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RECURSIVE BIORTHOGONAL DECOMPOSITION OF MULTIVARIATE FUNCTIONS AND NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

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Abstract

Recursive Biorthogonal Decomposition of Multivariate Functions and Nonlinear Partial Differential Equations

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We develop a numerical method for the decomposition of multivariate functions based on recursively applying biorthogonal decompositions in function spaces. The result is an approximation of the multivariate function by sums of products of univariate functions. Decompositions of this type can conveniently be visualized by binary trees and in some sense are a functional analog of the decompositions in tensor numerical methods that are obtained through sequences of matrix reshaping and singular value decomposition. The underlying theory of recursive biorthogonal decomposition in function spaces is developed and computational aspects are discussed. This decomposition is generalized to handle time dependence in such a way which allows for the decomposition and propagation of solutions to nonlinear time dependent partial differential equations. In this way we obtain a numerical solution for time dependent problems which remains on a low parametric manifold of constant rank for all time. We also discuss the addition and removal of time dependent modes during propagation to allow for robust adaptive solvers. Applications to prototype linear hyperbolic problems are presented and discussed.

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1 Introduction

1.1 Classical Numerical Methods: 'Curse of Dimensionality'

Time dependent partial differential equations (PDEs) arise in many areas of engineering, physical sciences and mathematics, most of which do not have obtainable analytical solutions. For this reason, numerical methods for PDEs are used often in many fields. There are a range of standard techniques available for low dimensional PDEs which have been studied extensively over the years, but there is a lack of techniques for high dimensional problems. Two prominent techniques for the numerical solution of low dimensional PDEs are classical finite difference methods and spectral methods. There is extensive amounts of literature on these two methods which study stability and convergene for a wide range of problems. However these methods are not viable for high dimensional problems since they suffer from what is called the 'curse of dimensionality'. This phrase is used to describe the exponential increase in computational complexity and storage cost of an algorithm with the number of dimensions d of the solution. Consequently these standard numerical techniques are not suitable for even moderate dimensional problems ($d \geq 4$). High dimensional PDEs are ubiquitous in science and engineering and therefore it is extremely desirable to have tools for solving such problems. With the increase in computing power over the years, reliable methods for time dependent problems which have improved scaling properties with respect to dimensionality have the potential of being widely applicable to many areas of scientific research. The goal of this thesis is to present a new method for the numerical solution of high dimensional time dependent PDEs which scales more favorably than classical methods with the number of dimensions

d. In doing so, we will also present a new decomposition for multivariate functions related to the decompositions in numerical tensor methods.

1.2 A Scalable Approach to Time Dependent Problems

In recent years, tensor numerical methods have been used as a tool to mitigate dimensionality problems rendering high dimensional problems tractable. The idea is to approximate multivariate functions and operators by projecting them onto a low parametric rank-structered manifold, see for example Khoromskij (2015a); Boelens et al. (2018). Tensor formats have proven to be capable of approximating a function related to d-dimensional data arrays of size N^d with complexity $\mathcal{O}(d \log N)$ De Lathauwer et al. (2000); Grasedyck (2009/10). However, there are inherent issues which arise when attempting to use tensor formats together with traditional numerical schemes for time dependent PDEs. For example, basic operations such as the addition of two tensors of ranks r_1 and r_2 in general results in a tensor of rank $r_1 + r_2$. Due to this fact, explicit numerical integration schemes with tensors must be injected with numerous truncation steps. The truncation of tensors is computationally expensive and perhaps more importantly, it is unknown how truncation effects the stability of numerical integration schemes. Tensor numerical methods provide a technique for data compression and have been used in many fields other than numerical solutions for PDEs. In all of its applications, analysis of methods using numerical tensors is notoriously difficult due to the complex sequence of operations[1] involved in truncating a tensor.

In this thesis we take a slightly different approach and develop a recursive decomposition for multivariate functions based on biorthogonal decompositions in function spaces. Each biorthogonal decomposition is determined by splitting variables into two disjoint subsets which, in a similar spirit to tensor numerical methods, can conveniently be visualized by binary trees. We consider two binary trees in particular which are analogous to the Tensor Train and Hierarchical Tucker formats of tensor numerical methods. We use recursive biorthogonal decompositions for the numerical solution

[1]Truncating tensors involves sequences of reshaping tensors into matrices and performing singular value decompositions on these matrices.

of high dimensional nonlinear time dependent PDEs of the form

$$\begin{cases} u(0,\boldsymbol{x}) = u_0(\boldsymbol{x}) \, , & \boldsymbol{x} \in D \, , \\ B(u(\boldsymbol{x})) = h(t,\boldsymbol{x}) \, , & \boldsymbol{x} \in \partial D \, , \end{cases} \tag{1.1}$$

where N is a separable differential operator of rank r_N, B is a linear differential operator, and D is a bounded domain in $\mathbb{R}^d$. By enforcing dynamic orthogonal (DO) or biorthogonal (BO) constraints on the hierarchy of biorthogonal modes obtained with the recursive decomposition, evolution equations for the modes are obtained. Thus we are able to propagate a solution to (1.1) on a tensor manifold of constant rank by solving time dependent PDEs of one spatial variable. The advantage of this approach over the numerical tensor approach is that there is a vast literature of stability and error analysis for the 1 dimensional PDEs we obtain. Also, our decomposition leverages on truncating infinite biorthogonal expansions for which error analysis is relatively straightforward. A consideration of propagating on a constant rank manifold is that the solution of (1.1) may not have an accurate representation on a constant rank manifold for all time. We will address issues that arise when attempting to increase the solution rank during propagation.

First we take a rigorous approach to the recursive subspace decomposition of time independent functions. In this way we obtain an approximation of a high dimensional functions by sums of products of univariate functions. We will also provide some error analysis of such decompositions. Next computational aspects of choosing a tensor format for the recursive biorthogonal decomposition is discussed. This is equivalent to choosing a binary tree which determines how spatial variables are split in each biorthogonal decomposition. We also describe a thresholding technique for determining how many biorthogonal modes to keep in each biorthogonal decomposition and provide a numerical example. Once the spatial decomposition has been established, the decomposition is extended to time dependent functions in a way which allows for the use of such an expansion for the numerical solution of PDEs of the form (1.1). This is accomplished by enforcing either a DO condition or a BO condition. We prove that the approximations resulting from these two conditions are equivalent in the sense that the components lie in the same finite dimensional function spaces. Finally we show how to use time dependent recursive subspace decompositions for the solution of PDEs of the form (1.1). Increasing and decreasing ranks is also discussed, and examples of solving prototype linear hyperbolic PDEs in 2, 4, and 50 spatial dimensions with these methods are presented and discussed.

2 Multivariate Function Decomposition

2.1 Time Independent Function Decomposition

Let us introduce a suitable mathematical setting for the decomposition of a multivariate function into a series expansion of univariate functions. Let D be a subset of $\mathbb{R}^d$ for some natural number d and

$$u : D \to \mathbb{R} \tag{2.1}$$

an element of a separable Hilbert space $\mathcal{H}$. We will consider the Sobolev space[1] $\mathcal{H} = H^2(D)$ in this thesis. We require $\mathcal{H}$ to be separable (i.e. admit a countable basis) so that it may be represented as a tensor product of two Hilbert spaces (Reed and Simon, 1980, p.51)

$$\mathcal{H} \simeq \mathcal{H}_1 \otimes \mathcal{H}_2. \tag{2.2}$$

The spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ may be specified by partitioning the spatial variables $\{x_1, \dots, x_d\}$ into two disjoint subsets. Consider the partition $\{x_1, x_2, \dots, x_d\} = \{x_1, \dots, x_p\} \dot{\cup} \{x_{p+1}, \dots, x_d\}$ which leads us to define the sets $D^{(1,\dots,p)} = D \cap (\mathbb{R}^p \times \varnothing^{d-p}) \subset \mathbb{R}^p$ and $D^{(p+1,\dots,d)} = D \cap (\varnothing^p \times \mathbb{R}^{d-p}) \subset \mathbb{R}^{d-p}$. In this particular setting, the Hilbert space $H^2(D)$ admits the following decomposition

$$H^2(D) = H^2(D^{(1,\dots,p)} \times D^{(p+1,\dots,d)}) \simeq H^2(D_1^{(1,\dots,p)}) \otimes H^2(D_1^{(p+1,\dots,d)}). \tag{2.3}$$

A representation of (2.1) in the tensor product space (2.3) has the general form

$$u^{(1,\dots,d)}(x_1, \dots, x_d) = \sum_{i,j=1}^{\infty} a_{ij} \varphi_i^{(1,\dots,p)}(x_1, \dots, x_p) \varphi_j^{(p+1,\dots,d)}(x_{p+1}, \dots, x_d) \tag{2.4}$$

[1] We choose this Sobolev space because of the applications to PDEs in Section 3. Another possible choice is $\mathcal{H} = L^2(D)$.

where $\varphi_i^{(1,\ldots,p)}$ and $\varphi_j^{(p+1,\ldots,d)}$ are orthonormal[2] basis functions of $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively. Notice that the superscripts in (2.4) denote which spatial components the function depends on. This will be the case throughout this thesis and for notational simplicity, the spatial arguments will be omitted when there is no ambiguity.

2.1.1 Biorthogonal Decomposition

With the isomorphism (2.3) established, we follow the approach of Aubry et al. (1991); Aubry and Lima (1995); Aubry (1991) to develop an operator theoretic framework which gaurantees the existence of a biorthogonal representation of u in the tensor product space (2.3). This framework is constructive in that it gives a method for the computation of biorthogonal decompositions. Define the operator

$$\begin{aligned} &U_u : H^2(D^{(1,\ldots,p)}) \to H^2(D^{(p+1,\ldots,d)})\ , \\ &\psi^{(1,\ldots,p)} \mapsto \int \cdots \int_{D^{(1,\ldots,p)}} u^{(1,\ldots,d)} \psi^{(1,\ldots,p)} dx_1 \cdots dx_p \end{aligned} \tag{2.5}$$

with adjoint operator given by

$$\begin{aligned} &U_u^* : H^2(D^{(p+1,\ldots,d)}) \to H^2(D^{(1,\ldots,p)})\ , \\ &\psi^{(p+1,\ldots,d)} \mapsto \int \cdots \int_{D^{(p+1,\ldots,d)}} \bar{u}^{(1,\ldots,d)} \psi^{(p+1,\ldots,d)} dx_{p+1} \cdots dx_d\ , \end{aligned} \tag{2.6}$$

where bar denotes complex conjugation. This is an integral operator with kernel specified by its subscript. We will shortly define a hierarchy of integral operators and it will be important to distinguish them by their kernels. Since u is square integrable, the operators U_u and U_u^* are compact. We can now introduce the two operators

$$R_u : H^2(D^{(p+1,\ldots,d)}) \to H^2(D^{(p+1,\ldots,d)})$$

such that

$$R_u = U_u U_u^*$$

and

$$L_u : H^2(D^{(1,\ldots,p)}) \to H^2(D^{(1,\ldots,p)})$$

[2]Orthonormality is relative to specific choices of inner products in $\mathcal{H}_1$ and $\mathcal{H}_2$.

such that

$$L_u = U_u^* U_u.$$

Remark 2.1.1. The operators L_u and R_u are compact since the composition of compact operators on a Hilbert space is compact. It follows that L_u and R_u both have discrete spectra (see e.g. (Kato, 1995, p.185)).

It is straightforward to show that

$$\begin{aligned} &R_u(\psi^{(p+1,\ldots,d)}) \\ &= \int \cdots \int_{D^{(p+1,\ldots,d)}} r_u(x_{p+1},\ldots,x_d,x'_{p+1},\ldots,x'_d)\psi^{(p+1,\ldots,d)}(x'_{p+1},\ldots,x'_d)dx'_{p+1}\cdots dx'_d \,, \end{aligned}$$

where r_u is the correlation function given by

$$\begin{aligned} &r_u(x_{p+1},\ldots,x_d,x'_{p+1},\ldots,x'_d) \\ &= \int \cdots \int_{D^{(1,\ldots,p)}} u(x_1,\ldots,x_p,x_{p+1},\ldots,x_d)\bar{u}(x_1,\ldots,x_p,x'_{p+1},\ldots,x'_d)dx_1\cdots x_p. \end{aligned}$$

Similarly

$$\begin{aligned} &L_u(\psi^{(1,\ldots,p)}) \\ &= \int \cdots \int_{D^{(1,\ldots,p)}} l_u(x_1,\ldots,x_p,x'_1,\ldots,x'_p)\psi^{(1,\ldots,p)}(x'_1,\ldots,x'_p)dx'_1\cdots dx'_p \,, \end{aligned} \tag{2.7}$$

where l_u is the correlation function given by

$$\begin{aligned} &l_u(x_1,\ldots,x_p,x'_1,\ldots,x'_p) \\ &= \int \cdots \int_{D^{(p+1,\ldots,d)}} u(x_1,\ldots,x_p,x_{p+1},\ldots x_d)\bar{u}(x'_1,\ldots,x'_p,x_{p+1},\ldots,x_d)dx_{p+1}\cdots dx_d. \end{aligned}$$

It is a classical demonstration in the theory of functional analysis of operators that there exists a canonical decomposition of u such that

$$u^{(1,\ldots,d)} = \sum_{k=1}^{\infty} \lambda_k \psi_k^{(1,\ldots,p)} \psi_k^{(p+1,\ldots,d)} \,, \tag{2.8}$$

where

$$\begin{aligned} &\lambda_1 \geq \lambda_2 \geq \cdots > 0 \,, \\ &\lim_{k\to\infty} \lambda_k = 0 \,, \\ &\langle \psi_i^{(1,\ldots,p)} \psi_j^{(1,\ldots,p)} \rangle = \langle \psi_i^{(p+1,\ldots,d)} \psi_j^{(p+1,\ldots,d)} \rangle = \delta_{ij}, \end{aligned} \tag{2.9}$$

and the series (2.8) converges in norm. This decomposition is called a biorthogonal decomposition of the function u. It is easy to see that the functions $\psi_k^{(1,\dots,p)}$ are eigenfunctions of the operator L_u with corresponding eigenvalue λ_k^2 and the functions $\psi_k^{(p+1,\dots,d)}$ are eigenfunctions of the operator R_u with corresponding eigenvalues λ_k^2

$$\begin{aligned} L_u(\psi_k^{(1,\dots,p)}) &= \lambda_k^2 \psi_k^{(1,\dots,p)} \ , \\ R_u(\psi_k^{(p+1,\dots,d)}) &= \lambda_k^2 \psi_k^{(p+1,\dots,d)}. \end{aligned} \tag{2.10}$$

In practice, we can solve the eigenvalue problem of smaller dimension[3] to obtain half of the modes and the eigenvalues. The other half of the modes can then be obtained by projecting u onto the eigenfunctions we have already computed

$$\begin{aligned} \psi_k^{(p+1,\dots,d)} &= \frac{1}{\lambda_k} \int \cdots \int_{D^{(1,\dots,p)}} u^{(1,\dots,d)} \psi_k^{(1,\dots,p)} dx_1 \cdots dx_p \\ \psi_k^{(1,\dots,p)} &= \frac{1}{\lambda_k} \int \cdots \int_{D^{(p+1,\dots,d)}} u^{(1,\dots,d)} \psi_k^{(p+1,\dots,d)} dx_{p+1} \cdots dx_d. \end{aligned} \tag{2.11}$$

2.1.2 Tensor Formats

In order to obtain a series expansion of u in terms of univariate functions, we apply the biorthogonal decomposition recursively. The way in which the variables are split in each step of the recursive decomposition (i.e. the choice of p) can conveniently be visualized by binary trees and is called a tensor format. We consider two tensor formats, Tensor Train and Hierarchical Tucker, with corresponding binary trees given in Figure 2.1.

Tensor Train

The Tensor Train format singles out one variable at a time. In order to obtain a Tensor Train decomposition of a d-variate function (2.1), begin by partitioning the variables in the following way $\{x_1, \dots, d\} = \{x_1\} \dot\cup \{x_2, \dots, x_d\}$ and perform a recursive biorthogonal decomposition (2.8). Then for each of the modes $\psi_{i_1}^{(2,\dots,d)}$, partition the variables as $\{x_2, \dots, d\} = \{x_2\} \dot\cup \{x_3, \dots, x_d\}$ and perform a biorthogonal decomposition for each of the $\psi_{i_1}^{(2,\dots,d)}$. In this way we obtain functions

[3] Provided that p is chosen such that $p \neq d - p$.

$\psi^{(3,\dots,d)}_{i_1 i_2}$. Proceeding recursively we obtain the following hierarchy of functions

$$u^{(1,\dots,d)} = \sum_{i_1=1}^{\infty} \lambda_{i_1} \psi^{(1)}_{i_1} \psi^{(2,\dots,d)}_{i_1} \tag{2.12}$$

$$\psi^{(2,\dots,d)}_{i_1} = \sum_{i_2=1}^{\infty} \lambda_{i_1 i_2} \psi^{(2)}_{i_1 i_2} \psi^{(3,\dots,d)}_{i_1 i_2} \tag{2.13}$$

$$\vdots$$

$$\psi^{(j,\dots,d)}_{i_1\cdots i_{j-1}} = \sum_{i_j=1}^{\infty} \lambda_{i_1\cdots i_j} \psi^{(j)}_{i_1\cdots i_j} \psi^{(j+1,\dots,d)}_{i_1\cdots i_j} \tag{2.14}$$

$$\vdots$$

$$\psi^{(d-1,d)}_{i_1\cdots i_{d-2}} = \sum_{i_{d-1}=1}^{\infty} \lambda_{i_1\cdots i_{d-1}} \psi^{(d-1)}_{i_1\cdots i_{d-1}} \psi^{(d)}_{i_1\cdots i_{d-1}}. \tag{2.15}$$

Each of the biorthogonal modes can be obtained by solving a sequence of 1 dimensional eigenfunction problems followed by projections. The eigenvalue problems using the notation developed above are

$$\begin{aligned} L_u(\psi^{(1)}_{i_1}) &= \lambda^2_{i_1} \psi^{(1)}_{i_1} , \\ L_{\psi^{(k-1)}_{i_1\cdots i_{k-1}}}(\psi^{(k)}_{i_1\cdots i_k}) &= \lambda^2_{i_1\cdots i_k} \psi^{(k)}_{i_1\cdots i_k} , \qquad k = 2,\dots,d-1 \end{aligned} \tag{2.16}$$

and the corresponding projections are given by

$$\begin{aligned} \psi^{(2,\dots,d)}_{i_1} &= \frac{1}{\lambda_{i_1}} \int_{D^{(1)}} u(x_1,\dots,x_d) \psi^{(1)}_{i_1} dx_1 \\ \psi^{(j+1,\dots,d)}_{i_1\cdots i_j} &= \frac{1}{\lambda_{i_1\cdots i_j}} \int_{D^{(j+1)}} \psi^{(j,\dots,d)}_{i_1\cdots i_{j-1}} \psi^{(j)}_{i_1\cdots i_j} dx_j \end{aligned} \tag{2.17}$$

In this format, we have the following series expansion

$$u^{(1,\dots,d)} = \sum_{i_1=1}^{\infty} \cdots \sum_{i_{d-1}=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1\cdots i_{d-1}} \psi^{(1)}_{i_1} \psi^{(2)}_{i_1 i_2} \cdots \psi^{(d-1)}_{i_1\cdots i_{d-1}} \psi^{(d)}_{i_1\cdots i_{d-1}}. \tag{2.18}$$

As can be seen from the hierarchy of biorthogonal decompositions (2.12)-(2.15), the Tensor Train format requires $d-1$ levels of biorthogonal decompositions to decompose a d-variate function, the number $d-1$ is referred to as the depth of the Tensor Train binary tree.

