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# Hierarchical tensor methods for high-dimensional nonlinear PDEs

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Workshop on Computational Issues in Nonlinear Control, Monterrey (CA)

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October 7, 2019

## Motivation

Consider the nonlinear optimal feedback control problem

$$\left\{ \begin{array}{l} \min_{\mathbf{u}(t, \mathbf{x})} F(\mathbf{x}(t_f)) + \int_t^{t_f} [h(\mathbf{x}(\tau)) + \mathbf{u}(\tau, \mathbf{x}(\tau))^T \mathbf{W} \mathbf{u}(\tau, \mathbf{x}(\tau))] d\tau \\ \text{subject to:} \\ \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{G}(\mathbf{x})\mathbf{u}(t, \mathbf{x}) \quad \mathbf{x}(t) = \mathbf{x} \end{array} \right. \quad \begin{array}{l} \text{open-loop: } \mathbf{u}(t) \\ \text{feedback: } \mathbf{u}(t, \mathbf{x}(t)) \end{array}$$

For each initial condition  $\mathbf{x}$  specified at time  $t$ , we define the **value function** (or cost-to-go)

$$V(t, \mathbf{x}) = \inf_{\mathbf{u}} \left\{ F(\mathbf{x}(t_f)) + \int_t^{t_f} [h(\mathbf{x}(\tau)) + \mathbf{u}(\tau, \mathbf{x}(\tau))^T \mathbf{W} \mathbf{u}(\tau, \mathbf{x}(\tau))] d\tau \right\} \quad (\mathbf{x} \text{ state at time } t)$$

It can be shown that the value function  $V(t, \mathbf{x})$  allows us to compute the optimal feedback control  $\mathbf{u}(t, \mathbf{x})$  as:

Optimal feedback control

$$\mathbf{u}^*(t, \mathbf{x}) = -\frac{1}{2} \mathbf{W}^{-1} \mathbf{G}^T(\mathbf{x}) \nabla V(t, \mathbf{x})$$

## Hamilton-Jacobi-Bellmann (HJB) equation

The value function  $V(t, \mathbf{x})$  satisfies the following HJB equation (here we set  $\mathbf{W} = \mathbf{I}$ )

$$\frac{\partial V(t, \mathbf{x})}{\partial t} + h(\mathbf{x}) + \mathbf{f}(\mathbf{x}) \cdot \nabla V(t, \mathbf{x}) = \frac{1}{4} \|\mathbf{G}^T(\mathbf{x}) \nabla V(t, \mathbf{x})\|_2^2 \quad V(t_f, \mathbf{x}) = F(\mathbf{x})$$

This equation can be solved pointwise by using the **method of characteristics**

$$\text{Two-point boundary value problem} \quad \begin{cases} \dot{\mathbf{x}}(\tau) = \mathbf{f}(\mathbf{x}) - \frac{1}{2} \mathbf{G}(\mathbf{x}) \mathbf{G}^T(\mathbf{x}) \boldsymbol{\lambda} & \mathbf{x}(0) = \mathbf{x}_0 \\ \dot{\boldsymbol{\lambda}}(\tau) = -\nabla h(\mathbf{x}) - \boldsymbol{\lambda}^T \left( \nabla \mathbf{f}(\mathbf{x}) - \frac{1}{2} \nabla (\mathbf{G}(\mathbf{x}) \mathbf{G}^T(\mathbf{x})) \boldsymbol{\lambda} \right) & \boldsymbol{\lambda}(t_f) = \nabla F(\mathbf{x}(t_f)) \\ \dot{v}(\tau) = h(\mathbf{x}) + \frac{1}{4} \boldsymbol{\lambda}^T \mathbf{G}(\mathbf{x}) \mathbf{G}^T(\mathbf{x}) \boldsymbol{\lambda} & v(0) = 0 \end{cases}$$

Here  $v(t)$  and  $\boldsymbol{\lambda}(t)$  represent, respectively, the **value function** and its **gradient** along the curve  $\mathbf{x}(t, \mathbf{x}_0)$

$$\boldsymbol{\lambda}(t) = \nabla V(t, \mathbf{x}(t, \mathbf{x}_0))$$

# Outline

## Hierarchical tensor expansions of high-dimensional functions

- Tensor-train format

## Dynamically orthogonal tensor methods for nonlinear PDEs

- DO-TT propagator
- Numerical applications to hyperbolic and parabolic PDE

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A. Dektor and D. Venturi, “Dynamically orthogonal tensor methods for high-dimensional nonlinear PDEs”, *arXiv* 1907.05924, 2019, pp. 1–39.

# Hierarchical bi-orthogonal decomposition of functions in separable measure spaces

Let us consider a domain  $\Omega \subset \mathbb{R}^d$  defined as a Cartesian product of  $d \geq 2$  one-dimensional sets

$$\Omega = \Omega_1 \times \cdots \times \Omega_d \quad \Omega_i \subset \mathbb{R}$$

On  $\Omega$  we define the scalar field  $u: \Omega \mapsto \mathbb{R}$ , which we assume to be an element of the Sobolev space

$$H^k(\Omega) = \{u \in L^2_\mu(\Omega) : D^\alpha u \in L^2_\mu(\Omega) \text{ for all } |\alpha| \leq k\}, \quad k = 0, 1, 2, \dots$$

$$D^\alpha u = \frac{\partial^{|\alpha|} u}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} \quad |\alpha| = \alpha_1 + \cdots + \alpha_d$$

We equip  $H^k(\Omega)$  with the inner product

$$\langle f, g \rangle_{H^k(\Omega)} = \sum_{|\alpha| \leq k} \int_{\Omega} D^\alpha f(\mathbf{x}) D^\alpha g(\mathbf{x}) \underbrace{\mu_1(x_1) \cdots \mu_d(x_d)}_{\mu(\mathbf{x}) \text{ (separable measure)}} d\mathbf{x}$$

