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POD for Linear-Quadratic Optimal Control

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1 The POD method

Throughout the lecture we suppose that X is a real Hilbert space (cf. [DR12, Definition 12.15]) endowed with the inner product $\langle\cdot\,,\cdot\rangle_X$ and the associated induced norm $\|\cdot\|_X = \langle\cdot\,,\cdot\rangle_X^{1/2}$. Furthermore, we assume that X is *separable*, i.e., X has a countable dense subset; [DR12, Definition 11.3]. This implies that X possesses a countable orthonormal basis; see, e.g., [DR12, Definition 12.30]. For the POD method in complex Hilbert spaces we refer to [Vol01], for instance.

1.1 The discrete variant of the POD method

For fixed $n, \wp \in \mathbb{N}$ let the so-called *snapshots* $y_1^k, \ldots, y_n^k \in X$ be given for $1 \le k \le \wp$. To avoid a trivial case we suppose that at least one of the y_j^k's is nonzero. Then, we introduce the finite dimensional, linear subspace

$$\mathcal{V}^n = \operatorname{span}\Big\{y_j^k \,\Big|\, 1 \le j \le n \text{ and } 1 \le k \le \wp\Big\} \subset X \tag{1.1}$$

with dimension $d^n \in \{1, \ldots, n\wp\} < \infty$. We call the set $\mathcal{V}^n$ *snapshot subspace*.

Remark 1.1. Later we will focus on the following application: Let $0 \le t_1 < t_2 < \ldots < t_n \le T$ be a given time grid in the interval $[0, T]$. To simplify of the presentation, the time grid is assumed to be equidistant with step-size $\Delta t = T/(n-1)$, i.e., $t_j = (j-1)\Delta t$. For nonequidistant grids we refer the reader to [KV02a, KV02b]. Suppose that we have trajectories $y^k \in C([0, T]; X)$, $1 \le k \le \wp$. Here, the Banach space $C([0, T]; X)$ contains all functions $\varphi : [0, T] \to X$, which are continuous on $[0, T]$ with the norm

$$\|\varphi\|_{C([0,T];X)} = \max\Big\{\|\varphi(t)\|_X \,\Big|\, t \in [0, T]\Big\} \quad \text{for } \varphi \in C([0, T]; X);$$

see, e.g., [Tro09, p. 114]. Let the snapshots be given as $y_j^k = y^k(t_j) \in X$ or $y_j^k \approx y^k(t_j) \in X$. In Sections 2 and 3 we will choose trajectories as solutions to evolution problems. $\Diamond$

In Section 1.3 we consider the case, where the number n is varied. Therefore, we emphasize this dependence by using the super index n. We distinguish two cases:

1) The separable Hilbert space X has finite dimension m. Then, X is isomorphic to $\mathbb{R}^m$. We set $\mathbb{I} = \{1, \ldots, m\}$. Clearly, we have $d^n \le \min(n\wp, m)$.
2) Since X is separable, each orthonormal basis of X has countably many elements. In this case X is isomorphic to the set ℓ_2 of sequences $\{x_i\}_{i\in\mathbb{N}}$ of real numbers which satisfy $\sum_{i=1}^\infty |x_i|^2 < \infty$; see [DR12, Beispiel 12.14-(ii)], for instance. Then, we define $\mathbb{I} = \mathbb{N}$.

The method of POD consists in choosing an orthonormal set $\{\psi_i\}_{i=1}^\ell$ in X such that for every $\ell \in \{1, \ldots, d^n\}$ the mean square error between the $n\wp$ elements y_j^k and their corresponding ℓ-th partial Fourier sum is minimized on average:

$$\min \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j^n \Big\|y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i\rangle_X\, \psi_i\Big\|_X^2 \text{ s.t. } \{\psi_i\}_{i=1}^\ell \subset X \text{ and } \langle\psi_i, \psi_j\rangle_X = \delta_{ij},\ 1 \le i, j \le \ell, \tag{$\mathbf{P}_n^\ell$}$$

where the α_j^n's denote positive weighting parameters and 's.t.' stands for 'subject to'. Here, the symbol δ_{ij} denotes the Kronecker symbol satisfying $\delta_{ii} = 1$ and $\delta_{ij} = 0$ for $i \ne j$. An optimal solution $\{\bar\psi_i^n\}_{i=1}^\ell$ to $(\mathbf{P}_n^\ell)$ is called a *POD basis* of *rank* ℓ, which can be extended to a complete orthonormal basis $\{\psi_i\}_{i\in\mathbb{I}}$ in the Hilbert space X. Notice that

$$
\begin{aligned}
&\Big\|y_j^k-\sum_{i=1}^\ell\langle y_j^k,\psi_i\rangle_X\,\psi_i\Big\|_X^2\\
&=\Big\langle y_j^k-\sum_{i=1}^\ell\langle y_j^k,\psi_i\rangle_X\,\psi_i,y_j^k-\sum_{l=1}^\ell\langle y_j^k,\psi_l\rangle_X\,\psi_l\Big\rangle_X\\
&=\|y_j^k\|_X^2-2\sum_{i=1}^\ell\langle y_j^k,\psi_i\rangle_X^2+\sum_{i=1}^\ell\sum_{l=1}^\ell\langle y_j^k,\psi_i\rangle_X\langle y_j^k,\psi_l\rangle_X\langle\psi_i,\psi_l\rangle_X\\
&=\|y_j^k\|_X^2-\sum_{i=1}^\ell\langle y_j^k,\psi_i\rangle_X^2
\end{aligned}
\tag{1.2}
$$

holds for any set $\{\psi_i\}_{i=1}^\ell\subset X$ satisfying $\langle\psi_i,\psi_j\rangle_X=\delta_{ij}$. Thus, $(\mathbf{P}_n^\ell)$ is equivalent with the maximization problem

$$
\max\sum_{k=1}^\wp\sum_{j=1}^n\alpha_j^n\sum_{i=1}^\ell\langle y_j^k,\psi_i\rangle_X^2\quad\text{s.t.}\quad\{\psi_i\}_{i=1}^\ell\subset X\text{ and }\langle\psi_i,\psi_j\rangle_X=\delta_{ij},\ 1\le i,j\le\ell. \tag{$\hat{\mathbf{P}}_n^\ell$}
$$

Suppose that $\{\psi_i\}_{i\in\mathbb{I}}$ is a complete orthonormal basis in X. Since X is separable, any $y_j^k\in X$, $1\le j\le n$ and $1\le k\le\wp$, can be written as

$$
y_j^k=\sum_{i\in\mathbb{I}}\langle y_j^k,\psi_i\rangle_X\,\psi_i \tag{1.3}
$$

and the (probably infinite) sum converges for all snapshots (even for all elements in X). Thus, the POD basis $\{\bar\psi_i^n\}_{i=1}^\ell$ of rank ℓ maximizes the absolute values of the first ℓ Fourier coefficients $\langle y_j^k,\psi_i\rangle_X$ for all $n\wp$ snapshots y_j^k in an average sense. Let us recall the following definition for linear operators in Banach spaces; cf. [DR11, Definition 10.16] and [DR12, Definition 13.18].