Hierarchical Tucker

In contrast with the Tensor Train format, the Hierarchical Tucker format splits sets of variables into equal size disjoint subsets whenever possible. In the case of $d = 2^n$ for some natural number n,

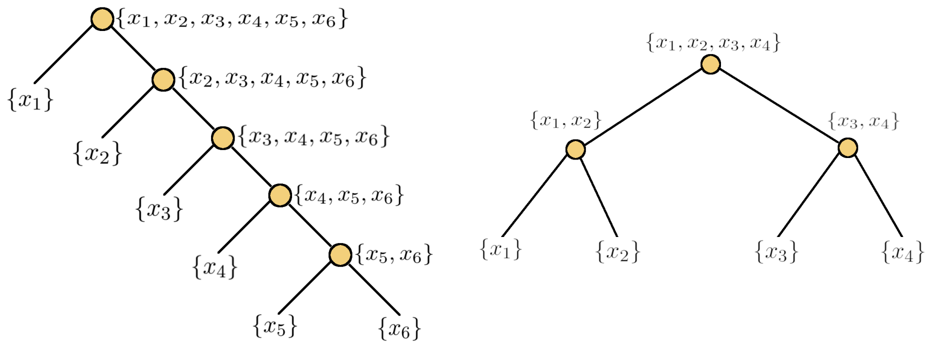

Figure 2.1: Binary trees corresponding to tensor formats. Left: Tensor Train for a 6 dimensional function. Right: Hierarchical Tucker for a 4 dimensional function.

the tree is balanced (i.e. every branch has the same depth). Other than the way in wich variables are split, the methodology of decomposing a function in the Hierarchical Tucker format is the same as in the Tensor Train format: a sequence of biorthogonal decompositions are applied recursively until we obtain an expansion in terms of univariate functions. To illustrate this format, let us unfold the hierarchy of biorthogonal modes of a d-variate function (2.1) when $d = 2^n$ in the Hierarchical Tucker format

$$u^{(1,\ldots,d)} = \sum_{i_1=1}^{\infty} \lambda_{i_1}^{(1,\ldots,\frac{d}{2})} \psi_{i_1}^{(1,\ldots,\frac{d}{2})} \psi_{i_1}^{(\frac{d}{2}+1,\ldots,d)} \tag{2.19}$$

$$\psi_{i_1}^{(1,\ldots,\frac{d}{2})} = \sum_{i_2=1}^{\infty} \lambda_{i_1 i_2}^{(1,\ldots,\frac{d}{4})} \psi_{i_1 i_2}^{(1,\ldots,\frac{d}{4})} \psi_{i_1 i_2}^{(\frac{d}{4}+1,\ldots,\frac{d}{2})} \tag{2.20}$$

$$\psi_{i_1}^{(\frac{d}{2}+1,\ldots,d)} = \sum_{i_2=1}^{\infty} \lambda_{i_1 i_2}^{(\frac{d}{2}+1,\ldots,\frac{3d}{4})} \psi_{i_1 i_2}^{(\frac{d}{2}+1,\ldots,\frac{3d}{4})} \psi_{i_1 i_2}^{(\frac{3d}{4}+1,\ldots,d)} \tag{2.21}$$

$$\vdots$$

$$\psi_{i_1\cdots i_{n-1}}^{(1,2)} = \sum_{i_n=1}^{\infty} \lambda_{i_1\cdots i_n}^{(1)} \psi_{i_1\cdots i_n}^{(1)} \psi_{i_1\cdots i_n}^{(2)} \tag{2.22}$$

$$\vdots$$

$$\psi_{i_1\cdots i_{n-1}}^{(d-1,d)} = \sum_{i_n=1}^{\infty} \lambda_{i_1\cdots i_n}^{(d-1)} \psi_{i_1\cdots i_n}^{(d-1)} \psi_{i_1\cdots i_n}^{(d)}. \tag{2.23}$$

In general, a Hierarchical Tucker tree is more shallow than a Tensor Train tree when decomposing functions of the same number of variables. The depth of a Hierarchical Tucker Tree for $d = 2^n$ is $n = \log_2(d)$. Similar to the Tensor Train format, a sequence of eigenfunction problems followed by projections can be used to obtain each of the modes in the decomposition above. However in this case the eigenfunction problems are higher dimensional and not compuationally tractable for large d. In the Hierarchical Tucker format, the approximate solution is represented by the series expansion

$$u^{(1,\dots,d)} = \sum_{i_1=1}^{\infty} \cdots \sum_{i_n=1}^{\infty} \lambda_{i_1}^{(1,\dots,\frac{d}{2})} \cdots \lambda_{i_1\cdots i_n}^{(d-1)} \psi_{i_1\cdots i_n}^{(1)} \psi_{i_1\cdots i_n}^{(2)} \cdots \psi_{i_1\cdots i_n}^{(d)}. \tag{2.24}$$

Remark 2.1.2. One may decompose a multivariate function by splitting variables in various ways at different levels of the decompositions. Any binary tree which has leaves containing one index leads to a series expansion in terms of functions of one spatial variable.

2.1.3 Error Analysis

In this section we develop two results related to the truncated recursive biorthogonal decomposition. The first is a Proposition which will be useful in Section 2.1.4 for establishing a thresholding criterion to truncate the infinite sums in expansions (2.18) and (2.24).

Proposition 2.1.1. *If $\psi \in L^2(D)$ with biorthogonal decomposition given by*

$$\psi(\boldsymbol{x}) = \sum_{i=1}^{\infty} \lambda_i \psi_i^{(l)}(\boldsymbol{x}_l)\psi_i^{(r)}(\boldsymbol{x}_r),$$

where $\psi_i^{(l)}(\boldsymbol{x}_l) \in L^2(D^{(l)})$ and $\psi_i^{(r)}(\boldsymbol{x}_r) \in L^2(D^{(r)})$, then $\sum_{i=1}^{\infty} \lambda_i^2 = \|\psi(\boldsymbol{x})\|_{L^2}$.

Proof. This result is easily obtained by using the orthonormality of the biorthogonal modes $\{\psi^{(l)}(\boldsymbol{x}_l)\}_{i=1}^{\infty}$ and $\{\psi^{(r)}(\boldsymbol{x}_r)\}_{i=1}^{\infty}$

$$\begin{aligned}
\|\psi(\boldsymbol{x})\|_{L^2} &= \int_D \psi(\boldsymbol{x})^2 d\boldsymbol{x} \\
&= \int_D (\sum_{i=1}^{\infty} \lambda_i \psi_i^{(l)}(\boldsymbol{x}_l)\psi_i^{(r)}(\boldsymbol{x}_r))^2 d\boldsymbol{x} \\
&= \sum_{i,j=1}^{\infty} \lambda_i \lambda_j \int_{D^{(l)}} \psi_i^{(l)}(\boldsymbol{x}_l)\psi_j^{(l)}(\boldsymbol{x}_l) d\boldsymbol{x}_l \int_{D^{(r)}} \psi_i^{(r)}(\boldsymbol{x}_r)\psi_j^{(r)}(\boldsymbol{x}_r) d\boldsymbol{x}_r \\
&= \sum_{i=1}^{\infty} \lambda_i^2.
\end{aligned}$$

□

Next we provide the exact L^2 error between an analytic Tensor Train series expansion of the form (2.18) and the truncated expansion

$$\tilde{u}^{(1,\dots,d)} = \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2(i_1)} \cdots \sum_{i_{d-1}=1}^{r_{d-1}(i_1,\dots,i_{d-2})} \lambda_{i_1} \cdots \lambda_{i_1\cdots i_{d-1}} \psi_{i_1}^{(1)} \psi_{i_1 i_2}^{(2)} \cdots \psi_{i_1\cdots i_{d-1}}^{(d-1)} \psi_{i_1\cdots i_{d-1}}^{(d)}. \quad (2.25)$$

Similar error analysis can be done for other tensor formats as well. These error results in the L^2 norm are analogous to the results mentioned by Schneider and Uschmajew Schneider and Uschmajew (2014), first proven by De Lathauwer et al. De Lathauwer et al. (2000), and later generalized by Grasedyck Grasedyck (2009/10) which bound the overall squared approximation error of multilinear singular value decompositions in the 2-norm by the sum (over the whole tree) of squares of deleted singular values. In order to simplify indexing and array bounds for truncated expansions such as (2.25), we will omit the array indices in the rank arrays. For example, we will write $\psi_{i_1\cdots i_k}^{(j_1,\dots,j_p)}$, $k = 1,\dots,r_k$ instead of $k = 1,\dots,r_k(i_1,\dots,i_{k-1})$ since the rank array indices are clear from the subscripts of the mode $\psi_{i_1\cdots i_k}^{(j_1,\dots,j_p)}$. In this notation, the truncated Tensor Train expansion (2.25) becomes

$$\tilde{u}^{(1,\dots,d)} = \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \cdots \sum_{i_{d-1}=1}^{r_{d-1}} \lambda_{i_1} \cdots \lambda_{i_1\cdots i_{d-1}} \psi_{i_1}^{(1)} \psi_{i_1 i_2}^{(2)} \cdots \psi_{i_1\cdots i_{d-1}}^{(d-1)} \psi_{i_1\cdots i_{d-1}}^{(d)}. \quad (2.26)$$

Theorem 2.1.1. *The squared error incurred by truncating the infinite expanion* (2.18) *to the finite expansion* (2.26) *is given by*

$$\begin{aligned} &\|u^{(1,\dots,d)} - \tilde{u}^{(1,\dots,d)}\|_{L^2}^2 \\ &= \sum_{i_1=r_1+1}^{\infty} \lambda_{i_1}^2 + \sum_{i_1=1}^{r_1} \sum_{i_2=r_2+1}^{\infty} \lambda_{i_1}^2 \lambda_{i_1 i_2}^2 + \cdots \\ &+ \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \cdots \sum_{i_{d-2}=1}^{r_{d-2}} \sum_{i_{d-1}=r_{d-1}+1}^{\infty} \lambda_{i_1}^2 \lambda_{i_1 i_2}^2 \cdots \lambda_{i_1\cdots i_{d-1}}^2. \end{aligned} \quad (2.27)$$

Proof. Rewrite (2.18) as

$$u^{(1,\dots,d)} = \sum_{i_1=1}^{\infty} \lambda_{i_1} \psi_{i_1}^{(1)} \sum_{i_2=1}^{\infty} \lambda_{i_1 i_2} \psi_{i_1 i_2}^{(2)} \cdots \sum_{i_{d-1}=1}^{\infty} \lambda_{i_1\cdots i_{d-1}} \psi_{i_1\cdots i_{d-1}}^{(d-1)} \psi_{i_1\cdots i_{d-1}}^{(d)} \quad (2.28)$$

then split each infinite sum into a finite sum and an infinite sum

$$\begin{aligned} u^{(1,\dots,d)} =& \Big(\sum_{i_1=1}^{r_1} \lambda_{i_1} \psi_{i_1}^{(1)} + \sum_{i_1=1}^{\infty} \lambda_{i_1} \psi_{i_1}^{(1)}\Big)\Big(\sum_{i_2=1}^{r_2} \lambda_{i_1 i_2} \psi_{i_1 i_2}^{(2)} + \sum_{i_2=1}^{\infty} \lambda_{i_1 i_2} \psi_{i_1 i_2}^{(2)}\Big) \cdots \\ & \cdots \Big(\sum_{i_{d-1}=1}^{r_{d-1}} \lambda_{i_1\cdots i_{d-1}} \psi_{i_1\cdots i_{d-1}}^{(d-1)} \psi_{i_1\cdots i_{d-1}}^{(d)} + \sum_{i_{d-1}=1}^{\infty} \lambda_{i_1\cdots i_{d-1}} \psi_{i_1\cdots i_{d-1}}^{(d-1)} \psi_{i_1\cdots i_{d-1}}^{(d)}\Big). \end{aligned} \quad (2.29)$$

We prove in Appendix A that by expanding the products in (2.29) the following expression is obtained

$$
\begin{aligned}
u^{(1,\dots,d)} = &\sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\cdots\sum_{i_{d-1}=1}^{r_{d-1}} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)} \\
&+ \sum_{i_1=r_1+1}^{\infty}\sum_{i_2=1}^{\infty}\cdots\sum_{i_{d-1}=1}^{\infty} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)} \\
&+ \sum_{i_1=1}^{r_1}\sum_{i_2=r_2+1}^{\infty}\sum_{i_3=1}^{\infty}\cdots\sum_{i_{d-1}=1}^{\infty} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)} \\
&+ \sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\sum_{i_3=r_3+1}^{\infty}\sum_{i_4=1}^{\infty}\cdots\sum_{i_{d-1}=1}^{\infty} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)} \\
&\qquad\vdots \\
&+ \sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\cdots\sum_{i_{d-2}=1}^{r_{d-2}}\sum_{i_{d-1}=r_{d-1}+1}^{\infty} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)}
\end{aligned}
\tag{2.30}
$$

where the first product of sums is precisely $\tilde{u}^{(1,\dots,d)}$. Now we have that

$$
\begin{aligned}
&\|u^{(1,\dots,d)} - \tilde{u}^{(1,\dots,d)}\|_{L^2}^2 \\
= &\ \| \sum_{i_1=r_1+1}^{\infty}\sum_{i_2=1}^{\infty}\cdots\sum_{i_{d-1}=1}^{\infty} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)} \\
&+ \sum_{i_1=1}^{r_1}\sum_{i_2=r_2+1}^{\infty}\sum_{i_3=1}^{\infty}\cdots\sum_{i_{d-1}=1}^{\infty} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)} \\
&+ \sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\sum_{i_3=r_3+1}^{\infty}\sum_{i_4=1}^{\infty}\cdots\sum_{i_{d-1}=1}^{\infty} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)} \\
&\qquad\vdots \\
&+ \sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\cdots\sum_{i_{d-2}=1}^{r_{d-2}}\sum_{i_{d-1}=r_{d-1}+1}^{\infty} \lambda_{i_1}\cdots\lambda_{i_1\cdots i_{d-1}}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_{d-1}}^{(d-1)}\psi_{i_1\cdots i_{d-1}}^{(d)}\|_{L^2}^2
\end{aligned}
$$

and using the orthogonality of each set of biorthogonal modes

$$
\begin{aligned}
&\|u^{(1,\dots,d)} - \tilde{u}^{(1,\dots,d)}\|_{L^2}^2 \\
&= \sum_{i_1=r_1+1}^{\infty} \sum_{i_2=1}^{\infty} \cdots \sum_{i_{d-1}=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{d-1}} \|\psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{d-1}}^{(d-1)} \psi_{i_1 \cdots i_{d-1}}^{(d)}\|_{L^2} \\
&+ \sum_{i_1=1}^{r_1} \sum_{i_2=r_2+1}^{\infty} \sum_{i_3=1}^{\infty} \cdots \sum_{i_{d-1}=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{d-1}} \|\psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{d-1}}^{(d-1)} \psi_{i_1 \cdots i_{d-1}}^{(d)}\|_{L^2} \\
&+ \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \sum_{i_3=r_3+1}^{\infty} \sum_{i_4=1}^{\infty} \cdots \sum_{i_{d-1}=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{d-1}} \|\psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{d-1}}^{(d-1)} \psi_{i_1 \cdots i_{d-1}}^{(d)}\|_{L^2} \\
&\qquad \vdots \\
&+ \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \cdots \sum_{i_{d-2}=1}^{r_{d-2}} \sum_{i_{d-1}=r_{d-1}+1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{d-1}} \|\psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{d-1}}^{(d-1)} \psi_{i_1 \cdots i_{d-1}}^{(d)}\|_{L^2}^2 .
\end{aligned}
$$

Finally using the orthonormality of each mode and Proposition 2.1.1 we obtain

$$
\begin{aligned}
&\|u^{(1,\dots,d)} - \tilde{u}^{(1,\dots,d)}\|_{L^2}^2 \\
&= \sum_{i_1=r_1+1}^{\infty} \lambda_{i_1}^2 + \sum_{i_1=1}^{r_1} \sum_{i_2=r_2+1}^{\infty} \lambda_{i_1}^2 \lambda_{i_1 i_2}^2 + \cdots \\
&+ \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \cdots \sum_{i_{d-2}=1}^{r_{d-2}} \sum_{i_{d-1}=r_{d-1}+1}^{\infty} \lambda_{i_1}^2 \lambda_{i_1 i_2}^2 \cdots \lambda_{i_1 \cdots i_{d-1}}^2 .
\end{aligned}
$$

□

2.1.4 Computing Recursive Biorthogonal Decompositions

In this section we explain some computational aspects of the recursive biorthogonal decompositions such as (2.18) and (2.24). In order to obtain such decompositions, one of two kernels must be computed either r_u or l_u and then a corresponding eigenfunction problem must be solved. In the Hierarchical Tucker format, computing r_u or l_u require evaluating integrals of the same dimension ($\frac{d}{2}$) which result in eigenfunction problems of the same dimension (also $\frac{d}{2}$). In this case there is no advantage in choosing to compute l_u over r_u. In the Tensor Train format, there are two options

- Compute r_u which requires evaluating a 1 dimensional integral, then solve the resulting $d-1$ dimensional eigenfunction problem. Following this, $d-1$ dimensional integrals must be computed to obtain the second half of the modes through projection.

