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Proper orthogonal decomposition: New approximation theory and a new computational approach

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PROPER ORTHOGONAL DECOMPOSITION: NEW APPROXIMATION THEORY AND A NEW COMPUTATIONAL APPROACH

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ABSTRACT

Proper orthogonal decomposition (POD) projection errors and error bounds for POD reduced order models of partial differential equations have been studied by many. In this research we obtain new results regarding POD data approximation theory and present a new difference quotient (DQ) approach for computing the POD modes of the data.

First, we improve on earlier results concerning POD projection errors by extending to a more general framework that allows for non-orthogonal POD projections and seminorms. We obtain new exact error formulas and convergence results for POD data approximation errors, and also prove new pointwise convergence results and error bounds for POD projections. We consider both the discrete and continuous cases of POD within this generalized framework. We also apply our results to several example problems, and show how the new results improve on previous work.

Next, we consider the relationship between POD, difference quotients (DQs), and pointwise ROM error bounds. It is known that including DQs is necessary in order to prove optimal pointwise in time error bounds for POD reduced order models of the heat equation. We introduce a new approach to including DQs in the POD procedure to further investigate the role DQs play in POD numerical analysis. Instead of computing the POD modes using all of the snapshot data and DQs, we only use the first snapshot along with all of the DQs and special POD weights. We show that this approach retains all of the numerical analysis benefits of the standard POD DQ approach, while using a POD data set that has half the number of snapshots as the standard POD DQ approach, i.e., the new approach is more computationally efficient. We illustrate our theoretical results with numerical experiments.

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1. INTRODUCTION

Proper orthogonal decomposition (POD) is a model order reduction technique for partial differential equations (PDEs) and other mathematical models. With this method, modes are computed from simulation or experimental data and a Galerkin projection is used with these modes to reduce the model. Because POD reduced order models often have very low dimension, they can be used to efficiently simulate computationally demanding problems. Therefore, POD has been used in many fields of study including fluid dynamics [2, 3, 4, 5, 6, 7, 8, 9, 10] and control theory [11, 12, 13]. For more information about POD and many known results, see, e.g., [14, 15, 16, 17]. Because of the wide use of POD in many application areas, it is of great interest to study the approximation errors in POD model order reduction procedures. Numerical analysis results for POD reduced order models of PDEs were first obtained by Kunisch and Volkwein [18, 19], and then by many others; see, e.g., [1, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34] and the references therein.

In this work we obtain new results regarding POD data approximation theory and present a new difference quotient (DQ) approach for computing the POD modes of the data.

Understanding POD data approximation errors is typically important for these numerical analysis works. To see this, let w be the solution of the mathematical model, let w_r be the solution of the POD reduced order model, and let π_r be a projection onto the span of the first r POD modes. Split the error as

$$w - w_r = \rho_r + \theta_r, \quad \rho_r = w - \pi_r w, \quad \theta_r = \pi_r w - w_r.$$

Energy estimates can often be used to bound θ_r by quantities including various norms of ρ_r, the POD data approximation error for that projection.

In [1], exact error formulas and convergence results were proven for norms of ρ_r involving two Hilbert spaces, where one space is a subset of the other. In that work, Singler considered the continuous POD setting and proved results for different combinations of POD spaces, projections, and norms. Shortly after [1], Iliescu and Wang [25] provided analogous error formulas for the discrete POD case, and many of the recent numerical analysis works mentioned above use results from [1, 25] or extensions of these results to other scenarios.

As POD is increasingly applied in a variety of situations, it becomes more useful to have error results that can be easily applied in a wide range of scenarios. Therefore, in Section 3 we extend POD data approximation results in [1, 25] to a generalized framework that allows us to treat non-orthogonal POD projections and seminorms. We prove new error formulas and convergence results for norms of quantities involving $\rho_r = w - \pi_r w$ with various POD projections π_r. We also prove new pointwise convergence results for different POD projections. Non-orthogonal POD projections have been used in the numerical analysis for POD reduced order models [24, 27]; however, the exact POD data approximation error formulas and convergence results obtained here are new. Exact POD data approximation errors using various seminorms have been obtained in some cases (see, e.g., [35, Section 3.3], [28, Lemma 3.1]); the general extension and convergence results in this work are new. Finally, some pointwise convergence results for POD projections were obtained in [1]; we obtain new error bounds and improved convergence results here.

The POD data approximation error formulas presented here are exact and do not require the use of POD inverse inequalities. We consider both the discrete and continuous cases for POD and generalize the setting in [1, 25] to allow a linear mapping between two Hilbert spaces to act on the data. We require minimal assumptions on the data, the linear operator, and the Hilbert spaces; the assumptions we do require are naturally satisfied in many applications and allow us to obtain convergence results even in the fully continuous case when the data has infinitely many positive POD eigenvalues. Note that most of the proof strategies in this work are new; some proofs do rely on techniques from [1, 36].

As mentioned above the widespread use of POD in applications has caused many researchers to study POD ROMs from a numerical analysis perspective. In order for POD to be beneficial for applications, researchers must understand how the various errors involved behave. To fully understand this for PDEs, three types of error must be considered: spatial discretization error, time discretization error, and ROM discretization error. The optimality of these errors is of particular concern. POD numerical analysis papers tend to focus on the time discretization error and the ROM discretization error since the spatial discretization error can typically be handled using existing techniques. For more information on these three types of error and the numerical analysis of POD, see the introduction of the recent work [37]. In this thesis, we focus only on the POD ROM errors which leads to an improved understanding of the numerical analysis of POD ROMs, particularly in regards to difference quotients and pointwise error bounds.

In Section 4 we focus on various approaches to creating POD modes from the data. Two of the most common existing methods are considered, and we introduce a new method. The first existing approach is a standard method to compute the POD modes and uses only the data, and the second existing approach utilizes both the data and the DQs of the data. Researchers originally started including DQs in the POD calculations to improve the numerical analysis results for POD reduced order models as in [18]. For other numerical analysis results for POD ROMs using difference quotients see [19, 38, 39, 40, 41]. Further, DQs have been used in many reduced order modeling applications including feedback control for PDEs [42], subdiffusion equations [41], modeling the dynamics of a spiking neuron [40], and partial-integro-differential equations in financial modeling [43]. For a variety of additional applications see [31, 44, 45, 46].

Researchers have been curious about the role DQs play in the behavior of the ROM and whether or not they should be included in the POD computations. In general, results on this topic were inconclusive. However in 2014, substantial progress was made by Iliescu and Wang in [38] towards understanding this. In [38] a notion of optimality was introduced and their results strongly suggested that DQs are needed to achieve optimal pointwise-in-time convergence rates. Recently in [37], further progress was made. In this work it is shown that a critical assumption often made when using standard POD without DQs is automatically guaranteed to be satisfied when DQs are included with the data. The notion of optimality introduced in [38] is extended, and it is shown that including difference quotients results in optimal POD projection errors and ROM errors. The second primary goal of the thesis is to further investigate and understand pointwise error bounds in the POD-ROM setting.

To do this, in Section 4 we introduce a new approach to deriving POD modes from the data. When using all of the data with all of the DQs, the resulting data set is linearly dependent, i.e. the data set being used contains redundant information. This also leads to more costly POD basis computations compared to standard POD without DQs. In order to improve this situation, we consider the following question: *Can we obtain all of the same numerical analysis benefits of using DQs with POD using a data set without redundancy?* We show that the answer is yes, if we choose the data set and POD weights in a correct way. For our new approach we use only the first data snapshot and all of the difference quotients. This new approach to using DQs with POD uses a data set without redundancy in the following sense: if the original set of M snapshots is linearly independent, then the data set used in our new DQ approach has dimension M and is also linearly independent. Using this new collection of data and special POD weights, we are not only able to approximate the DQs and the one regular snapshot, but all of the other regular snapshot data as well. With this method we also prove that we retain the numerical analysis benefits that come with having the DQs in the POD data set.

The material in this dissertation is mostly from the works [47] and [48]. Some small changes have been made to increase readability and unify information, notation, and results between the works.

2. BACKGROUND

In this section, we recall some functional analysis background material, the basic theory for discrete POD and continuous POD as well as results on the optimality of POD. For details and proofs for the basic discrete and continuous POD theory, see, e.g., [14, 15, 19, 49, 50, 51] and also Section 2.2.3.

2.1. FUNCTIONAL ANALYSIS BACKGROUND

Let V and W be Hilbert spaces with inner products[1] $(\cdot,\cdot)_V$ and $(\cdot,\cdot)_W$ and corresponding norms $\|\cdot\|_V$ and $\|\cdot\|_W$. Throughout this work, the scalar field $\mathbb{K}$ for all spaces is either $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$.

Linear Operators: Let $T : V \to W$ be a linear operator with domain $\mathcal{D}(T) \subset V$, range $\mathcal{R}(T) \subset W$, and null space $\ker(T) \subset V$. The *rank* of T is the dimension of $\mathcal{R}(T)$. The operator T is *bounded* if $\|Tv\|_W \leq M\|v\|_V$ for all $v \in \mathcal{D}(T)$. Throughout this thesis, we only consider bounded operators $T : V \to W$ that are defined on the whole space, so $\mathcal{D}(T) = V$. For such a bounded operator $T : V \to W$, the usual operator norm is given by $\|T\| = \sup\{\|Tv\|_W : v \in V, \|v\|_V = 1\}$. We also consider unbounded linear operators that are not defined everywhere, so that $\mathcal{D}(T) \neq V$. The operator T is *closed* if its graph, $\mathcal{G}(T) = \{(v, w) : v \in \mathcal{D}(T), w = Tv\}$, is closed in $V \times W$. If T is bounded (and everywhere defined), then T is closed. If T is closed and invertible, then T^{-1} is closed.

Adjoint Operators: The *Hilbert-adjoint operator* $T^* : W \to V$ satisfies $(Tv, w)_W = (v, T^*w)_V$ for all $v \in \mathcal{D}(T)$ and $w \in \mathcal{D}(T^*)$. If T is bounded, then T^* exists, is unique, and is also bounded. If T is densely defined, then T^* exists, is unique, and is closed; in addition, if T is closed, then T^* is densely defined. If $T : V \to W$ is invertible, then we let

[1]In this thesis, all inner products and sesquilinear forms are linear in the first argument and conjugate linear in the second argument.

$T^{-*}: V \to W$ denote the Hilbert adjoint operator of the inverse $T^{-1}: W \to V$. We note for T^* to exist we need T bounded or densely defined, and for T^{-*} to exist we need T^{-1} bounded or densely defined. We note these assumptions when necessary.

The following basic result is important in this work.

Lemma 2.1.1. *Let V and W be Hilbert spaces. If* $T: V \to W$ *is a bounded linear operator, then* $\ker(TT^*) = \ker(T^*)$ *and* $\ker(T^*T) = \ker(T)$.

Proof. We only prove the first one. Let $w \in \ker(TT^*)$. Then,

$$TT^*w = 0 \Rightarrow (TT^*w, w)_W = 0 \Rightarrow (T^*w, T^*w)_V = 0 \Rightarrow \|T^*w\|_V^2 = 0 \Rightarrow T^*w = 0.$$

Next, let $w \in \ker(T^*)$. Then $T^*w = 0 \Rightarrow TT^*w = 0$. □

Projections: A bounded linear operator $\Pi : V \to V$ is a *projection* onto $U = \mathcal{R}(\Pi)$ if $\Pi^2 = \Pi$. Then we have $\Pi v \in U$ for all $v \in V$ and $\Pi u = u$ for all $u \in U$. Also, Π is an *orthogonal projection* if $u = \Pi v \in U$ minimizes $\inf_{u \in U} \|v - u\|_V$ for any $v \in V$. A nontrivial orthogonal projection Π is automatically self-adjoint, i.e., $\Pi^* = \Pi$, and satisfies $\|\Pi\| = 1$. We consider non-orthogonal projections in this thesis, and therefore we do not assume a projection is orthogonal or self-adjoint unless explicitly specified. Sometimes, we assume a family of projections $\{\Pi_r\}$ is uniformly bounded in operator norm, i.e., there exists a constant C such that $\|\Pi_r\| \leq C$ for all r.

The Singular Value Decomposition of a Compact Operator: If $T : V \to W$ is a compact linear operator, with separable Hilbert spaces V and W, then T has a *singular value decomposition* (SVD). The positive singular values of T are defined to be the square roots of the positive eigenvalues of the self-adjoint nonnegative compact operators $TT^* : W \to W$ and $T^*T : V \to V$. Further, the nonzero eigenvalues of these operators are equal, and we consider zero a singular value of T if either operator has a zero eigenvalue. If the ordered singular values of T are given by $\mu_1 \geq \mu_2 \geq \cdots \geq 0$ (including repetitions), the orthonormal basis of eigenvectors of TT^* is given by $\{\psi_k\} \subset W$, and the orthonormal basis of eigenvectors of T^*T is given by $\{g_k\} \subset V$, then the singular value decomposition of T is the expansion given by

$$Tg = \sum_{k\geq 1} \mu_k (g, g_k)_V \psi_k$$

for all $g \in V$. If $\mu_k > 0$, then

$$Tg_k = \mu_k \psi_k \text{ and } T^* \psi_k = \mu_k g_k.$$

Also, the rank r truncated SVD $T_r : V \to W$ of T is defined for $g \in V$ by

$$T_r g := \sum_{k=1}^{r} \mu_k (g, g_k)_V \psi_k.$$

For more information, see, e.g., [52, Chapters VI–VIII], [53, Section V.2.3], [54, Chapter 30], [55, Sections VI.5–VI.6].

Hilbert-Schmidt Operators: Let $T : V \to W$ be a linear operator, with separable Hilbert spaces V and W, and let $\{g_k\}$ be any orthonormal basis for V. Define the *Hilbert-Schmidt norm* of T as

$$\|T\|_{\mathrm{HS}(V,W)} = \left(\sum_{k\geq 1} \|Tg_k\|_V^2 \right)^{1/2}. \tag{2.1}$$

If the sum converges we say the operator T is *Hilbert-Schmidt*. The Hilbert-Schmidt norm is independent of choice of orthonormal basis, every Hilbert-Schmidt operator is compact, $\|T\| \leq \|T\|_{\mathrm{HS}(V,W)}$, T is Hilbert-Schmidt if and only if T^* is Hilbert-Schmidt, and T is Hilbert-Schmidt if and only if $\sum_{k\geq 1} \sigma_k^2 < \infty$, where $\{\sigma_k\}$ are the singular values (including repetitions) of T. We also have

$$\|T\|_{\mathrm{HS}(V,W)}^2 = \|T^*\|_{\mathrm{HS}(W,V)}^2 = \sum_{k\geq 1} \sigma_k^2.$$

For more, see, e.g., [52, Chapter VIII], [53, Section V.2.4], [55, Section VI.6].

Bochner Spaces: Let O be an open subset of $\mathbb{R}^d$, for some $d \geq 1$. For $p \in [1, \infty)$, let $L^p(O; V)$ denote the Bochner space of (equivalence classes of) Lebesgue measurable functions $v : O \to V$ satisfying $\int_O \|v(t)\|_V^p \, dt < \infty$. For $p = 2$, $L^2(O; V)$ is a Hilbert space with inner product

$$(v, w)_{L^2(O;V)} = \int_O (v(t), w(t))_V \, dt.$$

The following theorem, see, e.g., [56, Theorem III.6.20] and [57, Theorem 4.2.10], allows us to bring a closed linear operator inside an integral.

Theorem 2.1.2. *Suppose $T : \mathcal{D}(T) \subset V \to W$ is a closed linear operator. If $v : O \to \mathcal{D}(T)$, $v \in L^1(O; V)$, and $Tv \in L^1(O; W)$, then*

$$\int_O v(t) \, dt \in \mathcal{D}(T) \quad \text{and} \quad T \int_O v(t) \, dt = \int_O Tv(t) \, dt.$$

2.2. PROPER ORTHOGONAL DECOMPOSITION

Now we introduce proper orthogonal decomposition for both the discrete and continuous time cases.

2.2.1. Discrete Case. Let X be a separable Hilbert space. For the discrete case, let s be a positive integer and assume the POD data is given by $\{w^j\}_{j=1}^s \subset X$. Let $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$, and define $S := \mathbb{K}_\Gamma^s$ with the weighted inner product given by

$$(u, v)_S = v^* \Gamma u = \sum_{j=1}^{s} \gamma_j u^j \overline{v^j},$$

where $u, v \in S$, $\Gamma = \mathrm{diag}(\gamma_1, \gamma_2, ..., \gamma_s)$, and the values $\{\gamma_j\}_{j=1}^s$ are positive weights. Note these weights commonly arise from integral approximations. Define the POD operator $K : S \to X$ by

$$K f = \sum_{j=1}^{s} \gamma_j f^j \, w^j, \quad f = [f^1, f^2, \ldots, f^s]^T. \tag{2.2}$$

Since K has finite dimensional range, it is a compact operator and has a singular value decomposition. Let $\{\sigma_k, f_k, \varphi_k\} \subset \mathbb{R} \times S \times X$ be the singular values and orthonormal singular vectors ordered so that $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$. Thus, the singular value decomposition is given by

$$Kf = \sum_{j \geq 1} \sigma_j (f, f_j)_S \varphi_j. \tag{2.3}$$

When $\sigma_k > 0$, we have

$$K f_k = \sigma_k \varphi_k, \quad \text{and} \quad K^* \varphi_k = \sigma_k f_k,$$

where $K^* : X \to S$ is the Hilbert adjoint operator given by

$$K^* x = [(x, w^1)_X, (x, w^2)_X, \ldots, (x, w^s)_X]^T.$$

For a positive integer r, define $X_r = \text{span}\{\varphi_k\}_{k=1}^r$. Let $\Pi_r^X : X \to X$ be the orthogonal projection onto X_r, i.e., for $x \in X$ fixed, $\Pi_r^X x \in X_r$ minimizes the approximation error $\|x - x_r\|_X$ over all choices of $x_r \in X_r$. Since $\{\varphi_k\}$ is an orthonormal set in X, we have the exact representation

$$\Pi_r^X x = \sum_{k=1}^{r} (x, \varphi_k)_X \varphi_k. \tag{2.4}$$

The singular vectors $\{\varphi_k\}$ are called the POD modes of the data $\{w^k\} \subset X$. The POD modes provide the best low rank approximation to the data in the following sense: we have

$$\sum_{k=1}^{s} \gamma_k \|w^k - \Pi_r^X w^k\|_X^2 = \sum_{k>r} \sigma_k^2, \tag{2.5}$$

and no other choice of an orthonormal basis in (2.4) gives a smaller value for the approximation error.

Definition 2.2.1. *We call the singular values* $\{\sigma_k\}$ *and singular vectors* $\{\varphi_k\} \subset X$ *of* K *the POD singular values and POD modes for the data* $\{w^j\}_{j=1}^s$*, respectively. We also call the eigenvalues* $\{\lambda_k\}$ *of the operator* $KK^* : X \to X$ *the POD eigenvalues for the data* $\{w^j\}_{j=1}^s$*. We let* s_X *denote the number of positive POD singular values (or positive POD eigenvalues) for the data* $\{w^j\}_{j=1}^s$*, i.e.,* $s_X = \operatorname{rank}(K)$.

From Section 2.1, we know $\lambda_k = \sigma_k^2$ whenever $\lambda_k > 0$. Also, we have $s_X \leq s < \infty$. It is possible for data to have a zero POD singular value, but have all positive POD eigenvalues; this can happen if $s > \dim(X)$.

2.2.2. Continuous Case. Similarly to the discrete case we define the POD operator $K : S \to X$ for the continuous case, where again X is a separable Hilbert space. Let d and m be positive integers and let $O \subset \mathbb{R}^d$ be an open set. Then define $S := L^2(O; \mathbb{K}^m)$, where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$. We note that $L^2(O)$ is separable (see, e.g., [58, Theorem 2.5-4]), and therefore so is S. Assume the POD data is given by $\{w^j\}_{j=1}^m \subset L^2(O; X)$.

Remark 2.2.2. *In POD applications the set* O *is frequently a time interval; however, researchers also take* O *to be a multidimensional parameter domain as well. Note that we could also consider multiple open sets,* $O_j \subset \mathbb{R}^{d_j}$*, and data* $w^j \in L^2(O_j; X)$ *for* $j = 1, \ldots, m$*. In this case, we would define* $S := L^2(O_1) \times \cdots \times L^2(O_m)$*. All results in this thesis hold for this case as well. The previous case is chosen to simplify notation.*

Define the POD operator $K : S \to X$ by

$$Kf = \sum_{j=1}^{m} \int_O f^j(t) w^j(t) \, dt, \quad f \in S. \tag{2.6}$$

Since $f \in S$, note that $f = [f^1, f^2, \ldots, f^m]^T$, where each $f^j \in L^2(O)$. As in the discrete case, we know that K is a compact operator and has a singular value decomposition. We let $\{\sigma_k, f_k, \varphi_k\} \subset \mathbb{R} \times S \times X$ denote the singular values and orthonormal singular vectors ordered so that $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$. The SVD of K is given as in the discrete case (2.3).

Thus, when $\sigma_k > 0$, we have

$$K f_k = \sigma_k \varphi_k, \quad \text{and} \quad K^* \varphi_k = \sigma_k f_k,$$

where $K^* : X \to S$ is the Hilbert adjoint operator defined by

$$[K^* x](t) = [(x, w^1(t))_X, (x, w^2(t))_X, \ldots, (x, w^m(t))_X]^T.$$

We define $X_r := \operatorname{span}\{\varphi_k\}_{k=1}^r$ and the orthogonal projection $\Pi_r^X : X \to X$ (2.4) as before. The data approximation error is given by

$$\sum_{j=1}^{m} \int_O \| w^j(t) - \Pi_r^X w^j(t) \|_X^2 \, dt = \sum_{k>r} \sigma_k^2, \tag{2.7}$$

and the error goes to zero as $r \to \infty$. As in the discrete case, no other orthonormal basis in (2.4) gives a smaller value for the error.

We define the POD singular values, POD modes, POD eigenvalues, and $s_X = \operatorname{rank}(K)$ as in Definition 2.2.1 for the discrete case. Again, it is possible for data to have a zero POD singular value, but have all positive POD eigenvalues; an example where X is infinite dimensional can be found in [36, Section 3.1, Example 3]. Also, if X is finite dimensional, then the data always has a zero POD singular value.

Note that while the discrete time case of POD is considered throughout the thesis, the continuous time case is only considered here and in Chapter 3.

2.2.3. Optimality of POD. Below, we present the discrete and continuous versions of a result regarding Hilbert-Schmidt norms and POD. The continuous case result is known (see, e.e., [59, Section 3.5], [60, Theorem 12.6.1], [61, Lemma 4.4]), although perhaps not exactly in this precise form. We provide a proofs of both results to be complete, and also since the results are crucial to this work. These lemmas are used to prove the optimality of POD below.