Definition 1.2. *Let $\mathcal{B}_1$, $\mathcal{B}_2$ be two real Banach spaces. The operator $\mathcal{T}:\mathcal{B}_1\to\mathcal{B}_2$ is called a* linear, bounded operator *if these two conditions are satisfied:*

1) *$\mathcal{T}(\alpha u+\beta v)=\alpha\mathcal{T}u+\beta\mathcal{T}v$ for all α, $\beta\in\mathbb{R}$ and u, $v\in\mathcal{B}_1$.*
2) *There exists a constant $c>0$ such that $\|\mathcal{T}u\|_{\mathcal{B}_2}\le c\,\|u\|_{\mathcal{B}_1}$ for all $u\in\mathcal{B}_1$.*

The set of all linear, bounded operators from $\mathcal{B}_1$ to $\mathcal{B}_2$ is denoted by $\mathcal{L}(\mathcal{B}_1,\mathcal{B}_2)$ which is a Banach space equipped with the operator norm

$$
\|\mathcal{T}\|_{\mathcal{L}(\mathcal{B}_1,\mathcal{B}_2)}=\sup_{\|u\|_{\mathcal{B}_1}=1}\|\mathcal{T}u\|_{\mathcal{B}_2}\quad\textit{for }\mathcal{T}\in\mathcal{L}(\mathcal{B}_1,\mathcal{B}_2).
$$

If $\mathcal{B}_1=\mathcal{B}_2$ holds, we briefly write $\mathcal{L}(\mathcal{B}_1)$ instead of $\mathcal{L}(\mathcal{B}_1,\mathcal{B}_2)$. The dual mapping *$\mathcal{T}':\mathcal{B}_2'\to\mathcal{B}_1'$ of an operator $\mathcal{T}\in\mathcal{L}(\mathcal{B}_1,\mathcal{B}_2)$ is defined as*

$$
\langle\mathcal{T}'f,u\rangle_{\mathcal{B}_1',\mathcal{B}_1}=\langle f,\mathcal{T}u\rangle_{\mathcal{B}_2',\mathcal{B}_2}\quad\textit{for all }(u,f)\in\mathcal{B}_1\times\mathcal{B}_2',
$$

where, for instance, $\langle\cdot\,,\cdot\rangle_{\mathcal{B}_1',\mathcal{B}_1}$ denotes the dual pairing of the space $\mathcal{B}_1$ with its dual space $\mathcal{B}_1'=\mathcal{L}(\mathcal{B}_1,\mathbb{R})$.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ denote two real Hilbert spaces. For a given $\mathcal{T}\in\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)$ the *adjoint operator* $\mathcal{T}^\star:\mathcal{H}_2\to\mathcal{H}_1$ is uniquely defined by

$$
\langle\mathcal{T}^\star v,u\rangle_{\mathcal{H}_1}=\langle v,\mathcal{T}u\rangle_{\mathcal{H}_2}=\langle\mathcal{T}u,v\rangle_{\mathcal{H}_2}\quad\text{for all }(u,v)\in\mathcal{H}_1\times\mathcal{H}_2.
$$

Let $\mathcal{J}_i : \mathcal{H}_i \to \mathcal{H}_i'$, $i = 1, 2$, denote the *Riesz isomorphisms* satisfying

$$\langle u, v\rangle_{\mathcal{H}_i} = \langle \mathcal{J}_i u, v\rangle_{\mathcal{H}_i',\mathcal{H}_i} \quad \text{for all } u, v \in \mathcal{H}_i.$$

Then, we have

$$\begin{aligned}\langle \mathcal{T}^\star v, u\rangle_{\mathcal{H}_1} &= \langle v, \mathcal{T}u\rangle_{\mathcal{H}_2} = \langle \mathcal{J}_2 v, \mathcal{T}u\rangle_{\mathcal{H}_2',\mathcal{H}_2} = \langle \mathcal{T}'\mathcal{J}_2 v, u\rangle_{\mathcal{H}_1',\mathcal{H}_1}\\ &= \langle \mathcal{J}_1^{-1}\mathcal{T}'\mathcal{J}_2 v, u\rangle_{\mathcal{H}_1} \quad \text{for all } (u, v) \in \mathcal{H}_1 \times \mathcal{H}_2.\end{aligned}$$

Consequently, $\mathcal{T}^\star = \mathcal{J}_1^{-1}\mathcal{T}'\mathcal{J}_2$ holds. Moreover, $(\mathcal{T}^\star)^\star = \mathcal{T}$ for every $\mathcal{T} \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$. If $\mathcal{T} = \mathcal{T}^\star$ holds, $\mathcal{T}$ is said to be *selfadjoint*. The operator $\mathcal{T} \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ is called *nonnegative* if $\langle \mathcal{T}u, u\rangle_{\mathcal{H}_2} \geq 0$ for all $u \in \mathcal{H}_1$. Finally, $\mathcal{T} \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ is called *compact* if for every bounded sequence $\{u_n\}_{n\in\mathbb{N}} \subset \mathcal{H}_1$ the sequence $\{\mathcal{T}u_n\}_{n\in\mathbb{N}} \subset \mathcal{H}_2$ contains a convergent subsequence.

Now we turn to $(\mathbf{P}_n^\ell)$ and $(\hat{\mathbf{P}}_n^\ell)$. We make use of the following lemma.

Lemma 1.3. *Let X be a (separable) real Hilbert space and $y_1^k, \ldots, y_n^k \in X$ are given snapshots for $1 \leq k \leq \wp$. Define the linear operator $\mathcal{R}^n : X \to X$ as follows:*

$$\mathcal{R}^n\psi = \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j^n \,\langle \psi, y_j^k\rangle_X\, y_j^k \quad \textit{for } \psi \in X \tag{1.4}$$

with positive weights $\alpha_1^n, \ldots, \alpha_n^n$. Then, $\mathcal{R}^n$ is a compact, nonnegative and selfadjoint operator.

Proof. It is clear that $\mathcal{R}^n$ is a linear operator. From

$$\|\mathcal{R}^n\psi\|_X \leq \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j^n \big|\langle \psi, y_j^k\rangle_X\big|\, \|y_j^k\|_X \quad \text{for } \psi \in X$$

and the *Cauchy-Schwarz inequality* [DR12, Satz 12.17]

$$\big|\langle \varphi, \phi\rangle_X\big| \leq \|\varphi\|_X\|\phi\|_X \quad \text{for } \varphi,\, \phi \in X$$

we conclude that $\mathcal{R}^n$ is bounded. Since $\mathcal{R}^n\psi \in \mathcal{V}^n$ holds for all $\psi \in X$, the range of $\mathcal{R}^n$ is finite dimensional. Thus, $\mathcal{R}^n$ is a *finite rank operator* which is compact; see [DR12, Satz 19,2-(iii)]. Next we show that $\mathcal{R}^n$ is nonnegative. For that purpose we choose an arbitrary element $\psi \in X$ and consider

$$\langle \mathcal{R}^n\psi, \psi\rangle_X = \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j^n \,\langle \psi, y_j^k\rangle_X \,\langle y_j^k, \psi\rangle_X = \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j^n \,\langle \psi, y_j^k\rangle_X^2 \geq 0.$$

Thus, $\mathcal{R}^n$ is nonnegative. For any $\psi, \tilde{\psi} \in X$ we derive

$$\begin{aligned}\langle \mathcal{R}^n\psi, \tilde{\psi}\rangle_X &= \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j^n \,\langle \psi, y_j^k\rangle_X \,\langle y_j^k, \tilde{\psi}\rangle_X = \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j^n \,\langle \tilde{\psi}, y_j^k\rangle_X \,\langle y_j^k, \psi\rangle_X\\ &= \langle \mathcal{R}^n\tilde{\psi}, \psi\rangle_X = \langle \psi, \mathcal{R}^n\tilde{\psi}\rangle_X.\end{aligned}$$

Thus, $\mathcal{R}^n$ is selfadjoint. □

Next we recall some important results from the spectral theory of operators (on infinite dimensional spaces). We begin with the following definition; see [DR12, Definition 13.22].

Definition 1.4. *Let $\mathcal{H}$ be a real Hilbert space and $\mathcal{T} \in \mathcal{L}(\mathcal{H})$.*

1) *A complex number λ belongs to the* resolvent set *$\rho(\mathcal{T})$ if $\lambda\mathcal{I}-\mathcal{T}$ is a bijection with a bounded inverse. Here, $\mathcal{I} \in \mathcal{L}(\mathcal{H})$ stands for the identity operator. If $\lambda \notin \rho(\mathcal{T})$, then λ is an element of the* spectrum *$\sigma(\mathcal{T})$ of $\mathcal{T}$.*

2) *Let $u \neq 0$ be a vector with $\mathcal{T}u = \lambda u$ for some $\lambda \in \mathbb{C}$. Then, u is said to be an* eigenvector *of $\mathcal{T}$. We call λ the corresponding* eigenvalue. *If λ is an eigenvalue, then $\lambda\mathcal{I} - \mathcal{T}$ is not injective. This implies $\lambda \in \sigma(\mathcal{T})$. The set of all eigenvalues is called the* point spectrum *of $\mathcal{T}$.*

We will make use of the next two essential theorems for compact operators; see [RS80, p. 203] and [DR12, Satz 19.7 and Satz 19.8].