- Compute l_u which requires evaluating a $d-1$ dimensional integral, then solve the resulting 1 dimensional eigenfunction problem. Following this, 1 dimensional integrals must be computed to obtain the second half of the modes through projection.

From a computational viewpoint, it is advantageous to choose the second option since high dimensional integrals can effectively be computed using Quasi-Monte Carlo methods Dick et al. (2013) and one dimensional eigenfunction problems reduce to matrix eigenvalue problems when collocated on a tensor product grid. Solving the 1 dimensional eigenfunction problem (2.16) using a collocation method with a tensor product grid containing M points in x_1 and M points in x_1', we can obtain at most M eigenfunctions and their corresponding eigenvalues. This leads to the decision of how many of these eigenfunctions should one keep. The thresholding technique which we now explain gives a criterion for choosing how many eigenfunction and eigenvalue pairs to keep in each level of the recursive biorthogonal decomposition for any tensor format.

Thresholding

Notice in the series expansions (2.18) and (2.24) we take products of eigenvalues from each level of the corresponding binary tree. With this in mind, it is reasonable to have a criterion which ensures that each of these eigenvalue products remains above a threshold value σ. To simplify notation we explain how to threshold for the recursive biorthogonal Tensor Train decompsition (2.18) and note that the same idea can be applied to any tensor format.

Begin by setting some threshold value σ for which we will enforce $\lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1\cdots i_{d-1}} \geq \sigma$. In the first biorthogonal decomposition (2.12), we keep all biorthogonal modes $\psi_{i_1}^{(1)}, \psi_{i_1}^{(2,\ldots,d)}$ with eigenvalues $\lambda_{i_1} \geq \sigma$, of which there will be a finite number r_1 because of property (2.9). For the biorthogonal decomposition of each $\psi_{i_1}^{(2,\ldots,d)}$ $(1 \leq i_1 \leq r_1)$ we set a new threshold $\sigma_1 = \frac{\sigma}{\lambda_{i_1}}$ and keep all modes $\psi_{i_1 i_2}^{(2)}, \psi_{i_1 i_2}^{(3,\ldots,d)}$ with eigenvalues $\lambda_{i_1 i_2} \geq \sigma_{i_1}$. Proceeding in this way, on the j^{th} level of biorthogonal decompositions we set thresholds $\sigma_{i_1\cdots i_j} = \frac{\sigma_{i_1\cdots i_{j-1}}}{\lambda_{i_1\cdots i_j}}$. It is acceptable to disregard modes corresponding to eigenvalues less than σ in the first biorthogonal decomposition since it is easy to show that

$$\lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{j-1}} \geq \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_j} \tag{2.31}$$

for all $j = 2, \ldots, d-1$. Indeed, Proposition 2.1.1 implies that $\lambda_{i_1 \cdots i_j} \leq 1$ for all $j = 2, \ldots, d-1$ from which (2.31) immediately follows. Another desirable consequence of Proposition 2.1.1 is that $\sigma_{i_1 \cdots i_{j-1}} \leq \sigma_{i_1 \cdots i_j}$ for all $j = 2, \ldots, d-1$.

As a result of thresholding in this way, each individual biorthogonal decomposition is truncated to a different number of modes. Continuing the example of the Tensor Train format, on the first level of the tree there is only one biorthogonal decomposition, the decomposition of $u^{(1,\ldots,d)}$, for which we keep r_1 modes. For each of the modes $\psi_{i_1}^{(2,\ldots,d)}$ ($i_1 = 1, \ldots, r_1$), the level 2 biorthogonal decompositions are performed with corresponding thresholds σ_{i_1}. In the biorthogonal decomposition of $\psi_{i_1}^{(2,\ldots,d)}$, we keep $r_2(i_1)$ modes. Thus the biorthogonal ranks for the second level are described by the vector r_2. For each of the $r_1 \sum_{i_1=1}^{r_1} r_2(i_1)$ modes $\psi_{i_1 i_2}^{(3,\ldots,d)}$, the level 3 biorthogonal decompositions are performed with corresponding thresholds $\sigma_{i_1 i_2}$. In the biorthogonal decomposition of $\psi_{i_1 i_2}^{(3,\ldots,d)}$ we keep $r_3(i_1, i_2)$ modes. Thus the biorthogonal ranks for the third level of the Tensor Train decomposition are described by a matrix. In general on the j^{th} level, a $j-1$ way array of ranks is obtained.

A Numerical Example

As a demonstration of the methods we have mentioned so far, we compute numerically a recursive biorthogonal decomposition[4] of the function

$$u(x_1, x_2, x_3) = e^{\sin(x_1 + 2x_2 + 3x_3)} + x_2 x_3 \,, \qquad (x_1, x_2, x_3) \in [-1, 1]^3. \tag{2.32}$$

First we collocate (2.32) on a 3 dimensional tensor product grid with 50 Gauss-Legendre points in each direction. The kernel of the first integral operator we consider is given by

$$l_u(x_1, x_1') = \int_{-1}^{1} \int_{-1}^{1} u(x_1, x_2, x_3) u(x_1', x_2, x_3) dx_2 dx_3$$

[4] For two and three dimensional functions Tensor Train and Hierarchical Tucker formats are equivalent.

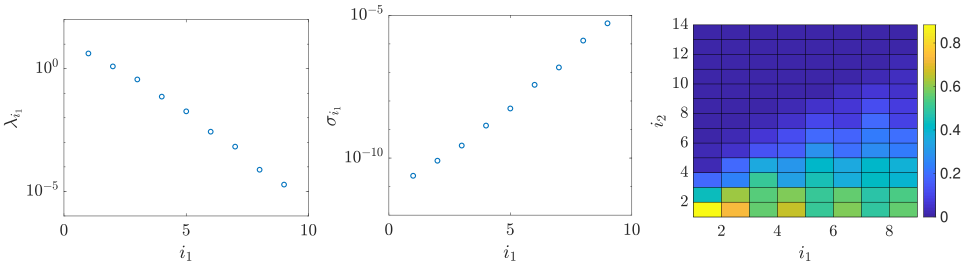

Figure 2.2: Left: Level 2 thresholds in the biorthogonal decomposition of (2.32) with level 1 threshold $\sigma = 10^{-10}$, Middle: Level 1 spectrum, Right: Level 2 spectrum.

which we compute with a tensor product quadrature rule corresponding to the chosen grid points. The x_1 modes are solutions of the eigenfunction problem

$$\int_{-1}^{1} l_u(x_1, x_1')\psi^{(1)}(x_1')dx_1' = \lambda^2 \psi^{(1)}(x_1). \tag{2.33}$$

We have l_u collocated on a 2 dimensional grid of Gauss-Legendre points, so the eigenfunctions $\psi^{(1)}$ in (2.33) collocated at Gauss-Legendre points with eigenvalue λ^2 are eigenvector and eigenvalue pairs of the matrix $l_u W$, where W is a diagonal matrix of Gauss-Legendre quadrature weights. Thus we obtain the 50 leading eigenvalues and collocated eigenfunctions of the operator L_u in (2.7). Following the thresholding technique explained above, we set $\sigma = 10^{-10}$ to determine how many level 1 eigenvalues and eigenfunctions to keep. It turns out that 9 eigenvalues are larger than σ, thus $r_1 = 9$. These 9 eigenvalues $\lambda_1, \dots, \lambda_9$ constitute the level 1 spectrum which is shown in the left plot of Figure 2.2, the corresponding eigenfunctions are $\psi_1^{(1)}, \dots, \psi_9^{(1)}$. The modes $\psi_1^{(2,3)}, \dots, \psi_9^{(2,3)}$ can now be obtained through projections as in (2.17)

$$\psi_j^{(2,3)} = \frac{1}{\lambda_j} \int_{-1}^{1} u(x_1, x_2, x_3)\psi_j^{(1)} dx_1. \tag{2.34}$$

We compute these integrals with Gauss-Legendre quadrature.

For each of the 9 modes $\psi_j^{(2,3)}$ we follow the same procedure used to obtain $\psi_j^{(1)}$ from u. That is, we compute the kernels

$$l_{\psi_j^{(2,3)}}(x_2, x_2') = \int_{-1}^{1} \psi^{(2,3)}(x_2, x_3)\psi^{(2,3)}(x_2', x_3)dx_3$$

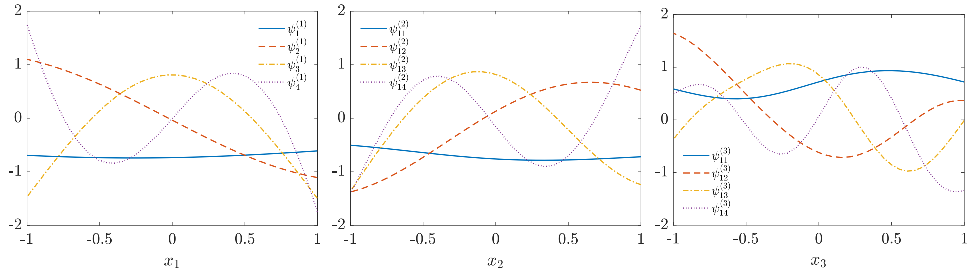

Figure 2.3: A few modes from the recursive biorthogonal decompostion of (2.32). Left: x_1 modes, middle: x_2 modes, right: x_3 modes.

with Gauss-Legendre quadrature. Then solve the eigenvalue problems

$$\int_{-1}^{1} l_{\psi_j^{(2,3)}}(x_2, x_2')\psi_j^{(2)}(x_2')dx_2' = \lambda_j^2 \psi_j^{(2)}$$

to obtain the first 50 collocated eigenfunctions and eigenvalues for each operator $L_{\psi_j^{(2,3)}}$, $j = 1, \ldots, 9$. To decide how many eigenvalues and eigenfunctions to keep for the operator $L_{\psi_j^{(2,3)}}$ we use the threshold $\sigma_j = \frac{\sigma}{\lambda_j}$. These threshold values are shown in the middle plot of Figure 2.2. This yields the vector of level 2 ranks $r_2 = [10, 11, 11, 13, 13, 13, 14, 13, 13]$. The level 2 spectra for all 9 modes can be seen in the right plot of Figure 2.2.

2.2 Time Dependent Function Decomposition

Now we consider the time dependent field

$$u : D \times [0, T] \to \mathbb{R} \tag{2.35}$$

for which at any fixed $t \in [0, T]$ we have that that $u(\boldsymbol{x}, t)$ is an element of the Sobolov space $H^2(D)$. Two possible methods for the decomposition of (2.35) are

- Provided that u is square integrable in t, we may treat t the same as a spatial variable and include it in the recursive biorthogonal decomposition.
- Perform a recursive biorthogonal decomposition in space at a fixed time $t_0 \in [0, T]$ to obtain one of the two decompositions (2.12)-(2.15) or (2.19)-(2.23). Then assume that each of the

modes in the recursive decomposition depends on time and develop evolution equations for each mode.

With the goal of using the recursive biorthogonal decomposition as an expansion of the solution to PDEs of the form (1.1), we develop the necessary theory for the second method in the Tensor Train format. The time redundancy that is introduced is overcome by enforcing either a dynamic orthogonality (DO) condition or a biorthogonal (BO) condition as done in Cheng et al. (2013a,b); Sapsis and Lermusiaux (2009); Choi et al. (2014); Babaee et al. (2017).

For the remainder of this thesis, we consider a decomposition of (2.35) of the form

$$\begin{aligned} &u^{(1,\dots,d)}(t) \\ &= \sum_{i_1=1}^{\infty}\cdots\sum_{i_{d-1}=1}^{\infty}\lambda_{i_1}(t)\cdots\lambda_{i_1\cdots i_{d-1}}(t)\psi^{(1)}_{i_1}(t)\psi^{(2)}_{i_1 i_2}(t)\cdots\psi^{(d-1)}_{i_1\cdots i_{d-1}}(t)\psi^{(d)}_{i_1\cdots i_{d-1}}(t). \end{aligned} \tag{2.36}$$

The rest of this chapter is devoted to deriving DO and BO evolution equations for the modes in (2.36) and showing that these two methods of propagating u on a low parametric manifold of constant rank are equivalent in the sense that the finite dimensional function spaces containing DO and BO components are the same. We also provide a numerical example of the DO propagator. In the following derivations every function is time dependent, so t is omitted from the function arguments. Superscripts indicate spatial dependencies so spatial arguments of functions are also omitted when there is no ambiguity. Angled brackets $\langle \bullet, \bullet \rangle$ denote an L^2 inner product over all spatial components for which the two inputs are defined. When the input arguments of $\langle \bullet, \bullet \rangle$ are vectors $\boldsymbol{f} = (f_1 \cdots f_m)^T$, $\boldsymbol{g} = (g_1 \cdots g_n)$, the result is an $m \times n$ matrix with entries $(\langle \boldsymbol{f}, \boldsymbol{g} \rangle)_{ij} = \langle f_i, g_j \rangle$.

2.2.1 DO Tensor Train Propagator

First we derive the DO evolution equations in the Tensor Train format. Using the notation in the recursive decomposition (2.12)-(2.15), we define the DO components as

$$\begin{aligned} \overset{\text{DO}(j)}{\psi}_{i_1\cdots i_j} &= \psi^{(j)}_{i_1\cdots i_j} \\ \overset{\text{DO}(j+1,\dots,d)}{\psi}_{i_1\cdots i_j} &= \lambda_{i_1\cdots i_j}\psi^{(j+1,\dots,d)}_{i_1\cdots i_j}. \end{aligned} \tag{2.37}$$

Notice that the right hand modes carry the eigenvalues in the DO components, this will be different for the BO components which will be defined in the following section. Enforce the dynamic constraints

$$\langle \frac{\partial \overset{\mathrm{DO}^{(j)}}{\psi}_{i_1\cdots i_{j-1}k}}{\partial t}, \overset{\mathrm{DO}^{(j)}}{\psi}_{i_1\cdots i_{j-1}p} \rangle = 0 \tag{2.38}$$

for all $k, p = 1, \ldots, r_j$. This condition implies that the $\{\overset{\mathrm{DO}^{(j)}}{\psi}_{i_1\cdots i_{j-1}1}, \ldots, \overset{\mathrm{DO}^{(j)}}{\psi}_{i_1\cdots i_{j-1}r_j}\}$ remain orthonormal with respect to the spatial inner product for all time. We do not enforce any conditions on the right hand modes, they will most often not remain orthogonal as they evolve. For ease of notation in the following derivation, we let $\psi^{(j)}_{i_1\cdots i_j} = \overset{\mathrm{DO}^{(j)}}{\psi}_{i_1\cdots i_j}$ and $\psi^{(j+1,\ldots,d)}_{i_1\cdots i_j} = \overset{\mathrm{DO}^{(j+1,\ldots,d)}}{\psi}_{i_1\cdots i_j}$.

To begin the derivation of the DO Tensor Train evolution equations, we differentiate the level 1 expansion

$$\sum_{i_1=1}^{r_1} \psi^{(1)}_{i_1} \psi^{(2,\ldots,d)}_{i_1} = u^{(1,\ldots,d)} \tag{2.39}$$

with respect to t to obtain

$$\sum_{i_1=1}^{r_1} \frac{\partial \psi^{(1)}_{i_1}}{\partial t} \psi^{(2,\ldots,d)}_{i_1} + \psi^{(1)}_{i_1} \frac{\partial \psi^{(2,\ldots,d)}_{i_1}}{\partial t} = \frac{\partial u^{(1,\ldots,d)}}{\partial t}. \tag{2.40}$$

Applying $\langle \bullet, \psi^{(1)}_{k_1} \rangle$ to (2.40) and utlizing the DO condition (2.38), we obtain evolution equations for half of the modes in (2.12)

$$\frac{\partial \psi^{(2,\ldots,d)}_{k_1}}{\partial t} = \langle \frac{\partial u^{(1,\ldots,d)}}{\partial t}, \psi^{(1)}_{k_1} \rangle := N^{\mathrm{DO}}_{k_1}. \tag{2.41}$$

To obtain evolution eqautions for the other half $\psi^{(1)}_{k_1}$, apply $\langle \bullet, \psi^{(2,\ldots d)}_{k_1} \rangle$ to (2.40) to obtain

$$\sum_{i_1=1}^{r_1} \frac{\partial \psi^{(1)}_{i_1}}{\partial t} \langle \psi^{(2,\ldots,d)}_{i_1}, \psi^{(2,\ldots,d)}_{k_1} \rangle + \psi^{(1)}_{i_1} \langle \frac{\partial \psi^{(2,\ldots,d)}_{i_1}}{\partial t}, \psi^{(2,\ldots,d)}_{k_1} \rangle = \langle \frac{\partial u^{(1,\ldots,d)}}{\partial t}, \psi^{(2,\ldots,d)}_{k_1} \rangle. \tag{2.42}$$

Then by applying $\langle \bullet, \psi^{(1)}_{k_1} \rangle$ to either (2.41) or (2.42) with we find that

$$\langle \frac{\partial \psi^{(2,\ldots,d)}_{k_1}}{\partial t}, \psi_{k_1} \rangle = \langle \langle \frac{\partial u^{(1,\ldots,d)}}{\partial t}, \psi^{(2,\ldots d)}_{k_1} \rangle, \psi^{(1)}_{k_1} \rangle. \tag{2.43}$$

Plugging (2.43) into (2.42) we obtain the evolution equations for the second half of the modes in (2.12)

$$\begin{aligned} &\sum_{i_1=1}^{r_1} \frac{\partial \psi^{(1)}_{i_1}}{\partial t} \langle \psi^{(2,\ldots,d)}_{i_1}, \psi^{(2,\ldots,d)}_{k_1} \rangle \\ &= \langle \frac{\partial u^{(1,\ldots,d)}}{\partial t}, \psi^{(2,\ldots,d)}_{k_1} \rangle - \sum_{i_1=1}^{r_1} \psi^{(1)}_{i_1} \langle \langle \frac{\partial u^{(1,\ldots,d)}}{\partial t}, \psi^{2,\ldots,d)}_{k_1} \rangle, \psi^{(1)}_{i_1} \rangle := M^{\mathrm{DO}}_{k_1}. \end{aligned} \tag{2.44}$$

These evolution equations can be expressed more succinctly by introducing the vector notation

$$\Psi^{(1)} = [\psi_1^{(1)} \cdots \psi_{r_1}^{(1)}]$$
$$\Psi^{(2,\dots,d)} = [\psi_1^{(2,\dots,d)} \cdots \psi_{r_1}^{(2,\dots,d)}]. \tag{2.45}$$

Now we may write

$$\frac{\partial}{\partial t}\Psi^{(1)} C = [M_1^{DO} \cdots M_{r_1}^{DO}]$$
$$\frac{\partial}{\partial t}\Psi^{(2,\dots,d)} = [N_1^{DO} \cdots N_{r_1}^{DO}] \tag{2.46}$$

where $(C)_{ij} = \langle \psi_i^{(2,\dots,d)}, \psi_j^{(2,\dots,d)} \rangle$.

