Dynamic tensor approximation of high-dimensional nonlinear PDEs

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Abstract

We present a new method based on functional tensor decomposition and dynamic tensor approximation to compute the solution of a high-dimensional time-dependent nonlinear partial differential equation (PDE). The idea of dynamic approximation is to project the time derivative of the PDE solution onto the tangent space of a low-rank functional tensor manifold at each time. Such a projection can be computed by minimizing a convex energy functional over the tangent space. This minimization problem yields the unique optimal velocity vector that allows us to integrate the PDE forward in time on a tensor manifold of constant rank.

In the case of initial/boundary value problems defined in real separable Hilbert spaces, this procedure yields evolution equations for the tensor modes in the form of a coupled system of one-dimensional time-dependent PDEs. We apply the dynamic tensor approximation to a four-dimensional Fokker–Planck equation with non-constant drift and diffusion coefficients, and demonstrate its accuracy in predicting relaxation to statistical equilibrium.

1. Introduction

High-dimensional partial differential equations (PDEs) arise in many areas of engineering, physical sciences and mathematics. Classical examples are equations involving probability density functions (PDFs) such as the Fokker–Planck equation [41], the Liouville equation [52, 15], or the Boltzmann equation [12, 18, 9]. More recently, high-dimensional PDEs have also become central to many new areas of application such as optimal mass transport [21, 53], random dynamical systems [51, 52], mean field games [19, 44], and functional-differential equations [50, 49].

Computing the solution to high-dimensional PDEs is a challenging problem that requires approximating high-dimensional functions, i.e., the solution to the PDE, and then developing appropriate numerical schemes to compute such functions accurately. Classical numerical methods based on tensor product representations are not viable in high-dimensions, as the number of degrees of freedom grows exponentially fast with the dimension. To address this problem there have been substantial research efforts in recent years on approximation theory for high-dimensional systems. Techniques such as sparse collocation [10, 14, 6, 20, 36], high-dimensional model representations [31, 11, 5], deep neural networks [39, 40, 54] and tensor methods [27, 4, 42, 8, 24, 30] were proposed to mitigate the exponential growth of the degrees of freedom, the computational cost and memory requirements. In recent work [17], we proposed a new method for solving high-dimensional time-dependent PDEs based on dynamically orthogonal tensor series expansions. The key idea is to represent the solution in terms of a hierarchy of Schmidt decompositions and then enforce dynamic orthogonality constraints on the tensor modes. In the case of initial/boundary value problems for PDEs defined in separable geometries, this procedure yields evolution equations for the dynamic tensor modes in the form of a coupled system of one-dimensional time-dependent PDEs.

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In this paper, we develop an extension of this approach based on the functional tensor train (FTT) expansion recently proposed by Bigoni, Engsig–Karup and Marzouk in [7]. In particular, we prove that FTT, combined with the set of hierarchical dynamic orthogonality constraints we introduced in [17], defines the best dynamic approximation of the solution to a nonlinear PDE on a smooth tensor manifold with constant rank. To describe what we mean by best dynamic approximation, consider the autonomous PDE

$$\frac{\partial u(x, t)}{\partial t} = N(u(x, t)), \quad u(x, 0) = u_0(x),$$

(1)

where $u : \Omega \times [0, T] \to \mathbb{R}$ is a $d$-dimensional (time-dependent) scalar field defined in the domain $\Omega \subseteq \mathbb{R}^d$ and $N$ is a nonlinear operator which may depend on the spatial variables, and may incorporate boundary conditions. Suppose that at some fixed time $t \in [0, T]$ the solution $u(x, t)$ belongs to a smooth manifold $M$ embedded in a real Hilbert space $H$. The best dynamic approximation aims at approximating $u(x, t)$ at a later time with a point lying on the manifold $M$ by determining the optimal vector in the tangent plane of $M$ that best approximates $\frac{\partial u(x, t)}{\partial t}$. This is achieved by solving the variational problem

$$\min_{v(x,t) \in T_{u(x,t)}} \left\| v(x,t) - \frac{\partial u(x,t)}{\partial t} \right\|_H = \min_{v(x,t) \in T_{u(x,t)}} \| v(x,t) - N(u(x,t)) \|_H. \quad (2)$$

Such an approximation is an infinite-dimensional analogue of the dynamical low–rank approximation on Euclidean manifolds considered by Lubich et al. for matrices [28, 37], Tucker tensors [29], and hierarchical tensors [33, 32].

This paper is organized as follows. In section 2 we briefly review the hierarchical Schmidt decomposition of multivariate functions (FTT format) and address its effective computation. In section 3 we prove that the set of constant-rank FTT tensors is a smooth Hilbert manifold, which therefore admits a tangent plane at each point. This result generalizes [46, Theorem 4] to tensor manifolds in infinite dimensions. In section 4 we parameterize the tangent space of the Hilbert manifold and derive a system of partial differential equations for the FTT cores corresponding to a given PDE. This system is shown to be the projection of the time derivative of the PDE solution onto the tangent space of the tensor manifold. In Section 5 we provide a numerical demonstration of the dynamic functional tensor train approximation for a four-dimensional Fokker–Planck equation with non-constant drift and diffusion coefficients. Finally, the main findings are summarized in section 6.

2. Functional tensor train (FTT) decomposition in real separable Hilbert spaces

Let $\Omega \subseteq \mathbb{R}^d$ be a Cartesian product of $d$ real intervals $\Omega_i = [a_i, b_i]$

$$\Omega = \prod_{i=1}^{d} \Omega_i,$$

(3)

$\mu$ a finite product measure on $\Omega$

$$\mu(x) = \prod_{i=1}^{d} \mu_i(x_i),$$

(4)

and

$$H = L^2_{\mu}(\Omega)$$

(5)

the standard weighted Hilbert space^n of square–integrable functions on $\Omega$. In this section we briefly review the functional tensor train decomposition [7, 22] of a multivariate function $u \in H$ in the setting of hierarchical bi-orthogonal series expansions [11, 2, 47, 48]. To this end, let $\Omega = \Omega_x \times \Omega_y$, $\mu = \mu_x \times \mu_y$ and

^nNote that the Hilbert space $H$ in equation (5) can be equivalently chosen to be a Sobolev space $W^{2,p}$ (see [17] for details).
$u(x, y) \in L^2_\mu(\Omega)$. The operator

$$T : L^2_{\mu_x}(\Omega_y) \to L^2_{\mu_y}(\Omega_x)$$

$$g \mapsto \int_{\Omega_y} u(x, y)g(y)d\mu_y(y)$$

(6)

is linear, bounded, and compact since $u$ is a Hilbert-Schmidt kernel. The formal adjoint operator of $T$ is given by

$$T^* : L^2_{\mu_y}(\Omega_x) \to L^2_{\mu_x}(\Omega_y)$$

$$h \mapsto \int_{\Omega_x} u(x, y)h(x)d\mu_x(x).$$

(7)

The composition operator $TT^* : L^2_{\mu_x}(\Omega_x) \to L^2_{\mu_y}(\Omega_x)$ is a self-adjoint compact Hermitian operator. The spectrum of $TT^*$, denoted as $\sigma(TT^*) = \{\lambda_1, \lambda_2, \ldots\}$, is countable with one accumulation point at 0, and satisfies

$$\sum_{i=1}^{\infty} \lambda_i < \infty.$$  

(8)

The normalized eigenfunction of $TT^*$ corresponding to $\lambda_i$, denoted by $\psi_i(x)$ is an element of $L^2_{\mu_x}(\Omega_x)$. The set $\{\psi_i\}_{i=1}^{\infty}$ is an orthonormal basis of $L^2_{\mu_x}(\Omega_x)$. The operator $T^*T : L^2_{\mu_y}(\Omega_y) \to L^2_{\mu_y}(\Omega_y)$ is also self-adjoint, compact, and Hermitian, and shares the same spectrum as $TT^*$, i.e., $\sigma(TT^*) = \sigma(T^*T)$. Its eigenfunctions $\{\varphi_i(y)\}_{i=1}^{\infty}$ form an orthonormal basis of $L^2_{\mu_y}(\Omega_y)$. It is a classical result in functional analysis that $u(x, y)$ can be expanded as (see [23][1][24])

$$u(x, y) = \sum_{i=1}^{\infty} \sqrt{\lambda_i} \psi_i(x) \varphi_i(y).$$

(9)

The functional tensor train (FTT) decomposition recently proposed in [7] can be developed in the setting of hierarchical bi-orthogonal expansions as follows. Let $u \in H$ and set $\Omega_x = \Omega_1$ and $\Omega_y = \Omega_2 \times \cdots \times \Omega_d$ in [6][7][10] to obtain

$$u(x) = \sum_{\alpha_1=1}^{\infty} \sqrt{\lambda_1(\alpha_1)} \psi_1(x; \alpha_1) \varphi_1(\alpha_1; x_2, \ldots, x_d).$$

(10)