# Hierarchical bi-orthogonal decomposition of functions in separable measure spaces

The Sobolev space  $H^k(\Omega)$  is separable

$$H^k(\Omega) = H^k(\Omega_1) \otimes \cdots \otimes H^k(\Omega_d)$$

The inner product within each subspace  $H^k(\Omega_p)$  can be defined as

$$\langle f, g \rangle_{H^k(\Omega_p)} = \sum_{\alpha=0}^k \int_{\Omega_p} \frac{\partial^\alpha f}{\partial x^\alpha} \frac{\partial^\alpha g}{\partial x^\alpha} \mu_p(x) dx \quad f, g \in H^k(\Omega_p).$$

More generally, the inner product in  $H^k(\Omega_{p,q})$ , where  $\Omega_{p,q} = \Omega_p \times \cdots \times \Omega_q$  can be defined as

$$\langle f, g \rangle_{H^k(\Omega_{p,q})} = \sum_{\alpha_p + \cdots + \alpha_q \leq k} \int_{\Omega_{p,q}} \frac{\partial^{\alpha_p + \cdots + \alpha_q} f}{\partial x_p^{\alpha_p} \cdots \partial x_q^{\alpha_q}} \frac{\partial^{\alpha_p + \cdots + \alpha_q} g}{\partial x_p^{\alpha_p} \cdots \partial x_q^{\alpha_q}} \mu_p(x_p) \cdots \mu_q(x_q) dx_p \cdots dx_q$$

# Hierarchical bi-orthogonal decomposition of functions in separable measure spaces

A representation of the function  $u(x_1, \dots, x_d)$  in the space  $H^k(\Omega_1) \otimes \dots \otimes H^k(\Omega_d)$  takes the form

$$u(x_1, \dots, x_d) = \sum_{i_1, \dots, i_d=1}^{\infty} a_{i_1 \dots i_d} \varphi_{i_1}^{(1)}(x_1) \cdots \varphi_{i_d}^{(d)}(x_d) \quad \varphi_{i_k}^{(k)}(x_k) \text{ orthonormal}$$

A truncation to  $r$  modes yields an expansion with  $r^d$  degrees of freedom (number of entries in  $a_{i_1 \dots i_d}$ )

$$d = 6 \quad r = 30 \quad \Rightarrow r^d = 590.49 \times 10^{12} \quad (73.81 \text{ TB})$$

To develop a more effective series expansion, we perform a sequence of bi-orthogonal decompositions as follows

$$\begin{aligned} H^k(\Omega) &= H^k(\Omega^1) \otimes H^k(\Omega^2 \times \dots \times \Omega^d) \\ &= H^k(\Omega^1) \otimes [H^k(\Omega^2) \otimes H^k(\Omega^3 \times \dots \times \Omega^d)] \\ &= H^k(\Omega^1) \otimes [H^k(\Omega^2) \otimes [H^k(\Omega^3) \otimes H^k(\Omega^4 \times \dots \times \Omega^d)]] \end{aligned}$$

...

(Tensor train format)

## Tensor-train format

In practice, we recursively single out one variable at a time until we obtain a product of 1D functions

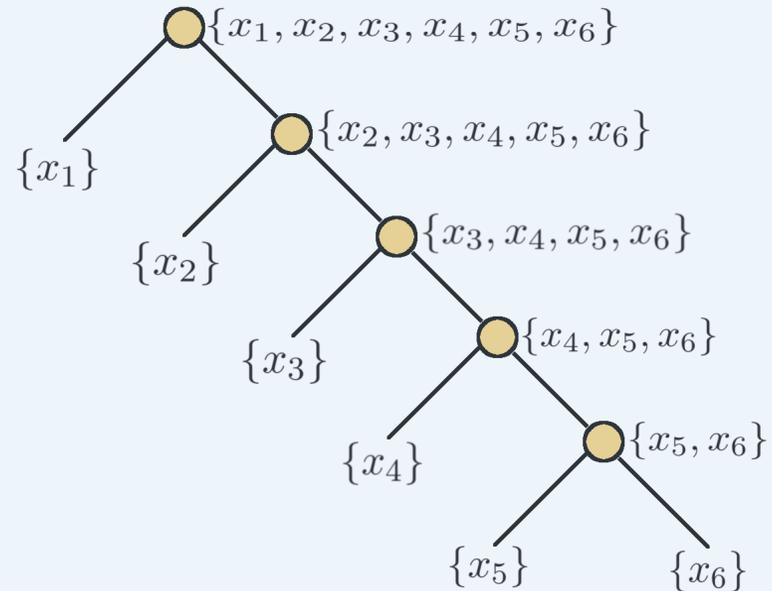
$$u(x_1, \dots, x_6) = \sum_{i_1=1}^{\infty} \lambda_{i_1} \psi_{i_1}^{(1)} \psi_{i_1}^{(2, \dots, 6)}$$

$$\psi_{i_1}^{(2, \dots, 6)} = \sum_{i_2=1}^{\infty} \lambda_{i_1 i_2} \psi_{i_1 i_2}^{(2)} \psi_{i_1 i_2}^{(3, \dots, 6)}$$

$$\psi_{i_1 i_2}^{(3, \dots, 6)} = \sum_{i_3=1}^{\infty} \lambda_{i_1 i_2 i_3} \psi_{i_1 i_2 i_3}^{(3)} \psi_{i_1 i_2 i_3}^{(4, \dots, 6)}$$

$$\psi_{i_1 i_2 i_3}^{(4, \dots, 6)} = \sum_{i_4=1}^{\infty} \lambda_{i_1 i_2 i_3 i_4} \psi_{i_1 i_2 i_3 i_4}^{(4)} \psi_{i_1 i_2 i_3 i_4}^{(5, 6)}$$

$$\psi_{i_1 i_2 i_3 i_4}^{(5, 6)} = \sum_{i_5=1}^{\infty} \lambda_{i_1 i_2 i_3 i_4 i_5} \psi_{i_1 i_2 i_3 i_4 i_5}^{(5)} \psi_{i_1 i_2 i_3 i_4 i_5}^{(6)}$$