Lemma 2.2.3. *For given data* $\{y^j\}_{j=1}^s \subset X$ *in the discrete case, the Hilbert-Schmidt norm of the POD operator* $K : S \to X$ *is given by*

$$\|K\|_{\mathrm{HS}(S,X)}^2 = \sum_{j=1}^s \gamma_j \|y^j\|_X^2.$$

Proof. Let $\{\xi_k\}_{k\geq 1}$ be an orthonormal basis for X. We have

$$\begin{aligned}\|K\|_{\mathrm{HS}(S,X)}^2 = \|K^*\|_{\mathrm{HS}(X,S)}^2 = \sum_{k\geq 1} \|K^*\xi_k\|_S^2 = \sum_{k\geq 1}\sum_{j=1}^s \gamma_j |(\xi_k, y^j)_X|^2 \\ = \sum_{j=1}^s \gamma_j \sum_{k\geq 1} |(\xi_k, y^j)_X|^2 = \sum_{j=1}^s \gamma_j \|y^j\|_X^2\end{aligned}$$

by Parseval's inequality. □

Lemma 2.2.4. *Let* Z *be a separable Hilbert space, and let* $S = L^2(O;\mathbb{K}^m)$*, where* O *is an open subset of* $\mathbb{R}^d$*. If* $K : S \to Z$ *is defined by*

$$Kf = \sum_{j=1}^m \int_O f^j(t) z^j(t)\, dt,$$

for $\{z^j\}_{j=1}^m \subset L^2(O;Z)$*, then* K *is Hilbert-Schmidt and*

$$\|K\|_{\mathrm{HS}(S,Z)}^2 = \sum_{j=1}^m \|z^j\|_{L^2(O;Z)}^2.$$

Proof. Let $\{\chi_i\}_{i\geq 1} \subset L^2(O)$ and $\{\xi_n\}_{n\geq 1} \subset Z$ be orthonormal bases. Therefore, $\{\overline{\chi}_i\}_{i\geq 1}$ is also an orthonormal basis for $L^2(O)$, and $\{\chi_i \xi_n\}_{i,n\geq 1}$ is an orthonormal basis for $L^2(O;Z)$ (see, e.g., [60, Theorem 12.6.1]).

For $\xi \in Z$, let $[K^*\xi]^j = (\xi, z^j(t))_Z$ denote the jth component of $K^*\xi \in S$. Working with the Hilbert adjoint operator K^* and using Parseval's equality gives

$$\|K^*\|_{\mathrm{HS}(S,Z)}^2 = \sum_{n\geq 1} \|K^*\xi_n\|_S^2$$

$$
\begin{aligned}
&= \sum_{j=1}^{m} \sum_{n \geq 1} \left\| [K^* \xi_n]^j \right\|_{L^2(O)}^2 \\
&= \sum_{j=1}^{m} \sum_{n,i \geq 1} \left| \left(\overline{\chi}_i, [K^* \xi_n]^j \right)_{L^2(O)} \right|^2 \\
&= \sum_{j=1}^{m} \sum_{n,i \geq 1} \left| \int_O \overline{\chi_i(t)}\, (z^j(t), \xi_n)_Z \, dt \right|^2 \\
&= \sum_{j=1}^{m} \sum_{n,i \geq 1} \left| \int_O (z^j(t), \chi_i(t) \xi_n)_Z \, dt \right|^2 \\
&= \sum_{j=1}^{m} \sum_{n,i \geq 1} \left| (z^j, \chi_i \xi_n)_{L^2(O;Z)} \right|^2 \\
&= \sum_{j=1}^{m} \| z^j \|_{L^2(O;Z)}^2 .
\end{aligned}
$$

□

To be complete, we present a brief proof of the optimality of POD for low rank data approximation in both the discrete and continuous cases. Our problem statement and proof strongly rely on the ideas from [50] and [49].

POD optimality problem: Let X be a separable Hilbert space, and let $S = \mathbb{K}_\Gamma^s$ in the discrete case or $S = L^2(O; \mathbb{K}^m)$ in the continuous case, where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$. Suppose we have given data $\{w^j\}_{j=1}^s \subset X$ in the discrete case or $\{w^j\}_{j=1}^m \subset L^2(O; X)$ in the continuous case. The POD optimality problem is to find coefficients $\{a_k\} \subset \mathbb{K}$ and basis elements $\{s_k\} \subset S$ and $\{\eta_k\} \subset X$ so that the rth order approximations

$$
\begin{aligned}
w_r^j &= \sum_{k=1}^{r} a_k s_k^j \eta_k && \text{for } j = 1, \dots, s \text{ (discrete case)}, \\
w_r^j(t) &= \sum_{k=1}^{r} a_k s_k^j(t) \eta_k && \text{for } j = 1, \dots, m \text{ (continuous case)},
\end{aligned}
$$

minimize the data approximation error

$$
E_r(w_r) = \sum_{j=1}^{s} \gamma_j \| w^j - w_r^j \|_X^2 \qquad \text{(discrete case)},
$$

$$E_r(w_r) = \sum_{j=1}^{m} \int_O \|w^j(t) - w_r^j(t)\|_X^2 \, dt \qquad \text{(continuous case).}$$

Remark 2.2.5. *In many papers on POD, the basis elements $\{\eta_k\} \subset X$ are required to be orthonormal, and w_r^j is also required to equal the orthogonal projection of w^j onto* $\mathrm{span}\{\eta_k\}_{k=1}^r$. *Therefore, the POD problem above allows more general approximations. The final result is the same.*

Notation: For given data $\{y^j\}_{j=1}^s \subset X$ in the discrete case or $\{y^j\}_{j=1}^m \subset L^2(O;X)$ in the continuous case, we let $K(y) : S \to X$ denote the POD operator for the data and we let $K^*(y) : X \to S$ denote the Hilbert adjoint operator of $K(y)$.

The proof of the next result follows directly from definitions and is omitted.

Lemma 2.2.6. *If the data is given by*

$$y^j = \sum_{k=1}^{p} \alpha_k s_k^j \eta_k \quad \textit{(discrete case)}, \qquad y^j(t) = \sum_{k=1}^{p} \alpha_k s_k^j(t) \eta_k, \quad \textit{(continuous case)}$$

for each j with $\{\alpha_k\} \subset \mathbb{K}$, $\{s_k\} \subset S$, and $\{\eta_k\} \subset X$, then the POD operator $K(y) : S \to X$ is given by

$$K(y)f = \sum_{k=1}^{p} \alpha_k (f, \overline{s_k})_S \eta_k, \qquad f \in S.$$

Now we prove the main optimality result. We rely on the fact that the rank r truncated SVD of $K(y)$ is the optimal rank r approximation to $K(y)$ in the Hilbert-Schmidt norm; see, e.g., [62, Section III.7, Theorem 7.1].

Theorem 2.2.7. *Let $\{w^j\}_{j=1}^s \subset X$ in the discrete case or $\{w^j\}_{j=1}^m \subset L^2(O;X)$ in the continuous case be given data, and let $\{\sigma_i, f_i, \varphi_i\} \subset \mathbb{R} \times S \times X$ be the ordered singular values of $K(w) : S \to X$ and the corresponding orthonormal bases of singular vectors. A solution of the POD problem is given by $\{w_r^j\}_{j=1}^s \subset X$ in the discrete case or $\{w_r^j\}_{j=1}^m \subset L^2(O;X)$ in the continuous case, where*

$$w_r^j = \sum_{k=1}^{r} \sigma_k \overline{f_k^j} \varphi_k = \sum_{k=1}^{r} \left(w^j, \varphi_k\right)_X \varphi_k \qquad \textit{(discrete case)},$$

$$w_r^j(t) = \sum_{k=1}^{r} \sigma_k \overline{f_k^j(t)} \varphi_k = \sum_{k=1}^{r} \left(w^j(t), \varphi_k\right)_X \varphi_k \qquad \textit{(continuous case).}$$

The minimum approximation error is given by

$$E_r^{\min} := E_r(w^r) = \sum_{k>r} \sigma_k^2 < \infty,$$

and $E_r^{\min} \to 0$ *as* r *increases.*

Proof. We first assume $r \leq s_X$ so that $\sigma_k > 0$ for $k = 1, \ldots, r$.

First, the equivalence of the two expressions for w_r^j comes from $K^*(w)\varphi_k = \sigma_k f_k$, $\sigma_k > 0$ for $k = 1, \ldots, r$, and the formulas for $K^*(w)$. Also, for $g \in S$, Lemma 2.2.6 implies

$$K(w_r)g = \sum_{k=1}^{r} \sigma_k (g, f_k)_S \varphi_k = K_r(w)g.$$

Therefore, $K(w^r) = K_r(w)$, where $K_r(w) : S \to X$ is the rth order truncated SVD of the POD operator $K(w) : S \to X$.

Next, by the Hilbert-Schmidt norm results Lemma 2.2.4 and Lemma 2.2.3 and since the POD operator is linear in the data we have

$$E_r(w^r) = \|K(w - w^r)\|_{\mathrm{HS}}^2 = \|K(w) - K(w^r)\|_{\mathrm{HS}}^2 = \|K(w) - K_r(w)\|_{\mathrm{HS}}^2 = \sum_{k>r} \sigma_k^2.$$

Also, since $\|K(w)\|_{\mathrm{HS}} = \sum_{k\geq 1} \sigma_k^2 < \infty$, we have $\sum_{k>r} \sigma_k^2 \to 0$ as r increases.

Now we show that this is the smallest value possible for the error. Let coefficients $\{a_k\} \subset \mathbb{K}$ and basis elements $\{s_k\} \subset S$ and $\{\eta_k\} \subset X$ be given, and define the rth order approximation

$$z_r^j = \sum_{k=1}^{r} \alpha_k s_k^j \eta_k \quad \text{(discrete case)}, \qquad z_r^j(t) = \sum_{k=1}^{p} \alpha_k s_k^j(t) \eta_k, \quad \text{(continuous case)}.$$

By Lemma 2.2.6, $K(z^r)$ has rank at most r. Therefore, we have

$$E_r(z^r) = \|K(w - z^r)\|_{\text{HS}}^2 = \|K(w) - K(z^r)\|_{\text{HS}}^2 \geq \sum_{k>r} \sigma_k^2.$$

Next, if $s_X < \infty$, then the result is true for $r = s_X$. Therefore, we have $w^j = w_{s_X}^j$ for all j, and this proves the result for $r > s_X$. □

3. NEW POD APPROXIMATION THEORY

3.1. ASSUMPTIONS AND NOTATION

In this section, assume X and Y are separable Hilbert spaces, and $L : \mathcal{D}(L) \subset X \to Y$ is a linear operator. We study POD error formulas and POD projections involving the data $\{w_j\}$ and the data $\{Lw_j\}$.

3.1.1. Discrete Case. Recall from Section 2.2.1 we consider data $\{w^j\}_{j=1}^s \subset X$ and the corresponding POD operator $K : S \to X$ defined by $Kf = \sum_{j=1}^s \gamma_j f^j w^j$, where $S = \mathbb{K}_\Gamma^s$ and $\mathbb{K}$ is either $\mathbb{R}$ or $\mathbb{C}$. The singular value decomposition of K is given by $Kf = \sum_{k\geq 1} \sigma_k (f, f_k)_S \varphi_k$. The set X_r is the span of $\{\varphi_k\}_{k=1}^r$, and $\Pi_r^X : X \to X$ is the orthogonal projection onto X_r.

To consider POD projections involving the data $\{Lw^j\}$, we make the following assumption:

> Main assumption: For the discrete case, we assume throughout the paper that (i) $\{w^j\}_{j=1}^s \subset \mathcal{D}(L)$, and also (ii) $\sigma_r > 0$ whenever we consider the projection Π_r^X.

Assumption (i) has two important consequences. First, since $w^j \in \mathcal{D}(L)$ for each j, we know the range of K is contained in $\mathcal{D}(L)$. Second, assumption (i) allows us to consider the POD operator $K^Y : S \to Y$ for the data $\{Lw^j\}_{j=1}^s \subset Y$ defined by

$$K^Y f = LKf = \sum_{j=1}^s \gamma_j f^j Lw^j, \quad f = [f^1, f^2, \ldots, f^s]^T. \tag{3.1}$$

Note that K^Y is the result of applying L to the POD operator K for the data $\{w^j\}$, i.e., $K^Y = LK$. Since K^Y has finite rank, it is compact and has a singular value decomposition. Define $s_Y = \text{rank}(K^Y)$ to be the number of positive singular values of K^Y. Note that assumption (i) is automatically satisfied if L is bounded.

For assumption (ii), note that if $\sigma_k > 0$, then assumption (i) implies the corresponding singular vector φ_k is in $\mathcal{D}(L)$ since

$$\varphi_k = \sigma_k^{-1} K f_k \in \mathcal{D}(L). \tag{3.2}$$

Since $\sigma_r > 0$, this implies $X_r \subset \mathcal{D}(L)$ and Π_r^X maps into $\mathcal{D}(L)$.

To guarantee the boundedness of certain POD projections, in some cases of Theorem 3.2.3 we need to assume the POD modes $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L)$ satisfy some additional regularity properties. These properties can be guaranteed by making additional regularity assumptions on the data.

First, the condition $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^{-*})$ is guaranteed to hold if we assume $\sigma_r > 0$ and $w^j \in \mathcal{D}(L^{-*})$ for each j. With this assumption, we know as above that $\mathcal{R}(K) \subset \mathcal{D}(L^{-*})$ and also $\varphi_k \in \mathcal{D}(L^{-*})$ whenever $\sigma_k > 0$. Since $\sigma_r > 0$, we can guarantee $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^{-*})$.

Next, a similar argument using (3.2) shows the condition $\{L\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^*)$ is guaranteed to hold if we assume $\sigma_r > 0$ and $Lw^j \in \mathcal{D}(L^*)$ for each j.

3.1.2. Continuous Case. The continuous case requires a few more assumptions than the discrete case. Recall $K : S \to X$, where $S := L^2(O; \mathbb{K}^m)$ and $\mathbb{K}$ is either $\mathbb{R}$ or $\mathbb{C}$. In order to define the POD operator K^Y and ensure $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L)$, we make the following assumption:

> Main assumption: For the continuous case, we assume throughout the paper that (i) $\{Lw^j\}_{j=1}^m \subset L^2(O; Y)$, and for all $f \in S$ we have $Kf \in \mathcal{D}(L)$ and
>
> $$LKf = \sum_{j=1}^m \int_O f^j(t) Lw^j(t)\, dt,$$
>
> and also (ii) $\sigma_r > 0$ whenever we consider the projection Π_r^X.

As in the discrete case, assumption (i) gives $\mathcal{R}(K) \subset \mathcal{D}(L)$ and allows us to define the (compact) POD operator $K^Y = LK$ for the data $\{Lw^j\}_{j=1}^m \subset L^2(\mathcal{O}; Y)$. As before, we let $s_Y = \text{rank}(K^Y)$ be the number of positive singular values of K^Y. Also as in the discrete case, assumptions (i) and (ii) imply $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L)$ and Π_r^X maps into $\mathcal{D}(L)$.

Remark 3.1.1. *There are three common conditions that guarantee assumption (i) holds.*

1. *If $L : X \to Y$ is bounded, the operator L can be pulled through the integral in the definition of K and assumption (i) clearly holds.*

2. *If each $w^j \in L^2(\mathcal{O}; X)$ takes the form*

$$w^j(t) = \sum_{\ell,k=1}^{n_j} a_{k\ell}^j g_k^j(t) x_{\ell j},$$

   where $a_{k\ell}^j$ are constants in $\mathbb{K}$, $g_k^j(t) \in L^2(\mathcal{O})$, and $x_{\ell j} \in \mathcal{D}(L)$, then it can be checked that assumption (i) holds. This condition is similar to the assumption made in the discrete case.

3. *If $L : \mathcal{D}(L) \subset X \to Y$ is closed, $w^j \in \mathcal{D}(L)$ a.e., and $Lw^j \in L^2(\mathcal{O}; Y)$ then Theorem 2.1.2 implies assumption (i) holds.*

Again, for certain cases of Theorem 3.2.3 we need to assume the POD modes $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L)$ satisfy some additional regularity properties. As in the discrete case, we can make additional assumptions on the data to satisfy these regularity properties.

We briefly mention conditions on the data similar to Remark 3.1.1, Item 3 that yield the needed regularity. First, if L^{-*} exists, it is closed. Therefore, $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^{-*})$ holds if we assume $\sigma_r > 0$, $w^j \in \mathcal{D}(L^{-*})$ a.e., and $\{L^{-*}w^j\}_{j=1}^m \in L^2(\mathcal{O}; Y)$. Second, if L^* exists, then it is closed. Therefore, $\{L\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^*)$ holds if we assume $\sigma_r > 0$, $Lw^j \in \mathcal{D}(L^*)$ a.e., and $\{L^*Lw^j\}_{j=1}^m \in L^2(\mathcal{O}; X)$.

We also note that the condition in Remark 3.1.1, Item 2 can be modified similarly to the discrete case to yield the required regularity.

3.2. POD PROPERTIES

Recall the standard POD orthogonal projection, $\Pi_r^X : X \to X$ given by (2.4), and the known POD data approximation error given by

$$\sum_{j=1}^{m} \int_O \|w^j(t) - \Pi_r^X w^j(t)\|_X^2 dt = \sum_{k>r} \sigma_k^2.$$

One of the goals of this dissertation is to find extensions of this error formula to other scenarios involving the linear operator $L : X \to Y$ and another sequence of projections, which need not be orthogonal.

Definition 3.2.1. *For a positive integer r with $\sigma_r > 0$, we define $Y_r := LX_r = \mathrm{span}\{L\varphi_k\}_{k=1}^r$ and we let $\Pi_r^Y : Y \to Y$ be a projection onto Y_r.*

Remark 3.2.2. *The condition $\sigma_r > 0$ implies $X_r \subset \mathcal{D}(L)$, so the definition makes sense. We assume throughout that $\sigma_r > 0$ whenever we consider Π_r^Y. It is important to note that unless stated otherwise we do not assume the projection Π_r^Y is orthogonal. To obtain convergence results as r increases, we sometimes need to require $\{\Pi_r^Y\}$ are uniformly bounded in operator norm. If $\{\Pi_r^Y\}$ are the orthogonal projections onto Y_r, then this condition is satisfied.*

3.2.1. Non-orthogonal POD Projections.

In Section 3.4, we consider pointwise convergence results for the linear operators $L^{-1}\Pi_r^Y L : X \to X$ and $L\Pi_r^X L^{-1} : Y \to Y$. Below, we give conditions that guarantee that these linear operators are bounded, or have bounded extensions, for r fixed. We note that when these operators are bounded we have $L^{-1}\Pi_r^Y L : X \to X$ is a projection onto $X_r = \mathrm{span}\{\varphi\}_{j=1}^r$ and $L\Pi_r^X L^{-1} : Y \to Y$ is a projection onto $Y_r = \mathrm{span}\{L\varphi\}_{j=1}^r$. Even if Π_r^Y is an orthogonal projection, these projections are typically non-orthogonal POD projection operators.

In the simplest case, if L and L^{-1} are bounded, then clearly $L^{-1}\Pi_r^Y L : X \to X$ and $L\Pi_r^X L^{-1} : Y \to Y$ are both bounded for each r. In this case, $\{L\Pi_r^X L^{-1}\}$ is uniformly bounded in operator norm, and $\{L^{-1}\Pi_r^Y L\}$ is also uniformly bounded when $\{\Pi_r^Y\}$ is uniformly bounded.

Below, we consider the case when either L or L^{-1} is unbounded. For each fixed r, we show $L^{-1}\Pi_r^Y L : X \to X$ is bounded when L is bounded, and $L\Pi_r^X L^{-1} : Y \to Y$ is bounded when L^{-1} is bounded. In other cases, we need certain assumptions to be satisfied to construct bounded extensions of the operators for each r. We do *not* show that these non-orthogonal POD projection operators are uniformly bounded in operator norm.

In specific cases, we need certain adjoint operators to exist, so we need the operators to be densely defined or bounded. For example, for the operator L^{-*} to exist we must assume that $\mathcal{D}(L^{-1})$ is dense in Y, or L^{-1} is bounded. These type of assumptions must be added to the second and fourth parts of the following theorem, in addition to results later in this section.

Theorem 3.2.3. *Assume L is invertible and $r > 0$ is fixed.*

1. *If L^{-1} is bounded, then $L\Pi_r^X L^{-1} : Y \to Y$ is bounded.*
2. *If $\mathcal{D}(L^{-1})$ is dense in Y and $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^{-*})$, the operator $L\Pi_r^X L^{-1} : Y \to Y$ can be extended to a bounded operator on Y.*
3. *If L is bounded, then $L^{-1}\Pi_r^Y L : X \to X$ is bounded.*
4. *Assume $\Pi_r^Y : Y \to Y$ is the orthogonal projection onto span$\{L\varphi_k\}_{k=1}^r$. If L^{-1} is bounded, $\mathcal{D}(L)$ is dense, and $\{L\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^*)$, then $L^{-1}\Pi_r^Y L : X \to X$ can be extended to a bounded operator on X.*

Remark 3.2.4. *In the second and fourth items, we assume the POD modes satisfy the regularity properties $\{\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^{-*})$ and $\{L\varphi_k\}_{k=1}^r \subset \mathcal{D}(L^*)$, respectively. See Section 3.1.1 and Section 3.1.2 for conditions on the data in the discrete and continuous cases that guarantee these properties hold.*

Proof. 1. Note

$$L\Pi_r^X L^{-1} y = \sum_{k=1}^{r} (L^{-1} y, \varphi_k)_X L\varphi_k. \tag{3.3}$$

Since L^{-1} is a bounded operator and $\varphi_k \in \mathcal{D}(L)$ for all k, the sum in (3.3) is well defined for all $y \in Y$. Also, it can be checked that

$$\|L\Pi_r^X L^{-1} y\|_Y \le c\|y\|_Y, \tag{3.4}$$

where the constant $c := \|L^{-1}\| \left(\sum_{k=1}^r \|L\varphi_k\|_Y^2\right)^{1/2}$ depends on r. This shows that the operator $L\Pi_r^X L^{-1}$ is bounded when L^{-1} is bounded.

2. The linear operator $L\Pi_r^X L^{-1} : Y \to Y$ is defined by (3.3) for all $y \in \mathcal{D}(L^{-1})$. Using the assumptions, we can rewrite (3.3) for $y \in \mathcal{D}(L^{-1})$ as

$$L\Pi_r^X L^{-1} y = \sum_{k=1}^r (y, L^{-*}\varphi_k)_X L\varphi_k. \tag{3.5}$$

It can be checked that (3.4) holds for all $y \in \mathcal{D}(L^{-1})$ with

$$c := \sum_{k=1}^r \|L^{-*}\varphi_k\|_X \|L\varphi_k\|_Y.$$

Note that (3.5) is well-defined for all $y \in Y$, and therefore yields a bounded linear extension of $L\Pi_r^X L^{-1} : Y \to Y$ to all of Y.