Theorem 1.5 (Riesz-Schauder)**.** *Let $\mathcal{H}$ be a real Hilbert space and $\mathcal{T} : \mathcal{H} \to \mathcal{H}$ a linear, compact operator. Then the spectrum $\sigma(\mathcal{T})$ is a discrete set having no limit points except perhaps 0. Furthermore, the space of eigenvectors corresponding to each nonzero $\lambda \in \sigma(\mathcal{T})$ is finite dimensional.*

Theorem 1.6 (Hilbert-Schmidt)**.** *Let $\mathcal{H}$ be a real separable Hilbert space and $\mathcal{T} : \mathcal{H} \to \mathcal{H}$ a linear, compact, selfadjoint operator. Then, there is a sequence of eigenvalues $\{\lambda_i\}_{i\in\mathbb{I}}$ and of an associated complete orthonormal basis $\{\psi_i\}_{i\in\mathbb{I}} \subset X$ satisfying*

$$\mathcal{T}\psi_i = \lambda_i\psi_i \quad \text{and} \quad \lambda_i \to 0 \text{ as } i \to \infty.$$

Since X is a separable real Hilbert space and $\mathcal{R}^n : X \to X$ is a linear, compact, nonnegative, selfadjoint operator (see Lemma 1.3), we can utilize Theorems 1.5 and 1.6: There exist a complete countable orthonormal basis $\{\bar\psi_i^n\}_{i\in\mathbb{I}}$ and a corresponding sequence of real eigenvalues $\{\bar\lambda_i^n\}_{i\in\mathbb{I}}$ satisfying

$$\mathcal{R}^n\bar\psi_i^n = \bar\lambda_i^n\bar\psi_i^n, \quad \bar\lambda_1^n \geq \ldots \geq \bar\lambda_{d^n} > \bar\lambda_{d^n+1} = \ldots = 0. \tag{1.5}$$

The spectrum of $\mathcal{R}^n$ is a pure point spectrum except for possibly 0. Each nonzero eigenvalue of $\mathcal{R}^n$ has finite multiplicity and 0 is the only possible accumulation point of the spectrum of $\mathcal{R}^n$.

Remark 1.7. From (1.4), (1.5) and $\|\psi\|_X = 1$ we infer that

$$\begin{aligned}\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\,\langle y_j^k, \bar\psi_i^n\rangle_X^2 &= \Big\langle \sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\,\langle y_j^k, \bar\psi_i^n\rangle_X y_j^k, \bar\psi_i^n\Big\rangle_X \\ &= \langle \mathcal{R}^n\bar\psi_i^n, \bar\psi_i^n\rangle_X = \bar\lambda_i^n \quad \text{for any } i \in \mathbb{I}.\end{aligned} \tag{1.6}$$

In particular, it follows that

$$\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\,\langle y_j^k, \bar\psi_i^n\rangle_X^2 = 0 \quad \text{for all } i > d^n. \tag{1.7}$$

Since $\{\bar\psi_i^n\}_{i\in\mathbb{I}}$ is a complete orthonormal basis and $\|y_j^k\|_X < \infty$ holds for $1 \leq k \leq \wp$, $1 \leq j \leq n$, we derive from (1.6) and (1.7) that

$$\begin{aligned}\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\,\|y_j^k\|_X^2 &= \sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{\nu\in\mathbb{I}}\langle y_j^k, \bar\psi_\nu^n\rangle_X^2 \\ &= \sum_{\nu\in\mathbb{I}}\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\,\langle y_j^k, \bar\psi_\nu^n\rangle_X^2 = \sum_{i\in\mathbb{I}}\bar\lambda_i^n = \sum_{i=1}^{d^n}\bar\lambda_i^n.\end{aligned} \tag{1.8}$$

By (1.8) the sum $\sum_{i\in\mathbb{I}}\bar\lambda_i^n$ is bounded. It follows from (1.2) that the objective of $(\mathbf{P}_n^\ell)$ can be written as

$$\begin{aligned}&\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\Big\|y_j^k - \sum_{i=1}^{\ell}\langle y_j^k, \bar\psi_i^n\rangle_X\,\bar\psi_i^n\Big\|_X^2 \\ &\quad = \sum_{i=1}^{d^n}\bar\lambda_i^n - \sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{i=1}^{\ell}\langle y_j^k, \bar\psi_i^n\rangle_X^2\end{aligned} \tag{1.9}$$

which we will use in the proof of Theorem 1.8. $\quad\Diamond$

Now we can formulate the main result for $(\mathbf{P}_n^\ell)$ and $(\hat{\mathbf{P}}_n^\ell)$.

Theorem 1.8. *Let X be a separable real Hilbert space, $y_1^k,\dots,y_n^k \in X$ for $1 \le k \le \wp$ and $\mathcal{R}^n : X \to X$ be defined by (1.4). Suppose that $\{\bar\lambda_i^n\}_{i\in\mathbb{I}}$ and $\{\bar\psi_i^n\}_{i\in\mathbb{I}}$ denote the nonnegative eigenvalues and associated orthonormal eigenfunctions of $\mathcal{R}^n$ satisfying (1.5). Then, for every $\ell \in \{1,\dots,d^n\}$ the first ℓ eigenfunctions $\{\bar\psi_i^n\}_{i=1}^\ell$ solve $(\mathbf{P}_n^\ell)$ and $(\hat{\mathbf{P}}_n^\ell)$. Moreover, the value of the cost evaluated at the optimal solution $\{\bar\psi_i^n\}_{i=1}^\ell$ satisfies*

$$\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\Big\|y_j^k-\sum_{i=1}^{\ell}\langle y_j^k,\bar\psi_i^n\rangle_X\,\bar\psi_i^n\Big\|_X^2=\sum_{i=\ell+1}^{d^n}\bar\lambda_i^n \tag{1.10}$$

and

$$\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{i=1}^{\ell}\langle y_j^k,\bar\psi_i^n\rangle_X^2=\sum_{i=1}^{\ell}\bar\lambda_i^n. \tag{1.11}$$

Proof. We prove the claim for $(\hat{\mathbf{P}}_n^\ell)$ by finite induction over $\ell \in \{1,\dots,d^n\}$.

1) The base case: Let $\ell = 1$ and $\psi \in X$ with $\|\psi\|_X = 1$. Since $\{\bar\psi_\nu^n\}_{\nu\in\mathbb{I}}$ is a complete orthonormal basis in X, we have the representation

$$\psi=\sum_{\nu\in\mathbb{I}}\langle\psi,\bar\psi_\nu^n\rangle_X\,\bar\psi_\nu^n. \tag{1.12}$$

Inserting this expression for ψ in the objective of $(\hat{\mathbf{P}}_n^\ell)$ we find that

$$\begin{aligned}
\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\,\langle y_j^k,\psi\rangle_X^2&=\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\Big\langle y_j^k,\sum_{\nu\in\mathbb{I}}\langle\psi,\bar\psi_\nu^n\rangle_X\,\bar\psi_\nu^n\Big\rangle_X^2\\
&=\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{\nu\in\mathbb{I}}\sum_{\mu\in\mathbb{I}}\Big(\langle y_j^k,\langle\psi,\bar\psi_\nu^n\rangle_X\,\bar\psi_\nu^n\rangle_X\langle y_j^k,\langle\psi,\bar\psi_\mu^n\rangle_X\,\bar\psi_\mu^n\rangle_X\Big)\\
&=\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{\nu\in\mathbb{I}}\sum_{\mu\in\mathbb{I}}\Big(\langle y_j^k,\bar\psi_\nu^n\rangle_X\langle y_j^k,\bar\psi_\mu^n\rangle_X\langle\psi,\bar\psi_\nu^n\rangle_X\langle\psi,\bar\psi_\mu^n\rangle_X\Big)\\
&=\sum_{\nu\in\mathbb{I}}\sum_{\mu\in\mathbb{I}}\bigg(\Big\langle\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\langle y_j^k,\bar\psi_\nu^n\rangle_X\,y_j^k,\bar\psi_\mu^n\Big\rangle_X\langle\psi,\bar\psi_\nu^n\rangle_X\langle\psi,\bar\psi_\mu^n\rangle_X\bigg).
\end{aligned}$$