We move to the next level of the Tensor Train tree and derive DO evolution equations for the level 2 modes. By following the same sequence of projections as done for the level 1 modes, we obtain

$$\frac{\partial \psi_{k_1 k_2}^{(3,\dots,d)}}{\partial t} = \langle N_{k_1}, \psi_{k_1 k_2}^{(2)} \rangle := N_{k_1 k_2}^{\text{DO}} \tag{2.47}$$

and

$$\sum_{i_2=1}^{r_2} \frac{\partial \psi_{k_1 i_2}^{(2)}}{\partial t} \langle \psi_{k_1 i_2}^{(3,\dots,d)}, \psi_{k_1 k_2}^{(3,\dots,d)} \rangle$$
$$= \langle N_{k_1}, \psi_{k_1 k_2}^{(3,\dots,d)} \rangle - \sum_{i_2=1}^{r_2} \psi_{k_1 i_2}^{(2)} \langle \langle N_{k_1}, \psi_{k_1 k_2}^{(3,\dots,d)} \rangle, \psi_{k_1 i_2}^{(2)} \rangle := M_{k_1 k_2}^{\text{DO}}. \tag{2.48}$$

Proceeding recursively in this manner, evolution equations for the entire Tensor Train tree are unfolded

$$\frac{\partial \psi_{k_1 \cdots k_j}^{(j+1,\dots,d)}}{\partial t} = \langle N_{k_1 \cdots k_{j-1}}, \psi_{k_1 \cdots k_j}^{(j+1,\dots,d)} \rangle := N_{k_1 \cdots k_j}^{\text{DO}}$$
$$\sum_{i_j=1}^{r_j} \frac{\partial \psi_{k_1 \cdots k_{j-1} i_j}}{\partial t} \langle \psi_{k_1 \cdots k_{j-1} i_j}^{(j+1,\dots,d)}, \psi_{k_1 \cdots k_j}^{(j+1,\dots,d)} \rangle$$
$$= \langle N_{k_1 \cdots k_{j-1}}, \psi_{k_1 \cdots k_j}^{(j+1,\dots,d)} \rangle - \sum_{i_j=1}^{r_j} \psi_{k_1 \cdots k_{j-1} i_j} \langle \langle N_{k_1 \cdots k_{j-1}}, \psi_{k_1 \cdots k_j}^{(j+1,\dots,d)} \rangle, \psi_{k_1 \cdots k_{j-1} i_j}^{(j)} \rangle := M_{k_1 \cdots k_j}^{\text{DO}}. \tag{2.49}$$

If we use the vector notation

$$\Psi_{i_1 \cdots i_{j-1}}^{(j)} = [\psi_{i_1 \cdots i_{j-1} 1}^{(j)} \cdots \psi_{i_1 \cdots i_{j-1} r_j}^{(j)}]$$
$$\Psi_{i_1 \cdots i_{j-1}}^{(j+1,\dots,d)} = [\psi_{i_1 \cdots i_{j-1} 1}^{(j+1,\dots,d)} \cdots \psi_{i_1 \cdots i_{j-1} r_j}^{(j+1,\dots,d)}] \tag{2.50}$$

then the evolution equations become

$$\frac{\partial}{\partial t}\Psi_{i_1 \cdots i_{j-1}}^{(j)} C_{i_1 \cdots i_{j-1}} = [M_{i_1 \cdots i_{j-1} 1}^{DO} \cdots M_{i_1 \cdots i_{j-1} r_j}^{DO}]$$
$$\frac{\partial}{\partial t}\Psi_{i_1 \cdots i_{j-1}}^{(j+1,\dots,d)} = [N_{i_1 \cdots i_{j-1} 1}^{DO} \cdots N_{i_1 \cdots i_{j-1} r_j}^{DO}] \tag{2.51}$$

Remark 2.2.1. The 'non-leaf' modes $\psi^{(j+1,\dots,d)}_{k_1\cdots k_j}$ can be constructed at any time as an expansion of 'leaf' modes

$$\psi^{(j+1,\dots,d)}_{k_1\cdots k_j} = \sum_{i_{j+1}=1}^{r_{j+1}} \cdots \sum_{i_{d-1}=1}^{r_{d-1}} \psi^{(j+1)}_{k_1\cdots k_j i_{j+1}} \cdots \psi^{(d-1)}_{k_1\cdots k_j i_{j+1}\cdots i_{d-1}} \psi^{(d)}_{k_1\cdots k_j i_{j+1}\cdots i_{d-1}} \tag{2.52}$$

as can the solution $\tilde{u}$ as in equation (2.18). Therefore it is sufficient to only propagate the evolution equations corresponding to the 'leaf' modes, these are the univariate functions in the biorthogonal hierarchy (2.12)-(2.15).

A Numerical Example

We demonstrate the DO propagator using the function

$$u(t, x_1, x_2, x_3) = (t+1)x_2x_3 + (t^2 - 10)x_1x_3 - (4\sin(t) + 3)x_1x_2x_3 \tag{2.53}$$

with $\boldsymbol{x} \in [-1, 1]^3$. We perform a recursive biorthogonal decomposition of $u(0, x_1, x_2, x_3)$ in exactly the same way as it is done in Section 2.1.4. We use 50 Gauss-Legendre quadrature points and set the threshold to $\sigma = 10^{-10}$. This allows us to obtain the DO components at $t = 0$ in the expansion

$$u(0, x_1, x_2, x_3) = \psi^{(1)}_1 \psi^{(2)}_{11} \psi^{(3)}_{11} + \psi^{(1)}_2 \psi^{(2)}_{21} \psi^{(3)}_{21}. \tag{2.54}$$

The rank of this recursive biorthogonal decomposition is $r_1 = 2$, $r_2 = (1, 1)$. The time derivative of u is

$$\frac{\partial u}{\partial t} = x_2x_3 + 2tx_1x_3 - 4\cos(t)x_1x_2x_3$$

and the DO evolution equations in this case are

$$\begin{aligned}
&\frac{\partial \psi^{(1)}_j}{\partial t} = \langle x_2x_3\psi^{(2,3)}_j\rangle + 2tx_1\langle x_3\psi^{(2,3)}_j\rangle - 4\cos(t)x_1\langle x_2x_3\psi^{(2,3)}_j\rangle \\
&-\sum_{p=1}^{r_1} \psi^{(1)}_p [\langle \psi^{(1)}_p\rangle\langle x_2x_3\psi^{(2,3)}\rangle + 2t\langle x_1\psi^{(1)}_p\rangle\langle x_3\psi^{(2,3)}\rangle - 4\cos(t)\langle x_1\psi^{(1)}_p\rangle\langle x_2x_3\psi^{(2,3)}\rangle] \\
&\frac{\partial \psi^{(2)}_{j1}}{\partial t}\langle \psi^{(3)}_{j1}\psi^{(3)}_{j1}\rangle = x_2\langle x_3\psi^{(3)}_{j1}\rangle\langle \psi^{(1)}_j\rangle + 2t\langle x_3\psi^{(3)}_{j1}\rangle\langle x_1\psi^{(1)}_j\rangle - 4\cos(t)x_2\langle x_3\psi^{(3)}_{j1}\rangle\langle x_1\psi^{(1)_j}\rangle \\
&-\psi^{(2)}_{j1}[\langle x_2\psi^{(2)}_{j1}\rangle\langle x_3\psi^{(3)}_{j1}\rangle\langle \psi^{(1)}_j\rangle + 2t\langle \psi^{(2)}_{j1}\rangle\langle x_3\psi^{(3)}_{j1}\rangle\langle x_1\psi^{(1)}_j\rangle - 4\cos(t)\langle x_2\psi^{(2)}_{j1}\rangle\langle x_3\psi^{(3)}_{j1}\rangle\langle x_1\psi^{(1)}_j\rangle] \\
&\frac{\partial \psi^{(3)}_{j1}}{\partial t} = x_3\langle x_2\psi^{(2)}_{jk}\rangle\langle \psi^{(1)}_j\rangle + 2tx_3\langle \psi^{(2)}_{j1}\rangle\langle x_1\psi^{(1)}_j\rangle - 4\cos(t)x_3\langle x_2\psi^{(2)}_{j1}\rangle\langle x_1\psi^{(1)}_j\rangle
\end{aligned} \tag{2.55}$$

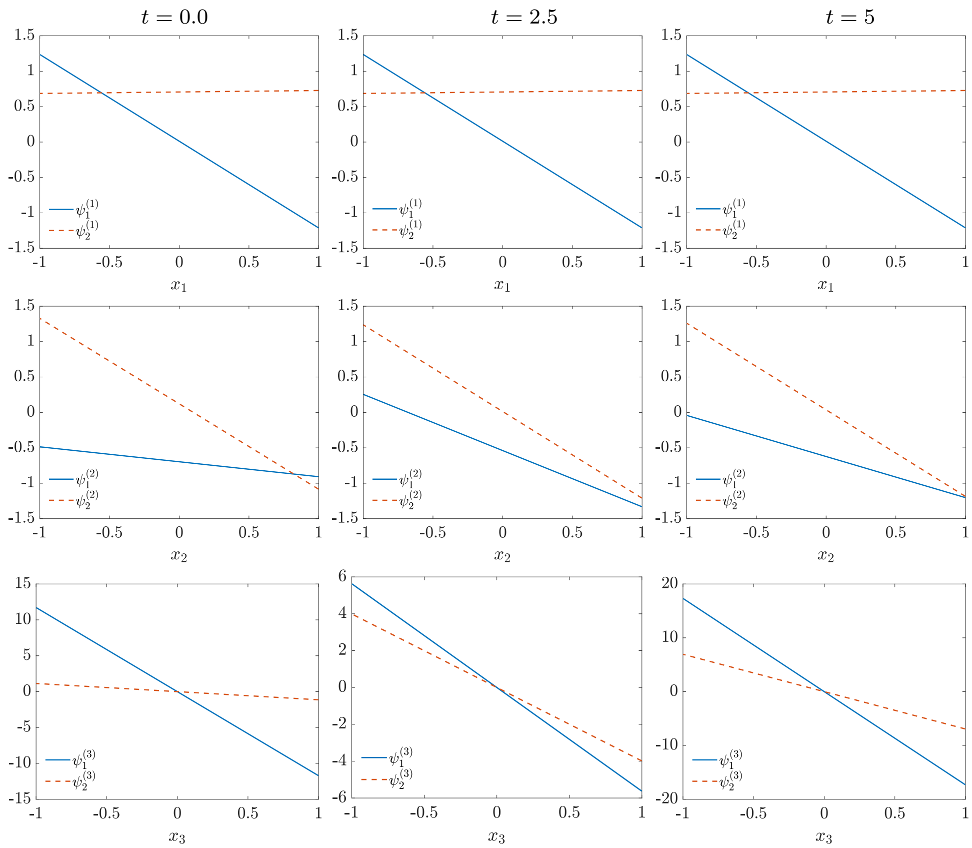

Figure 2.4: All 6 modes in the DO decomposition of (2.53) at a few snapshots in the time interval $[0, 5]$.

for $j = 1, 2$. Using a collocation method, the DO evolution equations become a system of ODEs. We solve the the ODE system numerically using an explicit RK4 method with adaptive time stepping and all integrals in (2.55) are computed with Gauss-Legendre quadrature. All 6 modes at various time snapshots in are plotted in Figure 2.4. The L^2 error of the approximation is shown in Figure 2.5.

Notice that the $u(t, x_1, x_2, x_3)$ is separable with rank $r_1 = 2$, $r_2 = (1, 1)$ for all time. This means that the solution can be accurately represented on a low paremtric manifold of constant rank for all time. We will see examples in Section 3.2 where one set of ranks $(r_1, \ldots, r_{d-1})$ may provide a sufficient representation of a function at initial time, but at a later time a different set of ranks are more suitable to represent the function. Techniques for adjusting rank are discussed in Section 3.1.

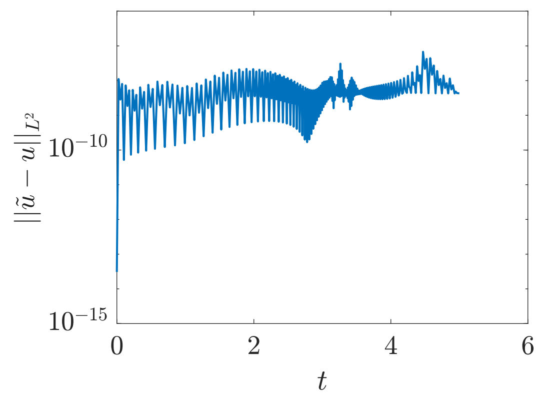

Figure 2.5: L^2 error of the DO approximation to (2.53)

.

2.2.2 BO Tensor Train Propagator

Using the decomposition (2.12) we define the BO components to be

$$\begin{aligned} \varphi^{(j)}_{i_1\cdots i_j} &= \lambda_{i_1\cdots i_j}\psi^{(j)}_{i_1\cdots i_j} \\ \varphi^{(j+1,\dots,d)}_{i_1\cdots i_j} &= \psi^{(j+1,\dots,d)}_{i_1\cdots i_j}. \end{aligned} \tag{2.56}$$

In contrast with DO components, it is the left hand modes of the BO components which carry the eigenvalue. We introduce the following vector notation to simplify the BO evolution equations

$$\begin{aligned} \Phi^{(j)}_{i_1\cdots i_{j-1}} &= (\varphi^{(j)}_{i_1\cdots i_{j-1}1}\cdots\varphi^{(j)}_{i_1\cdots i_{j-1}r_j}) \\ \Phi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}} &= (\varphi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}1}\cdots\varphi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}r_j}). \end{aligned} \tag{2.57}$$

In the BO setting, we enforce two static constraints

$$\langle\varphi^{(j)}_{i_1\dots i_{j-1}k},\varphi^{(j)}_{i_1\dots i_{j-1}p}\rangle = \lambda_{i_1\cdots i_{j-1}k}\delta_{kp} \tag{2.58}$$

$$\langle\varphi^{(j+1,\dots,d)}_{i_1\dots i_{j-1}k},\varphi^{(j+1,\dots,d)}_{i_1\dots i_{j-1}p}\rangle = \delta_{kp} \tag{2.59}$$

for all time. By projecting, BO Tensor Train evolution equations can be obtained. We omit the derivation of these evolution equations here but refer the reader to the derivations given in Cheng et al. (2013a,b)[5]. Define the following matrices and vectors to simplify the notation in the BO

[5]The derivation given in these papers takes place in probability spaces rather than L^2 or H^2 spaces, but the sequence of projections which lead to the BO evolution equations are the same.

evolution equations

$$
\begin{aligned}
\boldsymbol{h}_{i_1\cdots i_j} &= \langle N^{BO}_{i_1\cdots i_{j-1}}, \Phi^{(j)}_{i_1\cdots i_{j-1}}\rangle \\
\boldsymbol{p}_{i_1\cdots i_j} &= \langle N^{BO}_{i_1\cdots i_{j-1}}, \Phi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}}\rangle \\
\Lambda_{i_1\cdots i_j} &= \langle \Phi^{(j),T}_{i_1\cdots i_{j-1}}, \Phi^{(j)}_{i_1\cdots i_{j-1}}\rangle \\
G_{i_1\cdots i_j} &= \langle \Phi^{(j),T}_{i_1\cdots i_{j-1}} \langle N^{BO}_{i_1\cdots i_{j-1}}, \Phi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}}\rangle\rangle \\
M_{i_1\cdots i_j} &= \langle \Phi^{(j+1,\dots,d),T}_{i_1\cdots i_{j-1}}, \frac{\partial \Phi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}}}{\partial t}\rangle \\
S_{i_1\cdots i_j} &= \langle \Phi^{(j),T}_{i_1\cdots i_{j-1}}, \frac{\partial \Phi^{(j)}_{i_1\cdots i_{j-1}}}{\partial t}\rangle \\
(\Sigma_{i_1\cdots i_j})_{kp} &= \begin{cases} (S_{i_1\cdots i_j})_{kp}\,, & k \neq p\,, \\ 0\,, & k = p \end{cases}
\end{aligned}
\tag{2.60}
$$

for $j = 1, \dots, d-2$.

Remark 2.2.2. The matrices $\Sigma_{i_1\cdots i_j}$ are skew-symmetric since differentiating (2.58) with respect to time we find that $\langle \frac{\partial \phi^{(j)}_k}{\partial t}, \phi^{(j)}_p\rangle + \langle \phi^{(j)}_k, \frac{\partial \phi^{(j)}_p}{\partial t}\rangle = 0$ for $k \neq p$.

The tricky part of developing the BO evolution equations is determining the matrices $M_{i_1\cdots i_j}$ and $S_{i_1\cdots i_j}$. These matrices are not defined in the case of an eigenvalue crossing, that is if $\lambda_{i_1\cdots i_{j-1}k} = \lambda_{i_1\cdots i_{j-1}p}$ for $k \neq p$. Provided no eigenvalue crossings occur, the BO evolution equations are

$$
\begin{aligned}
\frac{\partial \Phi^{(j)}_{i_1\cdots i_{j-1}}}{\partial t} &= \Phi^{(j)}_{i_1\cdots i_{j-1}} M_{i_1\cdots i_j} + \boldsymbol{p}_{i_1\cdots i_j} = \left[M^{BO}_{i_1\cdots i_{j-1}1} \cdots M^{BO}_{i_1\cdots i_{j-1}i_{r_j}} \right] \\
\frac{\partial \Phi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}}}{\partial t} \Lambda_{i_1\cdots i_j} &= -\Phi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}} S^T_{i_1\cdots i_j} + \boldsymbol{h}_{i_1\cdots i_j} = \left[N^{BO}_{i_1\cdots i_{j-1}1} \cdots N^{BO}_{i_1\cdots i_{j-1}i_{r_j}} \right].
\end{aligned}
\tag{2.61}
$$

2.2.3 Equivalence of DO and BO Tensor Train Components

We now show that the DO Tensor Train decomposition and the BO Tensor Train decomposition are equivalent in the sense that they approximate a function using components from the same finite dimensional function spaces. We prove the equivalence for one biorthogonal decomposition following the method of Choi et al. (2014).