3. Since Π_r^Y is a projection onto $Y_r = \text{span}\{L\varphi\}_{j=1}^r$, we know for $y \in Y$ there exists constants $\{\alpha_j(y)\}$ depending on y such that $\Pi_r^Y y = \sum_{j=1}^r \alpha_j(y) L\varphi_j$. Then

$$\left\| \sum_{j=1}^r \alpha_j(y) L\varphi_j \right\|_Y = \|\Pi_r^Y y\|_Y \le \|\Pi_r^Y\| \|y\|_Y. \tag{3.6}$$

Also,

$$\left\| \sum_{j=1}^r \alpha_j(y) L\varphi_j \right\|_Y^2 = \sum_{j,k=1}^r \alpha_j(y)(L\varphi_j, L\varphi_k)_Y \overline{\alpha_k(y)} = \alpha(y)^* A_r \alpha(y),$$

where the star denotes complex conjugate, and

$$\alpha(y) = [\alpha_1(y), ..., \alpha_r(y)]^T \in \mathbb{K}^r, \quad [A_r]_{i,j} = (L\varphi_i, L\varphi_j)_Y.$$

Since L is invertible and $\{\varphi_j\}_{j=1}^r$ is a linearly independent set, we know $\{L\varphi_j\}_{j=1}^r$ is a linearly independent set; therefore, A_r is symmetric positive definite, which implies there exists $\beta > 0$ such that $\alpha^* A_r \alpha \geq \beta\|\alpha\|_{\mathbb{K}^r}^2$ for all $\alpha \in \mathbb{K}^r$. Note that β may depend on r. Together, the above implies that

$$\beta\|\alpha(y)\|_{\mathbb{K}^r}^2 \leq \left\| \sum_{j=1}^r \alpha_j(y) L\varphi_j \right\|_Y^2 \leq \|\Pi_r^Y\|^2 \|y\|_Y^2.$$

So,

$$\|\alpha(y)\|_{\mathbb{K}^r} \leq \beta^{-1/2} \|\Pi_r^Y\| \|y\|_Y. \tag{3.7}$$

In this case, $y = Lx$ and L is bounded and invertible; thus,

$$L^{-1}\Pi_r^Y(Lx) = L^{-1} \sum_{j=1}^r \alpha_j(Lx) L\varphi_j = \sum_{j=1}^r \alpha_j(Lx)\varphi_j$$

where the constants α_j now depend on Lx. Since $\{\varphi_j\} \subset X$ is orthonormal, we have

$$\begin{aligned} \|L^{-1}\Pi_r^Y Lx\|_X^2 &= \left\| \sum_{j=1}^r \alpha_j(Lx)\varphi_j \right\|_X^2 \\ &= \|\alpha(Lx)\|_{\mathbb{K}^r}^2 \\ &\leq \beta^{-1}\|\Pi_r^Y\|^2 \|Lx\|_Y^2 \\ &\leq \beta^{-1}\|\Pi_r^Y\|^2 \|L\|^2 \|x\|_X^2. \end{aligned}$$

Therefore, for all $x \in X$ we have

$$\|L^{-1}\Pi_r^Y Lx\|_X \leq c\|x\|_X, \tag{3.8}$$

where $c := \beta^{-1/2}\|\Pi_r^Y\|\|L\|$.

4. We obtain a representation of $L^{-1}\Pi_r^Y L$ as follows. First, note that the sets $\{L\varphi_k\}$ and $\{L^{-*}\varphi_k\}$ are biorthogonal, i.e., $(L\varphi_k, L^{-*}\varphi_j)_Y = \delta_{k,j}$, where $\delta_{k,j}$ is the Kronecker delta symbol. Recall from the proof of part 3 that $\Pi_r^Y y = \sum_{k=1}^r \alpha_k L\varphi_k$ for some scalars α_k that depend on y. We can calculate the values for α_k by noting

$$\left(\Pi_r^Y y, L^{-*}\varphi_j\right)_Y = \sum_{k=1}^r \alpha_k (L\varphi_k, L^{-*}\varphi_j)_Y = \alpha_j.$$

This yields

$$\Pi_r^Y y = \sum_{k=1}^r (\Pi_r^Y y, L^{-*}\varphi_k)_Y L\varphi_k = \sum_{k=1}^r (y, \Pi_r^Y L^{-*}\varphi_k)_Y L\varphi_k, \tag{3.9}$$

since Π_r^Y is orthogonal and therefore $(\Pi_r^Y)^* = \Pi_r^Y$.

By assumption, $\{L\varphi_j\} \subset \mathcal{D}(L^*)$ and so (3.9) implies $\Pi_r^Y y \in \mathcal{D}(L^*)$ for all $y \in Y$. This gives the following representation for any $x \in \mathcal{D}(L)$:

$$L^{-1}\Pi_r^Y L x = \sum_{k=1}^r (x, L^*\Pi_r^Y L^{-*}\varphi_k)_X \varphi_k. \tag{3.10}$$

Also, for all $x \in \mathcal{D}(L)$, the bound (3.8) holds with $c := \left(\sum_{k=1}^r \|L^*\Pi_r^Y L^{-*}\varphi_k\|_X^2\right)^{1/2}$. Equation (3.10) is well-defined for all $x \in X$, and therefore defines a bounded linear extension of $L^{-1}\Pi_r^Y L : X \to X$ to all of X.

□

3.2.2. POD Singular Values and POD Eigenvalues. The number of nonzero singular values (or eigenvalues) of the POD operators plays an important role throughout the thesis. It is also important to note the difference between singular values and eigenvalues. For a POD operator $K : S \to Z$, recall the POD eigenvalues are the eigenvalues of $KK^* : Z \to Z$, the POD singular values are the singular values of K, and $s_Z = \mathrm{rank}(K)$, i.e., s_Z is the number of positive POD singular values of K (or positive POD eigenvalues of KK^*). As discussed in Section 2.2, it is possible to have a zero POD singular value but to have all nonzero POD eigenvalues.

Below, we study various relationships between the POD eigenvalues and POD singular values for the data $\{w^j\}$ and the data $\{Lw^j\}$. Recall, $K : S \to X$ is the POD operator for the data $\{w^j\}$, and $K^Y = LK : S \to Y$ is the POD operator for the data $\{Lw^j\}$. Therefore, $s_X = \text{rank}(K)$ is the number of nonzero POD singular values (or POD eigenvalues) for the data $\{w^j\}$, and $s_Y = \text{rank}(K^Y)$ is the number of nonzero POD singular values (or POD eigenvalues) for the data $\{Lw^j\}$

First, we give a relationship between the POD eigenvalues and the null space of the adjoint POD operator. Then we also give some additional information about s_X and s_Y. There is also a relationship between the number of POD eigenvalues under the linear mapping L.

Lemma 3.2.5. *1. All of the POD eigenvalues for the data $\{w^j\}$ are nonzero if and only if $\ker(K^*) = \{0\}$. In this case, $X = \overline{\mathcal{R}(K)}$. In addition, if $s_X < \infty$, then $X = \mathcal{R}(K)$ and $\dim(X) = s_X$.*

2. *All of the POD eigenvalues for the data $\{Lw^j\}$ are nonzero if and only if $\ker((K^Y)^*) = \{0\}$. In this case, $Y = \overline{\mathcal{R}(K^Y)}$. In addition, if $s_Y < \infty$, then $Y = \mathcal{R}(K^Y)$ and $\dim(Y) = s_Y$.*

3. *The number of nonzero POD eigenvalues for $\{Lw^j\}$ is less than or equal to the number of nonzero POD eigenvalues for $\{w^j\}$. That is, $s_Y \le s_X$.*

4. *If L is invertible, then $s_X = s_Y$.*

Proof. The first two items are proven similarly. Here we show item 1.

1. Lemma 2.1.1 proves the first statement. To see the rest, note that $X = \ker(K^*) \oplus \overline{\mathcal{R}(K)}$ and $\ker(K^*) = \{0\}$ imply $X = \overline{\mathcal{R}(K)}$. Then if $s_X = \text{rank}(K) = \dim(\mathcal{R}(K))$ is finite, we have $\overline{\mathcal{R}(K)} = \mathcal{R}(K)$ and therefore $X = \mathcal{R}(K)$ and $\dim(X) = s_X$.

3. First, if $s_X = \infty$, we are done. Assume $s_X < \infty$. We know

$$Kf = \sum_{j=1}^{s_X} \sigma_j (f, f_j)_S \varphi_j,$$

and therefore

$$K^Y f = LKf = \sum_{j=1}^{s_X} \sigma_j (f, f_j)_S L\varphi_j.$$

Thus, $s_Y = \text{rank}(K^Y) \leq s_X$.

4. Because of item 3, we need only show $s_X \leq s_Y$. First, if $s_Y = \infty$, we are done. Assume $s_Y < \infty$. Let the singular value decomposition of K^Y be given by

$$K^Y f = LKf = \sum_{j=1}^{s_Y} \sigma_j^Y (f, f_j^Y)_S \varphi_j^Y.$$

Note that $\varphi_j^Y \in \mathcal{D}(L^{-1})$ whenever $\sigma_j^Y > 0$, since $\mathcal{D}(L^{-1}) = R(L)$ and

$$\varphi_j^Y = (\sigma_j^Y)^{-1} K^Y f_j^Y = (\sigma_j^Y)^{-1} LKf_j^Y.$$

Then, since L is invertible,

$$Kf = L^{-1}LKf = L^{-1}K^Y f = \sum_{j=1}^{s_Y} \sigma_j^Y (f, f_j^Y)_S L^{-1}\varphi_j^Y,$$

and therefore $s_X = \text{rank}(K) \leq s_Y$.

□

The following lemma gives further results about the connections between the two main sets of POD eigenvalues under consideration in this paper, i.e., the POD eigenvalues for the data $\{w^j\}$ and the data $\{Lw^j\}$. With extra assumptions, we can use the fact that all the POD eigenvalues are nonzero for one set of data to obtain the same conclusion for the other set of data.

Lemma 3.2.6. *1. If L is bounded, $\mathcal{R}(L)$ is dense in Y, and the POD eigenvalues for $\{w^j\}$ are all nonzero, then the POD eigenvalues for $\{Lw^j\}$ are all nonzero.*

2. If L^{-1} is bounded, $\mathcal{R}(L^{-1})$ is dense in X, and the POD eigenvalues for $\{Lw^j\}$ are all nonzero, then the POD eigenvalues for $\{w^j\}$ are all nonzero.

Proof. The proofs of the two items are similar; we only prove the first item.

Since $X = \ker(K^*) \oplus \overline{\mathcal{R}(K)}$ and $\ker(K^*) = \{0\}$ (Lemma 3.2.5, Item 1), we have $X = \overline{\mathcal{R}(K)}$. Let $\varepsilon > 0$ and let $y \in Y$. Since $\mathcal{R}(L)$ is dense in Y, there exists $x \in X$ such that $\|y - Lx\|_Y < \varepsilon/2$. Since $X = \overline{\mathcal{R}(K)}$, for this x there exists $f \in S$ such that $\|x - Kf\|_X < \varepsilon/(2\|L\|)$. This gives

$$\|y - LKf\|_Y < \|y - Lx\|_Y + \|Lx - LKf\|_Y < \frac{\varepsilon}{2} + \|L\|\frac{\varepsilon}{2\|L\|} < \varepsilon,$$

which shows $\overline{\mathcal{R}(K^Y)} = Y$ and $\ker((K^Y)^*) = \{0\}$. Thus, the POD eigenvalues for $\{Lw^j\}$ are all nonzero by Lemma 3.2.5, Item 2. □

3.3. ERROR FORMULAS

One goal of this thesis is to provide exact formulas for POD data approximation errors. The two main results of this section can be found in Theorem 3.3.2 and Theorem 3.3.4. The section is split between the discrete case, where we can use a more direct proof approach, and the continuous case, which requires more care since the data can have infinitely many nonzero POD eigenvalues.

The next lemma gives three different Hilbert-Schmidt norm approximation results involving the POD operator K for the data $\{w^j\}$ and the POD operator $K^Y = LK$ for the data $\{Lw^j\}$. The result will be of particular usefulness when discussing the continuous case in Section 3.3.2, but it applies to the discrete case as well. We also use this result throughout Section 3.4.

Lemma 3.3.1. *The Hilbert-Schmidt norm errors are given by*

$$\|LK - L\Pi_r^X K\|_{\mathrm{HS}(S,Y)}^2 = \sum_{k>r} \sigma_k^2 \|L\varphi_k\|_Y^2, \tag{3.11}$$

$$\|LK - \Pi_r^Y LK\|_{\mathrm{HS}(S,Y)}^2 = \sum_{k>r} \sigma_k^2 \|L\varphi_k - \Pi_r^Y L\varphi_k\|_Y^2, \tag{3.12}$$

and

$$\|K - L^{-1}\Pi_r^Y LK\|_{\mathrm{HS}(S,X)}^2 = \sum_{k>r} \sigma_k^2 \|\varphi_k - L^{-1}\Pi_r^Y L\varphi_k\|_X^2. \tag{3.13}$$

In the case $s_X = \infty$, the following convergence results hold. For (3.11)*: The error tends to zero as $r \to \infty$. For* (3.12)*: If $\{\Pi_r^Y\}$ is uniformly bounded in operator norm, then the error goes to zero as $r \to \infty$. For* (3.13)*: If L^{-1} is bounded and $\{\Pi_r^Y\}$ is uniformly bounded in operator norm, then the error tends to zero as $r \to \infty$. For* (3.13)*: If $\{L^{-1}\Pi_r^Y L\}$ is uniformly bounded in operator norm, then the error converges to zero as $r \to \infty$.*

Proof. Let $\{f_k\}$ be an orthonormal basis of S of eigenvectors of K^*K and let $\mathbb{J} = \{k : f_k \notin \ker(K^*K)\}$. Note that $Kf_k = 0$ for all $k \notin \mathbb{J}$, since $\ker(K^*K) = \ker(K)$ by Lemma 2.1.1. Also, $Kf_k = \sigma_k \varphi_k$ for all $k \in \mathbb{J}$. Then,

$$\begin{aligned}
\|LK - L\Pi_r^X K\|_{\mathrm{HS}(S,Y)}^2 &= \sum_{k\geq 1} \|(LK - L\Pi_r^X K) f_k\|_Y^2 \\
&= \sum_{k\in\mathbb{J}} \|(LK - L\Pi_r^X K) f_k\|_Y^2 \\
&= \sum_{k\in\mathbb{J}} \|L\sigma_k\varphi_k - L\Pi_r^X \sigma_k\varphi_k\|_Y^2 \\
&= \sum_{k>r,\, k\in\mathbb{J}} \sigma_k^2 \|L\varphi_k\|_Y^2,
\end{aligned}$$

where the last equality holds since $\Pi_r^X \varphi_k = \varphi_k$ for $k \leq r$ and $\Pi_r^X \varphi_k = 0$ for $k > r$. Also,

$$\sum_{k>r,\, k\in\mathbb{J}} \sigma_k^2 \|L\varphi_k\|_Y^2 = \sum_{k>r,\, k\in\mathbb{J}} \|LKf_k\|_Y^2 = \sum_{k>r,\, k\in\mathbb{J}} \|K^Y f_k\|_Y^2,$$

which converges to zero as $r \to \infty$ since K^Y is Hilbert-Schmidt. Next,

$$
\begin{aligned}
\|LK - \Pi_r^Y LK\|^2_{\mathrm{HS}(S,Y)} &= \sum_{k\geq 1} \|(LK - \Pi_r^Y LK) f_k\|_Y^2 \\
&= \sum_{k\in\mathbb{J}} \|L\sigma_k\varphi_k - \Pi_r^Y L\sigma_k\varphi_k\|_Y^2 \\
&= \sum_{k>r,\, k\in\mathbb{J}} \sigma_k^2 \|L\varphi_k - \Pi_r^Y L\varphi_k\|_Y^2,
\end{aligned}
$$

where the last equality holds since $\Pi_r^Y L\varphi_k = L\varphi_k$ for $k \leq r$. For convergence, note

$$
\begin{aligned}
\|LK - \Pi_r^Y LK\|^2_{\mathrm{HS}(S,Y)} &= \sum_{k>r,\, k\in\mathbb{J}} \|LKf_k - \Pi_r^Y LKf_k\|_Y^2 \\
&= \sum_{k>r,\, k\in\mathbb{J}} \|K^Y f_k - \Pi_r^Y K^Y f_k\|_Y^2 \\
&\leq \sum_{k>r,\, k\in\mathbb{J}} \|I - \Pi_r^Y\|^2 \, \|K^Y f_k\|_Y^2.
\end{aligned}
$$

Since $\|I - \Pi_r^Y\|$ is uniformly bounded and K^Y is Hilbert-Schmidt, the error converges to zero as $r \to \infty$.

Since $L^{-1}\Pi_r^Y L\varphi_k = L^{-1}L\varphi_k = \varphi_k$ for $k \leq r$, for the last equality we have

$$
\begin{aligned}
\|K - L^{-1}\Pi_r^Y LK\|^2_{\mathrm{HS}(S,X)} &= \sum_{k\in\mathbb{J}} \|\sigma_k\varphi_k - L^{-1}\Pi_r^Y L\sigma_k\varphi_k\|_X^2 \\
&= \sum_{k>r,\, k\in\mathbb{J}} \sigma_k^2 \|\varphi_k - L^{-1}\Pi_r^Y L\varphi_k\|_X^2.
\end{aligned}
$$

Assuming L^{-1} is bounded and $\{\Pi_r^Y\}$ is uniformly bounded, the convergence follows from

$$
\begin{aligned}
\|K - L^{-1}\Pi_r^Y LK\|^2_{\mathrm{HS}(S,X)} &= \sum_{k>r,\, k\in\mathbb{J}} \|L^{-1}(I - \Pi_r^Y)LKf_k\|_X^2 \\
&\leq \sum_{k>r,\, k\in\mathbb{J}} \|L^{-1}\|^2 \, \|I - \Pi_r^Y\|^2 \, \|K^Y f_k\|_Y^2
\end{aligned}
$$

in a similar manner to the previous case. For the second convergence case, we assume $\{L^{-1}\Pi_r^Y L\}$ is uniformly bounded in operator norm and we have

$$\|K - L^{-1}\Pi_r^Y LK\|_{\mathrm{HS}(S,X)}^2 = \sum_{k>r,\, k\in\mathbb{J}} \|(I - L^{-1}\Pi_r^Y L)Kf_k\|_X^2$$
$$\leq \sum_{k>r,\, k\in\mathbb{J}} \|I - L^{-1}\Pi_r^Y L\|^2 \, \|K^Y f_k\|_X^2,$$

which converges to zero as $r \to \infty$.

□

3.3.1. Discrete Case. First we introduce several representations that will be useful in the proof of Theorem 3.3.2 below. Recall, $s_X = \mathrm{rank}(K) < \infty$ is the number of nonzero POD singular values (or POD eigenvalues) for the data $\{w^j\}$. By the known POD error formula (2.5), we have

$$w^j = \Pi_{s_X}^X w^j = \sum_{k=1}^{s_X} \left(w^j, \varphi_k\right)_X \varphi_k \quad \text{and} \quad Lw^j = \sum_{k=1}^{s_X} \left(w^j, \varphi_k\right)_X L\varphi_k.$$

Note that since the sums are finite, $\{\varphi_k\} \subset \mathcal{D}(L)$, and L is linear we can pull L through the sums in this section without any additional assumptions. This is one point where the discrete and continuous cases differ.

Next, from Section 2.2.1 we know for all $j \leq s$ and $k \leq s_X$ we have

$$\left(w^j, \varphi_k\right)_X = \overline{(\varphi_k, w^j)_X} = \overline{(K^*\varphi_k)_j} = \sigma_k \overline{f_k^j},$$

where f_k^j denotes the jth component of the singular vector $f^k \in \mathbb{K}^s$. This gives

$$w^j = \sum_{k=1}^{s_X} \sigma_k \, \overline{f_k^j} \, \varphi_k \quad \text{and} \quad Lw^j = \sum_{k=1}^{s_X} \sigma_k \, \overline{f_k^j} \, L\varphi_k. \tag{3.14}$$

Also, recall $\{f^j\}$ are orthonormal in S, which yields

$$\sum_{j=1}^{s} \gamma_j \overline{f_k^j} f_\ell^j = (f_\ell, f_k)_S = \delta_{\ell,k}.$$

Theorem 3.3.2. *The data approximation errors are given by*

$$\sum_{j=1}^{s} \gamma_j \|Lw^j - L\Pi_r^X w^j\|_Y^2 = \sum_{k=r+1}^{s_X} \sigma_k^2 \|L\varphi_k\|_Y^2, \tag{3.15}$$

and

$$\sum_{j=1}^{s} \gamma_j \|Lw^j - \Pi_r^Y Lw^j\|_Y^2 = \sum_{k=r+1}^{s_X} \sigma_k^2 \|L\varphi_k - \Pi_r^Y L\varphi_k\|_Y^2. \tag{3.16}$$

Also, if L is invertible, then

$$\sum_{j=1}^{s} \gamma_j \|w^j - L^{-1}\Pi_r^Y Lw^j\|_X^2 = \sum_{k=r+1}^{s_X} \sigma_k^2 \|\varphi_k - L^{-1}\Pi_r^Y L\varphi_k\|_X^2. \tag{3.17}$$

Proof. We only prove (3.16). The proofs of the other two results are similar. First, note we can apply Π_r^Y to Lw^j given in (3.14) to get

$$Lw^j - \Pi_r^Y w^j = \sum_{k=1}^{s_X} \sigma_k \overline{f_k^j} \, (L\varphi_k - \Pi_r^Y L\varphi_k).$$

Then

$$\begin{aligned}
\sum_{j=1}^{s} \gamma_j \|Lw^j - \Pi_r^Y Lw^j\|_Y^2 &= \sum_{j=1}^{s} \gamma_j \left(\sum_{k=1}^{s_X} \sigma_k \overline{f_k^j} (L\varphi_k - \Pi_r^Y L\varphi_k), \sum_{\ell=1}^{s_X} \sigma_\ell \overline{f_\ell^j} (L\varphi_\ell - \Pi_r^Y L\varphi_\ell) \right)_Y \\
&= \sum_{j=1}^{s} \gamma_j \sum_{\ell,k=1}^{s_X} \sigma_k \sigma_\ell \overline{f_k^j} f_\ell^j \left(L\varphi_k - \Pi_r^Y L\varphi_k, L\varphi_\ell - \Pi_r^Y L\varphi_\ell \right)_Y \\
&= \sum_{\ell,k=1}^{s_X} \sigma_k \sigma_\ell \left(\sum_{j=1}^{s} \gamma_j \overline{f_k^j} f_\ell^j \right) \left(L\varphi_k - \Pi_r^Y L\varphi_k, L\varphi_\ell - \Pi_r^Y L\varphi_\ell \right)_Y \\
&= \sum_{k=1}^{s_X} \sigma_k^2 \left(L\varphi_k - \Pi_r^Y L\varphi_k, L\varphi_k - \Pi_r^Y L\varphi_k \right)_Y
\end{aligned}$$

$$= \sum_{k=1}^{s_X} \sigma_k^2 \| L\varphi_k - \Pi_r^Y L\varphi_k \|_Y^2.$$

Note that $\Pi_r^Y L\varphi_k = L\varphi_k$ for $k = 1, \ldots, r$ since Π_r^Y is a projection onto $Y_r = \mathrm{span}\{L\varphi_k\}_{k=1}^r$. Therefore,

$$\sum_{j=1}^{s} \gamma_j \| Lw^j - \Pi_r^Y Lw^j \|_Y^2 = \sum_{k=r+1}^{s_X} \sigma_k^2 \| L\varphi_k - \Pi_r^Y L\varphi_k \|_Y^2.$$

□

In Corollary 3.4.10, we focus on error bounds for approximating each individual data snapshot w^ℓ with various POD projections. Also, another way to prove Theorem 3.3.2 is to use the Hilbert Schmidt norm results in Lemma 3.3.1. The proof we give above requires less background. However, we do require Lemma 3.3.1 for the continuous case below.