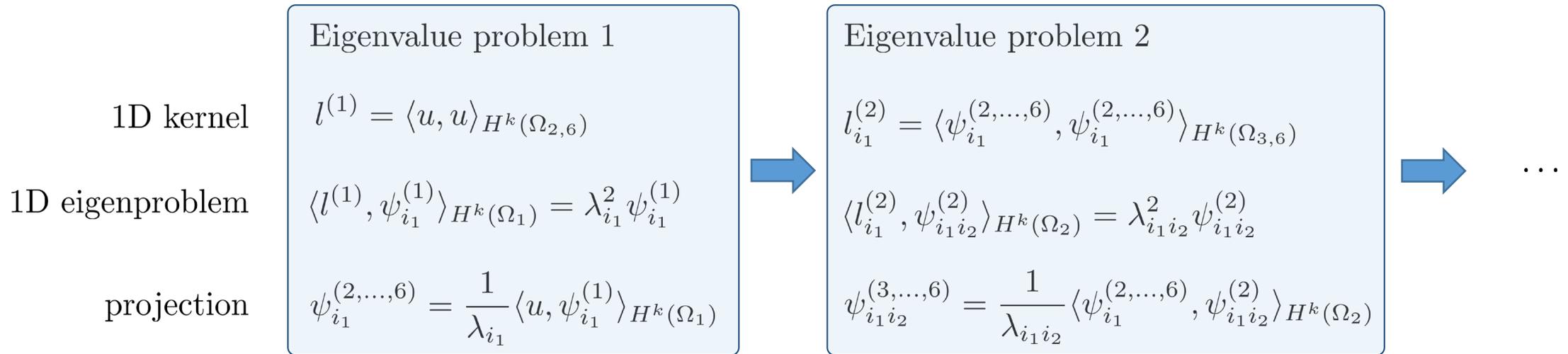
Binary tree representing the Tensor Train decomposition of a 6D function

## Tensor-train format

This yields the following expansion

$$u(x_1, \dots, x_6) \simeq \sum_{i_1=1}^{r_1} \cdots \sum_{i_5=1}^{r_5} \lambda_{i_1} \lambda_{i_1 i_2} \lambda_{i_1 i_2 i_3} \lambda_{i_1 i_2 i_3 i_4} \lambda_{i_1 i_2 i_3 i_4 i_5} \psi_{i_1}^{(1)} \psi_{i_1 i_2}^{(2)} \psi_{i_1 i_2 i_3}^{(3)} \psi_{i_1 i_2 i_3 i_4}^{(4)} \psi_{i_1 i_2 i_3 i_4 i_5}^{(5)} \psi_{i_1 i_2 i_3 i_4 i_5}^{(6)}$$

The eigenvalues  $\lambda_{i_1 \dots i_k}$  and the 1D tensor modes  $\psi_{i_1 \dots i_k}^{(k)}$  are obtained by solving a hierarchy of eigenvalue problems



## Tresholding the TT expansion

The eigenvalue  $\lambda_{i_1 \dots i_k}$  represents the energy of the 1D tensor mode  $\psi_{i_1 \dots i_k}^{(k)}$

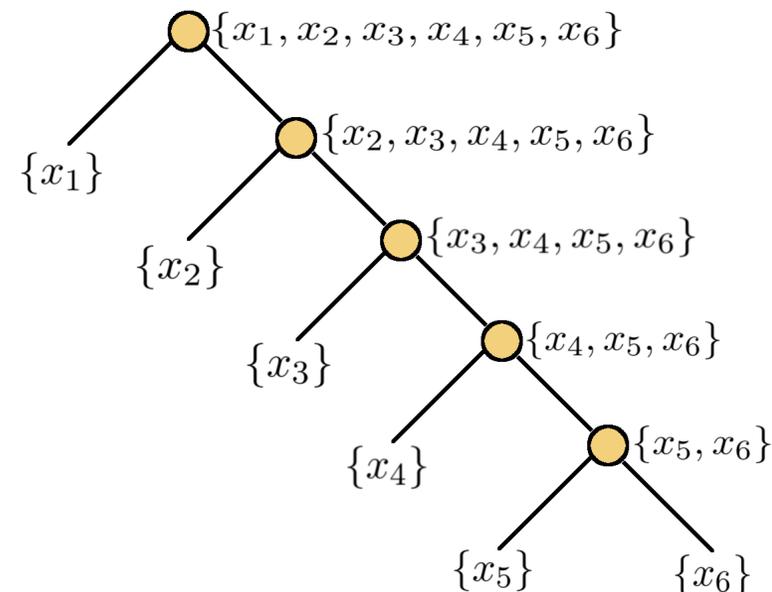
We begin by setting some treshold  $\sigma$

**level 1:** keep all eigenvalues  $\lambda_{i_1} \geq \sigma$

**level 2:** keep all eigenvalues  $\lambda_{i_1 i_2} \geq \sigma / \lambda_{i_1}$

$\vdots$

**level 5:** keep all eigenvalues  $\lambda_{i_1 i_2 i_3 i_4 i_5} \geq \sigma / \lambda_{i_1 i_2 i_3 i_4}$



Binary tree representing the Tensor Train decomposition of a 6D function

In this way, we guarantee that the the energy of each 6D mode is above the threshold  $\sigma$