Now we let $\Omega_x = \mathbb{N} \times \Omega_2$ and $\Omega_y = \Omega_3 \times \cdots \times \Omega_d$. From the orthonormality of $\{\varphi_1(\alpha_1, \cdot)\}_{\alpha_1=1}^{\infty}$ and the fact that $u \in L^2_{\mu}(\Omega)$ we have

$$\int_{\Omega_x \times \Omega_y} |\sqrt{\lambda_1(\alpha_1)} \varphi_1(\alpha_1; x_2, \ldots, x_d)|^2 d\tau(\alpha_1)d\mu_2(x_2) \cdots d\mu_d(x_d)$$

$$= \sum_{\alpha_1=1}^{\infty} \lambda_1(\alpha_1) \int_{\Omega_2 \times \cdots \Omega_d} |\varphi_1(\alpha_1; x_2, \ldots, x_d)|^2 d\mu_2(x_2) \cdots d\mu_d(x_d)$$

$$= \sum_{\alpha_1=1}^{\infty} \lambda_1(\alpha_1) < \infty,$$

(11)

i.e., $(\sqrt{\lambda_1} \varphi_1) \in L^2_{\times \mu_2 \times \cdots \times \mu_d}(X \times Y)$. Moreover, $\varphi_1(\alpha_1; x_2, \ldots, x_d)$ can be decomposed further by using an expansion of the form (9), i.e.,

$$\sqrt{\lambda_1(\alpha_1)} \varphi_1(\alpha_1; x_2, \ldots, x_d) = \sum_{\alpha_2=1}^{\infty} \sqrt{\lambda_2(\alpha_2)} \psi_2(\alpha_1; x_2; \alpha_2) \varphi_2(\alpha_2; x_3, \ldots, x_d).$$

(12)
Substituting this expression into (10) yields
\[
u(x) = \sum_{\alpha_1=1}^{\infty} \sum_{\alpha_2=1}^{\infty} \sqrt{\lambda_2(\alpha_2)} \psi_1(x_1; \alpha_1) \psi_2(\alpha_1; x_2; \alpha_2) \varphi_2(\alpha_2; x_3, \ldots, x_d).
\]

(13)

Proceeding recursively in this manner yields the following FTT expansion
\[
u(x) = \sum_{\alpha_1, \ldots, \alpha_d=1}^{\infty} \psi_1(\alpha_0; x_1; \alpha_1) \psi_2(\alpha_1; x_2; \alpha_2) \cdots \psi_d(\alpha_{d-1}; x_d; \alpha_d),
\]

(14)

where \(\alpha_0 = \alpha_d = 1\) and
\[
\psi_d(\alpha_{d-1}; x_d; \alpha_d) := \sqrt{\lambda_d(\alpha_{d-1})} \varphi_d(\alpha_{d-1}; x_d).
\]

By truncating the expansion (14) such that the largest singular values are retained we obtain
\[
u_{TT}(x) = \sum_{\alpha_0, \ldots, \alpha_d=1}^{r} \psi_1(\alpha_0; x_1; \alpha_1) \psi_2(\alpha_1; x_2; \alpha_2) \cdots \psi_d(\alpha_{d-1}; x_d; \alpha_d),
\]

(15)

where \(r = (1, r_1, \ldots, r_{d-1}, 1)\) is the TT-rank (or rank if the TT format is clear from context).

It is known that the truncated FTT expansion converges optimally with respect to the \(L^2_\Omega(\Omega)\) norm \[7\]. More precisely, for any given function \(u \in L^2_\Omega(\Omega)\) the FTT approximant \([15]\) minimizes the residual \(R_{TT} = \|u - u_{TT}\|_{L^2_\Omega(\Omega)}\) relative to independent variations of the functions \(\{\psi_i(\alpha_{i-1}; x_i; \alpha_i)\}\) on a tensor manifold with constant rank \(r\). It is convenient to write \([15]\) in a more compact form as
\[
u_{TT}(x) = \Psi_1(x_1) \Psi_2(x_2) \cdots \Psi_d(x_d),
\]

(16)

where \(\Psi_i(x_i)\) is a \(r_{i-1} \times r_i\) matrix with entries \([\Psi_i(x_i)]_{jk} = \psi_i(j; x_i; k)\). The matrix-valued functions \(\Psi_i(x_i)\) will be referred to as FTT cores. The spatial dependency is clear from the subscript of the core so we will often suppress the explicit dependence on the spatial variable \(x_i\) to simply write \(\Psi_i = \Psi_i(x_i)\) and \(\psi_i(\alpha_{i-1}, \alpha_i) = \psi_i(\alpha_{i-1}; x_i; \alpha_i)\). Rank \(r\) FTT decompositions can be computed at quadrature points by first discretizing \(u\) on a tensor product grid and then using a tensor product quadrature rule together with known algorithms for computing a discrete TT decomposition of a full tensor as discussed in \[7\].

At this point we summarize the main differences between the FTT series expansion \([15]\) and the series expansions we recently developed in \[17\]. With reference to the first level of the hierarchical TT decomposition, i.e., Eq. \([10]\), we notice that in the FTT setting the functions \(\varphi_i(\alpha_i; x_i, \ldots, x_d)\) are not decomposed independently (for each \(\alpha_i = 1, 2, \ldots\)) as in \[17\]. Instead, only one bi-orthogonal decomposition is performed on the average
\[
\overline{\varphi}_i(x_{i+1}, \ldots, x_d) = \sum_{\alpha_i=1}^{\infty} \varphi_i(\alpha_i; x_{i+1}, \ldots, x_d).
\]

(17)

This follows naturally from the assumption \(\varphi_i(\alpha_i, x_{i+1}, \ldots, x_d) \in L^2_{\tau \times N_{i+1} \times \cdots \times N_d}(\Omega \times \Omega_{i+1} \times \cdots \times \Omega_d)\), which includes a counting measure \(\tau\) that yields the summation in \(\varphi_i(\alpha_i, x_{i+1}, \ldots, x_d)\) as part of the inner product. On the other hand, the hierarchical expansion we studied in \[17\] treats \(\varphi_i(\alpha_i; x_{i+1}, \ldots, x_d)\) as an element of \(L^2_{\mu_{i+1} \cdots \mu_d}(\Omega_{i+1} \times \cdots \Omega_d)\) for each \(\alpha_i = 1, 2, \ldots\). Hence, a bi-orthogonal decomposition is performed on \(\varphi_i(\alpha_i, x_{i+1}, \ldots, x_d)\) for each \(\alpha_i\). Obviously, such decomposition requires many more computations but offers more information about the spectrum of the multivariate function at each level of the TT binary tree. Hereafter we proceed by considering the FTT decomposition \([15]\), but note that similar theoretical results can also be developed for the hierarchical series expansions we studied in \[17\].
3. The manifold of constant rank FTT tensors

In this section we prove that the space of constant rank FTT tensors is a smooth manifold, which therefore admits a tangent plane at each point. The tangent plane will be used in section 4 to develop an integration theory based on dynamic tensor approximation for time-dependent nonlinear PDEs. To prove that the space of constant rank FTT tensors is a smooth manifold, we follow a similar construction as presented in [35, 34]. Closely related work was presented in [13] in relation to Slater–type variational spaces in many particle Hartree–Fock theory. Also, the discrete analogues of the infinite-dimensional tensor manifolds discussed hereafter were studied in detail in [46, 26].

Let $\Psi, \tilde{\Psi} \in M_{r_1 \times r_2}(L^2_{\mu}(\Omega))$, where $M_{r_1 \times r_2}(L^2_{\mu}(\Omega))$ denotes the set of $r_1 \times r_2$ matrices with entries in $L^2_{\mu}(\Omega)$. Define the matrix

$$\begin{align*}
C_{\Psi, \tilde{\Psi}} = \left< \Psi^T, \tilde{\Psi} \right>_{L^2_{\mu}(\Omega)} \in M_{r_2 \times r_2}(\mathbb{R})
\end{align*}$$

with entries:

$$\left[ C_{\Psi, \tilde{\Psi}} \right]_{ij} = \sum_{k=1}^{r_1} \left< \psi(k; x; i), \tilde{\psi}(k; x; j) \right>_{L^2_{\mu}(\Omega)}.$$  \hspace{1cm} (18)

Denote by $V^{(i)}_{r_1 \times r_2}$ the set of all $\Psi_i \in M_{r_1 \times r_2}(L^2_{\mu_i}(\Omega))$ with the property that $C_{\Psi_i, \Psi_i}$ is invertible. We are interested in the following subset of $L^2_{\mu}(\Omega)$ consisting of rank-$r$ FTT tensors in $d$ dimensions

$$\bar{\mathcal{T}}_{r}^{(d)} = \{ u \in L^2_{\mu}(\Omega) : u = \Psi_1 \Psi_2 \cdots \Psi_d, \; \Psi_i \in V^{(i)}_{r_1 \times r_2}, \; \forall i = 1, 2, \ldots, d \}. \hspace{1cm} (20)$$

The set

$$V = V^{(1)}_{r_0 \times r_1} \times V^{(2)}_{r_1 \times r_2} \times \cdots \times V^{(d)}_{r_{d-1} \times r_d}$$

(21)

can be interpreted as a latent space for $\bar{\mathcal{T}}_{r}^{(d)}$ via the mapping

$$\pi : V \to \bar{\mathcal{T}}_{r}^{(d)} \quad \pi(\Psi_1, \Psi_2, \ldots, \Psi_d) = \Psi_1 \Psi_2 \cdots \Psi_d.$$  \hspace{1cm} (22)

Any tensor $u \in \bar{\mathcal{T}}_{r}^{(d)}$ has many representations in $V$, that is the map $\pi(\cdot)$ is not injective. The purpose of the following Lemma 3.1 and Proposition 3.1 is to characterize all elements of the space $V$ which have the same image under $\pi$.

**Lemma 3.1.** If $\{ \psi(\alpha_k; x; \alpha_j) \}_{\alpha_j=1}^{r} \; \{ \tilde{\psi}(\alpha_k; x; \alpha_j) \}_{\alpha_j=1}^{r}$ are two bases for the same finite dimensional subspace of $L^2_{\mu}(\mathbb{N} \times \Omega)$ then the matrix $C_{\Psi, \tilde{\Psi}}$ defined in (18) is invertible.