3.3.2. Continuous Case. For the continuous case we must consider the possibility that the number of nonzero POD eigenvalues is infinite. We approach this case differently from the discrete case above. We show each of the data approximation errors we consider is equal to one of the Hilbert-Schmidt norm errors from Lemma 3.3.1. Then we use that result to prove the convergence of the errors to zero in the case of an infinite number of nonzero POD eigenvalues.

For one case, we need to make an additional assumption on L^{-1}.

The L^{-1} assumption: We assume

1. $s_X < \infty$, or
2. $L^{-1}\Pi_r^Y LKf = \sum_{j=1}^m \int_O f^j(t) L^{-1}\Pi_r^Y Lw^j(t)dt$ for all $f \in S$.

Remark 3.3.3. *Note that if $s_X < \infty$, then the proof technique in Section 3.3.1 above can be used for the continuous cases, with some minor modifications to deal with the change in the space S. The second condition is similar to the main assumption made in Section 3.1.2. Any of the three common conditions in Remark 3.1.1 that guarantee the main assumption holds also imply that the second condition in the L^{-1} assumption holds.*

Theorem 3.3.4. *The data approximation errors are given by*

$$\sum_{j=1}^{m} \|Lw^j - L\Pi_r^X w^j\|_{L^2(O;Y)}^2 = \sum_{k>r} \sigma_k^2 \|L\varphi_k\|_Y^2 \tag{3.18}$$

and

$$\sum_{j=1}^{m} \|Lw^j - \Pi_r^Y Lw^j\|_{L^2(O;Y)}^2 = \sum_{k>r} \sigma_k^2 \|L\varphi_k - \Pi_r^Y L\varphi_k\|_Y^2. \tag{3.19}$$

Also if the L^{-1} assumption holds then

$$\sum_{j=1}^{m} \|w^j - L^{-1}\Pi_r^Y Lw^j\|_{L^2(O;X)}^2 = \sum_{k>r} \sigma_k^2 \|\varphi_k - L^{-1}\Pi_r^Y L\varphi_k\|_X^2. \tag{3.20}$$

In the case $s_X = \infty$, the following convergence results hold. For Equation (3.18)*: The error tends to zero as $r \to \infty$. For Equation* (3.19)*: If $\{\Pi_r^Y\}$ is uniformly bounded in operator norm, then the error goes to zero as $r \to \infty$. For* (3.20)*: If L^{-1} is bounded and $\{\Pi_r^Y\}$ is uniformly bounded in operator norm, then the error tends to zero as $r \to \infty$. For Equation* (3.20)*: If $\{L^{-1}\Pi_r^Y L\}$ is uniformly bounded in operator norm, then the error converges to zero as $r \to \infty$.*

Remark 3.3.5. *Note that the conditions for convergence for the case $s_X = \infty$ are exactly the conditions given in Lemma 3.3.1.*

Proof. We prove (3.18), and the associated convergence result. The proofs of the other equalities and convergence results are similar. We first show that the data approximation error has an integral representation, and then we use the two Hilbert-Schmidt results for POD operators to conclude.

By definition, for $f \in S$ we have

$$\begin{aligned} L\Pi_r^X Kf &= \sum_{k=1}^{r} (Kf, \varphi_k)_X L\varphi_k \\ &= \sum_{k=1}^{r} \left(\sum_{j=1}^{m} \int_O f^j(t) w^j(t)\, dt, \varphi_k \right)_X L\varphi_k \end{aligned}$$

$$= \sum_{j=1}^{m} \int_{O} f^j(t) \sum_{k=1}^{r} (w^j(t), \varphi_k)_X L\varphi_k dt$$
$$= \sum_{j=1}^{m} \int_{O} f^j(t) L w_r^j(t) dt,$$

where $w_r^j(t) = \Pi_r^X w^j(t) = \sum_{k=1}^{r} (w^j(t), \varphi_k)_X \varphi_k$. Because of the main assumption, we can pull the operator L inside the integral to give

$$(LK - L\Pi_r^X K)f = \int_{O} \sum_{j=1}^{m} f^j(t)[Lw^j(t) - Lw_r^j(t)]dt.$$

Since $Lw^j - Lw_r^j \in L^2(O;Y)$ for each j, by Lemma 2.2.4 we have

$$\sum_{j=1}^{m} \|Lw^j - L\Pi_r^X w^j\|_{L^2(O;Y)}^2 = \|LK - L\Pi_r^X K\|_{\mathrm{HS}(S,Y)}^2.$$

Lemma 3.3.1 proves both (3.18) and the convergence result in the case $s_X = \infty$.

Note for (3.20), for $f \in S$ the L^{-1} assumption gives

$$L^{-1}\Pi_r^Y LKf = \int_{O} \sum_{j=1}^{m} f^j(t) L^{-1}\Pi_r^Y Lw^j(t)dt, \tag{3.21}$$

and then we proceed similarly to establish the result. □

3.4. POINTWISE CONVERGENCE OF POD PROJECTIONS

Recall that $\{\varphi_k\}$ is an orthonormal basis for X, and therefore $\|\Pi_r^X x - x\|_X \to 0$ for all $x \in X$. In this section, we prove various types of pointwise convergence results for the other POD projections; namely, Π_r^Y from Section 3.2, and $L\Pi_r^X L^{-1}$ and $L^{-1}\Pi_r^Y L$ from Section 3.2.1. The majority of this section is not split into the discrete and continuous cases because the proofs are similar for both, and many of the results hold regardless of case. We do focus on the discrete case at the end of this section and address some assumptions made in the literature about approximations of each individual data snapshot using POD projections. Pointwise convergence results for these POD projections are easiest to obtain when L and L^{-1} are both bounded. We primarily focus on the case when either L or L^{-1} is unbounded.

Range conditions are an important factor in this section. When an element to be approximated by a POD projection is in the range of K or K^Y, we can often get better results. When certain conditions hold, we know these ranges exactly. Recall from Lemma 3.2.5, if all the POD eigenvalues for $\{w^j\}$ are nonzero and $s_X < \infty$, then we know $X = \mathcal{R}(K)$ and $\dim(X) = s_X$. Note that in this case, the Hilbert space X must be finite dimensional. If all the POD eigenvalues for $\{w^j\}$ are nonzero and $s_X = \infty$ (i.e., X must be infinite dimensional), then Lemma 3.2.5 only gives $X = \overline{\mathcal{R}(K)}$. We do not always obtain the better convergence results in this case. Similar statements hold for the spaces Y and $\mathcal{R}(K^Y)$. Also, as in Section 3.3, we sometimes need to consider different proof techniques in the case $s_X = \infty$.

We begin with a pointwise convergence result for Π_r^Y assuming L is bounded. For another pointwise convergence result for Π_r^Y with different assumptions, see Theorem 3.4.5 below.

Theorem 3.4.1. *Assume L is bounded and $\{\Pi_r^Y\}$ is uniformly bounded in operator norm. If $y \in \mathcal{R}(L)$, then $\Pi_r^Y y \longrightarrow y$ as r increases. In addition, if $\mathcal{R}(L)$ is dense in Y, then $\Pi_r^Y y \longrightarrow y$ for all $y \in Y$.*

Proof. Let $y \in \mathcal{R}(L)$, so that $y = Lx$ for some $x \in X$. Note that since $L\Pi_r^X x \in Y_r = \operatorname{span}\{L\varphi_k\}_{k=1}^r$ and Π_r^Y is a projection onto Y_r, we have $\Pi_r^Y L\Pi_r^X x = L\Pi_r^X x$. Then

$$\begin{aligned}
\|\Pi_r^Y y - y\|_Y &\leq \|\Pi_r^Y Lx - \Pi_r^Y L\Pi_r^X x\|_Y + \|\Pi_r^Y L\Pi_r^X x - Lx\|_Y \\
&= \|\Pi_r^Y Lx - \Pi_r^Y L\Pi_r^X x\|_Y + \|L\Pi_r^X x - Lx\|_Y \\
&\leq \|\Pi_r^Y L\| \|x - \Pi_r^X x\|_Y + \|L\| \|\Pi_r^X x - x\|_Y,
\end{aligned}$$

which converges to zero as r increases since $\Pi_r^X x \to x$ and $\{\Pi_r^Y\}$ is uniformly bounded in operator norm. The final result follows directly from the Banach-Steinhaus theorem (i.e., the principle of uniform boundedness). □

The next convergence result relies on the boundedness of either L or L^{-1} and certain range conditions involving L.

Theorem 3.4.2. *1. For any $y \in \mathcal{R}(L) = \mathcal{D}(L^{-1})$, if L is bounded, then $\|L\Pi_r^X L^{-1}y - y\|_Y \to 0$ as r increases. In addition, if $\mathcal{R}(L)$ is dense in Y and $\{L\Pi_r^X L^{-1}\}$ is uniformly bounded, then $L\Pi_r^X L^{-1}y \to y$ for all $y \in Y$.*

2. For any $x \in \mathcal{D}(L) = \mathcal{R}(L^{-1})$, if L^{-1} is bounded and $\Pi_r^Y y \to y$ for all $y \in Y$ as r increases, then $\|L^{-1}\Pi_r^Y Lx - x\|_X \to 0$ as r increases. In addition, if $\mathcal{D}(L)$ is dense in X and $\{L^{-1}\Pi_r^Y L\}$ is uniformly bounded, then $L^{-1}\Pi_r^Y Lx \to x$ for all $x \in X$.

Remark 3.4.3. *Note that Theorem 3.4.1 and Theorem 3.4.5 give two cases where the assumption $\Pi_r^Y y \to y$ for all $y \in Y$ holds. Also, the uniform boundedness of $\{L\Pi_r^X L^{-1}\}$ and $\{L^{-1}\Pi_r^Y L\}$ is not currently known, unless L and L^{-1} are both bounded. Note that when L and L^{-1} are both bounded, Theorem 3.4.1 gives $\Pi_r^Y y \to y$ for all $y \in Y$ whenever $\{\Pi_r^Y\}$ is uniformly bounded; therefore, in this case Theorem 3.4.2 gives $L\Pi_r^X L^{-1}y \to y$ for all $y \in Y$ and $L^{-1}\Pi_r^Y Lx \to x$ for all $x \in X$.*

Proof. We only prove the first result; the proof of the second is similar. Since $y \in \mathcal{R}(L)$ we have $y = Lx$ for some $x \in X$. Then

$$\begin{aligned}\|L\Pi_r^X L^{-1}y - y\|_Y &= \|L\Pi_r^X x - Lx\|_Y \\ &\leq \|L\|\,\|\Pi_r^X x - x\|_X,\end{aligned}$$

which converges to zero as r increases. The final convergence result again follows from the principle of uniform boundedness. □

Next, we consider how range conditions involving K and K^Y affect the convergence of POD projections. We are able to obtain convergence rates, and at most require either L or L^{-1} to be bounded. We begin with the POD projection Π_r^Y and then consider $L\Pi_r^X L^{-1}$ and $L^{-1}\Pi_r^Y L$. We use the following simple lemma multiple times below.

Lemma 3.4.4. *Assume $y \in \mathcal{R}(K^Y)$ so that $y = K^Y g = LKg$ for some $g \in S$. If*

$$y_N = LK_N g = L\Pi_N^X Kg, \tag{3.22}$$

then $y_N \to y$ as N increases.

Proof. As N increases,

$$\|y_N - y\|_Y = \|LKg - LK_N g\|_Y \leq \|LK - L\Pi_N^X K\|_{\mathrm{HS}(S,Y)}\|g\|_S \to 0$$

by Lemma 3.3.1. □

Recall from Lemma 3.2.5 that s_Y is always less than or equal to s_X. Thus if we assume $s_X < \infty$, we know that $s_Y < \infty$. For the following proofs, we consider whether s_X is finite or infinite.

Theorem 3.4.5. *Assume $\{\Pi_r^Y\}$ is uniformly bounded in operator norm whenever $s_X = \infty$. If $y = K^Y g$ for some $g \in S$, then $\Pi_r^Y y \to y$ as r increases and the following error bound holds:*

$$\|\Pi_r^Y y - y\|_Y \leq \sum_{k>r} \sigma_k |(g, f_k)_S| \, \|\Pi_r^Y L\varphi_k - L\varphi_k\|_Y. \tag{3.23}$$

Also, if the POD eigenvalues for the data $\{Lw^j\}$ are all nonzero, then $\Pi_r^Y y \to y$ for all $y \in Y$.

Proof. First consider the case $s_X < \infty$, and fix r. Assume $y = K^Y g = LKg$ for some $g \in S$. Thus,

$$\Pi_r^Y y = \Pi_r^Y K^Y g = \Pi_r^Y LKg = \sum_{k=1}^{s_X} \sigma_k (g, f_k)_S \Pi_r^Y L\varphi_k, \quad \text{and} \quad y = \sum_{k=1}^{s_X} \sigma_k (g, f_k)_S L\varphi_k. \tag{3.24}$$

Subtracting gives

$$\Pi_r^Y y - y = \sum_{k=1}^{s_X} \sigma_k (g, f_k)_S (\Pi_r^Y L\varphi_k - L\varphi_k) = \sum_{k=r+1}^{s_X} \sigma_k (g, f_k)_S (\Pi_r^Y L\varphi_k - L\varphi_k),$$

since $\Pi_r^Y L\varphi_k = L\varphi_k$ for $k = 1, ..., r$. The error bound (3.23) follows directly from this representation and the triangle inequality. Furthermore, since $s_X < \infty$, clearly $\Pi_r^Y y \to y$ as r increases for each $y \in \mathcal{R}(K^Y)$.

Next, assume the POD eigenvalues for the data $\{Lw^j\}$ are all nonzero. By Item 2 of Lemma 3.2.5, since $s_Y \leq s_X < \infty$ we have $Y = \mathcal{R}(K^Y)$. This gives $\Pi_r^Y y \to y$ for all $y \in Y$.

Now consider the case $s_X = \infty$, and fix r. For $y = K^Y g = LKg$ with $g \in S$ as above, recall the definition of $y_N = L\Pi_N^X Kg$ given in (3.22). We have

$$\begin{aligned} \|\Pi_r^Y y - y\|_Y &\leq \|\Pi_r^Y y - \Pi_r^Y y_N\|_Y + \|\Pi_r^Y y_N - y_N\|_Y + \|y_N - y\|_Y \\ &\leq \left(\|\Pi_r^Y\| + 1\right) \|y - y_N\|_Y + \|\Pi_r^Y y_N - y_N\|_Y. \end{aligned}$$

Note that for the second term, $\|\Pi_r^Y y_N - y_N\|_Y$, we can obtain representations for $\Pi_r^Y y_N$ and y_N similar to that in (3.24) above. Proceeding in the same way gives

$$\|\Pi_r^Y y_N - y_N\|_Y \leq \sum_{k=r+1}^{N} \sigma_k |(g, f_k)_S| \, \|\Pi_r^Y L\varphi_k - L\varphi_k\|_Y.$$

Since r is fixed and $y_N \to y$ as $N \to \infty$ (Lemma 3.4.4), the two inequalities above give

$$\|\Pi_r^Y y - y\|_Y \leq \sum_{k=r+1}^{\infty} \sigma_k |(g, f_k)_S| \, \|\Pi_r^Y L\varphi_k - L\varphi_k\|_Y.$$

For convergence, we have

$$\|\Pi_r^Y y - y\|_Y \leq \left(\sum_{k>r} |(g, f_k)_S|^2 \right)^{1/2} \left(\sum_{k>r} \sigma_k^2 \|\Pi_r^Y L\varphi_k - L\varphi_k\|_Y^2 \right)^{1/2}.$$

Since $\{f_k\}$ is an orthonormal basis for S, we know $\sum_{k>r} |(g, f_k)_S|^2$ goes to zero as r increases by Parseval's equality. Furthermore, since $\{\Pi_r^Y\}$ is uniformly bounded, Lemma 3.3.1 gives that $\sum_{k>r} \sigma_k^2 \|\Pi_r^Y L\varphi_k - L\varphi_k\|_Y^2$ goes to zero as r increases. This gives $\Pi_r^Y y \to y$ for each $y \in \mathcal{R}(K^Y)$.

Finally, assume the POD eigenvalues for the data $\{Lw^j\}$ are all nonzero. By Item 2 of Lemma 3.2.5, we have $\mathcal{R}(K^Y)$ is dense in Y. Since $\{\Pi_r^Y\}$ is uniformly bounded, the principle of uniform boundedness gives $\Pi_r^Y y \to y$ for all $y \in Y$. □

For the next two results we need to assume L or L^{-1} is bounded whenever $s_X = \infty$.

Theorem 3.4.6. *Assume $s_X < \infty$, or either L or L^{-1} is bounded. If $y = K^Y g$ for some $g \in S$, then*

$$\|y - L\Pi_r^X L^{-1} y\|_Y \leq \sum_{k>r} \sigma_k \, |(g, f_k)_S| \, \|L\varphi_k\|_Y \tag{3.25}$$

and the error converges to zero as r increases. Now assume $\{L\Pi_r^X L^{-1}\}$ is uniformly bounded in operator norm whenever $s_X = \infty$. If the POD eigenvalues for the data $\{Lw^j\}$ are all nonzero, then $L\Pi_r^X L^{-1} y \to y$ for all $y \in Y$.

Proof. Let $y = LKg$ for some $g \in S$, assume $s_X < \infty$, and fix r. As in the proof of Theorem 3.4.5, it can be shown that

$$\begin{aligned} y - L\Pi_r^X L^{-1} y &= LKg - L\Pi_r^X Kg \\ &= \sum_{k=1}^{s_X} \sigma_k (g, f_k)_S L\varphi_k - \sum_{k=1}^{r} \sigma_k (g, f_k)_S L\varphi_k \\ &= \sum_{k=r+1}^{s_X} \sigma_k (g, f_k)_S L\varphi_k. \end{aligned}$$

The triangle inequality gives the error bound (3.25). The convergence results for the case $s_X < \infty$ follow just as in the proof of Theorem 3.4.5.

Now consider the case $s_X = \infty$, assume $y = LKg$ for some $g \in S$, and fix r. Then for $y_N = L\Pi_N^X Kg$ as in (3.22), with $N \geq r$, we have

$$\|y - L\Pi_r^X L^{-1} y\|_Y \leq \|y - y_N\|_Y + \|y_N - L\Pi_r^X L^{-1} y_N\|_Y + \|L\Pi_r^X L^{-1} y_N - L\Pi_r^X L^{-1} y\|_Y.$$

Lemma 3.4.4 implies that the first term tends to zero as $N \to \infty$. For the second term, proceed as above and use $\Pi_r^X \Pi_N^X = \Pi_r^X$ (since $N \geq r$) to show

$$\|y_N - L\Pi_r^X L^{-1} y_N\|_Y \leq \sum_{k=r+1}^{N} \sigma_k \, |(g, f_k)_S| \, \|L\varphi_k\|_Y.$$

For the third term, first assume L is bounded. In this case,

$$\|L\Pi_r^X L^{-1} y_N - L\Pi_r^X L^{-1} y\|_Y \leq \|L\| \|\Pi_r^X\| \|L^{-1} y_N - L^{-1} y\|_X = \|L\| \|\Pi_r^X\| \|\Pi_N^X Kg - Kg\|_X,$$

which converges to zero as $N \to \infty$, since r is fixed. If instead L^{-1} is bounded, then $L\Pi_r^X L^{-1}$ is bounded by Theorem 3.2.3 and so

$$\|L\Pi_r^X L^{-1} y_N - L\Pi_r^X L^{-1} y\|_Y \leq \|L\Pi_r^X L^{-1}\| \|y_N - y\|_Y,$$

which converges to zero as $N \to \infty$ by Lemma 3.4.4, again since r is fixed. Combining the above results gives

$$\|y - L\Pi_r^X L^{-1} y\|_Y \leq \sum_{k=r+1}^{\infty} \sigma_k \, |(g, f_k)_S| \, \|L\varphi_k\|_Y.$$

For convergence, we proceed as in the proof of Theorem 3.4.5. We have

$$\|y - L\Pi_r^X L^{-1} y\|_Y \le \left(\sum_{k>r} |(g, f_k)_S|^2 \right)^{1/2} \left(\sum_{k>r} \sigma_k^2 \|L\varphi_k\|_Y^2 \right)^{1/2} .$$

We know $\sum_{k>r} |(g, f_k)_S|^2$ goes to zero as r increases by Parseval's equality. Furthermore, Lemma 3.3.1 gives that $\sum_{k>r} \sigma_k^2 \|L\varphi_k\|_Y^2$ goes to zero as r increases. This implies $L\Pi_r^X L^{-1} y \to y$ for each $y \in \mathcal{R}(K^Y)$. To show convergence for all $y \in Y$, we again use Item 2 of Lemma 3.2.5 and the principle of uniform boundedness. □

We omit the proof of the next result, as it is similar to the proof of the previous result, Theorem 3.4.6. Note that in Theorem 3.4.6 the error converges to zero for a fixed $y \in \mathcal{R}(K^Y)$ without any additional assumptions. In this next result, if $s_X = \infty$ we need to require additional conditions to guarantee that the error converges to zero for a fixed $x \in \mathcal{R}(K)$; these conditions come from Lemma 3.3.1.

Theorem 3.4.7. *Assume $s_X < \infty$ or either L or L^{-1} is bounded. If $x = Kg$ for some $g \in S$, then*

$$\|x - L^{-1}\Pi_r^Y Lx\|_X \le \sum_{k>r} \sigma_k |(g, f_k)_S| \, \|\varphi_k - L^{-1}\Pi_r^Y L\varphi_k\|_X. \tag{3.26}$$

If $s_X < \infty$, the error converges to zero as r increases. If $s_X = \infty$, then the error goes to zero as r increases when either (i) L^{-1} is bounded and $\{\Pi_r^Y\}$ is uniformly bounded or (ii) $\{L^{-1}\Pi_r^Y L\}$ is uniformly bounded. Now assume $\{L^{-1}\Pi_r^Y L\}$ is uniformly bounded in operator norm whenever $s_X = \infty$. If the POD eigenvalues for the data $\{w^j\}$ are all nonzero, then $L^{-1}\Pi_r^Y Lx \to x$ for all $x \in X$.

To be complete, we give an exact error formula and an error bound for approximations of elements in the range of K using the POD projection Π_r^X. This result gives an error bound for approximating each individual data snapshot in the discrete case.