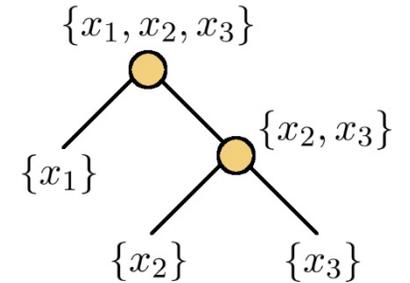
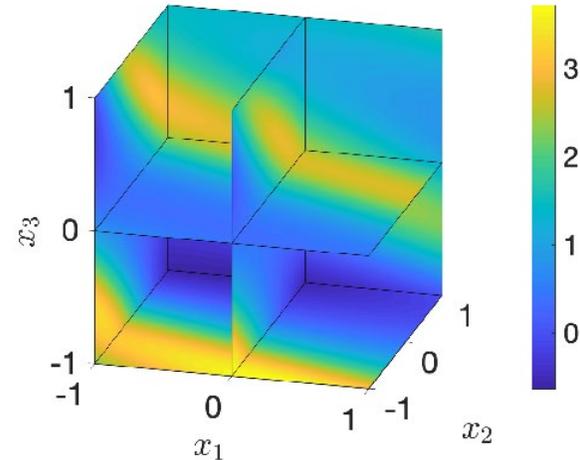
$$\lambda_{i_1} \lambda_{i_1 i_2} \lambda_{i_1 i_2 i_3} \lambda_{i_1 i_2 i_3 i_4} \lambda_{i_1 i_2 i_3 i_4 i_5} \geq \sigma$$

# TT decomposition: An example

Consider the 3D function

$$u = e^{\sin(x_1 + 2x_2 + 3x_3)} + x_2 x_3$$

$$u \simeq \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2(r_1)} \lambda_{i_1} \lambda_{i_1 i_2} \psi_{i_1}^{(1)} \psi_{i_1 i_2}^{(1)} \psi_{i_1 i_2}^{(3)}$$

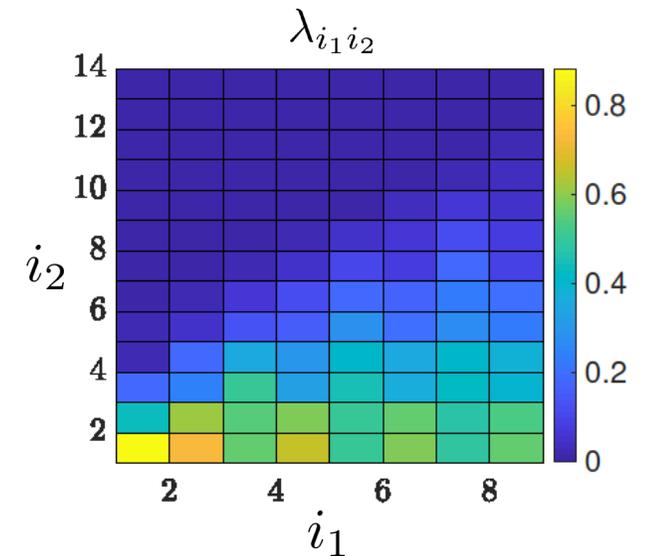
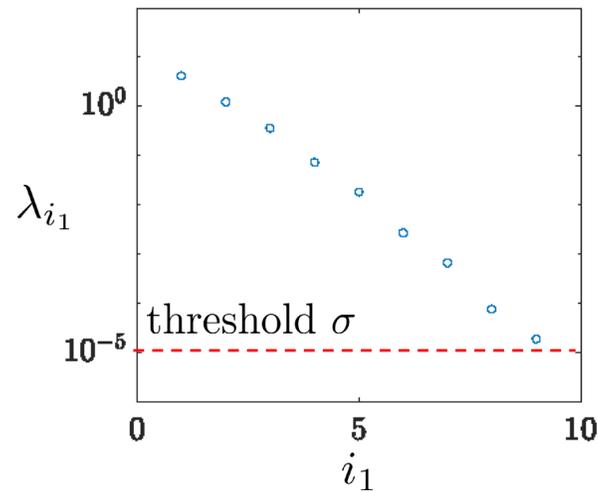


By using the tresholding method we obtain

$$\sigma = 10^{-5}$$

$$r_1 = 9$$

$$r_2(r_1) = [11, 11, 11, 11, 11, 11, 10, 6, 0]$$



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## Dynamically orthogonal tensor methods

Consider the nonlinear autonomous evolution equation

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = \mathcal{G}(u) \quad u(\mathbf{x}, 0) = u_0(\mathbf{x}) \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d$$

Here  $\mathcal{G}$  is a nonlinear operator which may incorporate boundary conditions. We look for a representation of the solution in the form

$$u(\mathbf{x}, t) \simeq \sum_{i_1=1}^{r_1} \cdots \sum_{i_{d-1}=r_{d-1}}^{\infty} \lambda_{i_1}(t) \cdots \lambda_{i_1 \cdots i_{d-1}}(t) \psi_{i_1}^{(1)}(t) \psi_{i_1 i_2}^{(2)}(t) \cdots \psi_{i_1 \cdots i_{d-1}}^{(d-1)}(t) \psi_{i_1 \cdots i_{d-1}}^{(d)}(t)$$

(Time-dependent TT expansion)

We assume that the time-dependent tensor modes satisfy

$$\left\langle \psi_{i_1 \cdots i_q}^{(q)}, \frac{\partial \psi_{i_1 \cdots i_q}^{(q)}}{\partial t} \right\rangle = 0 \quad (\text{Dynamic orthogonality condition})$$

Note that:  $\{\psi_{i_1 \cdots i_k}^{(k)}(0)\} \perp \Rightarrow \{\psi_{i_1 \cdots i_k}^{(k)}(t)\} \perp$