**Proof:** The matrix under consideration is given by

$$C_{\Psi, \tilde{\Psi}} = \begin{bmatrix}
\sum_{k=1}^{r} \left< \psi(k; x; 1), \tilde{\psi}(k; x; 1) \right>_{L^2_{\mu}(\Omega)} & \cdots & \sum_{k=1}^{r} \left< \psi(k; x; 1), \tilde{\psi}(k; x; r) \right>_{L^2_{\mu}(\Omega)} \\
\vdots & \ddots & \vdots \\
\sum_{k=1}^{r} \left< \psi(k; x; r), \tilde{\psi}(k; x; 1) \right>_{L^2_{\mu}(\Omega)} & \cdots & \sum_{k=1}^{r} \left< \psi(k; x; r), \tilde{\psi}(k; x; r) \right>_{L^2_{\mu}(\Omega)}
\end{bmatrix}.$$  \hspace{1cm} (23)

\[In equations (18) and (19) \left< \cdot, \cdot \right>_{L^2_{\mu}(\Omega)} \] denotes the standard inner product in $L^2_{\mu}(\Omega)$. \[\text{In equations (18) and (19) \left< \cdot, \cdot \right>_{L^2_{\mu}(\Omega)} \] denotes the standard inner product in $L^2_{\mu}(\Omega)$.\]
We will show that the columns of this matrix are linearly independent. To this end, consider the linear equation
\[
\sum_{i=1}^{r} v_i \left( \sum_{k=1}^{r} \langle \psi(k; x; 1), \tilde{\psi}(k; x; i) \rangle_{L^2_{\tau}(\Omega)} \right) = 0 \quad v_i \in \mathbb{R} \tag{24}
\]
the \(p\)-th row of which reads
\[
\sum_{k=1}^{r} \langle \psi(k; x; p), \sum_{i=1}^{r} v_i \tilde{\psi}(k; x; i) \rangle_{L^2_{\tau}(\Omega)} = 0 \quad p = 1, \ldots, r. \tag{25}
\]
If not all the \(v_i\) are equal to zero then (25) implies that \(\sum_{i=1}^{r} v_i \tilde{\psi}(k; x; i)\) is orthogonal to \(\psi(k; x; p)\) in \(L^2_{\tau \times \mu}(\mathbb{N} \times \Omega)\) and therefore linearly independent for all \(p = 1, \ldots, r\). This contradicts the assumption that \(\{\psi(i, j)\}_{j=1}^{r}, \{\tilde{\psi}(i, j)\}_{j=1}^{r}\) span the same finite dimensional subspace of \(L^2_{\tau \times \mu}(\mathbb{N} \times \Omega)\). Hence \(v_i\) are zero for every \(i = 1, \ldots, r\).

\[\Box\]

**Proposition 3.1.** Let \(\{\Psi_i\}_{i=1}^{d}, \{\tilde{\Psi}_i\}_{i=1}^{d}\) be elements of \(V\). Then
\[
\pi(\Psi_1, \ldots, \Psi_d) = \pi(\tilde{\Psi}_1, \ldots, \tilde{\Psi}_d) \tag{26}
\]
if and only if there exist matrices \(P_i \in GL_{r_i \times r_i}(\mathbb{R}) (i = 0, 1, \ldots, d)\) such that \(\Psi_i = P_i^{-1} \tilde{\Psi}_i P_i\) with \(P_0, P_d = 1\).

**Proof:** To prove the forward implication we proceed by induction on \(d\). For \(d = 2\) we have that
\[
\Psi_1 \Psi_2 = \tilde{\Psi}_1 \tilde{\Psi}_2 \tag{27}
\]
implies
\[
\Psi_1 = \tilde{\Psi}_1 C_{\Psi_2, \tilde{\Psi}_2}^{T} C_{\Psi_2, \Psi_2}^{-1} \tag{28}
\]
Set \(P_1 = C_{\Psi_2, \tilde{\Psi}_2}^{T} C_{\Psi_2, \Psi_2}^{-1}\) which is invertible since it is a change of basis matrix. Substituting \(\Psi_1 = \tilde{\Psi}_1 P_1\) into (27) we see that
\[
\tilde{\Psi}_1 P_1 \Psi_2 = \tilde{\Psi}_1 \tilde{\Psi}_2 \tag{29}
\]
which implies
\[
\Psi_2 = P_1^{-1} \tilde{\Psi}_2. \tag{30}
\]
This proves the proposition for \(d = 2\). Suppose that the proposition holds true for \(d - 1\) and that
\[
\Psi_1 \cdots \Psi_{d-1} = \tilde{\Psi}_1 \cdots \tilde{\Psi}_{d-1} \tag{31}
\]
Then,
\[
\Psi_1 \cdots \Psi_d = \tilde{\Psi}_1 \cdots \tilde{\Psi}_d. \tag{32}
\]
and we are guaranteed the existence of invertible matrices $P_1, \ldots, P_{d-2}$ such that
\[
\Psi_1 = \hat{\Psi}_1 P_1, \\
\vdots \\
\Psi_{d-2} = P_{d-3}^{-1} \hat{\Psi}_{d-2} P_{d-2}, \\
\Psi_{d-1} = P_{d-2}^{-1} \hat{\Psi}_{d-1} C_{\Psi_d}^{-1} C_{\Psi_d}^T P_{d-1}.
\]
Let $P_{d-1} = C_{\Psi_d}^{-1} C_{\Psi_d}^T$. Substituting equation (33) into (31) yields
\[
\hat{\Psi}_1 \cdots \hat{\Psi}_{d-2} \hat{\Psi}_{d-1} P_{d-1} \Psi_d = \tilde{\Psi}_1 \cdots \tilde{\Psi}_d, \\
P_{d-1}^{-1} \Psi_d = \tilde{\Psi}_d
\]
from which it follows that $P_{d-1}$ is invertible and
\[
\Psi_d = P_{d-1}^{-1} \tilde{\Psi}_d.
\]
This completes the proof.

With Proposition 3.1 in mind we define the group $^3$
\[
G = GL_{r_1 \times r_1}(\mathbb{R}) \times GL_{r_2 \times r_2}(\mathbb{R}) \times \cdots \times GL_{r_{d-1} \times r_{d-1}}(\mathbb{R})
\]
with group operation given by component-wise matrix multiplication. Let $G$ act on $V$ by
\[
(P_1, \ldots, P_{d-1}) \cdot (\Psi_1, \ldots, \Psi_d) = (\Psi_1 P_1, P_1^{-1} \Psi_2 P_2, \ldots, P_{d-1}^{-1} \Psi_d)
\]
for all $(P_1, \ldots, P_{d-1}) \in G$ and $(\Psi_1, \ldots, \Psi_d) \in V$. It is easy to see that this is action is free and transitive making $G, V, \Xi_r^{(d)}$ and $\pi$ a principal $G$-bundle \[43\]. In particular $V/G$ is isomorphic to $\Xi_r^{(d)}$ which allows us to equip $\Xi_r^{(d)}$ with a manifold structure. Thus, we can define its tangent space $T_u \Xi_r^{(d)}$ at a point $u \in \Xi_r^{(d)}$. We characterize such tangent space as the equivalence classes of velocities of smooth curves passing through the point $u$
\[
T_u \Xi_r^{(d)} = \left\{ \gamma'(s) \mid s = 0 : \gamma \in C^1\left((-\delta, \delta), \Xi_r^{(d)}\right), \gamma(0) = u \right\}.
\]
Here $C^1\left((-\delta, \delta), \Xi_r^{(d)}\right)$ is the space of continuously differentiable functions from the interval $(-\delta, \delta)$ to the space of constant rank FTT tensors $\Xi_r^{(d)}$. We conclude this section with the following Lemma which singles out a particular representation of $u \in \Xi_r^{(d)}$ for which the matrices $C_{\Psi_1, \Psi_i}$ (see Eqs. (18)-(19)) are diagonal.

**Lemma 3.2.** Given any FTT tensor $u \in \Xi_r^{(d)}$ there exist $\Psi_i \in V_{r_{i-1} \times r_i}^i$ $(i = 1, 2, \ldots, d)$ such that $u = \Psi_1 \Psi_2 \cdots \Psi_d$ and $C_{\Psi_1, \Psi_i} = I_{r_i \times r_i}$ for all $i = 1, \ldots, d - 1$.

**Proof:** Let us first represent $u \in \Xi_r^{(d)}$ relative to the tensor cores $\{\hat{\Psi}_1, \ldots, \hat{\Psi}_d\}$. Since $C_{\Psi_1, \hat{\Psi}_1}$ is symmetric there exists an orthogonal matrix $P_1$ such that $P_1^T C_{\hat{\Psi}_1, \Psi_1} P_1 = \Lambda_1$ is diagonal. Set $\Psi_1 = \hat{\Psi}_1 P_1 \Lambda_1^{-1/2}$ and $\hat{\Psi}_2 = \Lambda_1^{1/2} P_1^T \hat{\Psi}_2$ so that $C_{\Psi_1, \Psi_1} = I_{r_1 \times r_1}$ and $\Psi_1 \hat{\Psi}_2 \Psi_3 \cdots \hat{\Psi}_d = \hat{\Psi}_1 \cdots \hat{\Psi}_d$. The matrix $C_{\hat{\Psi}_2, \hat{\Psi}_2}$ is
\[In equation (36) $GL_{r_1 \times r_1}(\mathbb{R})$ denotes the general linear group of $r_1 \times r_1$ invertible matrices with real entries, together with the operation of ordinary matrix multiplication.