Theorem 3.4.8. *If $x = Kg$ for some $g \in S$, then*

$$\|x - \Pi_r^X x\|_X = \left(\sum_{k>r} \sigma_k^2 |(g, f_k)_S|^2 \right)^{1/2} \leq \sigma_{r+1} \|g\|_S. \tag{3.27}$$

Also, in the discrete case, for each $\ell = 1, \ldots, s$ we have

$$\|w^\ell - \Pi_r^X w^\ell\|_X \leq \gamma_\ell^{-1/2} \sigma_{r+1}. \tag{3.28}$$

Remark 3.4.9. *The bound* (3.28) *was obtained in [40, Proposition 3.1] for $X = \mathbb{R}^n$ and $\gamma_\ell = 1$ for all ℓ. Recall the constants $\{\gamma_\ell\}$ are the positive weights in the definition of the POD operator K in the discrete case; see Section 2.2.1.*

Proof. Using the SVD of K gives

$$x - \Pi_r^X x = \sum_{k>r} \sigma_k (g, f_k)_S \varphi_k.$$

Since $\|x - \Pi_r^X x\|_X^2 = (x - \Pi_r^X x, x - \Pi_r^X x)_X$ and $\{\varphi_k\}$ is an orthonormal basis for X, we immediately obtain the exact error formula in (3.27). To obtain the error bound in (3.27), use $\sigma_k \leq \sigma_{r+1}$ for all $k > r$ and also Parseval's equality.

Next, in the discrete case we have $w^\ell = Kg_\ell$ for each $\ell = 1, \ldots, s$, where $g_\ell = \gamma_\ell^{-1} e_\ell$ and e_ℓ is the ℓth standard unit vector for $\mathbb{K}^s$, i.e., the ℓth entry of e_ℓ is one and all other entries are zero. The error bound (3.28) follows from $\|g^\ell\|_S = \gamma_\ell^{-1/2}$ and (3.27). □

In Theorem 3.4.8, note that the quantity γ_ℓ^{-1} appears in the error bound (3.28) for approximating the snapshot w^ℓ. However, in applications it is typical that each weight γ_ℓ tends to zero as the number s of snapshots increases. Next, we use the above results to prove various approximation error bounds for each individual snapshot w^ℓ in the discrete case that do not depend on γ_ℓ^{-1}. Here, the bounds are only valid if r is sufficiently large. We note that these type of error bounds have been *assumed* to hold in the literature; Iliescu and Wang made this type of assumption in [25, Assumption 3.2] (with $\gamma_\ell = s^{-1}$ for all ℓ) in their analysis of a POD reduced order model of the Navier-Stokes equations, and many others have followed their approach.

Corollary 3.4.10. *In the discrete case, if r is sufficiently large, then for each $\ell = 1, \ldots, s$ we have*

$$\|w^\ell - \Pi_r^X w^\ell\|_X^2 \le \sigma_{r+1}^2, \tag{3.29a}$$

$$\|Lw^\ell - \Pi_r^Y Lw^\ell\|_Y^2 \le \sum_{k>r} \sigma_k^2 \|L\varphi_k - \Pi_r^Y L\varphi_k\|_Y^2, \tag{3.29b}$$

$$\|Lw^\ell - L\Pi_r^X w^\ell\|_Y^2 \le \sum_{k>r} \sigma_k^2 \|L\varphi_k\|_Y^2, \tag{3.29c}$$

$$\|w^\ell - L^{-1}\Pi_r^Y Lw^\ell\|_X^2 \le \sum_{k>r} \sigma_k^2 \|\varphi_k - L^{-1}\Pi_r^Y L\varphi_k\|_X^2. \tag{3.29d}$$

Proof. We only prove (3.29b); the proofs of the remaining inequalities are similar. As in the proof of Theorem 3.4.8, we know $w^\ell = Kg_\ell$ for each $\ell = 1, \ldots, s$, where $g_\ell = \gamma_\ell^{-1} e_\ell$. Using the error bound (3.23) in Theorem 3.4.5, the Cauchy-Schwarz inequality on the sum, and Parseval's inequality gives

$$\|Lw^\ell - \Pi_r^Y Lw^\ell\|_Y^2 \le \|g^\ell - \Pi_r^S g_\ell\|_S^2 \sum_{k>r} \sigma_k^2 \|L\varphi_k - \Pi_r^Y L\varphi_k\|_Y^2,$$

where $\Pi_r^S : S \to S$ is the orthogonal projection onto $S_r := \operatorname{span}\{f_k\}_{k=1}^r$. Since $\{f_k\}_{k\ge1}$ is an orthonormal basis for S, we know $\Pi_r^S g_\ell \to g_\ell$ for $\ell = 1, \ldots, s$. Since s is fixed, for all sufficiently large r we have $\|g_\ell - \Pi_r^S g_\ell\|_S \le 1$ for all $\ell = 1, \ldots, s$, and this completes the proof. □

3.5. EXAMPLES

In this section we present four examples illustrating these new results. Each example shows how to consider the problem in terms of our new framework. First, we consider a computational example in Section 3.5.1 to demonstrate the POD data approximation errors. Then we consider a few additional examples that relate to previous works.

For the examples in Section 3.5.2 and Section 3.5.3, we consider two separable Hilbert spaces, H and V, where V is a proper subset of H, and V is both continuously embedded[1] and dense in H. The linear operator L is a mapping between these two spaces. We assume we have the data $\{w^j\}_{j=1}^m \subset L^2(\mathcal{O};H) \cap L^2(\mathcal{O};V)$. We present the results for the continuous case only, but results for the discrete case can also be obtained using the theory in this work if desired.

3.5.1. Computational Example. Next, we briefly present numerical results for an example to demonstrate our new results. POD model order reduction is considered for this example in [29]; here, we focus on the POD data approximation errors. The new results are discussed in greater detail for other examples in Section 3.5.

Consider a nerve impulse model, the FitzHugh-Nagumo system in one dimension. The initial conditions for this model are zero and is given by

$$\begin{aligned}
\frac{\partial u(t,x)}{\partial t} &= \mu \frac{\partial^2 u(t,x)}{\partial x^2} - \frac{1}{\mu} v(t,x) + \frac{1}{\mu} f(u) + \frac{c}{\mu}, \quad 0 < x < 1, \\
\frac{\partial v(t,x)}{\partial t} &= b u(t,x) - \gamma v(t,x) + c, \quad 0 < x < 1,
\end{aligned}$$

where

$$f(u) = u(u - 0.1)(1 - u),$$

$\mu = 0.015$, $b = 0.5$, $\gamma = 2$, and $c = 0.05$. Further, the boundary conditions are given by

$$u_x(t,0) = -50000 t^3 e^{-15t} \quad \text{and} \quad u_x(t,1) = 0.$$

[1]i.e., there exists a constant $C_V > 0$ such that $\|v\|_H \leq C_V \|v\|_V$ for all $v \in V$

For this example, we take the Hilbert spaces $X = Y = L^2(0,1) \times L^2(0,1)$ with the usual inner product, and define the operator $L : X \to Y$ by

$$L \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} \partial_x u \\ \partial_x v \end{bmatrix}.$$

Note that here L is unbounded and closed, but not invertible. Thus, this operator satisfies the main assumption made for the continuous case. We let Π_r^Y be the orthogonal projection onto $Y_r = \text{span}\{L\varphi_k\}_{k=1}^r$, where $\{\varphi_k\} \subset X$ are the POD modes.

To approximate the solution of the PDE we used the interpolated coefficient finite element method with continuous piecewise linear basis functions from [29], and `ode23s` from MATLAB for the time stepping scheme. We approximated the solution using 100 equally spaced finite element nodes on the time interval $\mathcal{O} = (0, 10)$. Increasing the number of finite element nodes gave similar results below.

For the POD computations, the solution values were approximated at each time step, $w(t_k)$, where $w = [u, v]^T$, and a piecewise constant function in time was formed. The constant on each interval is given by the average of the solution at the current step and the solution at the next step, i.e., $0.5(w(t_{k+1}) + w(t_k))$. Note that for this problem we can calculate the POD eigenvalues, POD modes, and the data approximation errors exactly. Thus, comparisons between the actual approximation errors and the error formulas can be made.

In Tables 3.1 and 3.2 we present the errors from the relevant projections considered in Chapter 3 for $r = 4$ and $r = 12$. Note that errors for projections involving the inverse mapping L^{-1} are not included since L is not invertible for this example. In the tables, the actual error is the integral error measure and the error formula is the sum involving the POD singular values. The first line in the tables represents computations for the known error result (2.7). The second and third lines of the tables are computations for the new results

Table 3.1. Error Comparison with $r = 4$

POD Error Equation	Actual Error	Error Formula	Difference
Equation (2.7)	6.2755×10^{-5}	6.2792×10^{-5}	3.7584×10^{-8}
Equation (3.18)	2.1584×10^{-1}	2.1593×10^{-1}	9.1863×10^{-5}
Equation (3.19)	9.8536×10^{-3}	9.8541×10^{-3}	4.7712×10^{-7}

Table 3.2. Error Comparison with $r = 12$

POD Error Formula	Actual Error	Error Formula	Difference
Equation (2.7)	4.1453×10^{-8}	4.1487×10^{-8}	3.3661×10^{-11}
Equation (3.18)	2.2536×10^{-4}	2.2541×10^{-4}	5.2146×10^{-8}
Equation (3.19)	1.2664×10^{-5}	1.2668×10^{-5}	3.5150×10^{-9}

(3.18)-(3.19). The second line of each table gives the values for

$$\text{actual error } = \int_O \|Lw(t) - L\Pi_r^X w(t)\|_Y^2 dt, \quad \text{error formula } = \sum_{k>r} \sigma_k^2 \|L\varphi_k\|_Y^2,$$

while the third line of each table shows computational results for

$$\text{actual error } = \int_O \|Lw^j - \Pi_r^Y Lw^j\|_Y^2 dt, \quad \text{error formula } = \sum_{k>r} \sigma_k^2 \|L\varphi_k - \Pi_r^Y L\varphi\|_Y^2.$$

The differences in the computed values are likely due to round off errors. Note that as r increases the errors tend toward zero, as expected by the theory.

3.5.2. Examples From [1]. The first two examples are from [1]. Due to the above assumption on the data, the POD operator K can be viewed as a mapping into H or a mapping into V. One can obtain the SVD of $K : S \to H$ or the SVD of $K : S \to V$, i.e., one can choose $X = H$ or $X = V$. The different choices for X give different POD singular values, POD singular vectors, POD modes, and POD projections. In [1], the author considered both choices for X and four different POD projections between these spaces and gave exact expressions for the POD data approximation errors in the two different Hilbert space norms. We relate the notation and results for both the error formulas and pointwise convergence from the present work to [1]. We obtain better pointwise convergence results in this work. Also, O was only an interval in [1], but now we have O is an open subset of $\mathbb{R}^d$. For these first two examples, $Y_r = \text{span}\{L\varphi_k\}$ and $\Pi_r^Y : Y \to Y$ is the orthogonal projection onto Y_r. Note this implies $\{\Pi_r^Y\}$ is uniformly bounded in operator norm.

3.5.2.1. Example 1. For the first example, consider the case where $X = H$, $Y = V$, and $L : H \to V$ is defined by $Lv = v$ for all $v \in \mathcal{D}(L) = V$. The operator L is clearly invertible, and $L^{-1} : V \to H$ is given by $L^{-1}v = v$ for all $v \in V$. Note that $L^{-1} : V \to H$ is bounded due to the continuous embedding assumption. Also, the inverse of a bounded operator is closed, so L is closed. Furthermore, the assumption on the data gives $\{w^j\} \subset L^2(O; X)$ and $\{Lw^j\} \subset L^2(O; Y)$. Thus, we know that both the main assumption and the L^{-1} assumption hold.

Since $X = H$ and each set of singular vectors of the POD operator $K : S \to H$ are an orthonormal basis, we know the POD modes $\{\varphi_k\}$ are an orthonormal basis for H. Note that $X_r = \text{span}\{\varphi_k\}_{k=1}^r \subset H$, and $Y_r = \text{span}\{L\varphi_k\}_{k=1}^r = \text{span}\{\varphi_k\}_{k=1}^r \subset V$. Furthermore, the POD modes $\{\varphi_k\}$ may not be orthogonal in V. Also, the operator $K^Y = LK$ is simply the POD operator K viewed as a mapping from S to V. We take $\Pi_r^X : X \to X$ to be the orthogonal projection onto X_r, and $\Pi_r^Y : Y \to Y$ to be the orthogonal projection onto Y_r.

In order to discuss the POD projections we pay special attention to the spaces under consideration. Since $V \subset H$, the projections can be considered as mappings from V to V or from H to H. The projections considered in this work are related to the projections P_r^H and P_r^V in [1, Definition 3.2] as follows:

- $\Pi_r^X : X \to X$ is equal to the orthogonal projection $P_r^H : H \to H$.
- $\Pi_r^Y : Y \to Y$ is equal to the orthogonal projection $P_r^V : V \to V$.

- $L\Pi_r^X L^{-1} : Y \to Y$ is equal to the operator $P_r^H : V \to V$.
- $L^{-1}\Pi_r^Y L : X \to X$ is equal to the operator $P_r^V : H \to H$.

Now that we have the relationships between the projections, we compare the results. The error formulas presented here in Theorem 3.3.4 are essentially the same as the results in [1]. Again, the primary difference here is that O is an open subset of $\mathbb{R}^d$ instead of an interval. The POD data approximation errors from Theorem 3.3.4 become the following:

$$\sum_{j=1}^{m} \int_O \|w^j(t) - P_r^H w^j(t)\|_V^2 dt = \sum_{k>r} \sigma_k^2 \|\varphi_k\|_V^2, \tag{3.30}$$

$$\sum_{j=1}^{m} \int_O \|w^j(t) - P_r^V w^j(t)\|_V^2 dt = \sum_{k>r} \sigma_k^2 \|\varphi_k - P_r^V \varphi_k\|_V^2, \tag{3.31}$$

$$\sum_{j=1}^{m} \int_O \|w^j(t) - P_r^V w^j(t)\|_H^2 dt = \sum_{k>r} \sigma_k^2 \|\varphi_k - P_r^V \varphi_k\|_H^2. \tag{3.32}$$

In this example, all three sums converge to zero as r increases.

A larger improvement from [1] can be seen in the results concerning pointwise convergence of POD projections. To illustrate, we give the following result.

Proposition 3.5.1. *We have*

1. $\|P_r^V y - y\|_V \to 0$ *for all* $y \in \mathcal{R}(K)$*, and for* $y = Kg$ *we have*

$$\|P_r^V y - y\|_V \leq \sum_{k>r} \sigma_k |(g, f^k)_S| \, \|P_r^V \varphi_k - \varphi_k\|_V.$$

2. *If the POD eigenvalues for* $\{w^j\} \subset L^2(O; V)$ *are all nonzero, then* $P_r^V y \to y$ *in both* H *and* V *for all* $y \in V$.

3. $\|P_r^H y - y\|_V \to 0$ *for all* $y \in \mathcal{R}(K)$*, and for* $y = Kg$ *we have*

$$\|y - P_r^H y\|_V \leq \sum_{k>r} \sigma_k \, |(g, f^k)_S| \, \|\varphi_k\|_V.$$

4. $\|P_r^V x - x\|_H \to 0$ *for all* $x \in \mathcal{R}(K)$*, and for* $x = Kg$ *we have*

$$\|x - P_r^V x\|_H \leq \sum_{k>r} \sigma_k \, |(g, f^k)_S| \, \|\varphi_k - P_r^V \varphi_k\|_H.$$

Note that since Π_r^Y is orthogonal, item 1 and item 2 follow from Theorem 3.4.5 and item 2 of Theorem 3.4.2. Items 3 and 4 can be obtained from Theorem 3.4.6, Theorem 3.4.7, and the fact that L^{-1} is bounded.

The pointwise convergence results above are more complete and more sharp than the results in [1, Proposition 5.5]. First, item 2 is shown in [1, Proposition 5.5] under the assumption that all the POD singular values for $\{w^j\} \subset L^2(\mathcal{O}; V)$ are nonzero; as discussed in Section 2.2.2 this is a more restrictive assumption than the POD eigenvalues all being nonzero, as is required above. Next, the convergence result in item 3 is shown in [1, Proposition 5.5]; however, the error bound in item 3 is new. Also, items 1 and 4 are completely new.

For item 3, we note that an error bound was given in the proof of [1, Proposition 5.5]. However, that error bound does not converge to zero as fast as the error bound given in Theorem 3.4.6. Specifically, the error bound in [1] is a constant multiple of $(\sum_{k>r} |(g, f^k)_S|^2)^{1/2}$. However, the error bound in item 3 can be bounded above by

$$\|y - P_r^H y\|_V \leq \left(\sum_{k>r} |(g, f^k)_S|^2 \right)^{1/2} \left(\sum_{k>r} \sigma_k^2 \, \|\varphi_k\|_V^2 \right)^{1/2},$$

and both terms in parentheses tend to zero as r increases by Parseval's equality and Lemma 3.3.1 (see the proof of Theorem 3.4.6). Therefore, the error bound in item 3 is an improvement over the error bound in [1].

Finally, we consider boundedness of the non-orthogonal POD projections $P_r^H : V \to V$ and $P_r^V : H \to H$. For each fixed r, it is shown in [1, Lemma 3.3] that $P_r^H : V \to V$ is bounded. Singler did not consider the boundedness of $P_r^V : H \to H$ in [1]. Below, we use Theorem 3.2.3 to show $P_r^H : V \to V$ is bounded and also give a condition guaranteeing $P_r^V : H \to H$ has a bounded extension. However, we still do not know if these non-orthogonal POD projections are uniformly bounded in operator norm.

Define the linear operator $A : \mathcal{D}(A) \subset H \to H$ by

$$(Au, v)_H = (u, v)_V$$

for all $u \in \mathcal{D}(A)$ and $v \in V$ (see, e.g., [63, Section II.2]). We know A is closed. Now we apply this to our example. For all $x \in \mathcal{D}(L) = V$ and $y \in \mathcal{D}(L^*)$ we have

$$\begin{aligned} (x, L^* y)_H &= (Lx, y)_V = (x, y)_V \\ \Rightarrow (L^* y, x)_H &= (y, x)_V. \end{aligned}$$

Thus, $L^* = A$ and $\mathcal{D}(L^*) = \mathcal{D}(A)$. For PDE solution data we often have $\{Aw^j\} \subset L^2(O; H)$ for each j; see [63] for examples. In this case, since $\varphi_k = \sigma_k^{-1} K f^k$ we can use the Bochner integral result in Theorem 2.1.2 to show $\varphi_k \in \mathcal{D}(A)$ whenever $\sigma_k > 0$.

Therefore, since L^{-1} is bounded, item 1 and item 4 of Theorem 3.2.3 give the following result.

Proposition 3.5.2. *Let r be fixed. The operator $P_r^H : V \to V$ is bounded, and if $\{Aw^j\}_{j=1}^m \subset L^2(O; H)$, then the operator $P_r^V : H \to H$ can be extended to a bounded operator.*

3.5.2.2. Example 2. Next, consider the case where $X = V$, $Y = H$, and $L : V \to H$ is defined by by $Lv = v$ for all $v \in V$. Then $L^{-1} : H \to V$ is given by $L^{-1}v = v$ for all $v \in \mathcal{D}(L^{-1}) = V$. Note that in this case L is bounded by the continuous embedding property. Again, the assumption on the data gives $\{w^j\} \subset L^2(O; X)$ and $\{Lw^j\} \subset L^2(O; Y)$. Therefore, the main assumption and the L^{-1} assumption hold.

Since $X = V$, in this example the POD modes $\{\varphi_k\}$ are an orthonormal basis for V. We have $X_r = \text{span}\{\varphi_k\}_{k=1}^r \subset V$, and $Y_r = \text{span}\{L\varphi_k\}_{k=1}^r = \text{span}\{\varphi_k\}_{k=1}^r \subset H$. The POD modes $\{\varphi_k\}$ may not be orthogonal in H. The operator $K^Y = LK$ is the POD operator $K : S \to H$. As in Example 1, $\Pi_r^X : X \to X$ is the orthogonal projection onto X_r, and $\Pi_r^Y : Y \to Y$ is the orthogonal projection onto Y_r.

The projections in this work are related to the projections Q_r^H and Q_r^V from [1, Definition 3.2] as follows:

- $\Pi_r^X : X \to X$ is equal to the orthogonal projection $Q_r^V : V \to V$.
- $\Pi_r^Y : Y \to Y$ is equal to the orthogonal projection $Q_r^H : H \to H$.
- $L\Pi_r^X L^{-1} : Y \to Y$ is equal to the operator $Q_r^V : H \to H$.
- $L^{-1}\Pi_r^Y L : X \to X$ is equal to the operator $Q_r^H : V \to V$.

As before, the main data approximation error results in Theorem 3.3.4 become

$$\sum_{j=1}^m \int_O \|w^j(t) - Q_r^V w^j(t)\|_H^2 dt = \sum_{k>r} \sigma_k^2 \|\varphi_k\|_H^2,$$
$$\sum_{j=1}^m \int_O \|w^j(t) - Q_r^H w^j(t)\|_H^2 dt = \sum_{k>r} \sigma_k^2 \|\varphi_k - Q_r^H \varphi_k\|_H^2,$$
$$\sum_{j=1}^m \int_O \|w^j(t) - Q_r^H w^j(t)\|_V^2 dt = \sum_{k>r} \sigma_k^2 \|\varphi_k - Q_r^H \varphi_k\|_V^2.$$

Here the first two sums converge to zero as r increases. However, we cannot show convergence of the last sum. This is because we do not know L^{-1} is bounded or $\{Q_r^H\}$ is uniformly bounded as a family of operators mapping V to V. As before, the only improvement here compared to [1] is that O is not restricted to be an interval.

We also have the following pointwise convergence results.

Proposition 3.5.3. *As r increases we have*

1. $\|Q_r^H y - y\|_H \to 0$ *for all* $y \in H$*, and for* $y = Kg$ *we have*

$$\|Q_r^H y - y\|_H \leq \sum_{k>r} \sigma_k |(g, f^k)_S| \, \|Q_r^H \varphi_k - \varphi_k\|_H.$$

2. $\|Q_r^V y - y\|_H \to 0$ *for all* $y \in V$*, and for* $y = Kg$ *we have*

$$\|Q_r^V y - y\|_H \leq \sum_{k>r} \sigma_k |(g, f^k)_S| \, \|\varphi_k\|_H.$$

3. *For* $x = Kg$ *we have*

$$\|Q_r^H x - x\|_V \leq \sum_{k>r} \sigma_k |(g, f^k)_S| \|Q_r^H \varphi_k - \varphi_k\|_V.$$

If also $s_X < \infty$ *or* L^{-1} *is bounded, then the error goes to zero as* r *increases.*

Since L is bounded, item 1 follows from item 1 of Theorem 3.4.1 and also Theorem 3.4.5. Item 2 can be obtained from Theorem 3.4.6, using L is bounded. Theorem 3.4.7 gives item 3; note that we cannot guarantee convergence of the error without the extra assumptions since we only know L is bounded.

Again, these results improve on the results in [1, Proposition 5.5]. All of the error bounds are new. The convergence result in item 2 was not stated in [1], but it follows directly from the continuous embedding and $\|Q_r^V y - y\|_V \to 0$ for all $y \in V$. The convergence result in item 1 was given in [1, Proposition 5.5], however that work made the assumption that all the POD singular values for $\{w^j\} \subset L^2(O; V)$ are nonzero. Here, we proved the convergence result in item 1 without that assumption.

Next, we use the technique from Section 3.5.2.1 to determine the boundedness of the non-orthogonal POD projections $Q_r^H : V \to V$ and $Q_r^V : H \to H$. For this example, we have $A = L^{-*} = (L^{-1})^*$. Therefore, if $\{Aw^j\} \subset L^2(\mathcal{O}; H)$, then we have $\{\varphi_k\} \subset \mathcal{D}(L^{-*})$, just as in Section 3.5.2.1. Since L is bounded, items 2 and 3 of Theorem 3.2.3 give the following result.