Suppose that $\Phi^{(j)} = (\phi^{(j)}_1 \cdots \phi^{(j)}_r)$, $\Phi^{(j+1,\dots,d)} = (\phi^{(j+1,\dots,d)}_1 \cdots \phi^{(j+1,\dots,d)}_r)$ are biorthogonal components and consider the transformation

$$\begin{aligned}\Psi^{(j)} &= \Phi^{(j)}\Lambda^{-\frac{1}{2}}P \\ \Psi^{(j+1,\ldots,d)} &= \Phi^{(j+1,\ldots,d)}\Lambda^{\frac{1}{2}}P\end{aligned} \tag{2.62}$$

where $\Lambda = \langle \Phi^{(j)^T}\Phi^{(j)} \rangle$ and P satisfies the matrix differential equation

$$\begin{cases} \frac{dP}{dt} = -\Lambda^{-\frac{1}{2}}\Sigma\Lambda^{-\frac{1}{2}}P \\ P(0) = I_{r\times r} \end{cases} \tag{2.63}$$

with

$$\Sigma_{ij} = \begin{cases} S_{ij}\ , & i \neq j\ , \\ 0\ , & i = j\ , \end{cases}$$
$$S = \langle \Phi^{(j)^T}, \frac{\partial \Phi^{(j)}}{\partial t} \rangle \tag{2.64}$$

as in (2.60).

Theorem 2.2.1. *Provided there are no eigenvalue crossings, the linear transformation in* (2.62) *is invertible and defines a new set of components for which*

(i) $\Psi^{(j)}$ *is orthonormal,*

(ii) $\Psi^{(j)}\Psi^{(j+1,\ldots,d)^T} = \Phi^{(j)}\Phi^{(j+1,\ldots,d)^T}$

(iii) $\Psi^{(j)}$ *satisfies the DO condition* $\langle \frac{\partial \Psi^{(j)^T}}{\partial t}\Psi^{(j)} \rangle = 0_{r\times r}$.

Hence $\Psi^{(j)}, \Psi^{(j+1,\ldots,d)}$ *are DO components.*

Before proving the theorem we prove the following lemma.

Lemma 2.2.1. *The matrix* $P(t)$ *in* (2.63) *remains orthogonal for all* $t \geq 0$ *provided the initial condition* $P(0)$ *is orthogonal.*

Proof. Note that $F(t) = -\Lambda^{-\frac{1}{2}}\Sigma\Lambda^{-\frac{1}{2}}$ is skew-symmetric since Σ is skew-symmetric as seen in

Remark 2.2.2. Thus

$$\begin{aligned}\frac{d}{dt}(P^TP) &= \frac{dP^T}{dt}P + P^T\frac{dP}{dt} \\ &= (FP)^TP + P^TFP \\ &= P^T(F^T+F)P \\ &= 0_{r\times r}\end{aligned}$$

for all $t \geq 0$. $\square$

Now we prove the equivalence Theorem 2.2.1.

Proof. First, note that the transformations in (2.62) are in fact invertible by Lemma 2.2.1. To prove (i),

$$\begin{aligned}\Lambda &= \langle \Phi^{(j)^T}\Phi^{(j)}\rangle \\ &= \langle (\Psi^{(j)}P^T\Lambda^{\frac{1}{2}})^T\Psi^{(j)}P^T\Lambda^{\frac{1}{2}}\rangle \\ &= \langle \Lambda^{\frac{1}{2}}P\Psi^{(j)^T}\Psi^{(j)}P^T\Lambda^{\frac{1}{2}}\rangle \\ &= \Lambda^{\frac{1}{2}}P\langle\Psi^{(j)^T}\Psi^{(j)}\rangle P^T\Lambda^{\frac{1}{2}}.\end{aligned}$$

Multiply $P^T\Lambda^{-\frac{1}{2}}, \Lambda^{-\frac{1}{2}}P$ to the left and right hand sides respectively to obtain that

$$\begin{aligned}\langle\Psi^{(j)^T}\Psi^{(j)}\rangle &= P^T\Lambda^{-\frac{1}{2}}\Lambda\Lambda^{-\frac{1}{2}}P \\ &= I_{r\times r}\end{aligned}$$

which proves (i). We can prove (ii) by using (2.62)

$$\begin{aligned}\Phi^{(j)}\Phi^{(j+1,\ldots,d)^T} &= \Psi^{(j)}P^T\Lambda^{\frac{1}{2}}(\Psi^{(j+1,\ldots,d)}P^T\Lambda^{-\frac{1}{2}})^T \\ &= \Psi^{(j)}P^T\Lambda^{\frac{1}{2}}\Lambda^{-\frac{1}{2}}P\Psi^{(j+1,\ldots,d)} \\ &= \Psi^{(j)}\Psi^{(j+1,\ldots,d)^T}.\end{aligned}$$

To prove (iii) we differentiate the equality $\Phi^{(j)} = \Psi^{(j)}P^T\Lambda^{\frac{1}{2}}$ with respect to time

$$\begin{aligned}\frac{\partial\Phi^{(j)}}{\partial t} =& \frac{\partial\Psi^{(j)}}{\partial t}P^T\Lambda^{\frac{1}{2}} + \Psi^{(j)}\frac{\partial P^T}{\partial t}\Lambda^{\frac{1}{2}} + \frac{1}{2}\Psi^{(j)}P^T\Lambda^{-\frac{1}{2}}\frac{\partial\Lambda}{\partial t} \\ =& \frac{\partial\Psi^{(j)}}{\partial t}P^T\Lambda^{\frac{1}{2}} + \Psi^{(j)}P^T\Lambda^{-\frac{1}{2}}(S-2\Sigma)^T\end{aligned}$$

where the second equality follows from (2.63) and that $S = \Sigma + \frac{1}{2}\frac{\partial \Lambda}{\partial t}$. We have by definition (2.60) that

$$S = \langle \Phi^{(j)^T} \frac{\partial \Phi^{(j)}}{\partial t} \rangle$$

and using the expressions above for $\Phi^{(j)}$ and $\frac{\partial \Phi^{(j)}}{\partial t}$ yields

$$\begin{aligned} S &= \langle \Lambda^{\frac{1}{2}} P \Psi^{(j)^T} (\frac{\partial \Psi^{(j)}}{\partial t} P^T \Lambda^{\frac{1}{2}} + \Psi^{(j)} P^T \Lambda^{-\frac{1}{2}} (S - 2\Sigma)^T) \rangle \\ &= \langle \Lambda^{\frac{1}{2}} P \Psi^{(j)^T} \frac{\partial \Psi^{(j)}}{\partial t} P^T \Lambda^{\frac{1}{2}} \rangle + \langle \Lambda^{\frac{1}{2}} P \Psi^{(j)^T} \Psi^{(j)} P^T \Lambda^{-\frac{1}{2}} (S - 2\Sigma)^T \rangle \\ &= \Lambda^{\frac{1}{2}} P \langle \Psi^{(j)^T} \frac{\partial \Psi^{(j)}}{\partial t} \rangle P^T \Lambda^{\frac{1}{2}} + (S - 2\Sigma)^T. \end{aligned}$$

This implies that

$$\begin{aligned} \frac{1}{2} \Lambda^{\frac{1}{2}} P \langle \Psi^{(j)^T} \frac{\partial \Psi^{(j)}}{\partial t} \rangle P^T \Lambda^{\frac{1}{2}} &= \frac{S - S^T}{2} - \Sigma \\ &= 0_{r \times r} \end{aligned}$$

because Σ is the skew-symmetric part of S. We know that P and Λ are nonzero, thus it must be the case that

$$\langle \frac{\partial \Psi^{(j)^T}}{\partial t} \Psi^{(j)} \rangle = 0_{r \times r}.$$

□

With the equivalence between one set of BO and DO components established, we can discuss the effect of this transformation on a hierarchy of DO or BO components. An immediate consequence is that if this transformation is performed on the j^{th} level of a Tensor Train tree, each mode on levels above j remain unchanged. However such a transformation will require every mode below the j^{th} level to be recomputed. Moreover in the case of a BO hierarchy of modes, one has to be sure that there are no eigenvalue crossings in any of the biorthogonal decompositions.

3 Numerical Solutions of Nonlinear PDEs

Let us explain how to solve a PDE of the form (1.1) using an expansion of the solution of the form (2.36). The solution of (1.1) is given at time $t = 0$. Perform a recursive biorthogonal decomposition of the given initial condition to obtain initial conditions for the time dependent modes of u. The evolution equations for the modes are given in Section 2.2 with $\frac{\partial u}{\partial t}$ replaced with $N(u)$. If the operator N is not separable then the computation of inner products in the DO and BO Tensor Train evolution equations require computation of integrals in as many as $d-1$ variables. If we assume that N is a separable operator of rank r_N

$$N = \sum_{i=1}^{r_N} A_1^{(i)} \otimes \cdots \otimes A_d^{(i)}, \tag{3.1}$$

where $A_j^{(i)}$ operates only x_j, then the evolution equations can be evaluated with one dimensional integrals. Equations for $N_{k_1\cdots k_j}^{\mathrm{DO}}$ and $M_{k_1\cdots k_j}^{\mathrm{DO}}$ in (2.51) for operators of the form (3.1) are given in Appendix (B).

3.1 Addition and Removal of Modes

The solution to PDEs of the form (1.1) may not be accurately approximated by elements from a tensor manifold of constant rank for all time. It may be desirable to reduce the solution rank or increase the solution rank during mode propagation. Removing modes is straightforward since one can simply truncate the BO or DO decomposition on any level to a decomposition of smaller rank. Adding modes is a more subtle task. To illustrate the difficulties that arise we recall the DO and BO evolution equations from Section 2.2. In the DO case the evolution equations are

$$\begin{aligned} \frac{\partial}{\partial t}\Psi^{(j)}_{i_1\cdots i_{j-1}}C_{i_1\cdots i_{j-1}} &= [M^{DO}_{i_1\cdots i_{j-1}1}\cdots M^{DO}_{i_1\cdots i_{j-1}r_j}] \\ \frac{\partial}{\partial t}\Psi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}} &= [N^{DO}_{i_1\cdots i_{j-1}1}\cdots N^{DO}_{i_1\cdots i_{j-1}r_j}] \end{aligned} \tag{3.2}$$

and in the BO case the evolution equations are

$$\begin{aligned} \frac{\partial \Phi^{(j)}_{i_1\cdots i_{j-1}}}{\partial t} &= \Phi^{(j)}_{i_1\cdots i_{j-1}}M_{i_1\cdots i_j} + \boldsymbol{p}_{i_1\cdots i_j} = \left[M^{BO}_{i_1\cdots i_{j-1}1}\cdots M^{BO}_{i_1\cdots i_{j-1}i_{r_j}}\right] \\ \frac{\partial \Phi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}}}{\partial t}\Lambda_{i_1\cdots i_j} &= -\Phi^{(j+1,\dots,d)}_{i_1\cdots i_{j-1}}S^T_{i_1\cdots i_j} + \boldsymbol{h}_{i_1\cdots i_j} = \left[N^{BO}_{i_1\cdots i_{j-1}1}\cdots N^{BO}_{i_1\cdots i_{j-1}i_{r_j}}\right]. \end{aligned} \tag{3.3}$$

If the solution is approximated with a hierarchical rank which is too large at any level of the tree, the matrices in the evolution equations (3.2) and (3.3) corresponding to these modes become singular. If the solution is approximated with a rank that is too small, the approximation is not accurate. The amount of energy each mode contributes to the solution can be tracked by the eigenvalues of $\Lambda_{i_1\cdots i_j}$ in the BO setting and by the eigenvalues of the matrix $C_{i_1\cdots i_j}$ in the DO setting. Once a new mode is added with zero energy, one or more of the matrices $\Lambda_{i_1\cdots i_j}$ in the BO evolution equations or $C_{i_1\cdots i_j}$ in the DO evolution equations become singular. We consider three options to continue propagation in the presence of a new mode.

- Add a pair of modes (left and right) satisfying the orthogonality conditions of DO or BO (whichever condition is currently being enforced) with zero energy. Evolve the modes which do not require inverting the now singular matrix (right hand modes in the DO setting and left hand modes in the BO setting) for a short amount of time while keeping the other modes constant. At this point, the energy of the new mode comes up to some value λ_ϵ which is significantly smaller than the energy of the more developed modes. Now when the matrix is inverted to continue mode propagation of the modes which were fixed, we obtain a slow-fast system Bertram and Rubin (2017). The evolution of these modes remains slow-fast until the energy amongst all modes become more balanced.

- The technique presented in Babaee et al. (2017) is to add modes with small threshold energy ϵ. In this way a pseudo-inverse (PI) of the matrices in the DO and BO evolution equations is used to write the evolution equations in a form which can be solved with standard numerical methods. The system governing the evolution equations half of the modes at the time of mode addition again behave as a slow-fast system. This method is effective, however it does slightly pollute the solution at the time of adding the mode.

- Another technique which we propose is to switch from DO/BO evolution equations to an explicit time stepping scheme with numerical tensors Khoromskij (2015b); Grasedyck et al. (2013) for a number of timesteps, then restart the DO/BO evolution from a new initial condition. One time step using addition from numerical tensor methods results in a rank increase, a few timesteps with numerical tensor methods may be desirable depending on the problem, timestep size, and integration scheme. The larger rank tensor resulting from these timesteps can be truncated to a desirable rank using either truncation of numerical tensors or the thresholding technique explained in Section 2.1.4. In either case, a new set of biorthogonal modes must be obtained from the numerical tensor.

The first two approaches rely on enlarging the finite dimensional function space which the approximate solution lives in. The third approach is different from these two in that the new biorthogonal modes obtained from the numerical tensor need not lie in the same finite dimensional function space as the previous set of modes. In other words we are rerepresenting the solution in a more suitable finite dimensional function space. Moreover, we are not explicitly adding modes with low energy so this technique may or may not result in a slow-fast system. In Section 3.2 we demonstrate the second and third techniques for mode addition.

3.2 Numerical Examples

In this section we use the recursive biorthogonal decomposition in the Tensor Train format with DO constraints to solve prototype hyperbolic PDEs.

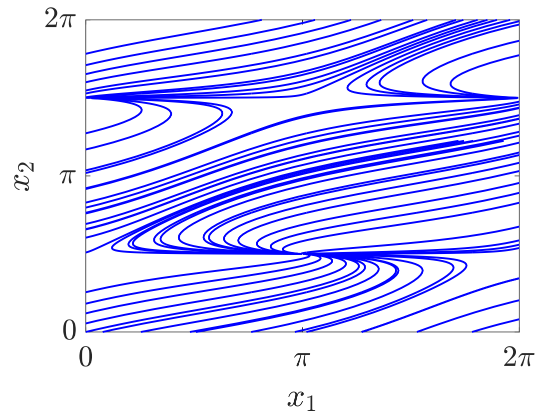

Figure 3.1: Trajectories of the characteristic system (3.5) corresponding to the PDE (3.4)

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3.2.1 2D Problem

Consider the time dependent PDE with two spatial dimensions

$$\begin{cases} \dfrac{\partial u(t,\boldsymbol{x})}{\partial t} = (\sin(x_1) + 3\cos(x_2))\dfrac{\partial u}{\partial x_1} + \cos(x_2)\dfrac{\partial u}{\partial x_2} \ , & \boldsymbol{x} \in [0, 2\pi]^2 \ , \ t \geq 0 \\ u_0(\boldsymbol{x}) = e^{\sin(x_1+x_2)} \ , & \boldsymbol{x} \in [0, 2\pi]^2 \end{cases} \tag{3.4}$$

subject to periodic boundary conditions in $[0, 2\pi]^2$. The analytical solution can be computed by using the method of characteristics. The solution to (3.4) remains constant along characteristic curves, so the dynamics of the characteristic system provide a view of the dynamics occuring in the time evolution of the solution of the PDE (3.4). The characteristic system of (3.4) is given by

$$\begin{aligned} \frac{dx_1}{dt} &= \sin(x_1) + 3\cos(x_2) \\ \frac{dx_2}{dt} &= \cos(x_2) \end{aligned} \tag{3.5}$$

and some trajectories are provided in Figure 3.1. We compute the characteristic curves numerically and use the resulting solution as the benchmark. Time snapshots of the anlytical solution are provided in the top row of Figure 3.5.