## DO-TT propagator

A substitution of the time-dependent TT expansion into the nonlinear PDE and subsequent projection onto the TT modes yields

$$\frac{\partial \Psi_{k_1 \dots k_j}^{(j+1, \dots, d)}}{\partial t} = N_{k_1 \dots k_j}^{(j+1, \dots, d)}, \quad \text{(System of 1D nonlinear PDEs)}$$

$$\sum_{i_j=1}^{r_j} \frac{\partial \psi_{k_1 \dots k_{j-1} i_j}^{(j)}}{\partial t} \langle \Psi_{k_1 \dots k_{j-1} i_j}^{(j+1, \dots, d)}, \Psi_{k_1 \dots k_j}^{(j+1, \dots, d)} \rangle$$

$$= \langle N_{k_1 \dots k_{j-1}}, \Psi_{k_1 \dots k_j}^{(j+1, \dots, d)} \rangle - \sum_{i_j=1}^{r_j} \psi_{k_1 \dots k_{j-1} i_j} \langle N_{k_1 \dots k_{j-1}}^{(j, \dots, d)}, \Psi_{k_1 \dots k_j}^{(j+1, \dots, d)} \psi_{k_1 \dots k_{j-1} i_j}^{(j)} \rangle$$

Here

$$\Psi_{k_1 \dots k_j}^{(j+1, \dots, d)} = \lambda_{k_1 \dots k_j}(t) \psi_{k_1 \dots k_j}^{(j+1, \dots, d)} \quad N_{k_1}^{(2, \dots, d)} = \langle \mathcal{G}(u), \psi_{k_1}^{(1)} \rangle \quad N_{k_1 \dots k_j}^{(j+1, \dots, d)} = \langle N_{k_1 \dots k_{j-1}}^{(j, \dots, d)} \psi_{k_1 \dots k_j}^{(j)} \rangle$$

The DO-TT propagator allows us to compute the solution of the PDE on a **smooth tensor manifold with constant rank**.

## One-step truncation algorithms vs DO-TT propoagators

Approximating the nonlinear PDE with respect to the space variables yields the system of ODEs

$$\frac{d\mathbf{u}(t)}{dt} = \mathbf{G}(\mathbf{u}) \quad \mathbf{u}(0) = \mathbf{u}_0$$

where  $\mathbf{u}: [0, T] \mapsto \mathbb{R}^{n_1 \times \dots \times n_d}$  is the solution tensor.

$$\mathbf{u}^{k+1} = \mathbf{u}^k + \frac{\Delta t}{2} [3\mathbf{G}(\mathbf{u}^k) - \mathbf{G}(\mathbf{u}^{k-1})] \quad (\text{AB2 integrator})$$

The iterated application of this scheme increases the tensor rank at each time step. In other words the rank of  $\mathbf{u}^{k+1}$  is larger than then rank of  $\mathbf{u}^k$  and  $\mathbf{u}^{k-1}$ . Hence, if we are interested in computing the solution on a tensor manifold with constant rank, we need to **retract** the solution back to such tensor manifold:

$$\mathbf{u}^{k+1} = \mathfrak{T}_r(\mathbf{u}^{k+1}) \quad \begin{array}{l} \text{rank truncation operator} \\ \text{(e.g. high-order SVD)} \end{array}$$

## Four-dimensional hyperbolic PDE

Consider the following initial value problem defined in the periodic hypercube  $[0, 2\pi]^4$

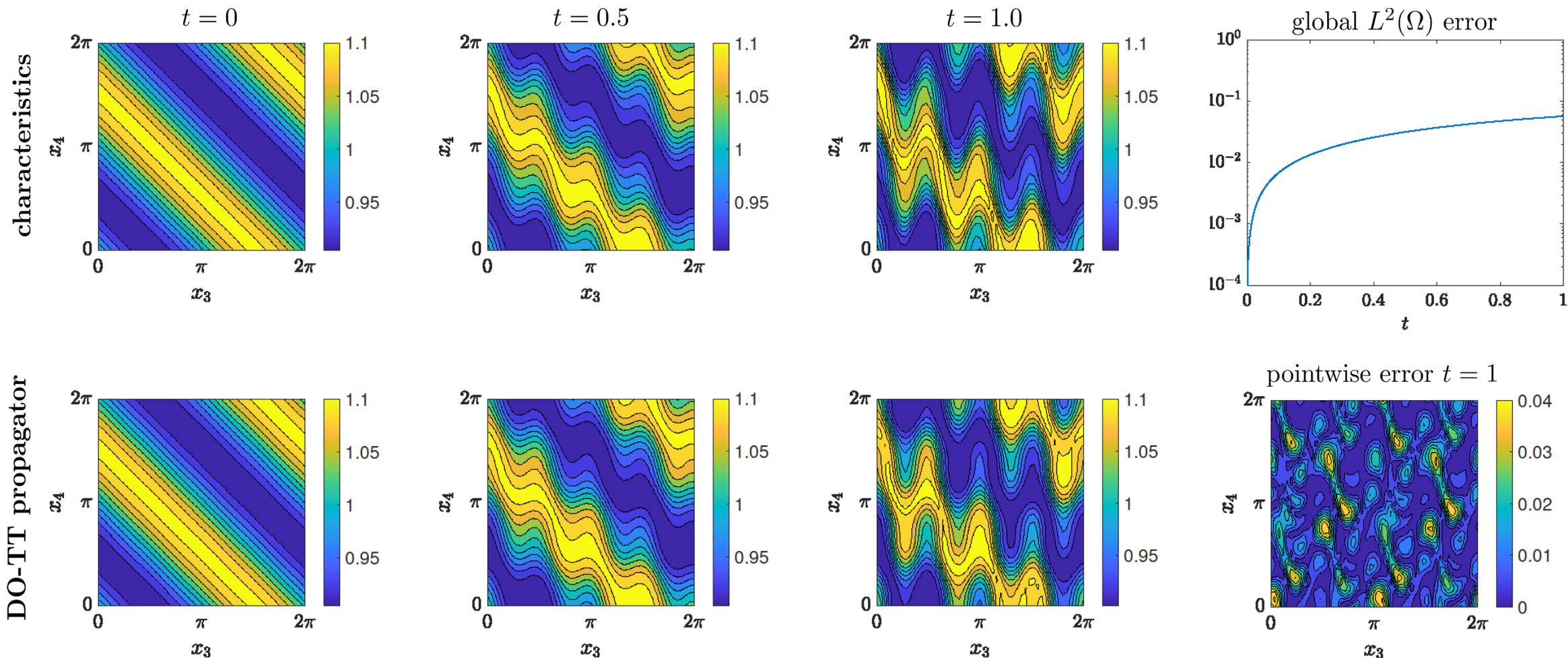
$$\begin{cases} \frac{\partial u(\mathbf{x}, t)}{\partial t} = \frac{1}{2} \cos(2x_2) \frac{\partial u(\mathbf{x}, t)}{\partial x_1} - \frac{1}{3} \sin(3x_3) \frac{\partial u(\mathbf{x}, t)}{\partial x_2} - \cos(4x_4) \frac{\partial u(\mathbf{x}, t)}{\partial x_3} + \frac{1}{2} \sin(x_1) \frac{\partial u(\mathbf{x}, t)}{\partial x_4} \\ u(\mathbf{x}, 0) = \exp \left[ -\frac{1}{10} \sin(x_1 + x_2 + x_3 + x_4) \right] \end{cases}$$