Proposition 3.5.4. *Let r be fixed. The operator $Q_r^H : V \to V$ is bounded, and if $\{Aw^j\}_{j=1}^m \subset L^2(\mathcal{O}; H)$, then the operator $Q_r^V : H \to H$ can be extended to a bounded operator on H.*

3.5.3. Non-orthogonal Projection Example. For the final example, we consider a case where Π_r^Y is not an orthogonal projection. In particular, we take Π_r^Y to be a Ritz projection, as considered in [24, 27]. All of our results for this case are new.

Consider the situation from Example 1 in Section 3.5.2.1: we have $X = H$, $Y = V$, and $L : X \to Y$ is defined by $Lv = v$ for all $v \in \mathcal{D}(L) = Y$. Assume we have a continuous elliptic sesquilinear form[2] $a : V \times V \to \mathbb{K}$. Define the projection $P_r^V : V \to V$ onto $V_r := Y_r = \text{span}\{L\varphi_k\} = \text{span}\{\varphi_k\} \subset V$ as follows: let $P_r^V u := u_r \in V_r$ be the unique solution of

$$a(u_r, v_r) = a(u, v_r) \quad \text{for all } v_r \in V_r.$$

The existence and uniqueness of such a solution is guaranteed by the Lax-Milgram Theorem. We take $\Pi_r^Y = P_r^V$.

Note that the main difference between this example and Example 1 is that the projection P_r^V is not the same. However, for this example it can be checked that the family of projections, $\{\Pi_r^Y\}$, is uniformly bounded. Therefore, the same pointwise convergence results and error formulas from Section 3.5.2.1 hold for this example with $P_r^V : V \to V$ defined as above. We note that these pointwise convergence results and error formulas are all new. Bounds on the POD data approximation errors can be found in Lemma 3.4 in [24]

[2] i.e., there exists constants $C_a, c_a > 0$ such that $|a(u, v)| \leq C_a \|u\|_V \|v\|_V$ and $c_a \|u\|_V^2 \leq \operatorname{Re} a(u, u)$ for all $u, v \in V$

and Lemma 2.9 in [27] in the discrete case; however, we have the exact formulas (3.30)-(3.32) for the POD data approximation errors in the continuous case. Again, analogous error formulas can be derived for the discrete case using our results.

4. A NEW APPROACH TO POD WITH DIFFERENCE QUOTIENTS

4.1. REVIEW OF EXISTING METHODS

Before presenting the new approach to proper orthogonal decomposition with difference quotients, we present current approaches to POD: the standard POD approach and standard POD with difference quotients approach. We compare our new method to known results about these established methods throughout the section. For details on the basics of POD see, e.g., [14, 15, 16, 19, 49, 50, 51].

First we establish some general notation. Let M and N be a positive integers and recall that X and Y are Hilbert spaces where the space X is called the POD space. In this chapter it is possible for $Y = X$. In the examples in this chapter for these Hilbert spaces we use the standard function spaces $L^2(\Omega)$ and $H_0^1(\Omega)$, where Ω is the spatial domain. In order to consider variable weights that often arise with numerical integration, we recall the definition from Section 2.2.1 of $S := \mathbb{K}_\Gamma^M$ with the weighted inner product given by

$$(g, h)_S = h^*\Gamma g = \sum_{j=1}^{M} \gamma_j g^j \overline{h^j}$$

where $g, h \in S$, $\Gamma = \text{diag}(\gamma_1, \gamma_2, \ldots, \gamma_M)$, and the values $\{\gamma_j\}_{j=1}^M$ are positive weights. In some instances it is beneficial to take the the positive weights to be certain specific values in order to approximate various time integrals.

For the POD reduced order modeling in this chapter, we consider data sets consisting of approximate solution data for a time dependent partial differential equation. Throughout, we consider the time interval $[0, T]$ with $T > 0$ a fixed positive constant. The approximate solution data will be given at times $t_n = (n - 1)\Delta t$, for $n = 1, \ldots, N$, where the time step is given by $\Delta t = \frac{T}{N-1}$. Note that while T is fixed, N can vary.

4.1.1. Standard POD. First we recall the standard POD approach as presented in Section 2.2.1. We present it here again with slightly different notation in order to use it for the remainder of the work.

Let $W = \{w^j\}_{j=1}^{M} \subset X$ be the POD data for some integer $M > 0$. We have the same POD operator as in Equation (2.2) which is

$$Kf = \sum_{j=1}^{M} \gamma_j f^j \, w^j, \quad f = [f^1, f^2, \ldots, f^M]^T. \tag{4.1}$$

We call this operator the standard POD operator. Further recall that the POD modes provide the best low rank approximation to the data. Thus we have the following formula as in Equation (2.5):

$$E_r = \sum_{j=1}^{M} \gamma_j \|w^j - \Pi_r^X w^j\|_X^2 = \sum_{k=r+1}^{s_X} \lambda_k \tag{4.2}$$

where $\{\lambda_k\}$ are the POD eigenvalues and s_X is the number of positive POD singular values.

For certain choices of weights $\{\gamma_i\}$ the error given in Equation (2.5) approximates a time integral, or a constant multiple of a time integral, as more and more time steps are used. Using various quadrature rules to determine the appropriate POD weights will lead to different time integral approximations. Allowing the weights to vary for the standard POD problem will also allow us to apply known results for this approach to new approaches.

The following lemma provides exact formulas for POD data approximation errors using other norms and other projections. We use this result later to provide POD data approximation results for other POD approaches. The proof of Lemma 4.1.1 is very similar to the proof of Theorem 3.3.2 above so we omit it here. For another similar result and proof see [37, Lemma 2.2].

Lemma 4.1.1. *Let* $X_r = \mathrm{span}\{\varphi_k\}_{k=1}^r$ *and* $\Pi_r^X : X \longrightarrow X$ *be the orthogonal projection onto* X_r*. Let* s_X *be the number of positive POD singular values for* K *defined in Equation* (2.2)*. If* Y *is a Hilbert space with* $W \subset Y$ *then*

$$\sum_{j=1}^{M} \gamma_j \|w^j - \Pi_r^X w^j\|_Y^2 = \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i\|_Y^2. \tag{4.3}$$

In addition if $\pi_r : Y \longrightarrow Y$ *is a bounded linear projection onto* X_r *then,*

$$\sum_{j=1}^{M} \gamma_j \|w^j - \pi_r w^j\|_Y^2 = \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - \pi_r \varphi_i\|_Y^2. \tag{4.4}$$

The standard POD approach does not have general bounds for pointwise errors, as shown in [37, Section 3].

4.1.2. POD with Difference Quotients. Another common approach to POD involves the use of difference quotients. Throughout this chapter, we refer to this method as the standard DQ approach. This approach has been studied by many including [18, 37, 38, 40, 64, 65]. We consider backward Euler for the time stepping scheme and the difference quotients.

Let $U = \{u^j\}_{j=1}^N \subset X$ be a given data set. Then the problem is to find an orthonormal basis minimizing the error

$$E_r^{DQ} = \sum_{j=1}^{N} \Delta t \|u^j - \Pi_r^X u^j\|_X^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \Pi_r^X \partial u^j\|_X^2 \tag{4.5}$$

where Δt is the time step and the difference quotients are given by

$$\partial u^j = \frac{u^{j+1} - u^j}{\Delta t}. \tag{4.6}$$

These difference quotients approximate the time derivative of the data in continuous time. The operator that provides the minimizing basis for the error in Equation (4.5) is $K_{DQ} : S \to X$ defined by

$$K_{DQ} f = \sum_{j=1}^{N} \Delta t f^j u^j + \sum_{j=1}^{N-1} \Delta t f^{N+j} \partial u^j. \tag{4.7}$$

This approach uses a total of $M = 2N - 1$ data snapshots which is nearly twice as many as the standard POD approach. Note for this operator we have $K_{DQ} f = K f$ where $w^i = u^i$ and $\gamma_i = \Delta t$ for $i = 1, \ldots N$, and also $w^{N+i} = \partial u^i$ and $\gamma_{N+i} = \Delta t$ for $i = 1, \ldots, N-1$. The resulting POD data set is $\{w^j\}_{j=1}^{M}$, where $M = 2N - 1$. Taking $\{\lambda_j^{DQ}\}_{j=1}^{2N-1}$ to be the POD eigenvalues and keeping the same notation $\{\varphi_j\}$ for the POD basis functions, we get similar results to those for the standard POD operator. When using this new set $\{w^j\}$ as the POD data set, we not only have a set that is nearly twice as large as the original but it can also be checked that the new set is linearly dependent. This redundancy is something we avoid with our new approach introduced in Section 4.2.

Remark 4.1.2. *While the weights can be taken to be any set of positive constants, for simplicity we take them to be the constant Δt. The results in this chapter can be extended to variable weights or other choices of constant weights. One popular choice of constant weight in the literature is M^{-1} as in [37, 38] where M represents the total number of data snapshots for the standard difference quotient approach to POD. Similarly to the standard POD case, with certain choices of weights, one can approximate time integrals with various quadrature rules.*

The following result is also similar to Lemma 2.4 in [37]. We provide it here for completeness.

Lemma 4.1.3. *Let $X_r = \mathrm{span}\{\varphi_k\}_{k=1}^r$ and $\Pi_r^X : X \longrightarrow X$ be the orthogonal projection onto X_r. Let s_X be the number of positive POD singular values for K_{DQ} defined in Equation* (4.7). *We have the following error formula:*

$$\sum_{j=1}^{N} \Delta t \|u^j - \Pi_r^X u^j\|_X^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \Pi_r^X \partial u^j\|_X^2 = \sum_{i=r+1}^{s_X} \lambda_i^{DQ}. \tag{4.8}$$

If Y is a Hilbert space with $U \subset Y$ then

$$\sum_{j=1}^{N} \Delta t \|u^j - \Pi_r^X u^j\|_Y^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \Pi_r^X \partial u^j\|_Y^2 = \sum_{i=r+1}^{s_X} \lambda_i^{DQ} \|\varphi_i\|_Y^2. \tag{4.9}$$

In addition, if $\pi_r : Y \longrightarrow Y$ is a bounded linear projection onto X_r then

$$\sum_{j=1}^{N} \Delta t \|u^j - \pi_r u^j\|_Y^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \pi_r \partial u^j\|_Y^2 = \sum_{i=r+1}^{s_X} \lambda_i^{DQ} \|\varphi_i - \pi_r \varphi_i\|_Y^2. \tag{4.10}$$

Proof. This result follows from Equation (2.5) and Lemma 4.1.1 by taking $\{\lambda_j^{DQ}\}_{j=1}^{s_X}$ as the POD eigenvalues for the POD operator in Equation (4.7). □

We have the following result about the pointwise error bounds for this POD case. A similar result with a different set of constant weights can be found in [37, Theorem 3.7]. The proof of the result below is similar so we omit it here. That theorem was key to obtaining the optimal pointwise POD ROM error bounds which were a main contribution of that work.

Theorem 4.1.4. *Let $X_r = \mathrm{span}\{\varphi_k\}_{k=1}^r$ and $\Pi_r^X : X \longrightarrow X$ be the orthogonal projection onto X_r. Let s_X be the number of positive POD singular values for K_{DQ}. We have*

$$\max_{1 \le j \le N} \|u^j - \Pi_r^X u^j\|_X^2 \le C \left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ} \right). \tag{4.11}$$

If Y is a Hilbert space with $U \subset Y$ then

$$\max_{1 \le j \le N} \|u^j - \Pi_r^X u^j\|_Y^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ} \|\varphi_i\|_Y^2\right). \tag{4.12}$$

If $\pi_r : Y \to Y$ is a bounded linear projection onto X_r then

$$\max_{1 \le j \le N} \|u^j - \pi_r u^j\|_Y^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ} \|\varphi_i - \pi_r \varphi_i\|_Y^2\right) \tag{4.13}$$

where $C = 2\max\{T^{-1}, T\}$.

In Section 4.2.2 we obtain a similar pointwise POD projection error result for the new POD approach described below in Section 4.2.

4.2. A NEW APPROACH

Next, we return to the question posed in the introduction: "Can we obtain all of the same numerical analysis benefits of using DQs with POD using a data set without redundancy?" We obtain a positive answer to this question by introducing a new POD problem and operator. Instead of including all of the POD data snapshots and all of the difference quotients as in Section 4.1.2, we include the first data snapshot and all of the difference quotients. Thus for the data $U = \{u^j\}_{j=1}^N \subset X$, the new POD problem is to minimize the error given by

$$E_r^{DQ1} = \|u^1 - \Pi_r^X u^1\|_X^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \Pi_r^X \partial u^j\|_X^2 \tag{4.14}$$

where the difference quotients are defined by Equation (4.6). Note that the POD error function in Equation (4.14) does not include the weighted sum of the errors of the regular snapshots; this contrasts with the POD approaches in Section 4.1, which both include such error terms, see Equation (2.5) and Equation (4.5). Furthermore, in the POD approaches in Section 4.1, we have exact error formulas for these error terms; see Lemma 4.1.1 and Lemma 4.1.3. In Section 4.2.2, we consider the weighted sum of the errors of the regular snapshots for this new approach and obtain an approximation error result in Corollary 4.2.5.

Note that with this approach we have a total of $N-1$ difference quotients. Together with the single snapshot, we have a total of N data snapshots for this POD problem. This is an improvement from the standard DQ approach to POD which has $2N-1$ data snapshots.

The minimum error can be found using the POD operator:

$$K_1 f = f^1 u^1 + \sum_{j=1}^{N-1} \Delta t f^{j+1} \partial u^j \tag{4.15}$$

We have $K_1 f = Kf$ where $w^1 = u^1$, $\gamma_1 = 1$, $\gamma_{i+1} = \Delta t$, and $w^{i+1} = \partial u^i$ for $i = 1, \ldots, N-1$. We choose to use the constant time step, Δt, as the weight for simplicity throughout. The results can be extended to include variable weights as well. Recall that for certain choices of weights one can approximate a time integral and the difference quotients approximate a time derivative.

Note that in contrast to the data set created for the standard POD approach with DQs, the data set for this new approach is linearly independent if the original data set is linearly independent as shown in Lemma 4.2.1.

Lemma 4.2.1. *If $\{u^i\}_{i=1}^N$ is linearly independent then $\{w^i\}_{i=1}^N$ given by $w^1 = u^1$ and $w^{i+1} = \partial u^i$ for $i = 1, \ldots, N-1$ is linearly independent.*

Proof. We show that if

$$c_1 w^1 + c_2 w^2 + \cdots + c_N w^N = 0$$

then $c_i = 0$ for all $i = 1, \ldots, N$. We have

$$c_1 u^1 + c_2 \left(\frac{u^2 - u^1}{\Delta t} \right) + \cdots + c_i \left(\frac{u^i - u^{i-1}}{\Delta t} \right) + \cdots + c_N \left(\frac{u^N - u^{N-1}}{\Delta t} \right) = 0$$

then

$$\left(c_1 - \frac{c_2}{\Delta t}\right) u^1 + \left(\frac{c_2}{\Delta t} - \frac{c_3}{\Delta t}\right) u^2 + \cdots + \left(\frac{c_{N-1}}{\Delta t} - \frac{c_N}{\Delta t}\right) u^{N-1} + \frac{c_N}{\Delta t} u^N = 0.$$

Since $\{u_i\}$ is linearly independent we know each of these coefficients must equal 0. Solving that system of equations leads to the conclusion that $c_i = 0$ for all $i = 1, \ldots, N$. □

If we let $\{\lambda_j^{DQ1}\}_{j=1}^N$ be the POD eigenvalues for this new POD approach, and let $\{\varphi_k\}_{k=1}^r$ be the POD modes for this data, we get the following error formulas given in Lemma 4.2.2.

Lemma 4.2.2. *Let* $X_r = \mathrm{span}\{\varphi_k\}_{k=1}^r$ *and* $\Pi_r^X : X \longrightarrow X$ *be the orthogonal projection onto* X_r. *Let* s_X *be the number of positive POD singular values for* K_1 *defined in Equation* (4.15). *We have the following formula for the data approximation error:*

$$\|u^1 - \Pi_r^X u^1\|_X^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \Pi_r^X \partial u^j\|_X^2 = \sum_{i=r+1}^{s_X} \lambda_i^{DQ1}. \tag{4.16}$$

If Y *is a Hilbert space with* $U \subset Y$ *then*

$$\|u^1 - \Pi_r^X u^1\|_Y^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \Pi_r^X \partial u^j\|_Y^2 = \sum_{i=r+1}^{s_X} \lambda_i^{DQ1} \|\varphi_i\|_Y^2. \tag{4.17}$$

If in addition $\pi_r : Y \longrightarrow Y$ *is a bounded linear projection onto* X_r *then,*

$$\|u^1 - \pi_r u^1\|_Y^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \pi_r \partial u^j\|_Y^2 = \sum_{i=r+1}^{s_X} \lambda_i^{DQ1} \|\varphi_i - \pi_r \varphi_i\|_Y^2. \tag{4.18}$$

Proof. This result follows from Equation (2.5) and Lemma 4.1.1 by taking $\{\lambda_j^{DQ1}\}_{j=1}^{s_X}$ as the POD eigenvalues for the POD operator in Equation (4.15). □

Preliminary computational results and pointwise error estimates for this new POD approach are discussed in Section 4.2.1 and Section 4.2.2 respectively.

4.2.1. Preliminary Computations. Before moving to our main results we perform some preliminary computations to test the new POD approach with difference quotients. For all computations in this chapter we consider the following test problem.

Test Problem: Consider the one dimensional heat equation

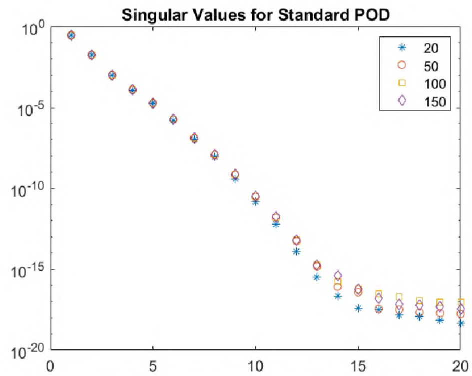
$$u_t - \nu u_{xx} = 0, \text{ in } \Omega \times [0, T]$$

$$u(x, 0) = e^x \sin(\pi x)$$

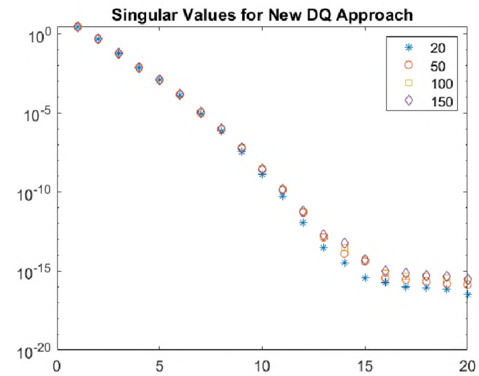
with $\nu = 1$, $\Omega = [0, 1]$, $T = 1$, and zero Dirichlet boundary conditions.

For the data $\{u^j\}$, we compute the solution using the finite element method with linear elements, equally spaced nodes, and backward Euler with a constant time step for the time stepping. The initial condition is taken to be the linear interpolation of the initial condition with respect to the finite element nodes. For this data and with the POD space $X = L^2(\Omega)$, we can calculate the POD modes, POD singular values, and the data approximation errors exactly which allows for comparison between the errors in the formulas from Lemma 4.2.2 and the actual approximation errors. In order to compute the singular value decomposition (SVD) of the POD operator, we use the technique described in [66, Section 2.2] with a minor modification to account for the POD weights. This procedure works well and is highly accurate for smaller data sets; for larger data sets one could use an incremental SVD approach or another related algorithm instead, see e.g. [66, 67, 68, 69, 70] and the references therein.

First we plot the singular values for both the standard POD and our new POD approach that includes one data snapshot and all of the difference quotients. For the standard POD computations we use the data set consisting of only the regular snapshots $\{w^j\}_{j=1}^N = \{u^j\}_{j=1}^N$ and we choose constant weights $\gamma_j = \Delta t$ for $j = 1, \ldots, N$. The singular value plots allow for a quick comparison between the two approaches to POD and are given in Figure 4.1. For each plot, we show the first 20 POD singular values for 20, 50, 100, and



(a) Standard POD



(b) New DQ POD

Figure 4.1. Plot of singular values of POD operators using different numbers of finite element nodes

150 finite element nodes when using 100 equally spaced time steps. The POD singular values decay at a similar rate which indicates that the POD basis for each case has a similar ability to approximate the data.

Next, we consider the data approximation error results given in Lemma 4.2.2 numerically. For these computations we take 200 equally spaced time steps and 100 equally spaced finite element nodes and compute the actual errors and the error formulas. Recall that $X = L^2(\Omega)$ is the POD space and note that here we take either $Y = H_0^1(\Omega)$ or $Y = L^2(\Omega)$. Also note the projection π_r is taken to be the Ritz projection, which we discuss in more detail in Section 4.3. The results are shown for all formulas of Lemma 4.2.2 in Table 4.1 for $r = 4$, $r = 6$, and $r = 8$. For example, the second row for each r value in the table gives the values for

$$\text{actual error } = \|u^1 - \Pi_r^X u^1\|_{H_0^1}^2 + \sum_{j=1}^{N-1} \Delta t \|\partial u^j - \Pi_r^X \partial u^j\|_{H_0^1}^2,$$

and

$$\text{error formula } = \sum_{i=r+1}^{s_X} \lambda_i^{DQ1} \|\varphi_k\|_{H_0^1}^2$$

Table 4.1. Actual Error vs. Error Formulas from Lemma 4.2.2 for New DQ POD

r value	Projection	Norm	Actual Error	Error Formula
4	Π_r^X	$L^2(\Omega)$	9.761e-06	9.761e-06
	Π_r^X	$H_0^1(\Omega)$	6.200e-03	6.200e-03
	π_r	$L^2(\Omega)$	1.736e-05	1.736e-05
	π_r	$H_0^1(\Omega)$	3.100e-03	3.100e-03
6	Π_r^X	$L^2(\Omega)$	5.482e-09	5.482e-09
	Π_r^X	$H_0^1(\Omega)$	1.036e-05	1.036e-05
	π_r	$L^2(\Omega)$	1.133e-08	1.133e-08
	π_r	$H_0^1(\Omega)$	5.159e-06	5.159e-06
8	Π_r^X	$L^2(\Omega)$	1.557e-12	1.557e-12
	Π_r^X	$H_0^1(\Omega)$	4.772e-09	4.772e-09
	π_r	$L^2(\Omega)$	3.481e-12	3.481e-12
	π_r	$H_0^1(\Omega)$	1.659e-09	1.659e-09

with the respective values for r. Round-off errors in the POD computations can cause very small imaginary parts to occur in the error formulas. Thus we report the absolute value of the computed error formulas. Note that the difference between the actual errors and the error formulas is unnoticeable to the given significant digits. These computational results verify what we show analytically. Similar results are achieved when using $X = H_0^1(\Omega)$.

Computational comparisons between all three of the methods can be found in Section 4.4.1 where we consider the errors in the reduced order models.