The numerical solution $\tilde{u}$ of (3.4) is computed using the Dynamically Orthogonal Tensor Train method. A biorthogonal decomposition is performed on the initial condition u_0 with threshold set to $\sigma = 10^{-13}$. We obtain 17 modes $(\psi_{i_1}^{(1)}, \psi_{i_1}^{(2)})_{i_1=1}^{17}$, each of which are collocated on an evenly

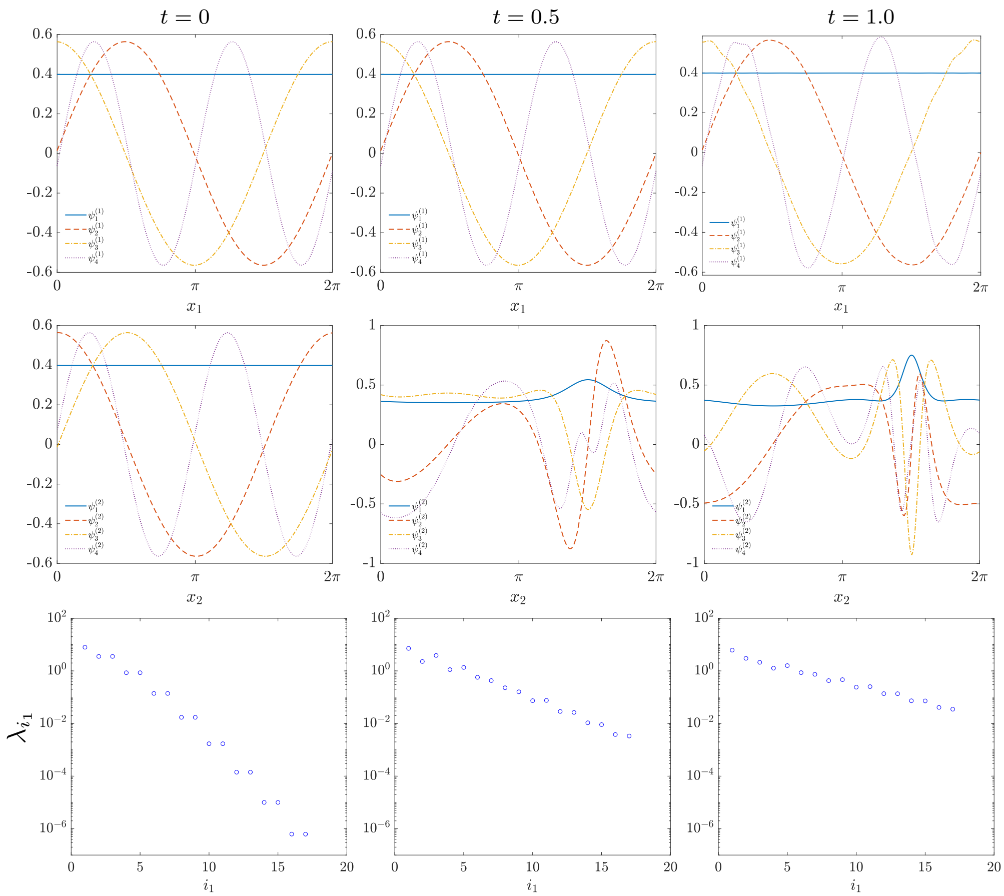

Figure 3.2: First four modes in the DO decomposition and the spectrum of the constant rank solution to (3.4) at times $t = 0.0$, $t = 0.5$, $t = 1.0$.

spaced grid with $M = 257$ points in $[0, 2\pi]$. The semi-discrete form of the DO evolution equations for (3.4) are given by

$$
\begin{aligned}
\frac{\partial \psi_j^{(2)}}{\partial t} &= \sum_{i_1=1}^{r_1} \{ \langle \sin(x_1) \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1} \psi_j^{(1)} \rangle \psi_{i_1}^{(2)} + 3 \langle \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1} \psi_j^{(1)} \rangle \psi_{i_1}^{(2)} \cos(x_2) \} + \cos(x_2) \frac{\partial \psi_j^{(2)}}{\partial x_2} \\
M_j &= \sum_{i_1=1}^{r_1} \{ \sin(x_1) \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1} \langle \psi_{i_1}^{(2)} \psi_j^{(2)} \rangle + 3 \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1} \langle \cos(x_2) \psi_{i_1}^{(2)} \psi_j^{(2)} \rangle + \psi_{i_1}^{(1)} \langle \cos(x_2) \frac{\partial \psi_{i_1}^{(2)}}{\partial x_2} \psi_j^{(2)} \rangle \\
&\quad - \sum_{p=1}^{r_1} \psi_p^{(1)} [\langle \sin(x_1) \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1} \psi_p^{(1)} \rangle \langle \psi_{i_1}^{(2)} \psi_j^{(2)} \rangle + 3 \langle \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1} \psi_p^{(1)} \rangle \langle \cos(x_2) \psi_{i_1}^{(2)} \psi_j^{(2)} \rangle \\
&\quad + \langle \psi_{i_1}^{(1)} \psi_p^{(1)} \rangle \langle \cos(x_2) \frac{\partial \psi_{i_1}^{(2)}}{\partial x_2} \psi_j^{(2)} \rangle] \} \\
&\frac{\partial}{\partial t} [\psi_1^{(1)} \cdots \psi_{r_1}^{(1)}] C = [M_1 \cdots M_{r_1}]
\end{aligned}
\tag{3.6}
$$

where $C_{ij} = \langle \psi_i^{(2)} \psi_j^{(2)} \rangle$, x_i are vectors of collocation points, $\frac{\partial}{\partial x_i}$ represent differentiation matri-

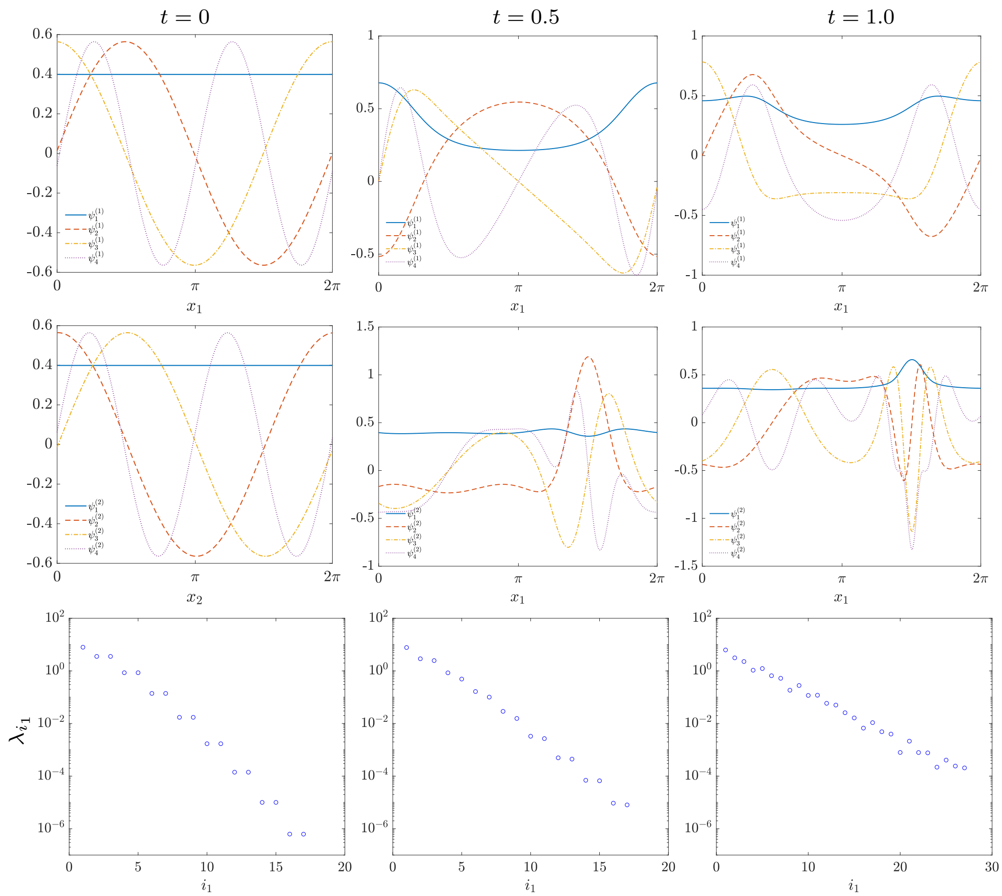

Figure 3.3: First four modes in the DO decomposition and the spectrum of the adaptive rank DO/BO numerical tensor hybrid solution to (3.4) at times $t = 0.0$, $t = 0.5$, $t = 1.0$.

ces, and inner products can be computed with a spectral quadrature rule. Put more succinctly, the evolution equations have been discretized in space with pseudospectral methods. The ODE system (3.6) is solved by first inverting the matrix C and then using an explicit RK4 scheme with time step $\Delta t = 10^{-3}$. We run one simulation with constant rank for all time, two simulations using the PI technique for addition of modes, and one simulation using the DO Tensor Train / numerical tensor hybrid scheme to add modes mentioned in Section 3.1. Time snapshots of the constant rank DO solution are provided in the middle row of Figure 3.5. Time snapshots of the pointwise error between the analytical solution and the constant rank DO solution are provided in the bottom row of Figure 3.5.

In the constant rank simulation, the slope of the error increases around $t = 0.5$ which

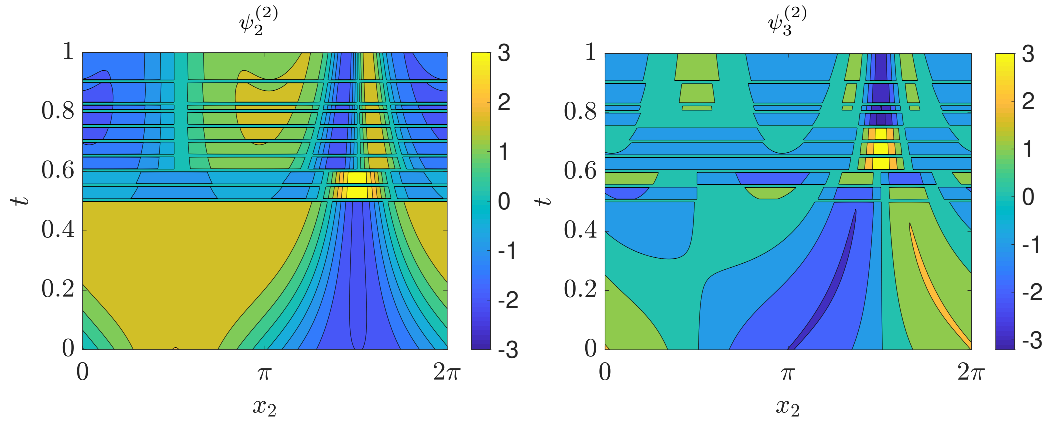

Figure 3.4: Discontinuities in the time evolution of modes obtained by using the DO Tensor Train / Numerical Tensor hybrid adaptive method for the solution of (3.4).

indicates that the solution can not be accurately represented with 17 modes. It can also be seen in the time evolution of the spectrum of the DO decomposition (Figure 3.2) that the solution requires more than 17 modes for an accurate approximation. Time snapshots of the first four modes and the full spectrum are plotted in Figure 3.2. In the first of the PI mode addition simulations, 6 modes are added beginning at $t = 0.5$ and in the second, 8 modes are added beginning at time $t = 0.5$. It can be seen from the error plot 3.6 that we are able to control the error by adding modes in this way.

In the DO Tensor Train / numerical tensor hybrid simulation we switch from the DO Tensor Train scheme to a numerical tensor method scheme at various $t \in [0.5, 1]$ and perform 10 time steps of explicit RK4 with the same time step $\Delta t = 10^{-3}$. The resulting 2-tensor is then decomposed using the biorthogonal decomposition with threshold $\sigma = 10^{-13}$ and a new set of modes are obtained. These new modes are propagated with the semi-discrete DO Tensor Train evolution equations (3.6). A few time snapshots of the first 4 modes and the full spectrum are plotted in Figure 3.3. In Figure 3.4 the time evolution of $\psi_2^{(2)}$ and $\psi_3^{(2)}$ are plotted. The horizontal bands correspond to time steps of numerical tensor methods for which there are no DO modes. After some of these bands the mode changes drastically indicating a discontinuity in the time evolution of the mode, a result of performing a new biorthogonal decomposition on the tensor. This DO Tensor Train / numerical tensor hybrid technique for adding modes performs slightly better than the PI

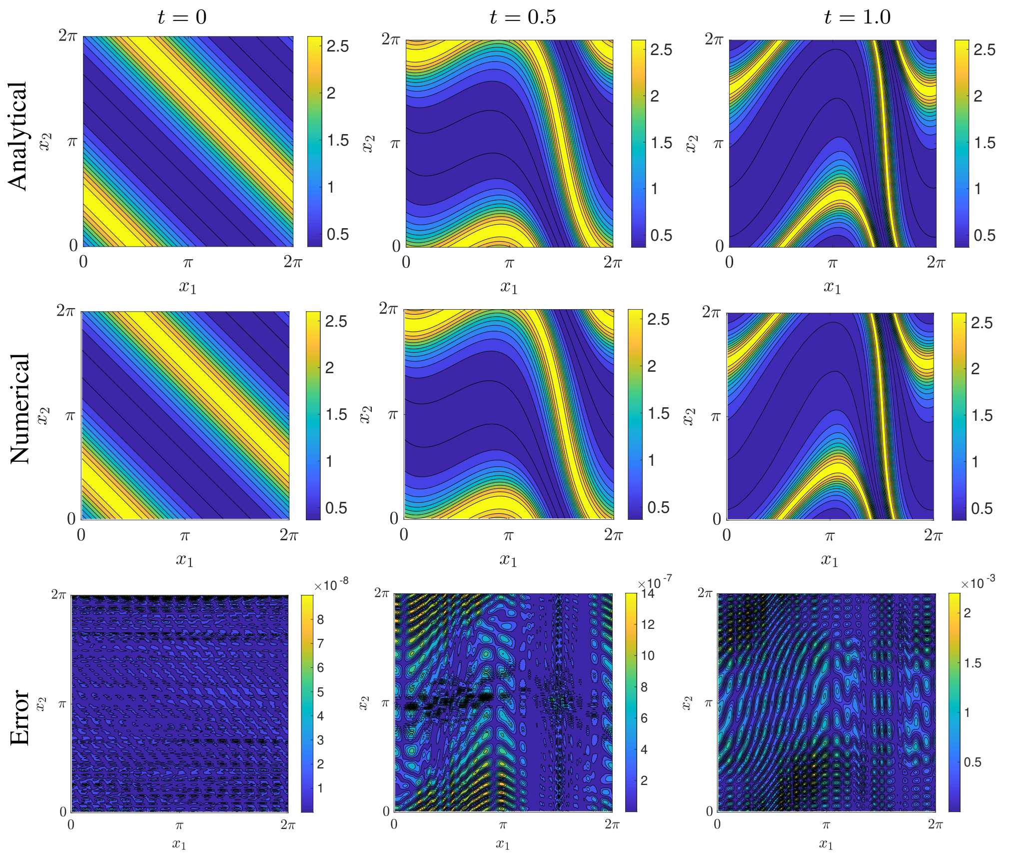

Figure 3.5: Time snapshots of the solution to (3.4) obtained using Method of Characteristics (top), Dynamically Orthogonal Tensor Train (middle), and the pointwise error (bottom).

technique.

3.2.2 4D Problem

Consider the 4 dimensional operator

$$N = \sum_{i,j=1}^{4} c_{ij} f_j(x_j) \frac{\partial}{\partial x_i} \tag{3.7}$$

where c_{ij} are real scalars and $f_j(x_j)$ are real valued functions. The DO Tensor Train evolution equations for this particular operator are given in Appendix B. For numerical demonstration, we set

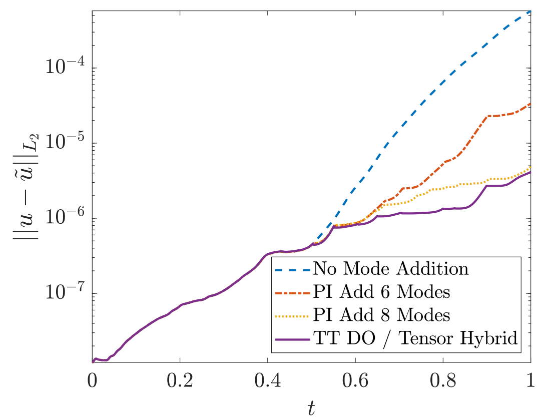

Figure 3.6: Error of Dynamically Orthogonal Tensor Train solution computed in the L^2 norm. One solution with constant modes for all time, one solution adding 6 modes at times $t = 0.5$, $t = 0.55$, $t = 0.6$, $t = 0.65$, $t = 0.7$, $t = 0.75$, and one solution adding 8 modes at times $t = 0.5$, $t = 0.55$, $t = 0.6$, $t = 0.65$, $t = 0.7$, $t = 0.75$, $t = 0.8$, $t = 0.825$, $t = 0.85$, $t = 0.9$.

the constant coefficient matrix

$$(c)_{ij} = \begin{bmatrix} 0 & 0.5 & 0 & 0 \\ 0 & 0 & -0.3 & 0 \\ 0 & 0 & 0 & -1 \\ 0.5 & 0 & 0 & 0 \end{bmatrix}$$

and variable coefficients

$$f_1(x_1) = \sin(x_1)$$

$$f_2(x_2) = \cos(2x_2)$$

$$f_3(x_3) = \sin(3x_3)$$

$$f_4(x_4) = \cos(4x_4).$$

The following PDE is solved using the method of characteristics to obtain an analytical solution

$$\begin{cases} \dfrac{\partial u(t, \boldsymbol{x})}{\partial t} = Nu\,, \qquad \boldsymbol{x} \in [0, 2\pi]^4\,,\ t \geq 0 \\ u(0, \boldsymbol{x}) = e^{-0.1\sin(x_1 + x_2 + x3 + x_4)}\,, \qquad \boldsymbol{x} \in [0, 2\pi]^4 \end{cases} \tag{3.8}$$

with periodic boundary conditions in the hypercube $[0, 2\pi]^4$.

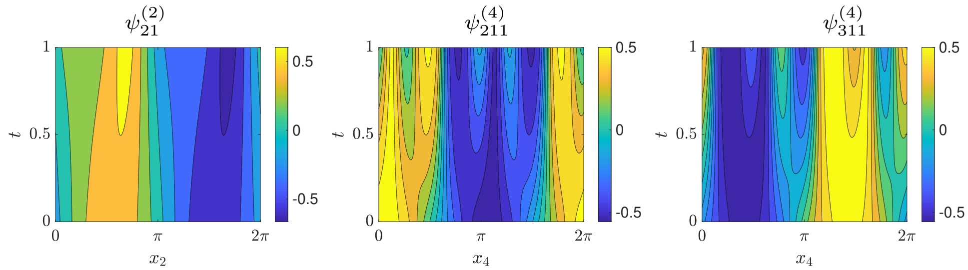

Figure 3.7: Time evolution of a few DO Tensor Train modes from the numerical solution of (3.8).

We also solve (3.8) using the DO Tensor Train method. A biorthogonal decomposition of the initial condition u_0 is performed with 20 collocation points and threshold set to $\sigma = 10^{-10}$. The following hierarchical rank arrays are obtained

$$r_1 = 9$$
$$r_2 = \begin{bmatrix} 1 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{bmatrix}$$
$$r_3 = \begin{bmatrix} 1 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \\ 0 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{bmatrix}^T$$

which we keep constant throughout mode propagation. The L^2 error between the analytic initial condition and the numerical approximation $\tilde{u}(0, \boldsymbol{x})$ obtained with the recursive biorthogonal decomposition in the Tensor Train format is on the order of 10^{-9}. After obtaining the initial biorthogonal modes at 20 collocation points, each mode is reinterpolated using trigonemetric interpolants. These interpolants are sampled at 200 evenly spaced collocation points in $[0, 2\pi]$. Using these points we obtain a semi-discrete form of the 4 dimensional DO evolution equations. This ODE system is solved using an explicit RK4 method with fixed time step $\Delta t = 10^{-3}$.