Utilizing (1.4), (1.5) and $\|\bar\psi_\nu^n\|_X = 1$ we find that

$$\begin{aligned}
\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\,\langle y_j^k,\psi\rangle_X^2&=\sum_{\nu\in\mathbb{I}}\sum_{\mu\in\mathbb{I}}\Big(\langle\bar\lambda_\nu^n\bar\psi_\nu^n,\bar\psi_\mu^n\rangle_X\langle\psi,\bar\psi_\nu^n\rangle_X\langle\psi,\bar\psi_\mu^n\rangle_X\Big)\\
&=\sum_{\nu\in\mathbb{I}}\bar\lambda_\nu^n\,\langle\psi,\bar\psi_\nu^n\rangle_X^2.
\end{aligned}$$

From $\bar\lambda_1^n \ge \bar\lambda_\nu^n$ for all $\nu \in \mathbb{I}$ and (1.6) we infer that

$$\begin{aligned}
\sum_{\nu\in\mathbb{I}}\bar\lambda_\nu^n\,\langle\psi,\bar\psi_\nu^n\rangle_X^2&\le\bar\lambda_1^n\sum_{\nu\in\mathbb{I}}\langle\psi,\bar\psi_\nu^n\rangle_X^2=\bar\lambda_1^n\,\|\psi\|_X^2=\bar\lambda_1^n\\
&=\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\,\langle y_j^k,\bar\psi_1^n\rangle_X^2,
\end{aligned}$$

i.e., $\bar\psi_1^n$ solves $(\hat{\mathbf{P}}_n^\ell)$ for $\ell = 1$ and (1.11) holds. This gives the base case. Notice that (1.9) and (1.11) imply (1.10).

2) The induction hypothesis: Now we suppose that

$$\begin{cases} \text{for any } \ell \in \{1,\dots,d^n-1\} \text{ the set } \{\bar\psi_i^n\}_{i=1}^\ell \subset X \text{ solve } (\hat{\mathbf{P}}_n^\ell) \\ \text{and } \displaystyle\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{i=1}^{\ell}\langle y_j^k,\bar\psi_i^n\rangle_X^2 = \sum_{i=1}^{\ell}\bar\lambda_i^n. \end{cases} \tag{1.13}$$

3) The induction step: We consider

$$\begin{cases} \max \displaystyle\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{i=1}^{\ell+1}\langle y_j^k,\psi_i\rangle_X^2 \\ \text{s.t. } \{\psi_i\}_{i=1}^{\ell+1}\subset X \text{ and } \langle\psi_i,\psi_j\rangle_X=\delta_{ij},\ 1\le i,j\le\ell+1. \end{cases} \tag{$\hat{\mathbf{P}}_n^{\ell+1}$}$$

By (1.13) the elements $\{\bar\psi_i^n\}_{i=1}^\ell$ maximize the term

$$\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{i=1}^{\ell}\langle y_j^k,\psi_i\rangle_X^2.$$

Thus, $(\hat{\mathbf{P}}_n^{\ell+1})$ is equivalent with

$$\begin{cases} \max \displaystyle\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\langle y_j^k,\psi\rangle_X^2 \\ \text{s.t. } \psi\in X \text{ and } \|\psi\|_X=1,\ \langle\psi,\bar\psi_i^n\rangle_X=0,\ 1\le i\le\ell. \end{cases} \tag{1.14}$$

Let $\psi\in X$ be given satisfying $\|\psi\|_X=1$ and $\langle\psi,\bar\psi_i^n\rangle_X=0$ for $i=1\dots,\ell$. Then, using the representation (1.12) and $\langle\psi,\bar\psi_i^n\rangle_X=0$ for $i=1\dots,\ell$, we derive as above

$$\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\langle y_j^k,\psi\rangle_X^2=\sum_{\nu\in\mathbb{I}}\bar\lambda_\nu^n\,\langle\psi,\bar\psi_\nu^n\rangle_X^2=\sum_{\nu>\ell}\bar\lambda_\nu^n\,\langle\psi,\bar\psi_\nu^n\rangle_X^2.$$

From $\bar\lambda_{\ell+1}^n\ge\bar\lambda_\nu^n$ for all $\nu\ge\ell+1$ and (1.6) we conclude that

$$\begin{aligned}\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\langle y_j^k,\psi\rangle_X^2&\le\bar\lambda_{\ell+1}^n\sum_{\nu>\ell}\langle\psi,\bar\psi_\nu^n\rangle_X^2\le\bar\lambda_{\ell+1}^n\sum_{\nu\in\mathbb{I}}\langle\psi,\bar\psi_\nu^n\rangle_X^2\\&=\bar\lambda_{\ell+1}^n\,\|\psi\|_X^2=\bar\lambda_{\ell+1}^n=\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\langle y_j^k,\bar\psi_{\ell+1}^n\rangle_X^2.\end{aligned}$$

Thus, $\bar\psi_{\ell+1}^n$ solves (1.14), which implies that $\{\bar\psi_i^n\}_{i=1}^{\ell+1}$ is a solution to $(\hat{\mathbf{P}}_n^{\ell+1})$ and

$$\sum_{k=1}^{\wp}\sum_{j=1}^{n}\alpha_j^n\sum_{i=1}^{\ell+1}\langle y_j^k,\bar\psi_i^n\rangle_X^2=\sum_{i=1}^{\ell+1}\bar\lambda_i^n.$$

Again, (1.9) and (1.11) imply (1.10).

It follows that the claim is proved. □

Remark 1.9. Theorem 1.8 can also be proved by using the theory of nonlinear programming; see [HLBR12, Vol01], for instance. In this case $(\hat{\mathbf{P}}_n^\ell)$ is considered as an equality constrained optimization problem. Applying a Lagrangian framework it turns out that (1.5) are first-order necessary optimality conditions for $(\hat{\mathbf{P}}_n^\ell)$. ◊

For the application of POD to concrete problems the choice of ℓ is certainly of central importance for applying POD. It appears that no general a-priori rules are available. Rather the choice of ℓ is based on heuristic considerations combined with observing the ratio of the modeled to the "total energy" contained in the snapshots $y_1^k, \ldots, y_n^k$, $1 \le k \le \wp$, which is expressed by

$$\mathcal{E}(\ell) = \frac{\sum_{i=1}^{\ell} \bar{\lambda}_i^n}{\sum_{i=1}^{d^n} \bar{\lambda}_i^n} \in [0, 1].$$

Utilizing (1.8) we have

$$\mathcal{E}(\ell) = \frac{\sum_{i=1}^{\ell} \bar{\lambda}_i^n}{\sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j^n \, \|y_j^k\|_X^2},$$

i.e., the computation of the eigenvalues $\{\bar{\lambda}_i\}_{i=\ell+1}^{d}$ is not necessary. This is utilized in numerical implementations when iterative eigenvalue solver are applied like, e.g., the Lanczos method; see [Ant05, Chapter 10], for instance.

In the following we will discuss three examples which illustrate that POD is strongly related to the singular value decomposition of matrices.