4.2.2. Pointwise Error Bounds. Using the technique from [37, Lemma 3.6] we establish the following lemma which allows us to directly prove the POD pointwise projection error bounds for the new DQ POD approach and an approximation error result for the weighted sum of the errors of the regular snapshots. These results are necessary to prove the reduced order model error bounds and show their optimality in Section 4.3.

Lemma 4.2.3. *Let $T > 0$, Z be a normed space, $\{z^j\}_{j=1}^N \subset Z$, and $\Delta t = T/(N-1)$. Then*

$$\max_{1\le j\le N} \|z^j\|_Z^2 \le C\left(\|z^1\|_Z^2 + \sum_{\ell=1}^{N-1} \Delta t \|\partial z^\ell\|_Z^2\right) \tag{4.19}$$

where $\partial z^\ell = \frac{z^{\ell+1}-z^\ell}{\Delta t}$ for $\ell = 1,\ldots,N-1$, and $C = 2\max\{T, 1\}$.

Proof. Note using $z^j = z^1 + \sum_{\ell=1}^{j-1} \Delta t(\partial z^\ell)$, we have

$$\|z^j\| \le \|z^1\| + \sum_{\ell=1}^{j-1} \Delta t\|\partial z^\ell\| \le \|z^1\| + \left(\sum_{\ell=1}^{j-1} \Delta t\right)^{1/2} \left(\sum_{\ell=1}^{N-1} \Delta t\|\partial z^\ell\|^2\right)^{1/2}.$$

Then

$$\|z^j\|^2 \le 2\|z^1\|^2 + 2\left(\sum_{\ell=1}^{j-1} \Delta t\right)\left(\sum_{\ell=1}^{N-1} \Delta t\|\partial z^\ell\|^2\right) \le 2\|z^1\|^2 + 2T\sum_{\ell=1}^{N-1} \Delta t\|\partial z^\ell\|^2$$

since $T = \sum_{j=1}^{N-1} \Delta t = (N-1)\Delta t$. Take the maximum over all j and the result follows. □

Next, we obtain a pointwise POD projection error result for the new POD DQ approach that is very similar to Theorem 4.1.4 for the standard POD DQ case.

Theorem 4.2.4. *Let $X_r = \text{span}\{\varphi_k\}_{k=1}^r$ and $\Pi_r^X : X \to X$ be the orthogonal projection onto X_r. Let s_X be the number of positive POD eigenvalues for $U = \{u^j\}_{j=1}^N$. Then*

$$\max_{1\le j\le N} \|u^j - \Pi_r^X u^j\|_X^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\right). \tag{4.20}$$

If Y is a Hilbert space with $U \subset Y$ then

$$\max_{1\le j\le N} \|u^j - \Pi_r^X u^j\|_Y^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\|\varphi_i\|_Y^2\right), \tag{4.21}$$

and in addition if $\pi_r : Y \to Y$ is a bounded linear projection onto X_r then

$$\max_{1\le j\le N} \|u^j - \pi_r u^j\|_Y^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\|\varphi_i - \pi_r\varphi_i\|_Y^2\right) \tag{4.22}$$

where $C = 2\max\{T, 1\}$.

Proof. To prove this theorem take $z^j = u^j - \Pi_r^X u^j$ or $z^j = u^j - \pi_r u^j$ with $Z = X$ or $Z = Y$ in Lemma 4.2.3. For example, if we let $z^j = u^j - \Pi_r^X u^j$ and $Z = X$, then

$$\max_{1\le j\le N} \|u^j - \Pi_r^X u^j\|_X^2 \le C\left(\|u^1 - \Pi_r^X u^1\|_X^2 + \sum_{\ell=1}^{N-1} \Delta t\|\partial u^\ell - \Pi_r^X \partial u^\ell\|_X^2\right) \tag{4.23}$$

Applying Lemma 4.2.2 for each of the three cases gives the result. □

Next, we use the above pointwise error bounds to obtain error bounds for the weighted sum of the errors of the regular snapshots.

Corollary 4.2.5. *Let $X_r = \operatorname{span}\{\varphi_k\}_{k=1}^r$ and $\Pi_r^X : X \to X$ be the orthogonal projection onto X_r. Let s_X be the number of positive POD eigenvalues for U then*

$$\sum_{j=1}^{N} \Delta t\|u^j - \Pi_r^X u^j\|_X^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\right). \tag{4.24}$$

If Y is a Hilbert space with $U \subset Y$ then

$$\sum_{j=1}^{N} \Delta t\|u^j - \Pi_r^X u^j\|_Y^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\|\varphi_i\|_Y^2\right). \tag{4.25}$$

If in addition $\pi_r : Y \to Y$ is a bounded linear projection onto X_r then

$$\sum_{j=1}^{N} \Delta t\|u^j - \pi_r u^j\|_Y^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\|\varphi_i - \pi_r\varphi_i\|_Y^2\right) \tag{4.26}$$

where $C = 4\max\{T^2, T\}$.

Proof. Since

$$N\Delta t = \frac{N}{N-1}[(N-1)\Delta t] = [N/(N-1)]T \leq 2T,$$

we have

$$\sum_{j=1}^{N} \Delta t \|u^j - \Pi_r^X u^j\|_X^2 \leq 2T \max_{1\leq j\leq N} \|u^j - \Pi_r^X u^j\|_X^2.$$

Theorem 4.2.4 gives Equation (4.24). The proofs of Equations (4.25) and (4.26) follow in the same way. □

These results are similar to those for the standard DQ approach while keeping redundancy out of the data set.

4.3. REDUCED ORDER MODELING

In this section we establish theory to compare the reduced order model solution to the backward Euler finite element solution for the heat equation using our new POD with DQs approach. In this section all POD computations are done using the new approach and all function spaces are assumed to be real. Our analysis and proof techniques strongly rely on the approach in [37, Section 4]. We provide proofs to make the work self-contained.

Let $\Omega \subset \mathbb{R}^d$ with $d \geq 1$ be an open bounded domain with Lipschitz continuous boundary, and define $V = H_0^1(\Omega)$. The space V is a Hilbert space with inner product $(g, h)_{H_0^1} = (\nabla g, \nabla h)_{L^2}$. We consider the weak formulation of the heat equation with homogeneous Dirichlet boundary conditions:

$$(\partial_t u, v)_{L^2} + \nu(\nabla u, \nabla v)_{L^2} = (f, v)_{L^2} \quad \forall v \in V \tag{4.27}$$

where $u(\cdot, 0) = u^1$ is the initial condition, ν is a positive constant, and f is a given forcing function. We project Equation (4.27) onto a standard conforming finite element space $V^h \subset V$ and apply backward Euler to obtain

$$\left(\frac{u^{n+1} - u^n}{\Delta t}, v\right)_{L^2} + \nu(\nabla u^{n+1}, \nabla v)_{L^2} = (f^{n+1}, v)_{L^2} \quad \forall v \in V^h. \tag{4.28}$$

We use the data set $\{u^n\}_{n=1}^N \subset V^h$ to compute the POD modes $\{\varphi_j\}_{j=1}^r \subset V^h$ using the new DQ approach with respect to the Hilbert space X. Below we take X to be either $X = L^2(\Omega)$ or $X = H_0^1(\Omega)$. Let $V_r^h = \text{span}\{\varphi_j\}_{j=1}^r$. Next, we develop the POD reduced order model of the heat equation by substituting u_r for the unknown u, using the Galerkin method, and projecting Equation (4.28) onto the space $V_r^h \subset V^h$. Thus we arrive at the following BE-POD-ROM:

$$\left(\frac{u_r^{n+1} - u_r^n}{\Delta t}, v_r\right)_{L^2} + \nu(\nabla u_r^{n+1}, \nabla v_r)_{L^2} = (f^{n+1}, v_r)_{L^2} \quad \forall v_r \in V_r^h. \tag{4.29}$$

We split the error, in the standard way, with

$$e^{n+1} = u^{n+1} - u_r^{n+1} = (u^{n+1} - \pi_r u^{n+1}) - (u_r^{n+1} - \pi_r u^{n+1}) = \eta^{n+1} - \phi_r^{n+1}$$

where π_r is a projection onto V_r^h, $\eta^{n+1} = u^{n+1} - \pi_r u^{n+1}$ is the POD projection error, and $\phi_r^{n+1} = u_r^{n+1} - \pi_r u^{n+1}$ is the discretization error. We subtract Equation (4.29) from Equation (4.28) and make the error substitution given above to get

$$\left(\frac{\phi_r^{n+1} - \phi_r^n}{\Delta t}, v_r\right)_{L^2} + \nu(\nabla \phi_r^{n+1}, \nabla v_r)_{L^2} = \left(\frac{\eta^{n+1} - \eta^n}{\Delta t}, v_r\right)_{L^2} + \nu(\nabla \eta^{n+1}, \nabla v_r)_{L^2} \quad \forall v_r \in V_r^h. \tag{4.30}$$

Remark 4.3.1. *The approach taken here is different than the one taken in [37]. In that work the authors compare the ROM solution u_r^n to the exact solution of the PDE $u(t_n)$. We can bound the error between the ROM solution and the exact solution using the triangle* *inequality*

$$\|u_r^n - u(t_n)\|_Y \leq \|u_r^n - u^n\|_Y + \|u^n - u(t_n)\|_Y$$

where Y is a Hilbert space. The current work focuses on bounding the ROM error term $\|u_r^n - u^n\|_Y$ with $Y = L^2(\Omega)$ or $Y = H_0^1(\Omega)$ and leaves the second term to be studied using well-known finite element theory.

For analysis and computations the initial condition is taken to be the POD projection of the given initial condition, i.e, $u_r^1 = \Pi_r^X u^1$. Other initial conditions are possible and have been considered in other works for the standard POD and DQ POD approaches. For example, in [37], the Ritz projection was used for the initial condition. We now consider each POD space, $L^2(\Omega)$ and $H_0^1(\Omega)$, separately.

4.3.1. POD Space: $L^2(\Omega)$. In this section, we take X to be the space $L^2(\Omega)$. The orthogonal projection onto V_r^h, $\Pi_r^X : L^2(\Omega) \to L^2(\Omega)$, is given by

$$\Pi_r^X u = \sum_{i=1}^{r} (u, \varphi_i)_{L^2} \varphi_i \tag{4.31}$$

and the set of POD modes $\{\varphi_i\}$ are orthogonal in $L^2(\Omega)$. Define π_r to be the Ritz projection R_r which satisfies

$$(\nabla(w - R_r w), \nabla v_r)_{L^2} = 0 \tag{4.32}$$

for all $v_r \in V_r^h$. Thus, for all $w \in V^h$ we have

$$\|w - R_r w\|_{H_0^1} = \inf_{v_r \in V_r^h} \|w - v_r\|_{H_0^1}.$$

Let $\eta_{Ritz}^{n+1} = u^{n+1} - R_r u^{n+1}$. Then Equation (4.30) becomes

$$\left(\frac{\phi_r^{n+1} - \phi_r^n}{\Delta t}, v_r\right)_{L^2} + \nu(\nabla\phi_r^{n+1}, \nabla v_r)_{L^2} = \left(\frac{\eta_{Ritz}^{n+1} - \eta_{Ritz}^n}{\Delta t}, v_r\right)_{L^2} \quad \forall v_r \in V_r^h. \tag{4.33}$$

Using this ROM error equation, we obtain the error bounds given below. Note, the constant C can change from step to step, but it does not depend on any discretization parameter. In Section 4.4.3 we investigate the final value of C computationally.

Theorem 4.3.2. *The pointwise L^2 solution error when the $L^2(\Omega)$ POD basis is used for the BE-POD-ROM is bounded by*

$$\max_k \|e^k\|^2_{L^2} \leq C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\|\varphi_i - R_r\varphi_i\|^2_{L^2} + \|\phi_r^1\|^2_{L^2}\right). \tag{4.34}$$

Proof. Taking $v_r = \phi_r^{n+1}$ in Equation (4.33) yields

$$\left(\frac{\phi_r^{n+1} - \phi_r^n}{\Delta t}, \phi_r^{n+1}\right)_{L^2} + \nu\|\nabla\phi_r^{n+1}\|^2_{L^2} = \left(\frac{\eta_{Ritz}^{n+1} - \eta_{Ritz}^n}{\Delta t}, \phi_r^{n+1}\right)_{L^2}. \tag{4.35}$$

Now, apply Cauchy-Schwartz followed by Young's inequality with a constant δ to get

$$\left(\frac{\phi_r^{n+1} - \phi_r^n}{\Delta t}, \phi_r^{n+1}\right)_{L^2} + \nu\|\nabla\phi_r^{n+1}\|^2_{L^2} \leq \frac{1}{4\delta}\|\partial\eta_{Ritz}^n\|^2_{L^2} + \delta\|\phi_r^{n+1}\|^2_{L^2}. \tag{4.36}$$

Finally apply a polarization identity, use the fact that $C\|\phi_r^{n+1}\|^2_{L^2} \leq \|\nabla\phi_r^{n+1}\|^2_{L^2}$, and rearrange to obtain

$$\left(\frac{1}{2\Delta t} - \delta + \frac{\nu}{C}\right)\|\phi_r^{n+1}\|^2_{L^2} - \frac{1}{2\Delta t}\|\phi_r^n\|^2_{L^2} \leq \frac{1}{4\delta}\|\partial\eta_{Ritz}^n\|^2_{L^2}. \tag{4.37}$$

Taking $\delta = \frac{\nu}{C}$ and multiplying by $2\Delta t$ we get

$$\|\phi_r^{n+1}\|^2_{L^2} - \|\phi_r^n\|^2_{L^2} \leq \frac{C\Delta t}{2\nu}\|\partial\eta_{Ritz}^n\|^2_{L^2}. \tag{4.38}$$

Summing from $n = 1$ to $n = k-1$, using $\|e^n\|^2_{L^2} \leq 2(\|\eta^n\|^2_{L^2} + \|\phi_r^n\|^2_{L^2})$, and rearranging once again gives

$$\|e^k\|^2_{L^2} \leq C\left(\Delta t\sum_{n=1}^{k-1}\|\partial\eta_{Ritz}^n\|^2_{L^2} + \|\eta_{Ritz}^k\|^2_{L^2} + \|\phi_r^1\|^2_{L^2}\right). \tag{4.39}$$

Then apply Lemma 4.2.2 and Theorem 4.2.4 with $Y = L^2(\Omega)$ and $\pi_r = R_r$ to get

$$\|e^k\|_{L^2}^2 \leq C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \|\phi_r^1\|_{L^2}^2\right). \tag{4.40}$$

Take the maximum over all k to get the result. □

Theorem 4.3.3. *The pointwise H_0^1 solution error when the $L^2(\Omega)$ POD basis is used for the BE-POD-ROM is bounded by*

$$\max_k \|\nabla e^k\|_{L^2}^2 \leq C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\left(\|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \|\nabla(\varphi_i - R_r\varphi_i)\|_{L^2}^2\right) + \|\phi_r^1\|_{H_0^1}^2\right). \tag{4.41}$$

Proof. Taking $v_r = \partial\phi_r^n$ in Equation (4.33) gives

$$\left(\frac{\phi_r^{n+1} - \phi_r^n}{\Delta t}, \partial\phi_r^n\right)_{L^2} + \nu\left(\nabla\phi_r^{n+1}, \nabla\partial\phi_r^n\right)_{L^2} = \left(\frac{\eta_{Ritz}^{n+1} - \eta_{Ritz}^n}{\Delta t}, \partial\phi_r^n\right)_{L^2}. \tag{4.42}$$

Rearranging and using the definition of $\partial\phi_r^n$ yields

$$\nu\left(\nabla\phi_r^{n+1}, \nabla\partial\phi_r^n\right)_{L^2} = \left(\frac{\eta_{Ritz}^{n+1} - \eta_{Ritz}^n}{\Delta t}, \partial\phi_r^n\right)_{L^2} - \|\partial\phi_r^n\|_{L^2}^2. \tag{4.43}$$

Then applying first the Cauchy-Schwartz inequality followed by Young's inequality with the constant δ we obtain

$$\begin{aligned}
\nu\left(\nabla\phi_r^{n+1}, \nabla\partial\phi_r^n\right)_{L^2} &\leq \left(\|\partial\eta_{Ritz}^n\|_{L^2}\|\partial\phi_r^{n+1}\|_{L^2}\right) - \|\partial\phi_r^n\|_{L^2}^2 \\
&\leq \left(\frac{1}{4\delta}\|\partial\eta_{Ritz}^n\|_{L^2}^2 + \delta\|\partial\phi_r^n\|_{L^2}^2\right) - \|\partial\phi_r^n\|_{L^2}^2 \\
&= \frac{1}{4\delta}\|\partial\eta_{Ritz}^n\|_{L^2}^2 + (\delta - 1)\|\partial\phi_r^n\|_{L^2}^2.
\end{aligned}$$

Taking the constant $\delta = 1$ yields

$$\nu\left(\nabla\phi_r^{n+1}, \nabla\partial\phi_r^n\right)_{L^2} \leq \frac{1}{4}\|\partial\eta_{Ritz}^n\|_{L^2}^2. \tag{4.44}$$

Also,

$$\Delta t \left(\nabla \phi_r^{n+1}, \nabla \partial \phi_r^n\right)_{L^2} = \frac{1}{2}\left(\|\nabla \phi_r^{n+1}\|_{L^2}^2 + \|\nabla \phi_r^{n+1} - \nabla \phi_r^n\|_{L^2}^2 - \|\nabla \phi_r^n\|_{L^2}^2\right). \tag{4.45}$$

Combining Equation (4.44) and Equation (4.45), summing over $n = 1, \ldots, k-1$, and using $\|\nabla e^k\|_{L^2}^2 \leq 2\left(\|\nabla \eta^k\|_{L^2}^2 + \|\nabla \phi_r^k\|_{L^2}^2\right)$ gives

$$\|\nabla e^k\|_{L^2}^2 \leq C\left(\Delta t \sum_{n=1}^{k-1} \|\partial \eta_{Ritz}^n\|_{L^2}^2 + \|\eta_{Ritz}^k\|_{H_0^1}^2 + \|\phi_r^1\|_{H_0^1}^2\right). \tag{4.46}$$

Then apply Lemma 4.2.2 and Theorem 4.2.4 with $Y = H_0^1(\Omega)$ and $\pi_r = R_r$ to get

$$\|\nabla e^k\|_{L^2}^2 \leq C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \sum_{i=r+1}^{s_X} \lambda_i^{DQ1}\|\varphi_i - R_r\varphi_i\|_{H_0^1}^2 + \|\phi_r^1\|_{H_0^1}^2\right). \tag{4.47}$$

Rearrange and take the maximum over all k to get the result. □

Theorem 4.3.4. *The pointwise solution norm error when the $L^2(\Omega)$ POD basis is used for the BE-POD-ROM is bounded by*

$$\|e^N\|_{L^2}^2 + \nu\Delta t \sum_{n=1}^{N-1} \|e^{n+1}\|_{H_0^1}^2 \leq C\left(\sum_{i=r+1}^{s_X} \lambda^{DQ1}(\|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \|\varphi_i - R_r\varphi_i\|_{H_0^1}^2) + \|\phi_r^1\|_{L^2}^2\right). \tag{4.48}$$

Proof. Taking ϕ_r^{n+1} in Equation (4.33), yields

$$\left(\frac{\phi_r^{n+1} - \phi_r^n}{\Delta t}, \phi_r^{n+1}\right)_{L^2} + \nu\|\nabla \phi_r^{n+1}\|_{L^2}^2 = \left(\frac{\eta_{Ritz}^{n+1} - \eta_{Ritz}^n}{\Delta t}, \phi_r^{n+1}\right)_{L^2}. \tag{4.49}$$

Now, apply the Cauchy-Schwartz inequality, Young's inequality, and a polarization identity to get

$$\frac{1}{2\Delta t}\left(\|\phi_r^{n+1}\|_{L^2}^2 - \|\phi_r^n\|_{L^2}^2\right) + \nu\|\nabla \phi_r^{n+1}\|_{L^2}^2 \leq \frac{1}{4\delta}\|\partial \eta_{Ritz}^n\|_{L^2}^2 + \delta\|\phi_r^{n+1}\|_{L^2}^2. \tag{4.50}$$

Now multiply by 2, apply the Poincaré inequality to the last term, and combine the resulting like terms:

$$\frac{1}{\Delta t}\left(\|\phi_r^{n+1}\|_{L^2}^2 - \|\phi_r^n\|_{L^2}^2\right) + 2\left(\nu - \delta C\right)\|\nabla\phi_r^{n+1}\|_{L^2}^2 \leq \frac{1}{2\delta}\|\partial\eta_{Ritz}^n\|_{L^2}^2. \tag{4.51}$$

Take $\delta = \frac{\nu}{2C}$ and multiply by Δt:

$$\|\phi_r^{n+1}\|_{L^2}^2 - \|\phi_r^n\|_{L^2}^2 + \nu\Delta t\|\nabla\phi_r^{n+1}\|_{L^2}^2 \leq \frac{C\Delta t}{\nu}\|\partial\eta_{Ritz}^n\|_{L^2}^2. \tag{4.52}$$

Sum from $n = 1$ to $k - 1$, rearrange, and take a maximum amoung the constants to obtain

$$\|\phi_r^k\|_{L^2}^2 + \nu\Delta t\sum_{n=1}^{k-1}\|\nabla\phi_r^{n+1}\|_{L^2}^2 \leq C\left(\Delta t\sum_{n=1}^{k-1}\|\partial\eta_{Ritz}^n\|_{L^2}^2 + \|\phi_r^1\|_{L^2}^2\right). \tag{4.53}$$

Using $\|e^n\|_{L^2}^2 \leq 2(\|\eta^n\|_{L^2}^2 + \|\phi_r^n\|_{L^2}^2)$ and rearranging gives

$$\begin{aligned}\|e^k\|_{L^2}^2 &+ \nu\Delta t\sum_{n=1}^{k-1}\|e^{n+1}\|_{H_0^1}^2 \\ &\leq C\left(\Delta t\sum_{n=1}^{k-1}\|\partial\eta_{Ritz}^n\|_{L^2}^2 + \|\eta_{Ritz}^k\|_{L^2}^2 + \Delta t\sum_{n=1}^{k-1}\|\eta_{Ritz}^{n+1}\|_{H_0^1}^2 + \|\phi_r^1\|_{L^2}^2\right).\end{aligned} \tag{4.54}$$

Finally, using Lemma 4.2.2, Theorem 4.2.4, and Corollary 4.2.5 with $\pi_r = R_r$ and both $Y = L^2(\Omega)$ and $Y = H_0^1(\Omega)$ yield

$$\|e^k\|_{L^2}^2 + \nu\Delta t\sum_{n=1}^{k-1}\|e^{n+1}\|_{H_0^1}^2 \leq C\left(\sum_{i=r+1}^{s_X}\lambda^{DQ1}(\|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \|\varphi_i - R_r\varphi_i\|_{H_0^1}^2) + \|\phi_r^1\|_{L^2}^2\right). \tag{4.55}$$

Taking $k = N$ yields the result. □

4.3.2. POD Space: $H_0^1(\Omega)$. Alternatively, we can take the POD space X to be $H_0^1(\Omega)$. The orthogonal projection onto V_r^h, $\Pi_r^X : H_0^1(\Omega) \to H_0^1(\Omega)$, is given by

$$\Pi_r^X u = \sum_{i=1}^{r} (u, \varphi_i)_{H_0^1} \varphi_i \tag{4.56}$$

and the set of POD modes $\{\varphi_i\}$ are orthogonal in $H_0^1(\Omega)$. Note that

$$\Pi_r^X \varphi_k = \sum_{i=1}^{r} (\varphi_k, \varphi_i)_{H_0^1} \varphi_i = 0$$

for $k > r$ since $\{\varphi_k\}$ are orthogonal in $H_0^1(\Omega)$. Further, since Π_r^X is orthogonal we have

$$\begin{aligned} &(w - \Pi_r^X w, v_r)_X = 0 \quad \forall v_r \in V_r^h \\ \implies &(w - \Pi_r^X w, v_r)_{H_0^1} = 0 \quad \forall v_r \in V_r^h \\ \implies &(\nabla(w - \Pi_r^X w), \nabla v_r)_{L^2} = 0 \quad \forall v_r \in V_r^h. \end{aligned}$$

Similarly to before we take π_r to be the Ritz projection, but in this case the Ritz projection is the orthogonal projection Π_r^X, and Equation (4.30) becomes

$$\left(\frac{\phi_r^{n+1} - \phi_r^n}{\Delta t}, v_r \right)_{L^2} + \nu (\nabla \phi_r^{n+1}, \nabla v_r)_{L^2} = \left(\frac{\eta_{Ritz}^{n+1} - \eta_{Ritz}^n}{\Delta t}, v_r \right)_{L^2} \quad \forall v_r \in V_r^h \tag{4.57}$$

where $\eta_{Ritz}^{n+1} = u^{n+1} - R_r u^{n+1} = u^{n+1} - \Pi_r^X u^{n+1}$. As before we can show error bounds for the L^2 and H_0^1 norm errors and the solution norm error.