7
symmetric so there exists an orthogonal matrix $P_2$ such that $P_2^T C_{\Psi_2, \Psi_2} P_2 = \Lambda_2$ is diagonal. Set $\Psi_2 = \Psi_2 P_2 \Lambda_2^{-1/2}$ and $\hat{\Psi}_3 = \Lambda_2^{-1/2} P_2^T \hat{\Psi}_3$ so that $C_{\Psi_2, \Psi_2} = I_{r_2 \times r_2}$ and $\Psi_1 \Psi_2 \hat{\Psi}_3 \psi \cdots \hat{\Psi}_d = \hat{\Psi}_1 \cdots \hat{\Psi}_d$. Proceed recursively in this way until $\Psi_1 \Psi_2 \cdots \hat{\Psi}_{d-1} \hat{\Psi}_d = \hat{\Psi}_1 \cdots \hat{\Psi}_d$ with $C_{\Psi_i, \psi_i} = I_{r_i \times r_i}$, $i = 1, \ldots, d - 1$. It is easy to check that the collection of cores \{\psi_1, \ldots, \psi_d\} satisfies the conclusion of the Lemma.

4. Dynamical approximation of PDEs on FTT tensor manifolds with constant rank

Computing the solution to high-dimensional PDEs has become central to many new areas of application such as optimal mass transport \cite{21, 53}, random dynamical systems \cite{51, 52}, mean field games \cite{19, 44}, and functional-differential equations \cite{50, 49}. In an abstract setting, such PDEs involve the computation of a function $u(x, t)$ governed by an autonomous evolution equation

$$
\begin{cases}
\frac{\partial u}{\partial t} = N(u), \\
u(x, 0) = u_0(x),
\end{cases}
$$

where $u : \Omega \times [0, T] \to \mathbb{R}$ is a $d$-dimensional (time-dependent) scalar field defined in the domain $\Omega \subseteq \mathbb{R}^d$ (see Eq. (3)) and $N$ is a nonlinear operator which may depend on the spatial variables and may incorporate boundary conditions.

We are interested in computing the best dynamic approximation of the solution to \eqref{39} on the tensor manifold $\Sigma_r^{(d)}$ for all $t \geq 0$. Such an approximation aims at determining the vector in the tangent plane of $\Sigma_r^{(d)}$ at the point $u$ that best approximates $\partial u / \partial t$ for each $u \in \Sigma_r^{(d)}$. One way to obtain the optimal vector in the tangent plane is by orthogonal projection which we now describe. For each $u \in L_\mu^2(\Omega)$ the tangent space $\mathcal{T}_u L_\mu^2(\Omega)$ is canonically isomorphic to $L_\mu^2(\Omega)$. Moreover, for each $u \in \Sigma_r^{(d)}$ the normal space to $\Sigma_r^{(d)}$ at the point $u$, denoted by $N_u \Sigma_r^{(d)}$, consists of all vectors in $L_\mu^2(\Omega)$ that are orthogonal to $\mathcal{T}_u \Sigma_r^{(d)}$ with respect to the inner product in $L_\mu^2(\Omega)$. The space $\mathcal{T}_u \Sigma_r^{(d)} \subseteq L_\mu^2(\Omega)$ is finite-dimensional and therefore it is closed. Thus, for each $u \in \Sigma_r^{(d)}$ the space $L_\mu^2(\Omega)$ admits the decomposition

$$L_\mu^2(\Omega) = \mathcal{T}_u \Sigma_r^{(d)} \oplus N_u \Sigma_r^{(d)}. \tag{40}$$

Assuming that the solution $u(x, t)$ to the PDE \eqref{39} lives on the manifold $\Sigma_r^{(d)}$ at time $t$, we have that its velocity $\partial u / \partial t = N(u)$ can be decomposed uniquely into a tangent component and a normal component with respect to $\Sigma_r^{(d)}$, i.e.,

$$N(u) = v + w, \quad v \in \mathcal{T}_u \Sigma_r^{(d)}, \quad w \in N_u \Sigma_r^{(d)}. \tag{41}$$

The orthogonal projection we are interested in computing for the best dynamic approximation is

$$P_u : L_\mu^2(\Omega) \to \mathcal{T}_u \Sigma_r^{(d)},
N(u) \mapsto P_u N(u). \tag{42}$$

In practice, we will compute the image of such a projection by solving the following minimization problem over the tangent space of $\Sigma_r^{(d)}$ at $u$

$$\min_{v(x, t) \in \mathcal{T}_u(x, t) \Sigma_r^{(d)}} \left\| v(x, t) - \frac{\partial u(x, t)}{\partial t} \right\|^2_{L_\mu^2(\Omega)} = \min_{v(x, t) \in \mathcal{T}_u(x, t) \Sigma_r^{(d)}} \| v(x, t) - N(u(x, t)) \|^2_{L_\mu^2(\Omega)} \tag{43}$$

for each fixed $t \in [0, T]$. From an optimization viewpoint the following proposition establishes the existence and uniqueness of the optimal tangent vector.
Proposition 4.1. If \( N(u) \not\in \Upsilon_r^{(d)} \) then there exists a unique solution to the minimization problem (43), i.e., a unique global minimum.

Proof: We first notice that the feasible set \( \mathcal{T}_u \Upsilon_r^{(d)} \) is a real vector space and thus a convex set. Next we show that the functional \( F[v] = \|v - N(u)\|_{L^2(\Omega)}^2 \) is strictly convex. Indeed, take \( v_1, v_2 \in \mathcal{T}_u \Upsilon_r^{(d)} \) distinct and \( q \in (0, 1) \). Then

\[
(F[qv_1 + (1 - q)v_2])^\frac{1}{2} = \|qv_1 + (1 - q)v_2 - N(u)\|_{L^2(\Omega)} \\
= \|q(v_1 - N(u)) + (1 - q)(v_2 - N(u))\|_{L^2(\Omega)} \\
\leq q\|v_1 - N(u)\| + (1 - q)\|v_2 - N(u)\|_{L^2(\Omega)},
\]

with equality if and only if there exists an \( \alpha > 0 \) such that \( q(v_1 - N(u)) = \alpha(1 - q)(v_2 - N(u)) \). However, this implies that \( v_1 - \beta v_2 = (1 - \beta)N(u) \) for some real number \( \beta \), whence \( N(u) \in \mathcal{T}_u \Upsilon_r^{(d)} \). Therefore if \( N(u) \not\in \mathcal{T}_u \Upsilon_r^{(d)} \) then the inequality in (44) is strict and the functional \( (F[v])^\frac{1}{2} \) is strictly convex. Since the function \( x^2 \) is strictly increasing on the image of \( F^{\frac{1}{2}} \) it follows that \( F \) is strictly convex and thus admits a unique global minimum over the feasible set \( \mathcal{T}_u \Upsilon_r^{(d)} \).

\[\square\]

It can easily be shown that the unique solution to the optimization problem (43) is \( P_u N(u) \). Next, we will use this optimization framework for computing the best tangent vector to integrate the PDE (39) forward in time on the manifold \( \Upsilon_r^{(d)} \). To this end, let us first assume that the initial condition \( u_0 \in \Upsilon_r^{(d)} \). If not, \( u_0 \) can be projected onto \( \Upsilon_r^{(d)} \) using the methods described in section 2. In both cases, this allows us to represent \( u_0(x) \) as

\[ u_0(x) = \Psi_1(0)\Psi_2(0) \cdots \Psi_d(0), \]

with \( C_{\Psi_i(0),\Psi_i(0)} = I_{x_i \times x_i} \) for \( i = 1, 2, \ldots, d - 1 \). A representation of this form (with diagonal matrices \( C_{\Psi_i(0),\Psi_i(0)} \)) always exists thanks to Lemma 3.2. To compute the unique solution of (43), we expand an arbitrary curve \( \gamma(s) \) of class \( C^1 \) on the manifold \( \Upsilon_r^{(d)} \) passing through the point \( u \in \Upsilon_r^{(d)} \) at \( s = 0 \) in terms of \( s \)-dependent FTT cores. This yields

\[
\gamma(s) = \Psi_1(s) \cdots \Psi_d(s) \\
= \sum_{\alpha_0, \ldots, \alpha_d = 1}^{r} \psi_1(s; \alpha_0, \alpha_1)\psi_2(s; \alpha_1, \alpha_2) \cdots \psi_d(s; \alpha_{d-1}, \alpha_d),
\]

which allows us to represent any element of the tangent space \( \mathcal{T}_u \Upsilon_r^{(d)} \) at \( u \) as

\[ v = \frac{\partial}{\partial s} [\Psi_1(s) \cdots \Psi_d(s)]_{s=0}, \]

with \( \Psi_1(0) \cdots \Psi_d(0) = u \). At this point we notice that minimizing the functional in (43) over the tangent space \( \mathcal{T}_u \Upsilon_r^{(d)} \) is equivalent to minimizing the same functional over the velocity of each of the FTT cores. For notational convenience, hereafter we omit evaluation at \( s = 0 \) of all quantities depending on the curve parameter \( s \). For example, we will write

\[ \psi_1(\alpha_{i-1}, \alpha_i) = \psi_1(s; \alpha_{i-1}, \alpha_i) \bigg|_{s=0}; \quad \frac{\partial \psi_1(\alpha_{i-1}, \alpha_i)}{\partial s} = \frac{\partial \psi_1(s; \alpha_{i-1}, \alpha_i)}{\partial s} \bigg|_{s=0}. \]
With this notation, the minimization problem (43) is equivalent to

$$
\min_{\psi_0, \ldots, \psi_d} \left\| \frac{\partial}{\partial s} \left( \sum_{\alpha_0, \ldots, \alpha_d=1}^r \psi_1(\alpha_0, \alpha_1)\psi_2(\alpha_1, \alpha_2) \cdots \psi_d(\alpha_{d-1}, \alpha_d) \right) - N(u) \right\|_{L^2_\mu(\Omega)}^2.
$$