Remark 1.10 (POD in Euclidean space $\mathbb{R}^m$)**.** Suppose that $X = \mathbb{R}^m$ with $m \in \mathbb{N}$ and $\wp = 1$ hold. Then we have n snapshot vectors $y_1, \ldots, y_n$ and introduce the rectangular matrix $Y = [y_1 \,|\, \ldots \,|\, y_n] \in \mathbb{R}^{m \times n}$ with rank $d^n \le \min(m, n)$. Choosing $\alpha_j^n = 1$ for $1 \le j \le n$ problem $(\mathbf{P}_n^\ell)$ has the form

$$\begin{cases} \min \displaystyle\sum_{j=1}^{n} \Big\| y_j - \sum_{i=1}^{\ell} (y_j^\top \psi_i) \psi_i \Big\|_{\mathbb{R}^m}^2 \\ \text{s.t. } \{\psi_i\}_{i=1}^{\ell} \subset \mathbb{R}^m \text{ and } \psi_i^\top \psi_j = \delta_{ij}, \ 1 \le i, j \le \ell, \end{cases} \tag{1.15}$$

where $\|\cdot\|_{\mathbb{R}^m}$ stands for the Euclidean norm in $\mathbb{R}^m$ and "$\top$" denotes the transpose of a given vector (or matrix). From

$$\big(\mathcal{R}^n \psi\big)_i = \Big(\sum_{j=1}^{n} (y_j^\top \psi) y_j \Big)_i = \sum_{j=1}^{n} \sum_{l=1}^{m} Y_{lj} \psi_l Y_{ij} = \big(YY^\top \psi\big)_i, \quad \psi \in \mathbb{R}^m,$$

for each component $1 \le i \le m$ we infer that (1.5) leads to the symmetric $m \times m$ eigenvalue problem

$$YY^\top \bar{\psi}_i^n = \bar{\lambda}_i^n \bar{\psi}_i^n, \quad \bar{\lambda}_1^n \ge \ldots \ge \bar{\lambda}_{d^n}^n > \bar{\lambda}_{d^n+1}^n = \ldots = \bar{\lambda}_m^n = 0. \tag{1.16}$$

Recall that (1.16) can be solved by utilizing the singular value decomposition (SVD) [Nob69]: There exist real numbers $\bar{\sigma}_1^n \ge \bar{\sigma}_2^n \ge \ldots \ge \bar{\sigma}_{d^n}^n > 0$ and orthogonal matrices $\Psi \in \mathbb{R}^{m \times m}$ with column vectors $\{\bar{\psi}_i^n\}_{i=1}^m$ and $\Phi \in \mathbb{R}^{n \times n}$ with column vectors $\{\bar{\phi}_i^n\}_{i=1}^n$ such that

$$\Psi^\top Y \Phi = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} =: \Sigma \in \mathbb{R}^{m \times n}, \tag{1.17}$$

where $D = \operatorname{diag}(\bar{\sigma}_1^n, \ldots, \bar{\sigma}_{d^n}^n) \in \mathbb{R}^{d \times d}$ and the zeros in (1.17) denote matrices of appropriate dimensions. Moreover the vectors $\{\bar{\psi}_i^n\}_{i=1}^d$ and $\{\bar{\phi}_i^n\}_{i=1}^d$ satisfy

$$Y \bar{\phi}_i^n = \bar{\sigma}_i^n \bar{\psi}_i^n \quad \text{and} \quad Y^\top \bar{\psi}_i^n = \bar{\sigma}_i^n \bar{\phi}_i^n \quad \text{for } i = 1, \ldots, d^n. \tag{1.18}$$

They are eigenvectors of $YY^\top$ and $Y^\top Y$, respectively, with eigenvalues $\bar{\lambda}_i^n = (\bar{\sigma}_i^n)^2 > 0$, $i = 1, \ldots, d^n$. The vectors $\{\bar{\psi}_i^n\}_{i=d^n+1}^m$ and $\{\bar{\phi}_i^n\}_{i=d^n+1}^n$ (if $d^n < m$ respectively $d^n < n$) are eigenvectors of $YY^\top$ and $Y^\top Y$ with eigenvalue 0. Consequently, in the case $n < m$ one can determine the POD basis of rank ℓ as follows: Compute the eigenvectors $\bar{\phi}_1^n, \ldots, \bar{\phi}_\ell^n \in \mathbb{R}^n$ by solving the symmetric $n \times n$ eigenvalue problem

$$Y^\top Y \bar{\phi}_i^n = \bar{\lambda}_i^n \bar{\phi}_i^n \quad \text{for } i = 1, \ldots, \ell$$

and set, by (1.18),

$$\bar{\psi}_i^n = \frac{1}{(\bar{\lambda}_i^n)^{1/2}}\, Y\bar{\phi}_i^n \quad \text{for } i = 1, \ldots, \ell.$$

For historical reasons this method of determing the POD-basis is sometimes called the *method of snapshots*; see [**?**]. On the other hand, if $m < n$ holds, we can obtain the POD basis by solving the $m \times m$ eigenvalue problem (1.16). If the matrix Y is badly scaled, we should avoid to build the matrix product $YY^\top$ (or $Y^\top Y$). In this case the SVD turns out to be more stable for the numerical computation of the POD basis of rank ℓ. $\quad\Diamond$

Remark 1.11 (POD in $\mathbb{R}^m$ with weighted inner product)**.** As in Remark 1.10 we choose $X = \mathbb{R}^m$ with $m \in \mathbb{R}^m$ and $\wp = 1$. Let $W \in \mathbb{R}^{m\times m}$ be a given symmetric, positive definite matrix. We supply $\mathbb{R}^m$ with the weighted inner product

$$\langle \psi, \tilde{\psi}\rangle_W = \psi^\top W\tilde{\psi} = \langle \psi, W\tilde{\psi}\rangle_{\mathbb{R}^m} = \langle W\psi, \tilde{\psi}\rangle_{\mathbb{R}^m} \quad \text{for } \psi, \tilde{\psi} \in \mathbb{R}^m.$$

Then, problem $(\mathbf{P}_n^\ell)$ has the form

$$\begin{cases} \min \displaystyle\sum_{j=1}^n \alpha_j^n \Big\| y_j - \sum_{i=1}^\ell \langle y_j, \psi_i\rangle_W\, \psi_i \Big\|_W^2 \\ \text{s.t. } \{\psi_i\}_{i=1}^\ell \subset \mathbb{R}^m \text{ and } \langle \psi_i, \psi_j\rangle_W = \delta_{ij},\ 1 \le i, j \le \ell. \end{cases}$$

As in Remark 1.10 we introduce the matrix $Y = [y_1 \,|\, \ldots \,|\, y_n] \in \mathbb{R}^{m\times n}$ with rank $d^n \le \min(m, n)$. Moreover, we define the diagonal matrix $D = \operatorname{diag}(\alpha_1^n, \ldots, \alpha_n^n) \in \mathbb{R}^{n\times n}$. We find that

$$\begin{aligned} \big(\mathcal{R}^n\psi\big)_i &= \Big(\sum_{j=1}^n \alpha_j^n \langle y_j, \psi\rangle_W\, y_j\Big)_i = \sum_{j=1}^n\sum_{l=1}^m\sum_{\nu=1}^m \alpha_j^n Y_{lj} W_{l\nu}\psi_\nu Y_{ij} \\ &= \big(YDY^\top W\psi\big)_i \quad \text{for } \psi \in \mathbb{R}^m, \end{aligned}$$

for each component $1 \le i \le m$. Consequently, (1.5) leads to the eigenvalue problem

$$YDY^\top W\bar{\psi}_i^n = \bar{\lambda}_i^n\bar{\psi}_i^n, \quad \bar{\lambda}_1^n \ge \ldots \ge \bar{\lambda}_{d^n}^n > \bar{\lambda}_{d^n+1}^n = \ldots = \bar{\lambda}_m^n = 0. \tag{1.19}$$

Since W is symmetric and positive definite, W possesses an eigenvalue decomposition of the form $W = QBQ^\top$, where $B = \operatorname{diag}(\beta_1, \ldots, \beta_m)$ contains the eigenvalues $\beta_1 \ge \ldots \ge \beta_m > 0$ of W and $Q \in \mathbb{R}^{m\times m}$ is an orthogonal matrix. We define

$$W^r = Q\operatorname{diag}(\beta_1^r, \ldots, \beta_m^r)Q^\top \quad \text{for } r \in \mathbb{R}.$$

Note that $(W^r)^{-1} = W^{-r}$ and $W^{r+s} = W^rW^s$ for r, $s \in \mathbb{R}$. Moreover, we have

$$\langle \psi, \tilde{\psi}\rangle_W = \langle W^{1/2}\psi, W^{1/2}\tilde{\psi}\rangle_{\mathbb{R}^m} \quad \text{for } \psi,\ \tilde{\psi} \in \mathbb{R}^m$$

and $\|\psi\|_W = \|W^{1/2}\psi\|_{\mathbb{R}^m}$ for $\psi \in \mathbb{R}^m$. Analogously, the matrix $D^{1/2}$ is defined. Inserting $\psi_i^n = W^{1/2}\bar{\psi}_i^n$ in (1.19), multiplying (1.19) by $W^{1/2}$ from the left and setting $\hat{Y} = W^{1/2}YD^{1/2}$ yield the symmetric $m \times m$ eigenvalue problem

$$\hat{Y}\hat{Y}^\top\psi_i^n = \bar{\lambda}_i^n\psi_i^n, \quad 1 \le i \le \ell.$$