Theorem 4.3.5. *The ROM solution errors when the $H_0^1(\Omega)$ POD basis is used for the BE-POD-ROM are bounded as follows:*

$$\max_k \|e^k\|_{L^2}^2 \leq C \left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1} \|\varphi_i\|_{L^2}^2 + \|\phi_r^1\|_{L^2}^2 \right), \tag{4.58}$$

$$\max_k \|\nabla e^k\|_{L^2}^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1}(\|\varphi_i\|_{L^2}^2 + 1) + \|\phi_r^1\|_{H_0^1}^2\right), \tag{4.59}$$

and

$$\|e^N\|_{L^2}^2 + \nu\Delta t \sum_{n=1}^{N-1} \|\nabla e^{n+1}\|_{L^2}^2 \le C\left(\sum_{i=r+1}^{s_X} \lambda^{DQ1}(1 + \|\varphi_i\|_{L^2}^2) + \|\phi_r^1\|_{L^2}^2\right). \tag{4.60}$$

Proof. Proceed as in the proofs of Theorem 4.3.2, Theorem 4.3.3, and Theorem 4.3.4 respectively, but now use $\eta_{Ritz} = u - \Pi_r^X u$ and the appropriate choices for Y in Theorem 4.2.4, Corollary 4.2.5, and Lemma 4.2.2. □

4.3.3. Optimality. In this section we investigate the optimality of this new approach to POD with difference quotients. To do so we follow the approach given in [37] but modify the optimality definitions given there to include the ROM error for the initial condition. For this portion of the thesis we focus on both of the POD ROM discretization errors and assume the time and spatial discretization errors are optimal. Thus, we ignore the latter errors in the equation given below. In this section we consider only the new approach as the standard difference quotient approach is discussed in [37]. The optimality of each error depends on both the POD space X and the error norm space Y. To give a precise definition of pointwise ROM error optimality, assume there exists a constant $C > 0$ that is independent of the discretization parameters such that the ROM errors $e^k = u^k - u_r^k$ for $k = 1, \ldots, N$ satisfy

$$\max_{1\le k\le N} \|e^k\|_Y^2 \le C\left(\Lambda_r + \Lambda_r^1\right) \tag{4.61}$$

where

- Λ_r is the ROM discretization error, and depends only on r, the POD eigenvalues, and the POD modes;
- Λ_r^1 is the ROM discretization error for the initial condition, and depends only on r, the POD eigenvalues, and the POD modes.

Let $X_r \subset X$ be the span of the first r POD modes, and assume $X_r \subset Y$. Let $\Pi_r^X : X \longrightarrow X$ be the orthogonal projection onto X_r and $\Pi_r^Y : Y \longrightarrow Y$ be the $Y-$orthogonal projection onto X_r. Further let s_X be the number of positive POD eigenvalues. In Definition 4.3.6 we extend the definitions of optimality provided in [37] to include the ROM discretization error for the initial condition.

Definition 4.3.6. *We say the total ROM discretization error, $\Lambda_r + \Lambda_r^1$, is*

- *optimal-I if there exists a constant C such that*

$$\Lambda_r + \Lambda_r^1 \leq C \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i\|_Y^2, \tag{4.62}$$

- *optimal-II if there exists a constant C such that*

$$\Lambda_r + \Lambda_r^1 \leq C \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - \Pi_r^Y \varphi_i\|_Y^2. \tag{4.63}$$

The constant C can depend on the solution data and the problem data, but does not depend on any discretization parameter.

Remark 4.3.7. *For a detailed discussion on the optimality types see [37]. Note that, as shown in [37, Proposition 4.8], optimal-II is stronger than optimal-I, and the two are equivalent if $X = Y$.*

First we consider the ROM error from the choice of initial condition by noting $\Lambda_r^1 = \|\phi_r^1\|_Y^2$ in Lemma 4.3.8 below.

Lemma 4.3.8. *Let the initial condition be the POD projection of the given initial condition, i.e. $u_r^1 = \Pi_r^X u^1$ so that $\phi_r^1 = u_r^1 - R_r u^1 = \Pi_r^X u^1 - R_r u^1$. If $X = L^2(\Omega)$ then*

$$\|\phi_r^1\|_{L^2}^2 \leq 2 \sum_{i=r+1}^{s_X} \lambda_i + 2 \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - R_r \varphi_i\|_{L^2}^2 \tag{4.64}$$

and

$$\|\phi_r^1\|_{H_0^1}^2 \leq 2 \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i\|_{H_0^1}^2 + 2 \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - R_r \varphi_i\|_{H_0^1}^2. \tag{4.65}$$

If $X = H_0^1(\Omega)$*, then*

$$\phi_r^1 = 0 \tag{4.66}$$

for either choice of space Y*.*

Proof. First consider the case $X = L^2(\Omega)$. We have

$$\begin{aligned}
\|\phi_r^1\|_Y^2 &= \|u_r^1 - R_r u^1\|_Y^2 \\
&= \|\Pi_r^X u^1 - R_r u^1\|_Y^2 \\
&\leq 2\|\Pi_r^X u^1 - u^1\|_Y^2 + 2\|u^1 - R_r u^1\|_{L^2}^2.
\end{aligned}$$

Using Lemma 4.2.2 with $Y = X = L^2(\Omega)$ and $\pi_r = R_r$ gives Equation (4.64) and with $Y = H_0^1(\Omega)$ and $\pi_r = R_r$ gives Equation (4.65). Finally if $X = H_0^1(\Omega)$, then $\Pi_r^X = R_r$ and Equation (4.66) follows by definition of π_r. □

This lemma allows us to investigate the total ROM discretization error in the following two theorems with the POD space taken to be L^2 and H_0^1 respectively.

Theorem 4.3.9. *If the* L^2 *POD basis is used, i.e.* $X = L^2(\Omega)$*, then the following hold:*

- *The pointwise ROM error in Equation* (4.34) *with the error norm* $Y = L^2$ *is optimal-I if there exists a constant C such that*

$$\|\varphi_i - R_r \varphi_i\|_{L^2} \leq C \tag{4.67}$$

  for $r + 1 \leq i \leq s_X$*. Note that in this case optimal-I is equivalent to optimal-II.*

- *The pointwise ROM error in Equation* (4.41) *with error norm* $Y = H_0^1$ *is optimal-I.*

Remark 4.3.10. *In [37, Theorem 4.10 (iv)], when using the* L^2 *POD basis with* $Y = H_0^1(\Omega)$ *but not considering the initial condition error the ROM error was optimal-II. When including the initial condition as the POD projection of the given initial condition, we obtain the* *weaker result that the error is optimal-I. Other choices of initial condition will yield different results. Further, the assumption Equation* (4.67) *is discussed in greater detail in [37, Section 4.2].*

Proof. For the first item

$$\begin{aligned}
\Lambda_r + \Lambda_r^1 &= \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \|\phi_r^1\|_{L^2}^2 \\
&\le \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - R_r\varphi_i\|_{L^2}^2 + 2\left(\sum_{i=r+1}^{s_X} \lambda_i + \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - R_r\varphi_i\|_{L^2}^2\right) \\
&\le C \sum_{i=r+1}^{s_X} \lambda_i \\
&= C \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i\|_{L^2}^2
\end{aligned}$$

using Lemma 4.3.8, the assumption in Equation (4.67), Theorem 4.2.4, and the L^2 orthonormality of the POD basis.

For the second item use the Poincaré inequality to get,

$$\begin{aligned}
\Lambda_r + \Lambda_r^1 &= \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \sum_{i=r+1}^{s_X} \lambda_i \|\nabla(\varphi_i - R_r\varphi_i)\|_{L^2}^2 + \|\phi_r^1\|_{H_0^1}^2 \\
&\le C \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - R_r\varphi_i\|_{H_0^1}^2 + \|\phi_r^1\|_{H_0^1}^2.
\end{aligned}$$

Lemma 4.3.8 and the orthogonality of the Ritz projection $R_r : H_0^1 \to H_0^1$ then yields

$$\Lambda_r + \Lambda_r^1 \le C \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i - R_r\varphi_i\|_{H_0^1}^2 + C \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i\|_{H_0^1}^2 \le C \sum_{i=r+1}^{s_X} \lambda_i \|\varphi_i\|_{H_0^1}^2.$$

Thus the error given in Equation (4.41) is optimal-I. □

Theorem 4.3.11. *If the H_0^1 POD basis is used, i.e. $X = H_0^1$, then the following results hold.*

- *The pointwise ROM error in Equation* (4.58) *with the error norm $Y = L^2$ is optimal-I.*

- *The pointwise ROM error in Equation* (4.58) *with error norm* $Y = L^2$ *is also optimal-II when*

$$\|\varphi_i\|_Y \leq C\|\varphi_i - \Pi_r^Y \varphi_i\|_Y \quad \textit{for } r+1 \leq i \leq s_X.$$

- *The pointwise ROM error in Equation* (4.59) *with the error norm* $Y = H_0^1$ *is optimal-I. Note that in this case optimal-I is equivalent to optimal-II.*

The proof of this result is similar to that of [37, Theorem 4.10] since from Lemma 4.3.8 we know $\phi_r^1 = 0$ for both $Y = L^2$ and $Y = H_0^1$. We omit the details. We note that the optimality results for the new POD DQ approach in Theorem 4.3.9 and Theorem 4.3.11 are very similar to [37, Theorem 4.10] for the standard POD DQ approach. In fact, the only fundamental difference in the results here was caused by our choice of the initial condition and including this in the optimality definition, as discussed in Remark 4.3.10.

4.4. NUMERICAL RESULTS

We now turn our attention to computational results. In this section we use the same test problem as in Section 4.2.1 to compute ROM solution errors in order to compare the new POD approach to the existing standard approaches. We also compute the scaling factors present in the bounds of the theoretical results from Theorem 4.2.4 and Section 4.3.

4.4.1. ROM Comparisons for the Three POD Approaches. First we find the ROM errors for the new POD DQ approach at the final time, i.e., the errors at $T = 1$. We compute both the L^2 norm error and the $H_0^1(\Omega)$ norm error. For this computation we use 100 finite element nodes, 100 time steps and 3 different values for r. Note that in all tables below we report the square of the norms for consistency with previous results. For comparison we also show the final time errors for the standard POD approach and the standard DQ POD approach. First we consider the case where the POD space is taken to be $X = L^2(\Omega)$. The results for the L^2 and H_0^1 errors can be found in Table 4.2 and Table 4.3

Table 4.2. ROM errors for the L^2 Norm at the final time

POD Space	r value	Standard POD	Standard DQ POD	New DQ POD
L^2	4	1.639e-08	1.206e-07	1.141e-07
	6	1.257e-10	1.148e-09	1.090e-09
	8	9.486e-13	9.144e-12	8.722e-12
H_0^1	4	1.851e-08	1.350e-07	1.276e-07
	6	1.324e-10	1.218e-09	1.156e-09
	8	9.999e-13	9.778e-12	9.323e-12

Table 4.3. ROM errors for the H_0^1 Norm at the final time

POD Space	r value	Standard POD	Standard DQ POD	New DQ POD
L^2	4	1.936e-07	1.340e-06	1.269e-06
	6	2.615e-09	2.364e-08	2.245e-08
	8	2.264e-11	2.123e-10	2.024e-10
H_0^1	4	2.171e-07	1.494e-06	1.413e-06
	6	2.755e-09	2.506e-08	2.379e-08
	8	2.396e-11	2.263e-10	2.157e-10

respectively. In Table 4.4, we compute the solution norm squared errors for this reduced order model using the same computation parameters. This solution norm error at the final time is given by Equation (4.68):

$$\|e^N\|_{L^2}^2 + \Delta t \sum_{n=1}^{N-1} \|\nabla e^{n+1}\|_{L^2}^2. \tag{4.68}$$

We also wish to compare the different POD approaches when we take the POD space to be $H_0^1(\Omega)$, i.e., $X = H_0^1(\Omega)$. All other parameters of the computation stay the same and the results can also be found in Table 4.2, Table 4.3, and Table 4.4. For both cases of the chosen POD space the errors behave similarly in all three approaches but are particularly close in the two approaches that utilize the difference quotients.

Table 4.4. ROM solution norm error Equation (4.68)

POD Space	r value	Standard POD	Standard DQ POD	New DQ POD
L^2	4	1.172e-07	2.441e-06	2.008e-06
	6	1.472e-11	4.373e-10	3.576e-10
	8	7.032e-16	2.227e-14	1.810e-14
H_0^1	4	1.135e-07	3.049e-06	2.525e-06
	6	1.467e-11	4.861e-10	3.996e-10
	8	6.984e-16	2.479e-14	2.032e-14

4.4.2. Pointwise Error Bounds. We want to compute the ratios generated by the theoretical results in Section 4.2.2. For these results we vary the number of time steps, while keeping everything else constant. This allows us to verify that the scaling factors are not dependent on the time step chosen. We performed similar experiments by varying other parameters and obtained similar results. We use 100 finite element nodes and an r value of 4. Both $X = L^2(\Omega)$ and $X = H_0^1(\Omega)$ are considered in this section. We use the data generated by the finite element method as described in Section 4.2.1 and compute the POD modes and POD singular values.

First, we consider the pointwise error bounds as in Theorem 4.2.4. The tables show the projection and the norm space Y that is used for each of the computations. Note that for these we have $\pi_r = R_r$ and either $Y = L^2(\Omega)$ or $Y = H_0^1(\Omega)$. For example, for the second result in Theorem 4.2.4 with $X = L^2(\Omega)$ and $Y = H_0^1(\Omega)$ we have

$$\text{scaling factor} = \left(\max_j \|u^j - \Pi_r^X u^j\|_Y^2\right) / \left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1} \|\varphi_i\|_Y^2\right).$$

Table 4.5. Scaling factors for Theorem 4.2.4 as Δt changes with $X = L^2(\Omega)$

Projection	Y	1/40	1/50	1/100	1/200	1/300
Π_r^X	$L^2(\Omega)$	6.0e-02	5.4e-02	4.0e-02	3.2e-02	2.9e-02
Π_r^X	$H_0^1(\Omega)$	5.6e-02	4.9e-02	3.3e-02	2.3e-02	1.8e-02
R_r	$L^2(\Omega)$	5.8e-02	5.2e-02	3.7e-02	2.9e-02	2.5e-02
R_r	$H_0^1(\Omega)$	5.5e-02	4.9e-02	3.2e-02	2.1e-02	1.6e-02

Table 4.6. Scaling factors for Theorem 4.2.4 as Δt changes with $X = H_0^1(\Omega)$

Projection	Y	1/40	1/50	1/100	1/200	1/300
Π_r^X	$L^2(\Omega)$	6.5e-02	5.8e-02	4.2e-02	3.1e-02	2.6e-02
Π_r^X	$H_0^1(\Omega)$	6.8e-02	6.2e-02	4.8e-02	4.0e-02	3.6e-02
R_r	$L^2(\Omega)$	6.5e-02	5.9e-02	4.3e-02	3.3e-02	2.8e-02
R_r	$H_0^1(\Omega)$	7.0e-02	6.4e-02	5.1e-02	4.4e-02	4.1e-02

The results for $X = L^2(\Omega)$ and $X = H_0^1(\Omega)$ are given in Table 4.5 and Table 4.6 respectively. We present the results with fixed values of $r = 4$ and 100 finite element nodes and varying values of Δt. Theoretically, we showed that the scaling factor should always be less that or equal to 2 (since $T = 1$ here). The computational results show that the scaling factor can be much less than that value.

4.4.3. ROM Error Bounds. Next we consider the reduced order model error bounds from Section 4.3. Again we use 100 finite element nodes and $r = 4$ with varying values of Δt. First define the following values:

$$\text{err}_1 = \max_k \|e^k\|_{L^2}^2,$$

$$\text{err}_2 = \max_k \|e^k\|_{H_0^1}^2,$$

and

$$\text{err}_3 = \|e^N\|_{L^2}^2 + \Delta t \sum_{n=1}^{N-1} \|\nabla e^{n+1}\|_{L^2}^2.$$

Table 4.7. Scaling factors as Δt changes for ROM errors

Δt	1/40	1/50	1/100	1/200	1/300
C_1	5.8e-02	5.1e-02	3.7e-02	2.8e-02	2.5e-02
C_2	1.0e-05	1.4e-05	2.9e-05	4.0e-05	4.3e-05
C_3	1.9e-06	2.4e-06	4.1e-05	5.2e-06	5.3e-06
C_4	6.7e-02	6.1-e02	4.7e-02	4.0e-02	3.6e-02
C_5	6.5e-02	5.8e-02	4.1e-02	3.0e-02	2.6e-02
C_6	1.1e-02	9.3e-03	5.7e-03	3.8e-03	3.1e-03

For the first set of scaling factors defined in Equation (4.69), Equation (4.70), and Equation (4.71) below we have $X = L^2(\Omega)$. We also compute the scaling factors for the results that use $X = H_0^1(\Omega)$ as the POD space. These scaling factors for the $X = H_0^1(\Omega)$ case are given by Equations (4.72) to (4.74). For these computations we once again vary the time steps and keep all other parameters constant. The results for both cases of POD basis space can be found in Table 4.7.

$$C_1 = \text{err}_1 / \left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1} \|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \|\phi_r^1\|_{L^2}^2 \right) \tag{4.69}$$

$$C_2 = \text{err}_2 / \left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1} \left(\|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \|\nabla(\varphi_i - R_r\varphi_i)\|_{L^2}^2 \right) + \|\phi_r^1\|_{H_0^1}^2 \right) \tag{4.70}$$

$$C_3 = \text{err}_3 / \left(\sum_{i=r+1}^{s_X} \lambda^{DQ1} (\|\varphi_i - R_r\varphi_i\|_{L^2}^2 + \|\nabla(\varphi_i - R_r\varphi_i)\|_{L^2}^2) + \|\phi_r^1\|_{L^2}^2 \right) \tag{4.71}$$

$$C_4 = \text{err}_1 / \left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1} \|\varphi_i\|_{L^2}^2 + \|\phi_r^1\|_{L^2}^2 \right) \tag{4.72}$$

$$C_5 = \mathrm{err}_2 / \left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1} (\|\varphi_i\|_{L^2}^2 + 1) + \|\phi_r^1\|_{H_0^1}^2 \right) \tag{4.73}$$

$$C_6 = \mathrm{err}_3 / \left(\sum_{i=r+1}^{s_X} \lambda_i^{DQ1} (1 + \|\varphi_i\|_{L^2}^2) + \|\phi_r^1\|_{L^2}^2 \right) \tag{4.74}$$

Note that changing the number of finite element nodes and keeping the number of time steps constant yields similar results. Theoretically we showed the scaling factors should remain bounded, and these computational results support that. For the computations in Section 4.4.2 and Section 4.4.3, we note that for larger values of r some of the projection errors, ROM errors, and error formulas become extremely small. In such cases some of the computed scaling factors are very large, but we believe this is caused by round off errors.

5. CONCLUSIONS

In this dissertation, we first prove new generalized error formulas for POD data approximation errors for both the discrete and continuous cases. We also show convergence of these errors under certain conditions and obtain new pointwise convergence results for POD projections. We demonstrate the application of our results to several example problems. We leave the application of these results to the numerical analysis of POD model order reduction methods for PDEs to be considered elsewhere.

Some open questions remain. When L^{-1} is unbounded, we have to assume uniform boundedness of the POD projections $\{L^{-1}\Pi_r^Y L\}$ to show that the error formula in (3.20) converges to zero as r increases. We do not know if there is a simpler condition that yields convergence of the approximation error. If L or L^{-1} is unbounded, we also do not know if the POD projections $\{L\Pi_r^X L^{-1}\}$ and $\{L^{-1}\Pi_r^Y L\}$ are uniformly bounded. Both of these issues have been discussed in the context of Example 2 in Section 3.5.2.2 in [1, 21]. The second issue has also been discussed in the context of Example 1 in Section 3.5.2.1 in [30, 39]; in these works, the H^1 stability of the L^2 POD projection is of interest.

Then, we introduce a new approach to POD using the difference quotients of the snapshot data. Specifically, we derive the POD modes from a data set that includes only the first snapshot and the regular difference quotients. This data set has approximately half the number of snapshots as the standard POD with DQ approach; also, this data set does not include redundant data when the snapshots are linearly independent. For this new approach to POD with DQs, we prove an approximation result for the weighted sum of the POD projection errors of the regular snapshots, and we also prove that we retain all of the numerical analysis benefits of using DQs that were shown in [37] for the standard POD with DQ approach. Our numerical experiments for a heat equation test problem show that this new approach produces similar reduced order model errors to other known POD approaches.

The latter part of this work focuses on numerical analysis results concerning pointwise POD projection errors and the optimality of pointwise in time ROM errors for our new approach to POD with DQs. Further investigation is needed to determine how this new approach compares to other standard POD methods in practical computations. The size of the ROM errors is not considered here and more research is needed to compare the size of the ROM error in this case with those of standard POD and standard DQ POD.

Also, we consider only one PDE and one choice of difference quotient. We focus on the heat equation and leave the Navier-Stokes equations and other more complicated PDEs to be considered elsewhere. Additionally, in this work we consider the difference quotients obtained when using backward Euler for time stepping. Other difference quotients are possible and have been used for snapshot collection in [31, 41, 46]. It is possible that results in this thesis can be extended to these other difference quotients, but we leave that to be considered elsewhere.

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