Of course, in view of Lemma 3.1 one curve \( \gamma(s) \) has many different expansions in terms of \( s \)-dependent FTT cores, which can be mapped into one another via collections of \( s \)-dependent invertible matrices. From Lemma 3.2, it is clear that any curve \( \gamma(s) \in C^1((-\delta, \delta), \mathbb{R}^d) \) passing through \( u \) at \( s = 0 \) admits the FTT decomposition \( \gamma(s) = \Psi_1(s) \cdots \Psi_d(s) \), where all auto-correlation matrices \( C_{\Psi_i, \Psi_i}(s)(i = 1, \ldots, d-1) \) are identity matrices for all for all \( s \in (-\delta, \delta) \), i.e.,

$$
C_{\Psi_i, \Psi_i}(s) = \langle \Psi_i^T(s), \Psi_i(s) \rangle_{L^2_{\mu_i}(\Omega_i)} = I_{r_i \times r_i}.
$$

Differentiating (50) with respect to \( s \) yields

$$
\left\langle \frac{\partial \Psi_i^T(s)}{\partial s}, \Psi_i(s) \right\rangle_{L^2_{\mu_i}(\Omega_i)} = - \left\langle \Psi_i^T(s), \frac{\partial \Psi_i(s)}{\partial s} \right\rangle_{L^2_{\mu_i}(\Omega_i)},
$$

which is attained when

$$
\left\langle \frac{\partial \Psi_i^T(s)}{\partial s}, \Psi_i(s) \right\rangle_{L^2_{\mu_i}(\Omega_i)} = 0_{r_i \times r_i}, \quad \forall s \in (-\delta, \delta).
$$

Enforcing (52) and prescribing (50) at \( s = 0 \) is equivalent to enforcing (50) for all \( s \in (-\delta, \delta) \). With this characterization of continuously differentiable curves \( \gamma(s) \) passing through \( u \in \mathbb{R}^d \), we can recast the minimization problem (49) in terms of FTT cores constrained by (52).

$$
\begin{aligned}
\min_{\psi_0, \ldots, \psi_d} \left\| \frac{\partial}{\partial s} \left( \sum_{\alpha_0, \ldots, \alpha_d=1}^r \psi_1(\alpha_0, \alpha_1)\psi_2(\alpha_1, \alpha_2) \cdots \psi_d(\alpha_{d-1}, \alpha_d) \right) - N(u) \right\|_{L^2_\mu(\Omega)}^2
\end{aligned}
$$

subject to:

$$
\left\langle \frac{\partial \psi_i(\alpha_i, -1, \alpha_i)}{\partial s}, \psi_i(\alpha_i, -1, \beta_i) \right\rangle_{L^2_{\mu_i}(\mathbb{R}^d \times N \times \Omega_i)} = 0 \quad \forall i = 1, 2, \ldots, d-1, \quad \alpha_i, \beta_i = 1, 2, \ldots, r_i,
$$

which by the discussion above still has the entire tangent space \( T_u \mathbb{R}^d \) as the feasible set. The minimization problem (53) is a convex optimization problem subject to linear equality constraints, which therefore is still convex. Hence, any local minimum is also a global minimum. Moreover a minimum of (53) provides the velocities of FTT cores which allow for the construction of the unique global minimum to the optimization problem (43) via equation (47). To solve (53) it is convenient to construct an action functional \( A \) that

---

4We are also assuming \( u = \Psi_1 \cdots \Psi_d \) is such that \( C_{\Psi_i, \Psi_i} = I_{r_i \times r_i} \) for \( i = 1, \ldots, d-1 \) so the constraint (50) is satisfied at \( s = 0 \).
introduces the constraints via Lagrange multipliers $\lambda_{\alpha_i \beta_i}^{(i)}$

$$A\left(\frac{\partial \psi_1(\alpha_0, \alpha_1)}{\partial s}, \ldots, \frac{\partial \psi_d(\alpha_{d-1}, \alpha_d)}{\partial s}\right) = \left\| \frac{\partial}{\partial s} \left[ \sum_{\alpha_0, \alpha_1, \ldots, \alpha_d=1}^r \psi_1(\alpha_0, \alpha_1)\psi_2(\alpha_1, \alpha_2) \cdots \psi_d(\alpha_{d-1}, \alpha_d) \right] - N(u) \right\|_{L^2_\tau(\Omega)}^2 + \sum_{i=1}^{d-1} \sum_{\alpha_i, \beta_i=1}^{r_i} \lambda_{\alpha_i \beta_i}^{(i)} \left\langle \frac{\partial \psi_i(\alpha_{i-1}, \alpha_i)}{\partial s}, \psi_i(\alpha_{i-1}, \beta_i) \right\rangle_{L^2_{\tau \times \mu_i}(\Omega \times \Omega_i)}.$$  

(54)

At this point, we have all elements to formulate the FTT propagator for the nonlinear PDE (39), which is the system of Euler-Lagrange equations corresponding to the unique global minimum of (54). Such propagator allows us to determine the best dynamic approximation of the solution to (39) on a FTT tensor manifold with constant rank.

**Theorem 4.1.** The unique global minimum of the functional (54) is attained at FTT tensor cores satisfying the PDE system

$$\frac{\partial \Psi_1}{\partial t} = \left[ \left\langle N(u), \Phi_1^T \right\rangle_{2^{\ldots}d} - \Psi_1 \left\langle \left\langle \Psi_1^T, N(u) \right\rangle_1, \Phi_1^T \right\rangle_{2^{\ldots}d} \right] C_{\Phi_1^T, \Phi_1^T}^{-1},$$

$$\frac{\partial \Psi_k}{\partial t} = \left[ \left\langle \Psi_{k-1}^T \cdots \Psi_1^T, N(u) \right\rangle_1, \cdots, \left\langle \Psi_{k-1}^T, N(u) \right\rangle_1 \right] C_{\Phi_k^T, \Phi_k^T}^{-1}, \quad k = 2, 3, \ldots, d - 1,$$

$$\frac{\partial \Psi_d}{\partial t} = \left\langle \Psi_{d-1}^T \cdots \Psi_1^T, N(u) \right\rangle_1.$$  

(55)

In these equations, $\langle \cdot, \cdot \rangle_{L^2_{\mu_k \times \cdots \times \mu_j}(\Omega_k \times \cdots \times \Omega_j)}$ and $\Phi_k$ is the multivariate FTT core in the $k$-th step of the FTT decomposition, i.e., the column vector that has components $\varphi_k(\alpha_k; x_{k+1}, \ldots, x_d)$ ($\alpha_k = 1, \ldots, r_k$) – see, e.g., Eq. (13).

We prove Theorem 4.1 in Appendix A. The PDE system (55) will be referred to as dynamically orthogonal functional tensor train (DO-FTT) propagator. As the solution evolves in time on the tensor manifold $\mathcal{T}_r^{(d)}$, it is possible for some of the cores to become linearly dependent. As a consequence, the auto-correlation matrices $C_{\Phi_k^T, \Phi_k^T}$ become singular and the equations (55) are no longer valid. In this case, the solution lives on a tensor manifold of smaller rank, say $\mathcal{T}_s^{(d)}$, where $s_i \leq r_i$ for all $i = 1, 2, \ldots, d$, and the dynamic tensor approximation can be constructed on $\mathcal{T}_s^{(d)}$. We conclude this section by emphasizing that it is possible to transform the dynamically orthogonal tensor cores $\Psi_i$ into bi-orthogonal cores (with corresponding bi-orthogonal equations) by adopting the proofs given in [17, 16]. In light of the discussion above on the optimality of the dynamically orthogonal FTT integrator on $\mathcal{T}_r^{(d)}$ and Lemma 3.1, it is clear that FTT with bi-orthogonal cores is also an optimal dynamic approximation on $\mathcal{T}_r^{(d)}$.

