication $\tilde{\boldsymbol{u}} = H_M y$
- Size $nM \times nM$, $nM = 4800$



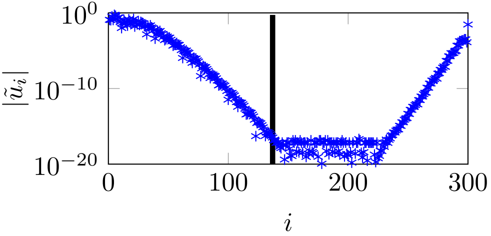

GMRES

- 44 iterations
- cutoff at $k = 137$

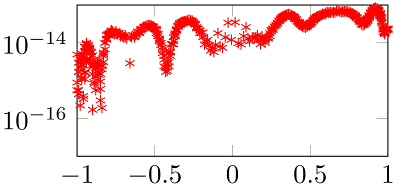


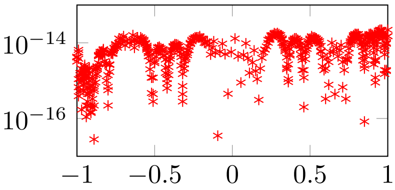
# Quality of approximation $M = 300$, cutoff $k = 137$

Coefficients:




For $\sum_{i=0}^{137} \tilde{u}_i p_i(t)$: $\text{err} = 4.1e-14$

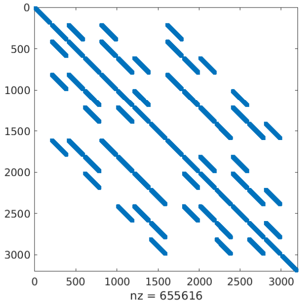


# Result $M = 200$ & cutoff at $k = 137$

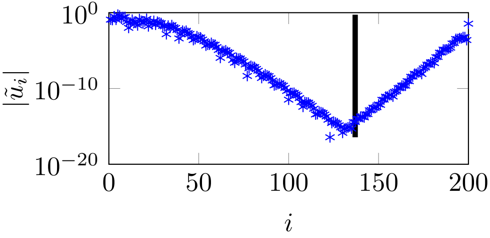
Approximation for $\tilde{u}(t) \approx \sum_{i=0}^{k} \tilde{u}_i p_i(t)$

- Solve system $(I_M - F_M)y = p$
- Multiplication $\tilde{\boldsymbol{u}} = H_M y$
- Size $nM \times nM$, $nM = 3200$



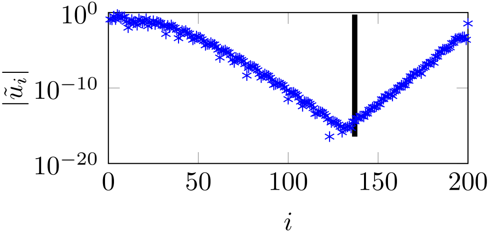

GMRES

- 44 iterations
- cutoff at $k = 137$

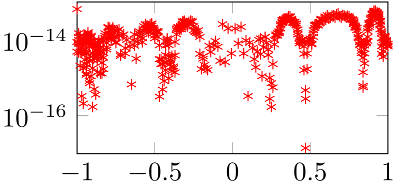


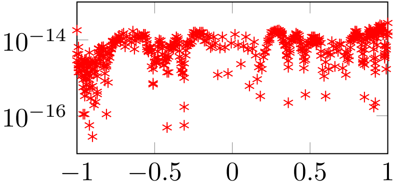
# Quality of approximation $M = 200$, cutoff $k = 137$

Coefficients:



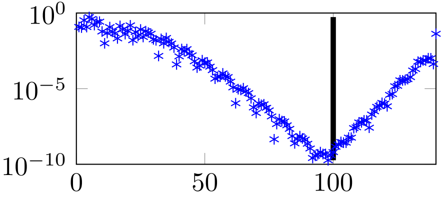

For $\sum_{i=0}^{137} \tilde{u}_i p_i(t)$: $\mathrm{err} = 4.7e - 14$



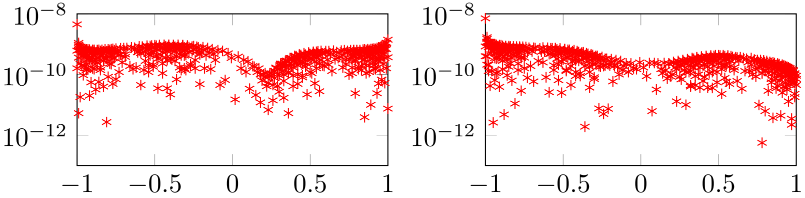



# Quality of approximation $M = 140$, cutoff $k = 100$

Coefficients:



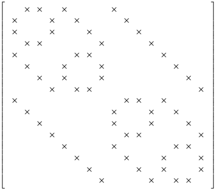

For $\sum_{i=0}^{100} \tilde{u}_i p_i(t)$: $\text{err} = 7.1e-9$



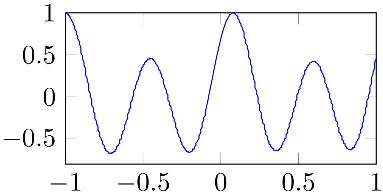
# Experiment 2 [Baligács, Bonhomme]