Note that

$$\hat{Y}^\top\hat{Y} = D^{1/2}Y^\top WYD^{1/2} \in \mathbb{R}^{n\times n}. \tag{1.20}$$

Thus, the POD basis $\{\bar{\psi}_i^n\}_{i=1}^\ell$ of rank ℓ can also be computed by the methods of snapshots as follows: First solve the symmetric $n \times n$ eigenvalue problem

$$\hat{Y}^\top\hat{Y}\phi_i^n = \bar{\lambda}_i^n\phi_i^n,\ 1 \le i \le \ell \quad \text{and} \quad \langle \phi_i^n, \phi_j^n\rangle_{\mathbb{R}^n} = \delta_{ij},\ 1 \le i, j \le \ell.$$

Then we set (by using the SVD of $\hat{Y}$)

$$\bar{\psi}_i^n = W^{-1/2}\psi_i^n = \frac{1}{\bar{\sigma}_i^n} W^{-1/2}\hat{Y}\phi_i^n = \frac{1}{\bar{\sigma}_i^n} Y D^{1/2}\phi_i^n, \quad 1 \le i \le \ell. \tag{1.21}$$

Note that

$$\langle \bar{\psi}_i^n, \bar{\psi}_j^n \rangle_W = (\bar{\psi}_i^n)^\top W \bar{\psi}_j^n = \frac{1}{\bar{\sigma}_i^n \bar{\sigma}_j^n} (\phi_i^n)^\top \underbrace{D^{1/2} Y^\top W Y D^{1/2}}_{=\hat{Y}^\top \hat{Y}} \phi_j^n = \delta_{ij}$$

for $1 \le i, j \le \ell$. Thus, the POD basis $\{\bar{\psi}_i^n\}_{i=1}^{\ell}$ of rank ℓ is orthonormal in $\mathbb{R}^m$ with respect to the inner product $\langle \cdot\,, \cdot \rangle_W$. We observe from (1.20) and (1.21) that the computation of $W^{1/2}$ and $W^{-1/2}$ is not required. For applications, where W is not just a diagonal matrix, the method of snapshots turns out to be more attractive with respect to the computational costs even if $m > n$ holds. $\Diamond$

Remark 1.12 (POD in $\mathbb{R}^m$ with multiple snapshots)**.** Let us discuss the more general case $\wp = 2$ in the setting of Remark 1.11. The extension for $\wp > 2$ is straightforward. We introduce the matrix $Y = [y_1^1 \,|\, \ldots \,|\, y_n^1 \,|\, y_1^2 \,|\, \ldots \,| y_n^2] \in \mathbb{R}^{m \times (n\wp)}$ with rank $d^n \le \min(m, n\wp)$. Then we find

$$\begin{aligned}
\mathcal{R}^n \psi &= \sum_{j=1}^n \Big(\alpha_j^n \, \langle y_j^1, \psi \rangle_W \, y_j^1 + \alpha_j^n \, \langle y_j^2, \psi \rangle_W \, y_j^2 \Big) \\
&= Y \underbrace{\begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}}_{=:\tilde{D} \in \mathbb{R}^{(n\wp)\times(n\wp)}} Y^\top W \psi = Y \tilde{D} Y^\top W \psi \quad \text{for } \psi \in \mathbb{R}^m.
\end{aligned}$$

Hence, (1.5) corresponds to the eigenvalue problem

$$Y \tilde{D} Y^\top W \bar{\psi}_i^n = \bar{\lambda}_i^n \bar{\psi}_i^n, \quad \bar{\lambda}_1^n \ge \ldots \ge \bar{\lambda}_{d^n}^n > \bar{\lambda}_{d^n+1}^n = \ldots = \bar{\lambda}_m^n = 0. \tag{1.22}$$

Setting $\psi_i^n = W^{1/2}\bar{\psi}_i^n$ in (1.22) and multiplying by $W^{1/2}$ from the left yield

$$W^{1/2} Y \tilde{D} Y^\top W^{1/2} \psi_i^n = \bar{\lambda}_i^n \psi_i^n. \tag{1.23}$$

Let $\hat{Y} = W^{1/2} Y \tilde{D}^{1/2} \in \mathbb{R}^{m \times (n\wp)}$. Using $W^\top = W$ as well as $\tilde{D}^\top = \tilde{D}$ we infer from (1.23) that the POD basis $\{\bar{\psi}_i^n\}_{i=1}^{\ell}$ of rank ℓ is given by the symmetric $m \times m$ eigenvalue problem

$$\hat{Y}\hat{Y}^\top \psi_i^n = \bar{\lambda}_i^n \psi_i^n, \ 1 \le i \le \ell, \quad \text{and} \quad \langle \psi_i^n, \psi_j^n \rangle_{\mathbb{R}^m} = \delta_{ij}, \ 1 \le i, j \le \ell$$

and $\bar{\psi}_i^n = W^{-1/2}\psi_i^n$. Note that

$$\hat{Y}^\top \hat{Y} = \tilde{D}^{1/2} Y^\top W Y \tilde{D}^{1/2} \in \mathbb{R}^{(n\wp)\times(n\wp)}.$$

Thus, the POD basis of rank ℓ can also be computed by the methods of snapshots as follows: First solve the symmetric $(n\wp) \times (n\wp)$ eigenvalue problem

$$\hat{Y}^\top \hat{Y} \phi_i^n = \bar{\lambda}_i^n \phi_i, \ 1 \le i \le \ell \quad \text{and} \quad \langle \phi_i^n, \phi_j^n \rangle_{\mathbb{R}^{n\wp}} = \delta_{ij}, \ 1 \le i, j \le \ell.$$

Then we set (by SVD)

$$\bar{\psi}_i^n = W^{-1/2}\psi_i^n = \frac{1}{\bar{\sigma}_i^n} W^{-1/2}\hat{Y}\phi_i^n = \frac{1}{\bar{\sigma}_i^n} Y \tilde{D}^{1/2} \phi_i^n$$

for $1 \le i \le \ell$. $\Diamond$

1.2 The continuous variant of the POD method

As in Remark 1.1 tet $0 \le t_1 < t_2 < \ldots < t_n \le T$ be a given time grid in the interval $[0, T]$ with equidistant with step-size $\Delta t = T/(n-1)$, i.e., $t_j = (j-1)\Delta t$. Suppose that we have trajectories $y^k \in C([0, T]; X)$, $1 \le k \le \wp$. Let the snapshots be given as $y_j^k = y^k(t_j) \in X$ or $y_j^k \approx y^k(t_j) \in X$. Then, the snapshot subspace $\mathcal{V}^n$ introduced in (1.1) depends on the chosen time instances $\{t_j\}_{j=1}^n$. Consequently, the POD basis $\{\bar\psi_i^n\}_{i=1}^\ell$ of rank ℓ as well as the corresponding eigenvalues $\{\bar\lambda_i^n\}_{i=1}^\ell$ depend also on the time instances (which has already been indicated by the superindex n). Moreover, we have not discussed so far what is the motivation to introduce the positive weights $\{\alpha_j^n\}_{j=1}^n$ in $(\mathbf{P}_n^\ell)$. For this reason we proceed by investigating the following two questions:

- How to choose good time instances for the snapshots?
- What are appropriate positive weights $\{\alpha_j^n\}_{j=1}^n$?