5. An application to the Fokker–Planck equation

In this section we demonstrate the dynamically orthogonal FTT integrator (55) on a four-dimensional ($d = 4$) Fokker–Planck equation with non-constant drift and diffusion coefficients. As is well known [41],

---

5By selecting a collection of time-dependent invertible matrices $P_i(s) \in \text{GL}_{r_i \times r_i}(\mathbb{R})$, $i = 2, 3, \ldots, d - 1$, defined by the
the Fokker–Planck equation describes the evolution of the probability density function (PDF) of the state vector solving the Itô stochastic differential equation (SDE)

\[ dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dW_t. \]  (57)

Here, \( X_t \) is the \( d \)-dimensional state vector, \( \mu(X_t, t) \) is the \( d \)-dimensional drift, \( \sigma(X_t, t) \) is an \( d \times m \) matrix and \( W_t \) is an \( m \)-dimensional standard Wiener process. The Fokker–Planck equation that corresponds to (57) has the form

\[ \frac{\partial p(x, t)}{\partial t} = \mathcal{L}(x, t)p(x, t), \quad p(x, 0) = p_0(x), \]  (58)

where \( p_0(x) \) is the PDF of the initial state \( X_0 \), \( \mathcal{L} \) is a second-order linear differential operator defined as

\[ \mathcal{L}(x, t)p(x, t) = -\sum_{k=1}^{d} \frac{\partial}{\partial x_k} (\mu_k(x, t)p(x, t)) + \sum_{k,j=1}^{d} \frac{\partial^2}{\partial x_k \partial x_j} (D_{ij}(x, t)p(x, t)), \]  (59)

and \( D(x, t) = \sigma(x, t)\sigma(x, t)^T/2 \) is the diffusion tensor. For our numerical demonstration we set

\[ \mu(x) = \alpha \begin{bmatrix} \sin(x_1) \\ \sin(x_3) \\ \sin(x_4) \\ \sin(x_1) \end{bmatrix}, \quad \sigma(x) = \sqrt{2} \beta \begin{bmatrix} g(x_2) & 0 & 0 & 0 \\ 0 & g(x_3) & 0 & 0 \\ 0 & 0 & g(x_4) & 0 \\ 0 & 0 & 0 & g(x_1) \end{bmatrix}, \]  (60)

where we define \( g(x) = \sqrt{1 + k \sin(x)} \). With the drift and diffusion matrices chosen in (60) the operator (59) takes the form

\[
\mathcal{L} = -\alpha \left( \cos(x_1) \sin(x_1) \frac{\partial}{\partial x_1} + \sin(x_3) \frac{\partial}{\partial x_2} + \sin(x_4) \frac{\partial}{\partial x_3} + \sin(x_1) \frac{\partial}{\partial x_4} \right) \\
+ \beta \left( \frac{\partial^2}{\partial x_1^2} + (1 + k \sin(x_2)) \frac{\partial^2}{\partial x_2^2} + (1 + k \sin(x_3)) \frac{\partial^2}{\partial x_3^2} + (1 + k \sin(x_1)) \frac{\partial^2}{\partial x_4^2} \right).
\]  (61)

This is a linear, time-independent separable operator of rank 9, since it can be written as

\[ \mathcal{L} = \sum_{i=1}^{9} L_i^{(1)} \otimes L_i^{(2)} \otimes L_i^{(3)} \otimes L_i^{(4)}, \]  (62)

where each \( L_i^{(j)} \) operates on \( x_j \) only. Specifically, we have

\[
L_1^{(1)} = -\alpha \cos(x_1), \quad L_2^{(1)} = -\alpha \sin(x_1) \frac{\partial}{\partial x_1}, \quad L_3^{(1)} = -\alpha \frac{\partial}{\partial x_2}, \quad L_4^{(1)} = \alpha \sin(x_3), \\
L_5^{(1)} = \beta \frac{\partial^2}{\partial x_3^2}, \quad L_6^{(1)} = 1 + k \sin(x_2), \quad L_7^{(1)} = \beta \frac{\partial^2}{\partial x_2^2}, \quad L_8^{(1)} = 1 + k \sin(x_4), \\
L_9^{(1)} = 1 + k \sin(x_1).
\]  (63)

matrix differential equation

\[
\begin{cases}
\frac{dP(s)}{ds} = G_t(P_t) \\
P_t(0) = P_{0,0}
\end{cases}
\]  (56)

it is possible to develop evolution equations different than (55) for \( \Psi_i(s) \), which still solve the minimization problem (49). In fact all possible solutions to (59) can be obtained in this way.
and all other unspecified $L_i^{(j)}$ are identity operators. We set the parameters in (60) as $\alpha = 0.1$, $\beta = 2.0$, $k = 1.0$ and consider the domain $\Omega = [0, 2\pi]^4$ with periodic boundary conditions. The initial PDF is set as

$$p_0(x) = \frac{\exp(\cos(x_1 + x_2 + x_3 + x_4))}{\| \exp(\cos(x_1 + x_2 + x_3 + x_4)) \|_{L^1(\Omega)}}. \quad (64)$$

To compute the FTT decomposition of $p_0(x)$ we first discretize it on a tensor product grid of 21 evenly-spaced Fourier points in each variable $x_j$ (194481 total points). The discrete tensor is then decomposed in the TT format using the TT-toolbox [38] with appropriate quadrature weights (see [7, §4.4]) and threshold set to $(21/2\pi)^4 \epsilon$. In particular, we set $\epsilon = \{10^{-8}, 10^{-5}, 10^{-3}\}$ to obtain

$$p_0(x, \epsilon) = \sum_{\alpha_0, \ldots, \alpha_4 = 1}^{r(\epsilon)} \Psi_1(0)\Psi_2(0)\Psi_3(0)\Psi_4(0), \quad (65)$$

with FTT ranks

$$r(10^{-8}) = \begin{bmatrix} 1 \\ 15 \\ 15 \\ 1 \end{bmatrix}, \quad r(10^{-5}) = \begin{bmatrix} 1 \\ 9 \\ 9 \\ 5 \end{bmatrix}, \quad r(10^{-3}) = \begin{bmatrix} 1 \\ 5 \\ 5 \\ 1 \end{bmatrix}. \quad (66)$$

To obtain a benchmark solution with which to compare the DO-FTT solution, the PDE (58) with initial condition (65) is solved on a full tensor product grid of points on the hypercube $\Omega = [0, 2\pi]^4$ with 21 evenly spaced points in each direction. Derivatives in the operator $L$ are computed with pseudo-spectral differentiation matrices [25], and the resulting semi-discrete approximation (ODE system) is integrated with explicit four stage fourth order Runge Kutta method using time step $\Delta t = 10^{-3}$. The numerical solution we obtained in this way is denoted by $p_f(x, t)$. In Figure 1 (middle row) we plot the two-dimensional marginal

$$p(x_1, x_2, t) = \int_0^{2\pi} \int_0^{2\pi} p(x_1, x_2, x_3, x_4, t) dx_3 dx_4$$

at $t = 0.1$, $t = 0.5$ and $t = 1$. 5.1. Fokker–Planck equation on the FTT tensor manifold

Next, we study the DO-FTT propagator (55) for the Fokker–Planck equation (58) with separable operator of the form (62). To write down such propagator explicitly, we adopt the convention that an operator applied to a matrix of functions acts on each entry of the matrix. With this convention, we obtain the
Figure 1: Time snapshots of the marginal PDF $p(x_1, x_2, t)$ of the solution to (58) computed with the DO-FTT propagator (top), on a full tensor product grid (middle) and and their pointwise error (bottom). The initial condition is obtained by decomposing (64) as a TT-tensor with threshold $\epsilon = 10^{-8}$.

The following evolution equations for the tensor cores

$$
\frac{\partial \Psi_1}{\partial t} = \sum_{i=1}^{9} \left[ L_i^{(1)} \Psi_1 \left( L_i^{(2,3,4)} \Phi_1, \Phi_1^T \right)_{2,3,4} - \Psi_1 \left( L_i^{(1)} \Psi_1 \right)_{1} \left( L_i^{(2,3,4)} \Phi_1, \Phi_1^T \right)_{2,3,4} \right] C_{\phi_1^T, \phi_1}^{-1},
$$

$$
\frac{\partial \Psi_2}{\partial t} = \sum_{i=1}^{9} \left[ \Psi_2 \left( L_i^{(1)} \Psi_1 \right)_{1} \left( L_i^{(2,3,4)} \Phi_2, \Phi_2^T \right)_{3,4} - \Psi_2 \left( L_i^{(1)} \Psi_1 \right)_{1} \left( L_i^{(2,3,4)} \Phi_2, \Phi_2^T \right)_{3,4} \right] C_{\phi_2^T, \phi_2}^{-1},
$$

$$
\frac{\partial \Psi_3}{\partial t} = \sum_{i=1}^{9} \left[ \Psi_3 \left( L_i^{(1)} \Psi_1 \right)_{1} \left( L_i^{(2,3,4)} \Phi_3, \Phi_4 \right)_{3} \left( L_i^{(4)} \Psi_4, \Psi_4^T \right)_{4} - \Psi_3 \left( L_i^{(1)} \Psi_1 \right)_{1} \left( L_i^{(2,3,4)} \Phi_3, \Phi_4 \right)_{3} \left( L_i^{(4)} \Psi_4, \Psi_4^T \right)_{4} \right] C_{\phi_4^T, \phi_4}^{-1},
$$

$$
\frac{\partial \Psi_4}{\partial t} = \sum_{i=1}^{9} \left[ \Psi_4 \left( L_i^{(1)} \Psi_1 \right)_{1} \left( L_i^{(2,3,4)} \Phi_2 L_i^{(3)} \Psi_3 \right)_{1,2,3} \left( L_i^{(4)} \Psi_4, \Psi_4^T \right)_{4} \right] C_{\phi_4^T, \phi_4}^{-1}.
$$

(68)
Figure 2: Error between the DO-FTT solution and the solution computed on a full tensor product grid to the Fokker–Planck equation (58) (a). Error between the DO tangent vector to $T_4^{(4)}$ and $\mathcal{L}_{PTT}(t)$ (b). We plot results corresponding to FTT decompositions of the initial condition with different thresholds $\epsilon$.

Figure 3: Time evolution of the DO-FTT solution rank for each simulation. Note that $r_0, r_4$ are excluded since they are always constantly equal to 1.