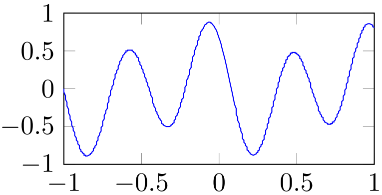
Setup:

- $\ell = 4$ spins $\rightarrow 16 \times 16$
- uncoupled spins under a pulse wave
- $H(t) = A + B(0.5 + \cos(4t) + \sin(10t) - 0.4\sin(16t)) + C(\sin(4t) + \cos(8t) + 2\sin(12t))$
- time $t \in [0, 1e{-2}]$
- Structure $B$ and $C$



Solution $\hat{u}(t)$

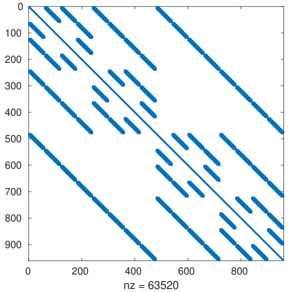


# Result $M = 60$ & cutoff at $k = 44$

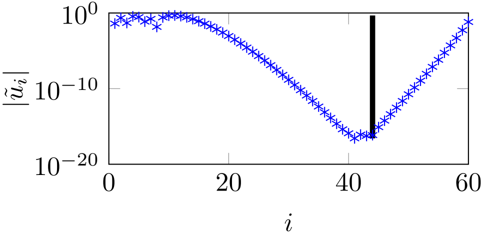
Approximation for $\tilde{u}(t) \approx \sum_{i=0}^{k} \tilde{u}_i p_i(t)$

- Solve system $(I_M - F_M)y = p$
- Multiplication $\tilde{\boldsymbol{u}} = H_M y$
- Size $nM \times nM$, $nM = 3200$



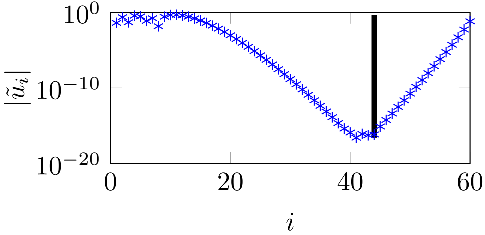

GMRES

- 59 iterations
- cutoff at $i = 44$

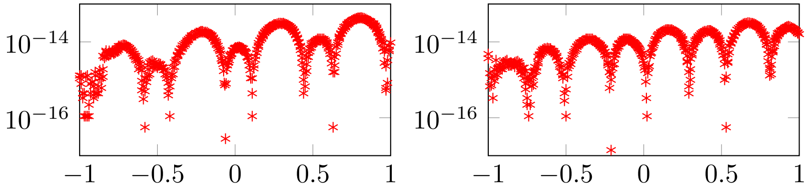


# Quality of approximation $M = 60$, cutoff $k = 44$

Coefficients:




For $\sum_{i=0}^{44} \tilde{u}_i p_i(t)$: $\mathrm{err} = 4.4e - 14$



# Recap

ODE: $\frac{d}{dt}U(t) = A(t)U(t)$

- New expression for $U(t) = U(t, -1)$:
  $U(t, s) = \Theta(t - s) \star (1_\star - A(t)\Theta(t - s))^{\star -1}$
- Legendre series: $\tilde{\boldsymbol{u}} = U_M p$, with $U_M = H_M(I - F_M)^{-1}$
- Bandedness $\Rightarrow$ recover decay of coefficients
- Efficient if:
  - fast solution linear system (Krylov + preconditioner!)
  - good estimation of $M$

# Recap

ODE: $\frac{d}{dt}U(t) = A(t)U(t)$

- New expression for $U(t) = U(t, -1)$:
  $U(t, s) = \Theta(t - s) \star (1_\star - A(t)\Theta(t - s))^{\star -1}$
- Legendre series: $\tilde{\boldsymbol{u}} = U_M p$, with $U_M = H_M(I - F_M)^{-1}$
- Bandedness $\Rightarrow$ recover decay of coefficients
- Efficient if:
  - fast solution linear system (Krylov + preconditioner!)
  - good estimation of $M$

Future work

# References


- S. P., N. V-B, paper in preparation
- P-L. Giscard, S. Pozza., *Lanczos-like method for the time-ordered exponential*, arXiv:1909.03437 [math.NA].
- P-L. Giscard, S. Pozza., *Lanczos-like algorithm for the time-ordered exponential: The $*$-inverse problem*, Applications of Mathematics, 2020.
- P-L. Giscard, S. Pozza, *Tridiagonalization of systems of coupled linear differential equations with variable coefficients by a Lanczos-like method*, Linear Algebra and its Applications, 2020.
- E. Baligács and C. Bonhomme, github.com/BaligacsEni/TOMEexamples.git, 2022.


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)*.


Thank you for your attention!