Thresholding the TT decomposition of the initial condition with  $\sigma = 10^{-5}$  yields

$$u(\mathbf{x}, 0) \simeq \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2(r_1)} \sum_{i_3=1}^{r_3(r_2)} \lambda_{i_1}(0) \lambda_{i_1 i_2}(0) \lambda_{i_1 i_2 i_3}(0) \psi_{i_1}^{(1)}(0) \psi_{i_1 i_2}^{(2)}(0) \psi_{i_1 i_2 i_3}^{(3)}(0) \psi_{i_1 i_2 i_3}^{(4)}(0)$$

$$r_1 = 9 \quad r_2 = [1 \quad 2 \quad 2] \quad r_3 = \begin{bmatrix} 1 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \\ 0 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{bmatrix}$$

# Four-dimensional hyperbolic PDE

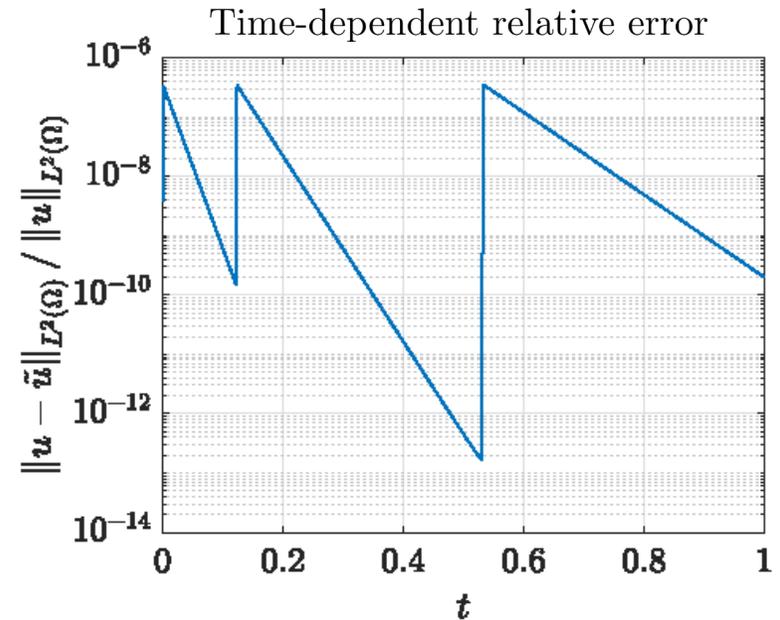
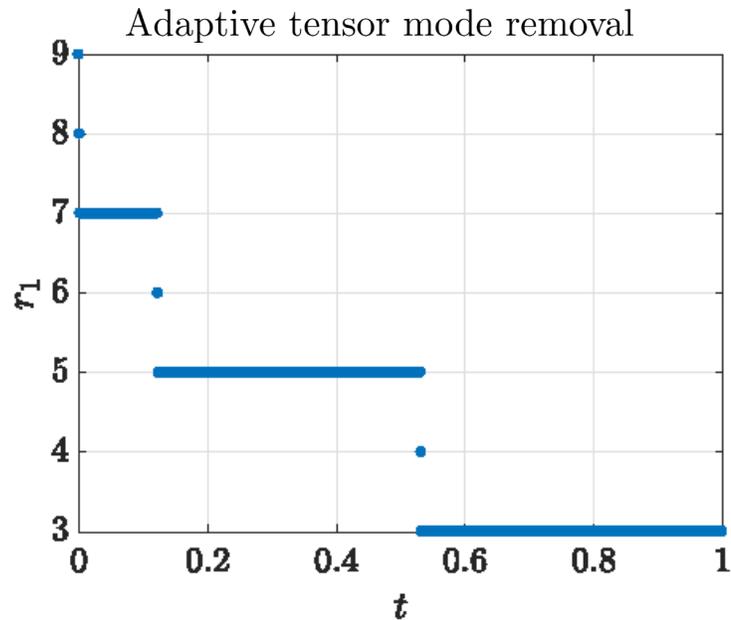


Time snapshots of 2D slide ( $x_1 = 2.95, x_2 = 2.95$ ) of the DO-TT and semi-analytical solution.