This PDE system governs the dynamics of the solution to the Fokker–Planck equation (58) with separable operator (62) on the FTT tensor manifold $T_4^{(4)}$. The rank $r$ can be adjusted adaptively in time [17, 3], to guarantee a prescribed accuracy of the FTT solution. The numerical solution to the PDE system (68) is computed with an explicit four–stages Runge-Kutta method with time step $\Delta t = 10^{-3}$, and a Fourier pseudo-spectral discretization [25] on 21 evenly–spaced collocation points in each spatial variable. In Figure 1 (top) we plot a few temporal snapshots of the marginal PDF (67) $p(x_1, x_2, t)$ we obtained using the DO-FTT temporal integrator. The $L^2(\Omega)$ error between the benchmark solution and the DO-FTT solution is plotted in Figure 2(a) for initial conditions decomposed with different thresholds $\epsilon$ (see Eqs. (65)-(66)).

With the velocity of each core $\partial \Psi_i/\partial t$ ($i = 1, 2, 3, 4$) at time $t$ given by the DO-FTT system (68) we can construct the optimal tangent vector $v_{PTT}(t)$ to the manifold $T_4^{(4)}$ at the point $p_{PTT}(x, t)$

$$v_{PTT}(t) = \frac{\partial \Psi_1}{\partial t} \Psi_2 \Psi_3 \Psi_4 + \Psi_1 \frac{\partial \Psi_2}{\partial t} \Psi_3 \Psi_4 + \Psi_1 \Psi_2 \frac{\partial \Psi_3}{\partial t} \Psi_4 + \Psi_1 \Psi_2 \Psi_3 \frac{\partial \Psi_4}{\partial t}.$$ (69)

In Figure 2(b) we plot the $L^2_{\mu}(\Omega)$ norm of $v_{PTT}(t) - \mathcal{L}_{PTT}(t)$ at each time $t$.

Note that the norm of $v_{PTT}(t) - \mathcal{L}_{PTT}(t)$ is the norm of the normal component of $\mathcal{L}_{PTT}(t)$ at the point $p_{PTT}(t)$ with respect to the manifold $T_4^{(4)}$ (see Eq. 411). Such a norm measures the deviation between the
temporal derivative of the DO-FTT solution $p_{TT}(x,t)$ and the temporal derivative defined by $Lp_{TT}(x,t)$ (right hand side of the Fokker–Planck equation). This provides an indication of whether the vector in the tangent plane of $T_r^{(4)}$ at $p_{TT}(x,t)$ is pointing in the right direction, and if the rank $r = (r_1, r_2, r_3, r_4)$ is sufficient to resolve the dynamics. Note that the rank is initially set by $\epsilon$ (see Eq. (66)). As $p_{TT}(x,t)$ propagates forward in time the energy of FTT modes (tensor cores) decays due to the diffusion term in the Fokker–Planck equation. If no action is taken to reduce solution rank, low energy modes will lead to ill-conditioned (possibly singular) matrices $C_{\phi^T_j,\phi^T_i}$ resulting in instabilities of the DO-FTT propagator (68). To ensure this does not happen the energy of each FTT mode is tracked and if the energy of one mode falls below the threshold $\epsilon$ then the FTT decomposition is recomputed with threshold $\epsilon$. For each of the three simulations we run, $\epsilon$ is kept constant throughout the integrating period $t \in [0, 1]$ and set at $\epsilon = \{10^{-8}, 10^{-5}, 10^{-3}\}$. In Figure 3 we plot the time evolution of the solution ranks we obtained for each of the three simulations.

6. Summary

We developed a new method based on functional tensor decomposition and dynamic tensor approximation to compute the solution of high-dimensional time-dependent nonlinear PDEs in real separable Hilbert spaces. The method is built upon the functional tensor train (FTT) expansion proposed by Bigoni et al. in [7], combined with dynamic tensor approximation. This yields an infinite-dimensional analogue of the dynamic low–rank approximation on Euclidean manifolds studied by Lubich et al. for matrices [28, 37], and for hierarchical tensors [33, 32]. The idea of dynamic approximation is to project the time derivative of the PDE solution onto the tangent space of a low-rank functional tensor manifold at each time. Using the set of hierarchical dynamic orthogonality constraints we recently introduced in [17] we computed the projection needed for dynamic approximation by minimizing a convex energy functional over the tangent space. The unique optimal velocity vector obtained in this way allows us to integrate the PDE forward in time on a tensor manifold of constant rank. In the case of initial/boundary value problems defined in separable geometries, this procedure yields evolution equations for the tensor modes in the form of a coupled system of one-dimensional time-dependent PDEs. We applied the proposed tensor method to a four-dimensional Fokker–Planck equation with non-constant drift and diffusion coefficients, and demonstrated its accuracy in predicting relaxation to statistical equilibrium.

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Appendix A. Proof of Theorem 4.1

The functional $\mathcal{A}$ in (54) is convex and thus a critical point is necessarily a global minimum. To find such a critical point set the first variation of $\mathcal{A}$ with respect to $\partial \psi_j(\xi_{j-1}, \xi_j) / \partial s$ in the direction $\eta_j(\xi_{j-1}, \xi_j)$

\[
\frac{d}{d\epsilon} \mathcal{A} \left( \frac{\partial \psi_j(\xi_{j-1}, \xi_j)}{\partial s} + \epsilon \eta_j(\xi_{j-1}, \xi_j) \right) \bigg|_{\epsilon=0} (A.1)
\]

equal to zero for all $\eta_j(\xi_{j-1}, \xi) \in L^2_{\mu_j}(\Omega_j)$. Note that we have available the dynamic constraints