The solution to the PDE (3.8) does not have constant hierarchical rank arrays for all $t \in [0, 1]$ which is evident by the error plot in Figure 3.9. However with the relatively low hierarchical ranks r_2, r_3 (in the sense that the maximum element of both rank arrays does not exceed 2) obtained from the initial condition, we still obtain a reasonable approximation to the solution of (3.8) for all $t \in [0, 1]$.

Slices in the x_3, x_4 plane of the analytical solution, numerical solution, and pointwise

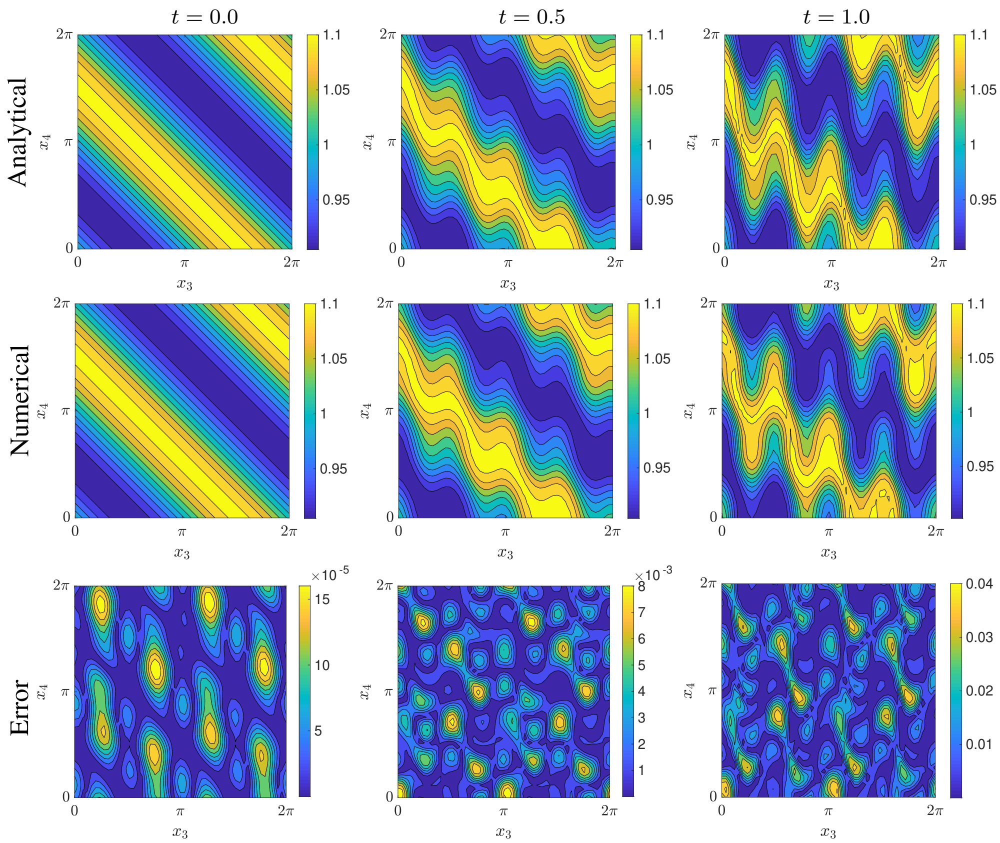

Figure 3.8: Time snapshots of slices of the solution to (3.4) obtained using Method of Characteristics (top), Dynamically Orthogonal Tensor Train (middle), and the pointwise error (bottom).

error are provided in Figure 3.8. In these slices we have fixed $x_1 = 0$ and $x_2 = 0$.

3.2.3 50D Problem

Consider the constant coefficient advection problem with rank 1 separable initial condition

$$\begin{cases} \dfrac{\partial u}{\partial t} = \displaystyle\sum_{j=1}^{50} f_j(x_j) \frac{\partial u}{\partial x_j}\,, \qquad x \in [0, 2\pi]^{50}\,, t \geq 0 \\ u(0, \boldsymbol{x}) = \displaystyle\prod_{j=1}^{50} \psi_0^{(j)}(x_j) \end{cases} \tag{3.9}$$

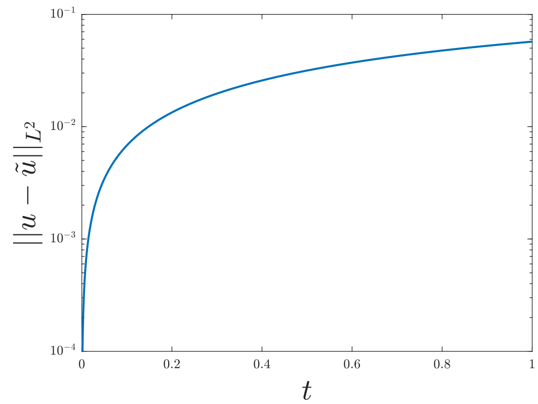

Figure 3.9: L^2 error of the DO Tensor Train approximation of the solution to (3.8)

subject to periodic boundary conditions in $[0, 2\pi]^{50}$. The DO evolution equations corresponding to the PDE (3.9) are

$$\begin{aligned}\frac{\partial \psi^{(j)}}{\partial t} &= f_j(x_j)\frac{\partial \psi^{(j)}}{\partial x_j} - f_j(x_j)\psi^{(j)}\langle \frac{\partial \psi^{(j)}}{\partial x_j}\psi^{(j)}\rangle \,, \qquad j = 1, 2, \ldots, 49 \\ \frac{\partial \psi^{(50)}}{\partial t} &= \sum_{j=1}^{49} f_j(x_j)\langle \frac{\partial \psi^{(j)}}{\partial x_j}\psi^{(j)}\rangle \psi^{(50)}.\end{aligned} \tag{3.10}$$

We set the coefficients to be constant $f_j(x_j) = j$ and the components of the initial conditions to be

$$\begin{aligned}\psi_0^{(j)}(x_j) &= \frac{\sin(x_j)}{\sqrt{\pi}} \,, \qquad j = 1, \ldots, 49 \\ \psi_0^{(50)}(x_{50}) &= 10^7(3 + \sin(x_{50})).\end{aligned} \tag{3.11}$$

which satisfy the DO conditions. The numerical solution is easily obtained by the method of characteristics. The characterstic system is given by The characterstic system given by

$$\frac{dx_j}{dt} = f_j(x_j) \,,$$

thus the characterstic curves in this case are lines. The analytical solution is given by

$$u(t, \boldsymbol{x}) = \prod_{j=1}^{50} \psi_0^{(j)}(x_j + jt). \tag{3.12}$$

We compute DO Tensor Train solution $\tilde{u}$ to (3.9)

$$\tilde{u} = \prod_{j=1}^{50} \psi^{(j)}(t). \tag{3.13}$$

Since the initial condition is already separated into biorthogonal components, there is no need to compute a recursive biorthogonal decomposition. We can simply propagate the given components.

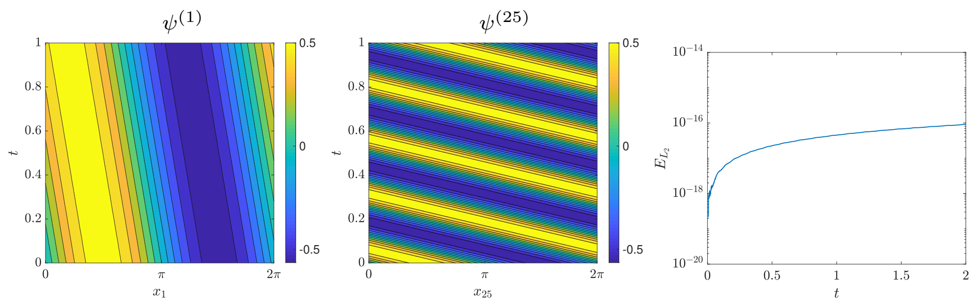

Figure 3.10: Time evolution of x_1 mode (left), time evolution of x_2 mode (middle), error of DO Tensor Train solution to (3.9) computed in the L^2 norm (right).

Using pseudospectral methods with 60 collocation points we obtain a semidiscrete form of the evolution equations (3.10). We solve the resulting ODE system with an explicit RK4 method using a fixed time step $\Delta t = 10^{-3}$. We know by looking at the analytical solution that the solution to (3.9) remains rank 1 for all time. Thus there is no need to add modes during mode propagation, and the L^2 error can be computed by computing one dimensional integrals as follows

$$
\begin{aligned}
&E_{L^2}(t) = \langle (u-\tilde{u})^2 \rangle^{\frac{1}{2}} \\
&= \langle (\prod_{j=1}^{50} \psi_0^{(j)}(x_j + jt) - \prod_{j=1}^{50} \psi^{(j)}(t))^2 \rangle^{\frac{1}{2}} \\
&= \langle \prod_{j=1}^{50} \psi_0^{(j)}(x_j + jt)^2 + \prod_{j=1}^{50} \psi^{(j)}(t)^2 - 2 \prod_{j=1}^{50} \psi_0^{(j)}(x_j + jt)\psi^{(j)}(t) \rangle^{\frac{1}{2}} \\
&= [\prod_{j=1}^{50} \int_0^{2\pi} \psi_0^{(j)}(x_j + jt)^2 dx_j + \prod_{j=1}^{50} \int_0^{2\pi} \psi^{(j)}(t)^2 dx_j - 2 \prod_{j=1}^{50} \int_0^{2\pi} \psi_0^{(j)}(x_j + jt)\psi^{(j)}(t) dx_j]^{\frac{1}{2}}.
\end{aligned}
$$

3.3 Summary

We have presented a new method for the decomposition of high dimensional time independent multivariate functions based on recursively applying biorthogonal decompositions. These decompositions can be seen as a continuous version of the decompositions from numerical tensor methods. Then we generalized the recursive biorthogonal decomposition to handle time dependence in such a way which makes the decomposition suitable for the numerical solution of high dimensional PDEs. Thus developing a new method for solving PDEs numerically which scales more favorably than classical finite difference and spectral methods.

The reason methods presented in this thesis may be preferable to tensor numerical methods for high dimensional time dependent problems is the following:

- The truncated recursive biorthogonal decomposition is subject to existing approximation results allowing for effective error analysis of the function approximation.
- Our method reduces high dimensional time dependent problems to one dimensional problems for which convergence and stability analysis is well understood. Convergence and stability of numerical tensor methods for time dependent problems is not well understood.

The methods we have presented can also be used in tandem with numerical tensor methods as we have explained in Section 3.1 and demonstrated in Section 3.2.

The purpose of this thesis was to develop the theory of a new multivariate function decomposition and its applications to solutions of time dependent PDEs, then demonstrate its effectiveness by using the methods to solve some prototype problems. In future work, we plan to develop the function approximation theory further to obtain deeper convergence results for various classes of multivariate functions. We plan to study the effect of applying the DO/BO equivalence transformation to the j^{th} level of components on the subsequent levels of the recursive biorthogonal decomposition. We also plan to use these methods to solve problems arising in physics and control theory in moderate to high dimensions. To this end, we will explore the development of high performance code which implements the methods explained in this thesis. Another application of these methods which will be explored is its use in the approximation of functionals and functional equations.

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Appendix A

This Appendix is dedicated to completing the proof of Theorem 2.1.1. The result which we prove is stated in the following Proposition.

Proposition A.0.1. *We have the following expansion of products of sums*

$$\begin{aligned}
&(\sum_{i_1=1}^{r_1}\lambda_{i_1}\psi_{i_1}^{(1)}+\sum_{i_1=1}^{\infty}\lambda_{i_1}\psi_{i_1}^{(1)})(\sum_{i_2=1}^{r_2}\lambda_{i_1i_2}\psi_{i_1i_2}^{(2)}+\sum_{i_2=1}^{\infty}\lambda_{i_1i_2}\psi_{i_1i_2}^{(2)})\cdots\\
&\cdots(\sum_{i_j=1}^{r_j}\lambda_{i_1\cdots i_j}\psi_{i_1\cdots i_j}^{(j)}+\sum_{i_j=1}^{\infty}\lambda_{i_1\cdots i_j}\psi_{i_1\cdots i_j}^{(j)})\\
=&\sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\cdots\sum_{i_j=1}^{r_j}\lambda_{i_1}\cdots\lambda_{i_1\cdots i_j}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_j}^{(j)}\\
+&\sum_{i_1=r_1+1}^{\infty}\sum_{i_2=1}^{\infty}\cdots\sum_{i_j=1}^{\infty}\lambda_{i_1}\cdots\lambda_{i_1\cdots i_j}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_j}^{(j)}\\
+&\sum_{i_1=1}^{r_1}\sum_{i_2=r_2+1}^{\infty}\sum_{i_3=1}^{\infty}\cdots\sum_{i_j=1}^{\infty}\lambda_{i_1}\cdots\lambda_{i_1\cdots i_j}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_j}^{(j)}\\
+&\sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\sum_{i_3=r_3+1}^{\infty}\sum_{i_4=1}^{\infty}\cdots\sum_{i_j=1}^{\infty}\lambda_{i_1}\cdots\lambda_{i_1\cdots i_j}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_j}^{(j)}\\
&\vdots\\
+&\sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\cdots\sum_{i_{j-1}=1}^{r_{j-1}}\sum_{i_j=r_j+1}^{\infty}\lambda_{i_1}\cdots\lambda_{i_1\cdots i_j}\psi_{i_1}^{(1)}\cdots\psi_{i_1\cdots i_j}^{(j)}
\end{aligned} \tag{A.1}$$

Proof. The proof is done by induction on j. For $j = 1$ the result is trivial. Assume the result holds for $k = j - 1$. Then

$$
\begin{aligned}
&(\sum_{i_1=1}^{r_1} \lambda_{i_1} \psi_{i_1}^{(1)} + \sum_{i_1=1}^{\infty} \lambda_{i_1} \psi_{i_1}^{(1)})(\sum_{i_2=1}^{r_2} \lambda_{i_1 i_2} \psi_{i_1 i_2}^{(2)} + \sum_{i_2=1}^{\infty} \lambda_{i_1 i_2} \psi_{i_1 i_2}^{(2)}) \cdots \\
&\cdots (\sum_{i_{j-1}=1}^{r_{j-1}} \lambda_{i_1 \cdots i_{j-1}} \psi_{i_1 \cdots i_{j-1}}^{(j-1)} + \sum_{i_{j-1}=1}^{\infty} \lambda_{i_1 \cdots i_{j-1}} \psi_{i_1 \cdots i_{j-1}}^{(j-1)}) \\
=&(\sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \cdots \sum_{i_{j-1}=1}^{r_{j-1}} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{j-1}} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{j-1}}^{(j-1)} \\
+& \sum_{i_1=r_1+1}^{\infty} \sum_{i_2=1}^{\infty} \cdots \sum_{i_{j-1}=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{j-1}} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{j-1}}^{(j-1)} \\
+& \sum_{i_1=1}^{r_1} \sum_{i_2=r_2+1}^{\infty} \sum_{i_3=1}^{\infty} \cdots \sum_{i_{j-1}=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{j-1}} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{j-1}}^{(j-1)} \\
+& \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \sum_{i_3=r_3+1}^{\infty} \sum_{i_4=1}^{\infty} \cdots \sum_{i_{j-1}=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{j-1}} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{j-1}}^{(j-1)} \\
&\vdots \\
+& \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \cdots \sum_{i_{j-2}=1}^{r_{j-2}} \sum_{i_{j-1}=r_{j-1}+1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_{j-1}} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_{j-1}}^{(j-1)}) \qquad \text{(A.2)} \\
&(\sum_{i_j=1}^{r_j} \lambda_{i_1 \cdots i_j} \psi_{i_1 \cdots i_j}^{(j)} + \sum_{i_j=1}^{\infty} \lambda_{i_1 \cdots i_j} \psi_{i_1 \cdots i_j}^{(j)}) \\
=& \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \cdots \sum_{i_j=1}^{r_j} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_j} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_j}^{(j)} \\
+& \sum_{i_1=r_1+1}^{\infty} \sum_{i_2=1}^{\infty} \cdots \sum_{i_j=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_j} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_j}^{(j)} \\
+& \sum_{i_1=1}^{r_1} \sum_{i_2=r_2+1}^{\infty} \sum_{i_3=1}^{\infty} \cdots \sum_{i_j=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_j} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_j}^{(j)} \\
+& \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \sum_{i_3=r_3+1}^{\infty} \sum_{i_4=1}^{\infty} \cdots \sum_{i_j=1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_j} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_j}^{(j)} \\
&\vdots \\
+& \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \cdots \sum_{i_{j-1}=1}^{r_{j-1}} \sum_{i_j=r_j+1}^{\infty} \lambda_{i_1} \cdots \lambda_{i_1 \cdots i_j} \psi_{i_1}^{(1)} \cdots \psi_{i_1 \cdots i_j}^{(j)}
\end{aligned}
$$