# Four-dimensional parabolic PDE

Consider the following initial value problem defined in the periodic hypercube  $[0, 2\pi]^4$

$$\begin{cases} \frac{\partial u(\mathbf{x}, t)}{\partial t} = \sum_{j=1}^4 \frac{\partial^2 u(\mathbf{x}, t)}{\partial x_j^2} \\ u(\mathbf{x}, 0) = \exp\left[-\frac{1}{10} \sin(x_1 + x_2 + x_3 + x_4)\right] \end{cases}$$



## Fifty-dimensional hyperbolic PDE

Consider the following initial value problem defined in the periodic hypercube  $[0, 2\pi]^{50}$

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = \sum_{j=1}^{50} j \frac{\partial u(\mathbf{x}, t)}{\partial x_j} \quad u(\mathbf{x}, 0) = \prod_{j=1}^{50} \psi_0^{(j)}(x_j)$$

The analytical solution to this problem is easily obtained as

$$u(\mathbf{x}, t) = \prod_{j=1}^{50} \psi_0^{(j)}(x_j - jt)$$

Note that the analytical solution is rank-one at each time. Hence, we look for a rank-one TT representation of the solution as

$$u(\mathbf{x}, t) \simeq \prod_{j=1}^{50} \psi^{(j)}(t)$$

# Fifty-dimensional hyperbolic PDE

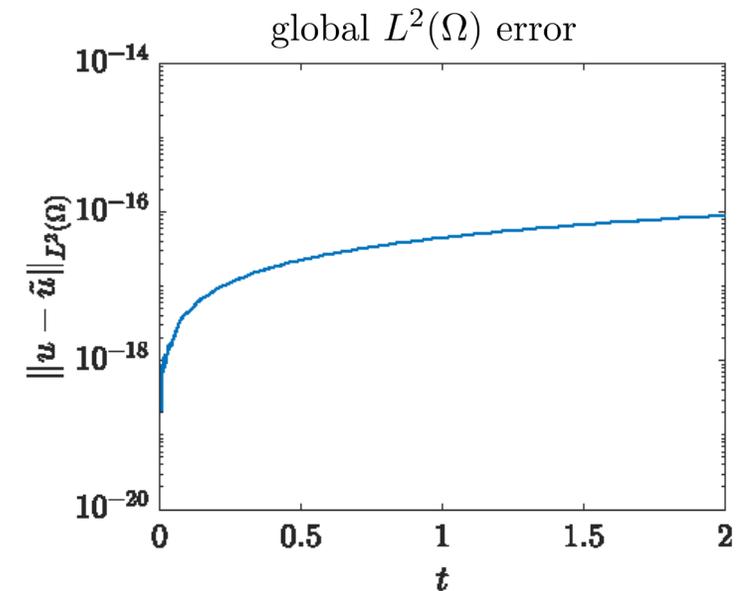
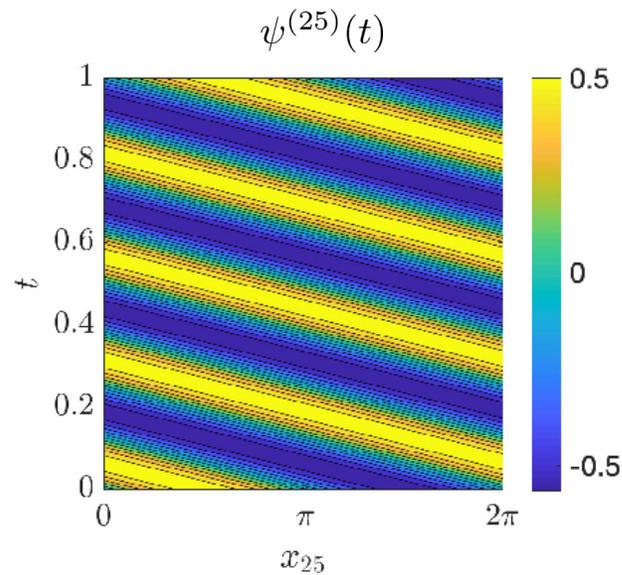
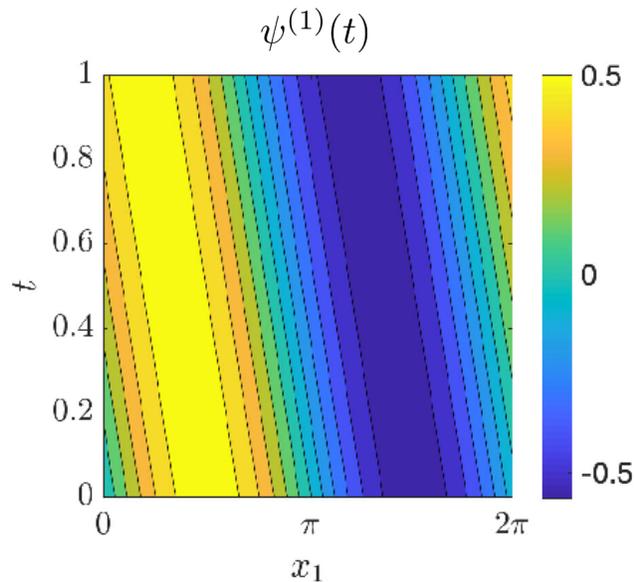
The DO-TT propagator is

$$\frac{\partial \psi^{(j)}}{\partial t} = j \frac{\partial \psi^{(j)}}{\partial x_j} - j \psi^{(j)} \left\langle \frac{\partial \psi^{(j)}}{\partial x_j} \psi^{(j)} \right\rangle$$

$$\frac{\partial \psi^{(50)}}{\partial t} = \sum_{j=1}^{49} j \left\langle \frac{\partial \psi^{(j)}}{\partial x_j} \psi^{(j)} \right\rangle \psi^{(50)}$$

$$\psi_0^{(j)}(x_j) = \frac{\sin(x_j)}{\sqrt{\pi}} \quad (j = 1, \dots, 49)$$

$$\psi_0^{(50)}(x_{50}) = 10^7 (3 + \sin(x_{50}))$$



## Fifty-dimensional parabolic PDE

Consider the following initial value problem defined in the periodic hypercube  $[0, 2\pi]^{50}$