\[
\left< \frac{\partial \psi_j(\cdot, \alpha_j)}{\partial s}, \psi_j(\cdot, \beta_j) \right>_{L^2_{\mu_j}(\Omega_j)} = 0, \quad \forall j = 1, \ldots, d-1, \quad \alpha_j, \beta_j = 1, \ldots, r_j, (A.2)
\]
and the static constraints
\[ \langle \psi_j(\cdot, \alpha_j), \psi_j(\cdot, \beta_j) \rangle_{L^2_{\mathcal{X} \times \mathcal{Y}}(\mathbb{N} \times \Omega_j)} = \delta_{\alpha_j, \beta_j}, \quad \forall j = 1, \ldots, d - 1, \quad \alpha_j, \beta_j = 1, \ldots, r_j, \tag{A.3} \]
which are implied by the dynamic constraints as long as the cores \( \Psi_1(s), \ldots, \Psi_{d-1}(s) \) all have identity auto-correlation matrices at some time (say at \( s = 0 \)). For \( j = 1 \) we obtain
\[
\left[ \frac{\delta \psi_1(\xi_0, \xi_1)}{\partial s} \right] A \eta_1(\xi_0, \xi_1) \\
= 2 \left( \frac{\partial}{\partial s} \sum_{\alpha, \alpha_1 = 1}^{r_0, r_1} \psi_1(\alpha_0, \alpha_1) \varphi_1(\alpha_1) \right) - N(u), \eta_1(\xi_0, \xi_1) \varphi_1(\xi_1) \right)_{1,2,\ldots,d} \\
+ \sum_{\alpha_1 = 1}^{r_j} \lambda_{\xi_0, \xi_1}^{(1)} \left( \eta_1(\xi_0, \xi_1), \psi_1(\xi_0, \alpha_1) \right)_{1} \\
= 0, \\
\]
whence the fundamental lemma of calculus of variations implies
\[
2 \left( \frac{\partial}{\partial s} \sum_{\alpha, \alpha_1 = 1}^{r_0, r_1} \psi_1(\alpha_0, \alpha_1) \varphi_1(\alpha_1) \right) - N(u), \varphi_1(\xi_1) \right)_{2,\ldots,d} + \sum_{\alpha_1 = 1}^{r_j} \lambda_{\xi_0, \xi_1}^{(1)} \psi_1(\xi_0, \alpha_1) = 0. \tag{A.5} \]
Rearranging terms we obtain
\[
\sum_{\alpha, \alpha_1 = 1}^{r_0, r_1} \left( \frac{\partial \psi_1(\alpha_0, \alpha_1)}{\partial s} \right) \left( \varphi_1(\alpha_1), \varphi_1(\xi_1) \right)_{2,\ldots,d} + \psi_1(\alpha_0, \alpha_1) \left( \frac{\partial \varphi_1(\alpha_1)}{\partial s}, \varphi_1(\xi_1) \right)_{2,\ldots,d} \\
= \left( N(u), \varphi_1(\xi_1) \right)_{2,\ldots,d} - \frac{1}{2} \sum_{\alpha_1 = 1}^{r_j} \lambda_{\xi_0, \xi_1}^{(1)} \psi_1(\xi_0, \alpha_1). \tag{A.6} \]
Taking \( \langle \cdot, \psi_1(\alpha_0, \xi_1') \rangle_{L^2_{\mathcal{X} \times \mathcal{Y}}(\mathbb{N} \times \Omega_1)} \) of the previous equation and utilizing the dynamic and static constraints, we solve for the Lagrange multiplier
\[
\lambda_{\xi_0, \xi_1}^{(1)} = \left( N(u), \psi_1(1, \xi_1') \varphi_1(\xi_1) \right)_{1,\ldots,d} - \left( \frac{\partial \varphi_1(\xi_1)}{\partial s}, \varphi_1(\xi_1) \right)_{2,\ldots,d}. \tag{A.7} \]
Substituting (A.7) into (A.6) and rearranging terms we obtain
\[
\sum_{\alpha_1 = 1}^{r_1} \frac{\partial \psi_1(1, \alpha_1)}{\partial s} \left( \varphi_1(\alpha_1), \varphi_1(\xi_1) \right)_{2,\ldots,d} \\
= \left( N(u), \varphi_1(\xi_1) \right)_{2,\ldots,d} - \sum_{\alpha_1 = 1}^{r_1} \psi_1(1, \alpha_1) \left( N(u), \psi_1(1, \alpha_1) \varphi_1(\xi_1) \right)_{1,\ldots,d}. \tag{A.8} \]
Using the matrix–vector notation for tensor cores and inverting the auto-correlation matrix on the left hand side yields the equation for \( \partial \Psi_j / \partial s \) in (A.11). For \( j = 2, \ldots, d - 1 \) we have that
\[
\left[ \delta \omega_{j,j-1} A \right] \eta_j(x_j, j, -j) = 2 \frac{\partial}{\partial s} \left[ \sum_{\alpha_0, \ldots, \alpha_j=1}^{r_0, \ldots, r_j} \psi_1(\alpha_0, \alpha_1) \cdot \psi_j(\alpha_j-1, \alpha_j) \varphi_j(\alpha_j) \right] - N(u),
\]
\[
\sum_{\alpha_0, \ldots, \alpha_j-2=1}^{r_0, \ldots, r_j-2} \psi_1(\alpha_0, \alpha_1) \cdot \psi_j(\alpha_j-2, \xi_j-1) \eta_j(\xi_j, j) \varphi_j(\xi_j) \bigg|_{1,2,\ldots,d}
\]
\[
+ \sum_{\alpha_j=1}^{r_j} \lambda_{\xi, j, \alpha} \left( \eta_j(\xi_j, j), \psi_j(\xi_j, j) \right) \bigg|_{j}. \tag{A.9}
\]
Moreover, utilizing the fundamental lemma of calculus of variations and rearranging terms we obtain
\[
\left\langle \sum_{\alpha_0, \ldots, \alpha_j-2=1}^{r_0, \ldots, r_j-2} \frac{\partial}{\partial s} \left[ \psi_j(\alpha_0, \alpha_1) \cdot \psi_j(\alpha_j-1, \alpha_j) \varphi_j(\alpha_j) \right] \right\rangle
\]
\[
\sum_{\alpha_0, \ldots, \alpha_j-2=1}^{r_0, \ldots, r_j-2} \psi_1(\alpha_0, \alpha_1) \cdot \psi_j(\alpha_j-2, \xi_j-1) \varphi_j(\xi_j) \bigg|_{1,2,\ldots,d}
\]
\[
= \left\langle N(u), \sum_{\alpha_0, \ldots, \alpha_j-2=1}^{r_0, \ldots, r_j-2} \psi_1(\alpha_0, \alpha_1) \cdot \psi_j(\alpha_j-2, \xi_j-1) \varphi_j(\xi_j) \right\rangle \bigg|_{1,2,\ldots,d}
\]
\[
- \frac{1}{2} \sum_{\alpha_j=1}^{r_j} \lambda_{\xi, j, \alpha} \psi_j(\xi_j, j). \tag{A.10}
\]
Utilizing the dynamic orthogonality condition (52) and the orthonormality for all \( t \) on the left hand side of (A.10) we obtain
\[
\sum_{\alpha_j} \left( \frac{\psi_j(\xi_j, j, \alpha_j)}{\partial s} \left( \varphi_j(\alpha_j), \varphi_j(\xi_j) \right) \right)_{j+1,\ldots,d} + \psi_j(\xi_j, j, \alpha_j) \left( \frac{\partial \varphi_j(\alpha_j)}{\partial s}, \varphi_j(\xi_j) \right)_{j+1,\ldots,d}
\]
\[
= \left\langle N(u_0), \sum_{\alpha_0, \ldots, \alpha_j-2=1}^{r_0, \ldots, r_j-2} \psi_1(\alpha_0, \alpha_1) \cdot \psi_j(\alpha_j-2, \xi_j-1) \varphi_j(\xi_j) \right\rangle \bigg|_{1,2,\ldots,d}
\]
\[
- \frac{1}{2} \sum_{\alpha_j=1}^{r_j} \lambda_{\xi, j, \alpha} \psi_j(\xi_j, j). \tag{A.11}
\]
Taking \( \langle \cdot, \psi_j(\alpha_j-1, \xi_j) \rangle_{L^2_{\mathbb{R}^x} \times \mu_j (\mathbb{N} \times \Omega_j)} \) of the previous equation and utilizing the constraints we find
\[
\lambda_{\xi_j, \epsilon_j}^{(j)} = 2 \left[ \sum_{\alpha_0, \ldots, \alpha_j=1}^{r_0, \ldots, r_j} \left( \left\langle N(u), \psi_1(\alpha_0, \alpha_1) \cdot \psi_j(\alpha_j-2, \xi_j-1) \psi_j(\alpha_j-1, \xi_j) \varphi_j(\xi_j) \right\rangle \right|_{1,2,\ldots,d} \right]
\]
\[
- \left( \frac{\partial \varphi_j(\xi_j, j)}{\partial s}, \varphi_j(\xi_j) \right)_{j+1,\ldots,d} \right]\]
Plugging \(A.12\) into \(A.11\) and simplifying we obtain

\[
\sum_{\alpha_j=1}^{r_j} \frac{\partial \psi_j(\xi_{j-1}, \alpha_j)}{\partial s} \left< \varphi_j(\alpha_j), \varphi_j(\xi_j) \right>_{j+1,...,d}
\]

\[
= \sum_{\alpha_0,...,\alpha_{j-2}=1}^{r_0,...,r_{j-2}} \left< N(u), \psi_1(\alpha_0, \alpha_1) \cdots \psi_{j-1}(\alpha_{j-2}, \xi_{j-1}) \varphi_j(\xi_j) \right>_{1,...,j-1,j+1,...,d} 
\]

\[
- \sum_{\alpha_0,...,\alpha_{j}=1}^{r_0,...,r_{j}} \psi_j(\xi_{j-1}, \alpha_j) \left< N(u), \psi_1(\alpha_0, \alpha_1) \cdots \psi_{j-1}(\alpha_{j-2}, \xi_{j-1}) \psi_j(\alpha_{j-1}, \alpha_{j}) \varphi_j(\xi_j) \right>_{1,...,d}.
\]

Using the matrix vector notation for tensor cores and inverting the auto-correlation matrix on the left hand side yields the equation for \(\partial \Psi_j / \partial s\) in (55). For \(j = d\) we obtain

\[
\left[ \delta \frac{\partial \varphi_d(\xi_0, \xi_1)}{\partial s} A \right] \eta_d(\xi_{d-1}, \xi_d) 
\]

\[
= 2 \left< \frac{\partial}{\partial s} \left[ \sum_{\alpha_0,...,\alpha_{d}=1}^{r_0,...,r_{d-1}} \psi_1(\alpha_0, \alpha_1) \cdots \psi_d(\alpha_{d-1}, \alpha_d) \right] - N(u), \right. 
\]

\[
\left. \sum_{\alpha_0,...,\alpha_{d-2}=1}^{r_0,...,r_{d-1}} \psi_1(\alpha_0, \alpha_1) \cdots \psi_{d-1}(\alpha_{d-2}, \xi_{d-1}) \eta_d(\xi_{d-1}, \xi_d) \right>_{1,2,...,d} 
\]

\[
= 0, \quad \forall \eta_d(\xi_{d-1}, \xi_d) \in L^2_{\mu_d}(\Omega_1),
\]

whence the fundamental lemma of calculus of variations implies

\[
\left< \frac{\partial}{\partial s} \left[ \sum_{\alpha_0,...,\alpha_{d}=1}^{r_0,...,r_{d-1}} \psi_1(\alpha_0, \alpha_1) \cdots \psi_d(\alpha_{d-1}, \alpha_d) \right] - N(u), \right. 
\]

\[
\left. \sum_{\alpha_0,...,\alpha_{d-2}=1}^{r_0,...,r_{d-1}} \psi_1(\alpha_0, \alpha_1) \cdots \psi_{d-1}(\alpha_{d-2}, \xi_{d-1}) \right>_{1,...,d-1} = 0. 
\]

Rearranging terms we obtain

\[
\left< \frac{\partial}{\partial s} \left[ \sum_{\alpha_0,...,\alpha_{d}=1}^{r_0,...,r_{d-1}} \psi_1(\alpha_0, \alpha_1) \cdots \psi_d(\alpha_{d-1}, \alpha_d) \right], \sum_{\alpha_0,...,\alpha_{d-2}=1}^{r_0,...,r_{d-1}} \psi_1(\alpha_0, \alpha_1) \cdots \psi_{d-1}(\alpha_{d-2}, \xi_{d-1}) \right>_{1,...,d-1} 
\]

\[
= \left< N(u), \sum_{\alpha_0,...,\alpha_{d-2}=1}^{r_0,...,r_{d-1}} \psi_1(\alpha_0, \alpha_1) \cdots \psi_{d-1}(\alpha_{d-2}, \xi_{d-1}) \right>_{1,...,d-1}. 
\]

Using the dynamic and static orthogonality constraints we obtain

\[
\frac{\partial \psi_d(\xi_{d-1}, 1)}{\partial s} = \left< N(u), \sum_{\alpha_0,...,\alpha_{d-2}=1}^{r_0,...,r_{d-1}} \psi_1(\alpha_0, \alpha_1) \cdots \psi_{d-1}(\alpha_{d-2}, \xi_{d-1}) \right>_{1,...,d-1}. 
\]

Writing this expression in matrix-vector notation the desired equation for \(\partial \Psi_d / \partial s\) is obtained.
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