To address these two questions we will introduce a *continuous version* of POD. In Section 1.1 we have introduced the operator $\mathcal{R}^n$ in (1.4). By $\{\bar\psi_i^n\}_{i\in\mathbb{I}}$ and $\{\bar\lambda_i^n\}_{i\in\mathbb{I}}$ we have denoted the eigenfunctions and eigenvalues for $\mathcal{R}^n$ satisfying (1.5). Moreover, we have set $d^n = \dim \mathcal{V}^n$ for the dimension of the snapshot set. Let us now introduce the snapshot set by

$$\mathcal{V} = \operatorname{span}\Big\{ y^k(t) \,|\, t \in [0, T] \text{ and } 1 \le k \le \wp \Big\} \subset X$$

with dimension $d \le \infty$. For any $\ell \le d$ we are interested in determining a POD basis of rank ℓ which minimizes the mean square error between the trajectories y^k and the corresponding ℓ-th partial Fourier sums on average in the time interval $[0, T]$:

$$\begin{cases} \min \displaystyle\sum_{k=1}^{\wp} \int_0^T \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \psi_i \rangle_X \, \psi_i \Big\|_X^2 \, \mathrm{d}t \\ \text{s.t. } \{\psi_i\}_{i=1}^\ell \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i, j \le \ell. \end{cases} \tag{$\mathbf{P}^\ell$}$$

An optimal solution $\{\bar\psi_i\}_{i=1}^\ell$ to $(\mathbf{P}^\ell)$ is called a *POD basis of rank* ℓ. Analogous to $(\hat{\mathbf{P}}_n^\ell)$ we can – instead of $(\mathbf{P}^\ell)$ – consider the problem

$$\begin{cases} \max \displaystyle\sum_{k=1}^{\wp} \int_0^T \sum_{i=1}^{\ell} \langle y^k(t), \psi_i \rangle_X^2 \, \mathrm{d}t \\ \text{s.t. } \{\psi_i\}_{i=1}^\ell \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i, j \le \ell. \end{cases} \tag{$\hat{\mathbf{P}}^\ell$}$$

A solution to $(\mathbf{P}^\ell)$ and to $(\hat{\mathbf{P}}^\ell)$ can be characterized by an eigenvalue problem for the linear integral operator $\mathcal{R} : X \to X$ given as

$$\mathcal{R}\psi = \sum_{k=1}^{\wp} \int_0^T \langle y^k(t), \psi \rangle_X \, y^k(t) \, \mathrm{d}t \quad \text{for } \psi \in X. \tag{1.24}$$

For the given real Hilbert space X we denote by $L^2(0, T; X)$ the Hilbert space of square integrable functions $t \mapsto \varphi(t) \in X$ so that [**?**, p. 114]

- the mapping $t \mapsto \varphi(t)$ is measurable for $t \in [0, T]$ and
- $\|\varphi\|_{L^2(0,T;X)} = \Big(\displaystyle\int_0^T \|\varphi(t)\|_X^2 \, \mathrm{d}t \Big)^{1/2} < \infty.$

Recall that $\varphi : [0, T] \to X$ is called *measurable* if there exists a sequence $\{\varphi_n\}_{n\in\mathbb{N}}$ of step functions $\varphi_n : [0, T] \to X$ satisfying $\varphi(t) = \lim_{n\to\infty} \varphi_n(t)$ for almost all $t \in [0, T]$. The standard inner product on $L^2(0, T; X)$ is given by

$$\langle \varphi, \psi \rangle_{L^2(0,T;X)} = \int_0^T \langle \varphi(t), \phi(t) \rangle_X \, \mathrm{d}t \quad \text{for } \varphi, \phi \in L^2(0, T; X).$$

Lemma 1.13. *Let X be a (separable) real Hilbert space and $y^k \in L^2(0,T;X)$, $1 \le k \le \wp$, be given snapshot trajectories. Then, the operator $\mathcal{R}$ introduced in* (1.24) *is compact, nonnegative and selfadjoint.*

Proof. First we write $\mathcal{R}$ as a product of an operator and its Hilbert space adjoint. For that purpose let us define the linear operator $\mathcal{Y} : L^2(0,T;\mathbb{R}^\wp) \to X$ by

$$\mathcal{Y}\phi = \sum_{k=1}^{\wp} \int_0^T \phi^k(t) y^k(t)\,\mathrm{d}t \quad \text{for } \phi = (\phi^1, \ldots, \phi^\wp) \in L^2(0,T;\mathbb{R}^\wp). \tag{1.25}$$

Utilizing the Cauchy-Schwarz inequality [DR12, Satz 12.17] and $y^k \in L^2(0,T;X)$ for $1 \le k \le \wp$ we infer that

$$\begin{aligned}
\|\mathcal{Y}\phi\|_X &\le \sum_{k=1}^{\wp} \int_0^T \big|\phi^k(t)\big| \|y^k(t)\|_X \,\mathrm{d}t \le \sum_{k=1}^{\wp} \|\phi^k\|_{L^2(0,T)} \|y^k\|_{L^2(0,T;X)} \\
&\le \bigg(\sum_{k=1}^{\wp} \|\phi^k\|^2_{L^2(0,T)}\bigg)^{1/2} \bigg(\sum_{k=1}^{\wp} \|y^k\|^2_{L^2(0,T;X)}\bigg)^{1/2} \\
&= C_{\mathcal{Y}} \, \|\phi\|_{L^2(0,T;\mathbb{R}^\wp)} \quad \text{for any } \phi \in L^2(0,T;\mathbb{R}^\wp),
\end{aligned}$$

where we set $C_{\mathcal{Y}} = (\sum_{k=1}^{\wp} \|y^k\|^2_{L^2(0,T;X)})^{1/2} < \infty$. Hence, the operator $\mathcal{Y}$ is bounded. Its Hilbert space adjoint $\mathcal{Y}^\star : X \to L^2(0,T;\mathbb{R}^\wp)$ satisfies

$$\langle \mathcal{Y}^\star \psi, \phi \rangle_{L^2(0,T;\mathbb{R}^\wp)} = \langle \psi, \mathcal{Y}\phi \rangle_X \quad \text{for } \psi \in X \text{ and } \phi \in L^2(0,T;\mathbb{R}^\wp).$$

Since we derive

$$\begin{aligned}
\langle \mathcal{Y}^\star \psi, \phi \rangle_{L^2(0,T;\mathbb{R}^\wp)} &= \langle \psi, \mathcal{Y}\phi \rangle_X = \bigg\langle \psi, \sum_{k=1}^{\wp} \int_0^T \phi^k(t) y^k(t)\,\mathrm{d}t \bigg\rangle_X \\
&= \sum_{k=1}^{\wp} \int_0^T \langle \psi, y^k(t) \rangle_X \phi^k(t)\,\mathrm{d}t = \Big\langle \big(\langle \psi, y^k(\cdot) \rangle_X\big)_{1 \le k \le \wp}, \phi \Big\rangle_{L^2(0,T;\mathbb{R}^\wp)}
\end{aligned}$$

for $\psi \in X$ and $\phi \in L^2(0,T;\mathbb{R}^\wp)$, the adjoint operator is given by

$$(\mathcal{Y}^\star \psi)(t) = \begin{pmatrix} \langle \psi, y^1(t) \rangle_X \\ \vdots \\ \langle \psi, y^\wp(t) \rangle_X \end{pmatrix} \quad \text{for } \psi \in X \text{ and } t \in [0,T] \text{ a.e.},$$

where 'a.e.' stands for 'almost everywhere'. From (1.4) and

$$\big(\mathcal{Y}\mathcal{Y}^\star\big)\psi = \mathcal{Y} \begin{pmatrix} \langle \psi, y^1(\cdot) \rangle_X \\ \vdots \\ \langle \psi, y^\wp(\cdot) \rangle_X \end{pmatrix} = \sum_{k=1}^{\wp} \int_0^T \langle \psi, y^k(t) \rangle_X y^k(t)\,\mathrm{d}t \quad \text{for } \psi \in X$$

we infer that $\mathcal{R} = \mathcal{Y}\mathcal{Y}^\star$ holds. Since the operator $\mathcal{Y}$ is bounded, its adjoint and therefore $\mathcal{R} = \mathcal{Y}\mathcal{Y}^\star$ are bounded operators. To prove that $\mathcal{R}$ is compact, we show that $\mathcal{Y}^\star$ is compact. Let $\{\chi_n\}_{n\in\mathbb{N}} \subset X$ be sequence converging weakly to an element $\chi \in X$, i.e.,

$$\lim_{n\to\infty} \langle \chi_n, \psi \rangle_X = \langle \chi, \psi \rangle_X \quad \text{for all } \psi \in X.$$