□

Appendix B

In this Appendix we provide DO Tensor Train evolution equation components for a general separable differential operator of the form (3.1) and the specific 4 dimensional operator (3.7). Expressions for the components of the DO Tensor Train evolution equations (2.51) are given by

$$
\begin{aligned}
M_{k_1\cdots k_p} &= \sum_{i=1}^{r_L} \sum_{i_1\cdots i_p=1}^{r_1\cdots r_p} \{\prod_{j=1}^{p-1} \langle A_j^{(i)}(\psi^{(j)}_{i_1\cdots i_j}), \psi_{k_1\cdots k_j}\rangle A_p^{(i)}(\psi^{(p)}_{i_1\cdots i_p}) \\
&\langle \bigotimes_{j=p+1}^{d} A_j^{(i)}(\psi^{(p+1,\ldots,d)}_{i_1\cdots i_p}), \phi_{k_0\cdots k_p}\rangle \\
&- \sum_{l=1}^{r_p} \psi^{(p)}_{k_1\cdots k_{p-1}l} \prod_{j=1}^{p-1} \langle A_j^{(i)}(\psi^{(j)}_{i_1\cdots i_j}), \psi^{(j)}_{k_1\cdots k_j}\rangle \langle A_p^{(i)}(\psi^{(p)}_{i_1\cdots i_p}), \psi^{(p)}_{k_1\cdots k_{p-1}l}\rangle \\
&\langle \bigotimes_{j=p+1}^{d} A_j^{(i)}(\psi^{(p+1,\ldots,d)}_{i_1\cdots i_p}), \psi^{(p+1,\ldots,d)}_{k_1\cdots k_p}\rangle\}\ , \\
N_{k_1\cdots k_p} &= \sum_{i=1}^{r_L} \sum_{i_1\cdots i_p=1}^{r_1\cdots r_p} \prod_{j=1}^{p} \langle A_j^{(i)}(\psi^{(j)}_{i_1\cdots i_j}), \psi^{(j)}_{k_1\cdots k_j}\rangle \bigotimes_{j=p+1}^{d} A_j^{(i)}(\psi^{(p+1,\ldots,d)}_{i_1\cdots i_p})
\end{aligned}
$$

for $p = 1, 2, \ldots, d-1$, $k_p = 1, \ldots, r_p$. In the four dimensional case, if we let N take the form (3.7) then

$$N_{k_1} = \sum_{i_1=1}^{r_1} \{ c_{11} \langle f_1 \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1}, \psi_{k_1}^{(1)} \rangle \psi_{i_1}^{(2,3,4))} + \sum_{j=2}^{4} c_{1j} \langle \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1}, \psi_{k_1}^{(1)} \rangle f_j \psi_{i_1}^{(2,3,4)}$$
$$+ \sum_{i=2}^{4} c_{i1} \langle f_1 \psi_{i_1}^{(1)}, \psi_{k_1}^{(1)} \rangle \frac{\partial \psi_{i_1}^{(2,3,4)}}{\partial x_i} + \sum_{i,j=2}^{4} c_{ij} f_j \frac{\partial \psi_{k_1}^{(2,3,4)}}{\partial x_i} \}$$
$$M_{k_1} = \sum_{i_1=1}^{r_1} \{ c_{11} f_1 \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1} \langle \psi_{i_1}^{(2,3,4)}, \psi_{k_1}^{(2,3,4)} \rangle + \sum_{i=2}^{4} c_{i1} f_1 \psi_{i_1}^{(1)} \langle \frac{\partial \psi_{i_1}^{(2,3,4)}}{\partial x_i}, \psi_{k_1}^{(2,3,4)} \rangle$$
$$+ \sum_{j=2}^{4} c_{1j} \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1} \langle f_j \psi_{i_1}^{(2,3,4)}, \psi_{k_1}^{(2,3,4)} \rangle + \sum_{i,j=2}^{4} c_{ij} \psi_{i_1}^{(1)} \langle f_j \frac{\partial \psi_{i_1}^{(2,3,4)}}{\partial x_i}, \psi_{k_1}^{(2,3,4)} \rangle$$
$$- \sum_{l=1}^{r_1} \psi_l^{(1)} [c_{11} \langle f_1 \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1}, \psi_l^{(1)} \rangle \langle \psi_{i_1}^{(2,3,4)}, \psi_{k_1}^{(2,3,4)} \rangle + \sum_{i=2}^{4} c_{i1} \langle f_1 \psi_{i_1}^{(1)}, \psi_l^{(1)} \rangle \langle \frac{\partial \psi_{i_1}^{(2,3,4)}}{\partial x_i}, \psi_{k_1}^{(2,3,4)} \rangle$$
$$+ \sum_{j=2}^{4} c_{1j} \langle \frac{\partial \psi_{i_1}^{(1)}}{\partial x_1}, \psi_l^{(1)} \rangle \langle f_j \psi_{i_1}^{(2,3,4)}, \psi_{k_1}^{(2,3,4)} \rangle + \sum_{i,j=2}^{4} c_{ij} \langle \psi_{i_1}^{(1)}, \psi_l^{(1)} \rangle \langle f_j \frac{\partial \psi_{i_1}^{(2,3,4)}}{\partial x_i}, \psi_{k_1}^{(2,3,4)} \rangle] \}$$

$$N_{k_1k_2} = \sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\{c_{11}\langle f_1\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle\langle\psi_{i_1i_2}^{(2)},\psi_{k_1k_2}^{(2)}\rangle\psi_{i_1i_2}^{(3,4)}+$$

$$c_{12}\langle\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle\langle f_2\psi_{i_1i_2}^{(2)},\psi_{k_1k_2}^{(2)}\rangle\psi_{i_1i_2}^{(3,4)}$$

$$+ c_{21}\langle f_1\psi_{i_1}^{(1)},\psi_{k_1}^{(1)}\rangle\langle\frac{\partial\psi_{i_1i_2}^{(2)}}{\partial x_2},\psi_{k_1k_2}^{(2)}\rangle\psi_{i_1i_2}^{(3,4)} + \sum_{i=3}^{4} c_{i1}\langle f_1\psi_{i_1}^{(1)},\psi_{k_1}^{(1)}\rangle\langle\psi_{i_1i_2}^{(2)},\psi_{k_1k_2}^{(2)}\rangle\frac{\partial\psi_{i_1i_2}^{(3,4)}}{\partial x_i}$$

$$+ \sum_{j=3}^{4} c_{1j}\langle\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle\langle\psi_{i_1i_2}^{(2)},\psi_{k_1k_2}^{(2)}\rangle f_j\psi_{i_1i_2}^{(3,4)}\} + \sum_{i_2=1}^{r_2}\{c_{22}\langle f_2\frac{\partial\psi_{k_1i_2}^{(2)}}{\partial x_2},\psi_{k_1k_2}^{(2)}\rangle\psi_{k_1i_2}^{(3,4)}$$

$$+ \sum_{i=3}^{4} c_{i2}\langle f_2\psi_{k_1i_2}^{(2)},\psi_{k_1k_2}^{(2)}\rangle\frac{\partial\psi_{k_1i_2}^{(3,4)}}{\partial x_i} + \sum_{j=3}^{4} c_{2j}\langle\frac{\partial\psi_{k_1i_2}^{(2)}}{\partial x_2},\psi_{k_1k_2}^{(2)}\rangle f_j\psi_{k_1i_2}^{(3,4)}\} + \sum_{i,j=3}^{4} c_{ij}f_j\frac{\partial\psi_{k_1k_2}^{(3,4)}}{\partial x_i}$$

$$M_{k_1k_2} = \sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\{c_{11}\langle f_1\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle\psi_{i_1i_2}^{(2)}\langle\psi_{i_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle+$$

$$c_{12}\langle\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle f_2\psi_{i_1i_2}^{(2)}\langle\psi_{i_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ c_{21}\langle f_1\psi_{i_1}^{(1)},\psi_{k_1}^{(1)}\rangle\frac{\partial\psi_{i_1i_2}^{(2)}}{\partial x_2}\langle\psi_{i_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle + \sum_{i=3}^{4} c_{i1}\langle f_1\psi_{i_1}^{(1)},\psi_{k_1}^{(1)}\rangle\psi_{i_1i_2}^{(2)}\langle\frac{\partial\psi_{i_1i_2}^{(3,4)}}{\partial x_i},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ \sum_{j=3}^{4} c_{1j}\langle\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle\psi_{i_1i_2}^{(2)}\langle f_j\psi_{i_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle\} + \sum_{i_2=1}^{r_2}\{c_{22}f_2\frac{\partial\psi_{k_1i_2}^{(2)}}{\partial x_2}\langle\psi_{k_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ \sum_{i=3}^{4} c_{i2}f_2\psi_{k_1i_2}^{(2)}\langle\frac{\partial\psi_{k_1i_2}^{(3,4)}}{\partial x_i},\psi_{k_1k_2}^{(3,4)}\rangle + \sum_{j=3}^{4} c_{2j}\frac{\partial\psi_{k_1i_2}^{(2)}}{\partial x_2}\langle f_j\psi_{k_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ \sum_{i,j=3}^{4} c_{ij}\psi_{i_1k_2}^{(2)}\langle f_j\frac{\partial\psi_{k_1i_2}^{(3,4)}}{\partial x_i},\psi_{k_1k_2}^{(3,4)}\rangle\}$$

$$- \sum_{l=1}^{r_2}\psi_{k_1l}^{(2)}\sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\{c_{11}\langle f_1\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle\langle\psi_{i_1i_2}^{(2)},\psi_{k_1l}^{(2)}\rangle\langle\psi_{i_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ c_{12}\langle\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle\langle f_2\psi_{i_1i_2}^{(2)},\psi_{k_1l}^{(2)}\rangle\langle\psi_{i_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ c_{21}\langle f_1\psi_{i_1}^{(1)},\psi_{k_1}^{(1)}\rangle\langle\frac{\partial\psi_{i_1i_2}^{(2)}}{\partial x_2},\psi_{k_1l}^{(2)}\rangle\langle\psi_{i_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ \sum_{i=3}^{4} c_{i1}\langle f_1\psi_{i_1}^{(1)},\psi_{k_1}^{(1)}\rangle\langle\psi_{i_1i_2}^{(2)},\psi_{k_1l}^{(2)}\rangle\langle\frac{\partial\psi_{i_1i_2}^{(3,4)}}{\partial x_i},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ \sum_{j=3}^{4} c_{1j}\langle\frac{\partial\psi_{i_1}^{(1)}}{\partial x_1},\psi_{k_1}^{(1)}\rangle\langle\psi_{i_1i_2}^{(2)},\psi_{k_1l}^{(2)}\rangle\langle f_j\psi_{i_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle\}$$

$$+ \sum_{i_2=1}^{r_2}\{c_{22}\langle f_2\frac{\partial\psi_{k_1i_2}^{(2)}}{\partial x_2},\psi_{k_1l}^{(2)}\rangle\langle\psi_{k_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ \sum_{i=3}^{4} c_{i2}\langle f_2\psi_{k_1i_2}^{(2)},\psi_{k_1l}^{(2)}\rangle\langle\frac{\partial\psi_{k_1i_2}^{(3,4)}}{\partial x_i},\psi_{k_1k_2}^{(3,4)}\rangle + \sum_{j=3}^{4} c_{2j}\langle\frac{\partial\psi_{k_1i_2}^{(2)}}{\partial x_2},\psi_{k_1l}^{(2)}\rangle\langle f_j\psi_{k_1i_2}^{(3,4)},\psi_{k_1k_2}^{(3,4)}\rangle$$

$$+ \sum_{i,j=3}^{4} c_{ij}\langle\psi_{i_1k_2}^{(2)},\psi_{k_1l}^{(2)}\rangle\langle f_j\frac{\partial\psi_{k_1i_2}^{(3,4)}}{\partial x_i},\psi_{k_1k_2}^{(3,4)}\rangle\}$$

$$
\begin{aligned}
N_{k_1k_2k_3} = &\sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\sum_{i_3=1}^{r_3}\{c_{11}\langle f_1\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(4)}_{i_1i_2i_3}\\
&+ c_{12}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle f_2\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(4)}_{i_1i_2i_3}\\
&+ c_{21}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\frac{\partial\psi^{(2)}_{i_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(4)}_{i_1i_2i_3}\\
&+ c_{13}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle f_3\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(4)}_{i_1i_2i_3}\\
&+ c_{31}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\frac{\partial\psi^{(3)}_{i_1i_2i_3}}{\partial x_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(4)}_{i_1i_2i_3}\\
&+ c_{14}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle f_4\psi^{(4)}_{i_1i_2i_3}\\
&+ c_{41}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\frac{\partial\psi^{(4)}_{i_1i_2i_3}}{\partial x_4}\}\\
&+ \sum_{i_2=1}^{r_2}\sum_{i_3=1}^{r_3}\{c_{22}\langle f_2\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{k_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(4)}_{k_1i_2i_3}\\
&+ c_{32}\langle f_2\psi^{(2)}_{k_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\frac{\partial\psi^{(3)}_{k_1i_2i_3}}{\partial x_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(4)}_{k_1i_2i_3}\\
&+ c_{23}\langle\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\langle f_3\psi^{(3)}_{k_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(4)}_{k_1i_2i_3}\\
&+ c_{24}\langle\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{k_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle f_4\psi^{(4)}_{k_1i_2i_3}\\
&+ c_{42}\langle f_2\psi^{(2)}_{k_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{k_1i_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\frac{\partial\psi^{(4)}_{k_1i_2i_3}}{\partial x_4}\}\\
&+ \sum_{i_3=1}^{r_3}\{c_{33}\langle f_3\frac{\partial\psi^{(3)}_{k_1k_2i_3}}{\partial x_3},\psi^{(3)}_{k_1k_2k_3}\rangle\psi^{(3)}_{k_1k_2i_3}\\
&+ c_{34}\langle\frac{\partial\psi^{(3)}_{k_1k_2i_3}}{\partial x_3},\psi^{(3)}_{k_1k_2k_3}\rangle f_4\psi^{(4)}_{k_1k_2i_3}\\
&+ c_{43}\langle f_3\psi^{(3)}_{k_1k_2i_3},\psi^{(3)}_{k_1k_2k_3}\rangle\frac{\partial\psi^{(4)}_{k_1k_2i_3}}{\partial x_4}\} + c_{44}f_4\frac{\partial\psi^{(4)}_{k_1k_2k_3}}{\partial x_4}
\end{aligned}
$$

$$
\begin{aligned}
M_{k_1k_2k_3} &= \sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\sum_{i_3=1}^{r_3}\{c_{11}\langle f_1\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\psi^{(3)}_{i_1i_2i_3}\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{12}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle f_2\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\psi^{(3)}_{i_1i_2i_3}\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{21}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\frac{\partial\psi^{(2)}_{i_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\psi^{(3)}_{i_1i_2i_3}\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{13}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle f_3\psi^{(3)}_{i_1i_2i_3}\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{31}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\frac{\partial\psi^{(3)}_{i_1i_2i_3}}{\partial x_3}\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{14}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\psi^{(3)}_{i_1i_2i_3}\langle f_4\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{41}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\psi^{(3)}_{i_1i_2i_3}\langle\frac{\partial\psi^{(4)}_{i_1i_2i_3}}{\partial x_4},\psi^{(4)}_{k_1k_2k_3}\rangle\}\\
&+ \sum_{i_2=1}^{r_2}\sum_{i_3=1}^{r_3}\{c_{22}\langle f_2\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\psi^{(3)}_{k_1i_2i_3}\langle\psi^{(4)}_{k_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{32}\langle f_2\psi^{(2)}_{k_1i_2},\psi^{(2)}_{k_1k_2}\rangle\frac{\partial\psi^{(3)}_{k_1i_2i_3}}{\partial x_3}\langle\psi^{(4)}_{k_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{23}\langle\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle f_3\psi^{(3)}_{k_1i_2i_3}\langle\psi^{(4)}_{k_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{24}\langle\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\psi^{(3)}_{k_1i_2i_3}\langle f_4\psi^{(4)}_{k_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{42}\langle f_2\psi^{(2)}_{k_1i_2},\psi^{(2)}_{k_1k_2}\rangle\psi^{(3)}_{k_1i_2i_3}\langle\frac{\partial\psi^{(4)}_{k_1i_2i_3}}{\partial x_4},\psi^{(4)}_{k_1k_2k_3}\rangle\}\\
&+ \sum_{i_3=1}^{r_3}\{c_{33}f_3\frac{\partial\psi^{(3)}_{k_1k_2i_3}}{\partial x_3}\langle\psi^{(4)}_{k_1k_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{34}\frac{\partial\psi^{(3)}_{k_1k_2i_3}}{\partial x_3}\langle f_4\psi^{(4)}_{k_1k_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+ c_{43}f_3\psi^{(3)}_{k_1k_2i_3}\langle\frac{\partial\psi^{(4)}_{k_1k_2i_3}}{\partial x_4},\psi^{(4)}_{k_1k_2k_3}\rangle + c_{44}\psi^{(3)}_{k_1k_2i_3}\langle f_4\frac{\partial\psi^{(4)}_{k_1k_2i_3}}{\partial x_4},\psi^{(4)}_{k_1k_2k_3}\rangle\}
\end{aligned}
$$

$$
\begin{aligned}
&-\sum_{l=1}^{r_3}\psi^{(3)}_{k_1k_2l}\sum_{i_1=1}^{r_1}\sum_{i_2=1}^{r_2}\sum_{i_3=1}^{r_3}\{c_{11}\langle f_1\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{12}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle_{x_1}\langle f_2\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{21}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\frac{\partial\psi^{(2)}_{i_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{13}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle f_3\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{31}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\frac{\partial\psi^{(3)}_{i_1i_2i_3}}{\partial x_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{14}\langle\frac{\partial\psi^{(1)}_{i_1}}{\partial x_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle f_4\psi^{(4)}_{i_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{41}\langle f_1\psi^{(1)}_{i_1},\psi^{(1)}_{k_1}\rangle\langle\psi^{(2)}_{i_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{i_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\frac{\partial\psi^{(4)}_{i_1i_2i_3}}{\partial x_4},\psi^{(4)}_{k_1k_2k_3}\rangle\}\\
&+\sum_{i_2=1}^{r_2}\sum_{i_3=1}^{r_3}\{c_{22}\langle f_2\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{k_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{k_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{32}\langle f_2\psi^{(2)}_{k_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\frac{\partial\psi^{(3)}_{k_1i_2i_3}}{\partial x_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{k_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{23}\langle\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\langle f_3\psi^{(3)}_{k_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{k_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{24}\langle\frac{\partial\psi^{(2)}_{k_1i_2}}{\partial x_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{k_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle f_4\psi^{(4)}_{k_1i_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{42}\langle f_2\psi^{(2)}_{k_1i_2},\psi^{(2)}_{k_1k_2}\rangle\langle\psi^{(3)}_{k_1i_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\frac{\partial\psi^{(4)}_{k_1i_2i_3}}{\partial x_4},\psi^{(4)}_{k_1k_2k_3}\rangle\}\\
&+\sum_{i_3=1}^{r_3}\{c_{33}\langle f_3\frac{\partial\psi^{(3)}_{k_1k_2i_3}}{\partial x_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\psi^{(4)}_{k_1k_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{34}\langle\frac{\partial\psi^{(3)}_{k_1k_2i_3}}{\partial x_3},\psi^{(3)}_{k_1k_2l}\rangle\langle f_4\psi^{(4)}_{k_1k_2i_3},\psi^{(4)}_{k_1k_2k_3}\rangle\\
&+c_{43}\langle f_3\psi^{(3)}_{k_1k_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle\frac{\partial\psi^{(4)}_{k_1k_2i_3}}{\partial x_4},\psi^{(4)}_{k_1k_2k_3}\rangle+\\
&c_{44}\langle\psi^{(3)}_{k_1k_2i_3},\psi^{(3)}_{k_1k_2l}\rangle\langle f_4\frac{\partial\psi^{(4)}_{k_1k_2i_3}}{\partial x_4},\psi^{(4)}_{k_1k_2k_3}\rangle\}.
\end{aligned}
$$

Note that the $\psi^{(j,\ldots,4)}_{i_1\cdots i_{j-1}}$ are separable functions so that all the inner products can be computed with one dimensional integrals.