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = \sum_{j=1}^{50} \frac{\partial^2 u(\mathbf{x}, t)}{\partial x_j^2} \quad u(\mathbf{x}, 0) = \prod_{j=1}^{50} \psi_0^{(j)}(x_j)$$

The analytical solution to this problem is easily obtained as

$$u(\mathbf{x}, t) = \prod_{j=1}^{50} \psi_0^{(j)}(x_j) e^{-50t}$$

Note that the analytical solution is rank-one at each time. Hence, we look for a rank-one TT representation of the solution as

$$u(\mathbf{x}, t) \simeq \prod_{j=1}^{50} \psi^{(j)}(t)$$

# Fifty-dimensional hyperbolic PDE

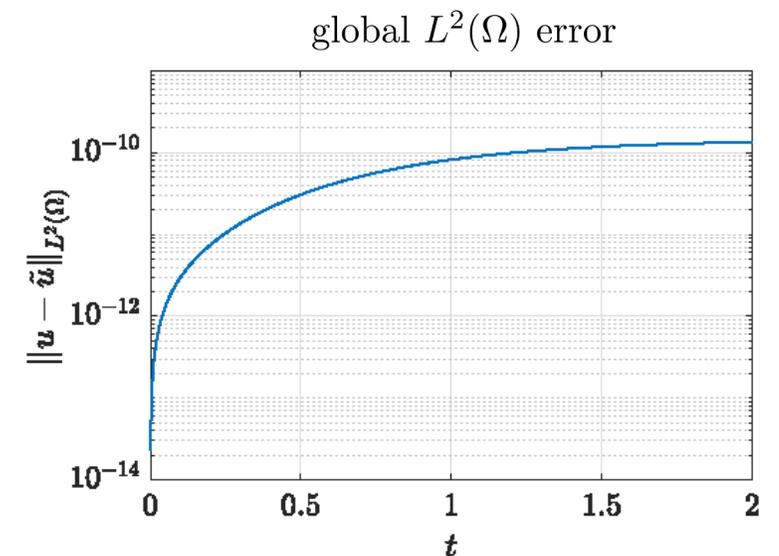
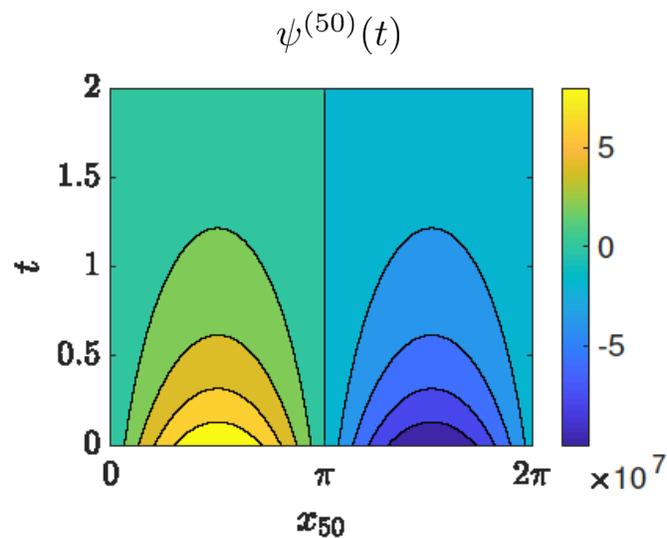
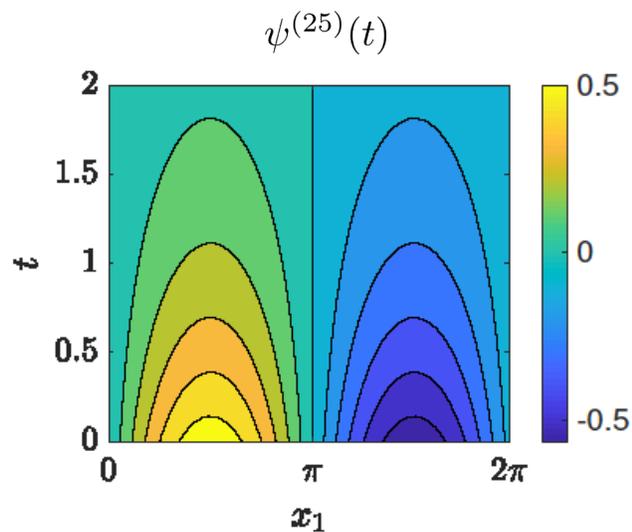
The DO-TT propagator is

$$\frac{\partial \psi^{(j)}}{\partial t} = \frac{\partial^2 \psi^{(j)}}{\partial x_j^2} - \psi^{(j)} \left\langle \frac{\partial^2 \psi^{(j)}}{\partial x_j^2} \psi^{(j)} \right\rangle$$

$$\frac{\partial \psi^{(50)}}{\partial t} = \sum_{j=1}^{49} \left\langle \frac{\partial^2 \psi^{(j)}}{\partial x_j^2} \psi^{(j)} \right\rangle \psi^{(50)}$$

$$\psi_0^{(j)} = \frac{\sin(x_j)}{\sqrt{\pi}} \quad (j = 1, \dots, 49)$$

$$\psi_0^{(50)} = 10^7 \sin(x_{50})$$



## Summary

1. I presented a new method to compute the numerical solution of high-dimensional nonlinear PDEs on low-rank tensor manifolds with no need for computational expensive rank reduction techniques.
2. The new method relies on a hierarchical decomposition of the solution space in terms of sequences of nested subspaces of smaller dimensions, which can be conveniently visualized in terms of binary trees.
3. By enforcing dynamic orthogonality on the tensor modes at each level of the binary tree, it is possible to obtain coupled evolutions equations - i.e., a system of nonlinear PDE - representing the dynamics of solution on a smooth tensor manifold with constant rank.
4. I demonstrated the accuracy of the new dynamically orthogonal tensor method in prototype applications involving simple parabolic and hyperbolic linear PDEs.

**Thank you for your attention**