This implies that

$$\lim_{n\to\infty} (\mathcal{Y}^\star \chi_n)(t) = \lim_{n\to\infty} \begin{pmatrix} \langle \chi_n, y^1(t) \rangle_X \\ \vdots \\ \langle \chi_n, y^\wp(t) \rangle_X \end{pmatrix} = \begin{pmatrix} \langle \chi, y^1(t) \rangle_X \\ \vdots \\ \langle \chi, y^\wp(t) \rangle_X \end{pmatrix} = \big(\mathcal{Y}^\star \chi\big)(t)$$

for $t \in [0,T]$ a.e. Thus, the sequence $\{\mathcal{Y}^\star \chi_n\}_{n\in\mathbb{N}}$ converges weakly to $\mathcal{Y}^\star\chi$ in $L^2(0,T;\mathbb{R}^\wp)$. Consequently, $\mathcal{R} = \mathcal{Y}\mathcal{Y}^\star$ is compact. From

$$\begin{aligned}\langle \mathcal{R}\psi, \psi\rangle_X &= \left\langle \sum_{k=1}^{\wp} \int_0^T \langle \psi, y^k(t)\rangle_X\, y^k(t)\,\mathrm{d}t, \psi \right\rangle_X \\ &= \sum_{k=1}^{\wp} \int_0^T \big|\langle \psi, y^k(t)\rangle_X\big|^2\,\mathrm{d}t \geq 0 \quad \text{for all } \psi \in X\end{aligned}$$

we infer that $\mathcal{R}$ is nonnegative. Finally, we have $\mathcal{R}^\star = (\mathcal{Y}\mathcal{Y}^\star)^\star = \mathcal{R}$, i.e. $\mathcal{R}$ is selfadjoint. □

Remark 1.14. It follows from the proof of Lemma 1.13 that $\mathcal{K} = \mathcal{Y}^\star\mathcal{Y} : L^2(0,T;\mathbb{R}^\wp) \to L^2(0,T;\mathbb{R}^\wp)$ is compact as well. We find that

$$\big(\mathcal{K}\phi\big)(t) = \begin{pmatrix} \sum\limits_{k=1}^{\wp} \int_0^T \langle y^k(s), y^1(t)\rangle_X \phi^k(s)\,\mathrm{d}s \\ \vdots \\ \sum\limits_{k=1}^{\wp} \int_0^T \langle y^k(s), y^\wp(t)\rangle_X \phi^k(s)\,\mathrm{d}s \end{pmatrix}, \quad \phi \in L^2(0,T;\mathbb{R}^\wp).$$

The compactness of $\mathcal{K}$ can also be shown as follow: Notice that the kernel function

$$r_{ik}(s,t) = \langle y^k(s), y^i(t)\rangle_X, \quad (s,t) \in [0,T]\times[0,T] \text{ and } 1 \leq i,k \leq \wp,$$

belongs to $L^2(0,T)\times L^2(0,T)$. Here, we shortly write $L^2(0,T)$ for $L^2(0,T;\mathbb{R})$. Then, it follows from [DR12, Beispiel 19.3] that the linear integral operator $\mathcal{K}_{ik} : L^2(0,T) \to L^2(0,T)$ defined by

$$\mathcal{K}_{ik}(t) = \int_0^T r_{ik}(s,t)\phi(s)\,\mathrm{d}s, \quad \phi \in L^2(0,T),$$

is compact. This implies, that the operator $\sum_{k=1}^{\wp} \mathcal{K}_{ik}$ is compact for $1 \leq i \leq \wp$ as well. ◊

In the next theorem we formulate how the solution to ($\mathbf{P}^\ell$) and ($\hat{\mathbf{P}}^\ell$) can be found.

Theorem 1.15. *Let X be a separable real Hilbert space and $y^k \in L^2(0,T;X)$ are given trajectories for $1 \leq k \leq \wp$. Suppose that the linear operator $\mathcal{R}$ is defined by* (1.24)*. Then, there exist nonnegative eigenvalues $\{\bar\lambda_i\}_{i\in\mathbb{I}}$ and associated orthonomal eigenfunctions $\{\bar\psi_i\}_{i\in\mathbb{I}}$ satisfying*

$$\mathcal{R}\bar\psi_i = \bar\lambda_i\bar\psi_i, \;\; \bar\lambda_1 \geq \ldots \geq \bar\lambda_d > \bar\lambda_{d+1} = \ldots = 0. \tag{1.26}$$

For every $\ell \in \{1,\ldots,d\}$ the first ℓ eigenfunctions $\{\bar\psi_i\}_{i=1}^\ell$ solve ($\mathbf{P}^\ell$) *and* ($\hat{\mathbf{P}}^\ell$)*. Moreover, the value of the objectives evaluated at the optimal solution $\{\bar\psi_i\}_{i=1}^\ell$ satisfies*

$$\sum_{k=1}^{\wp} \int_0^T \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \bar\psi_i\rangle_X\, \bar\psi_i \Big\|_X^2\,\mathrm{d}t = \sum_{i=\ell+1}^{d} \bar\lambda_i \tag{1.27}$$

and

$$\sum_{k=1}^{\wp} \int_0^T \sum_{i=1}^{\ell} \langle y^k(t), \bar\psi_i\rangle_X^2\,\mathrm{d}t = \sum_{i=1}^{\ell} \bar\lambda_i, \tag{1.28}$$

respectively.

Proof. The existence of sequences $\{\bar\lambda_i\}_{i\in\mathbb{I}}$ of eigenvalues and $\{\bar\psi_i\}_{i\in\mathbb{I}}$ of associated eigenfunctions satisfying (1.26) follows from Lemma 1.13, Theorem 1.5 and Theorem 1.6. Analogous to the proof of Theorem 1.8 in Section 1.1 one can show that $\{\bar\psi_i\}_{i=1}^\ell$ solves ($\mathbf{P}^\ell$) as well as ($\hat{\mathbf{P}}^\ell$) and that (1.27) respectively (1.28) are valid. □

Remark 1.16. Similar to (1.6) we have

$$\sum_{k=1}^{\wp} \int_0^T \|y^k(t)\|_X^2 \,\mathrm{d}t = \sum_{i=1}^{d} \bar\lambda_i. \tag{1.29}$$

In fact,

$$\mathcal{R}\bar\psi_i = \sum_{k=1}^{\wp} \int_0^T \langle y^k(t), \bar\psi_i\rangle_X \, y^k(t) \,\mathrm{d}t \quad \text{for every } i \in \mathbb{I}.$$

Taking the inner product with $\bar\psi_i$, using (1.26) and summing over i we get

$$\sum_{i=1}^{d}\sum_{k=1}^{\wp} \int_0^T \langle y^k(t), \bar\psi_i\rangle_X^2 \,\mathrm{d}t = \sum_{i=1}^{d} \langle \mathcal{R}\bar\psi_i, \bar\psi_i\rangle_X = \sum_{i=1}^{d} \bar\lambda_i.$$

Expanding each $y^k(t) \in X$ in terms of $\{\bar\psi_i\}_{i\in\mathbb{I}}$ for each $1 \le k \le \wp$ we have

$$y^k(t) = \sum_{i=1}^{d} \langle y^k(t), \bar\psi_i\rangle_X \, \bar\psi_i$$

and hence

$$\sum_{k=1}^{\wp} \int_0^T \|y^k(t)\|_X^2 \,\mathrm{d}t = \sum_{k=1}^{\wp}\sum_{i=1}^{d} \int_0^T \langle y^k(t), \bar\psi_i\rangle_X^2 \,\mathrm{d}t = \sum_{i=1}^{d} \bar\lambda_i,$$

which is (1.29). ◊

Remark 1.17 (Singular value decomposition)**.** Suppose that $y^k \in L^2(0,T;X)$ holds. By Theorem 1.15 there exist nonnegative eigenvalues $\{\bar\lambda_i\}_{i\in\mathbb{I}}$ and associated orthonomal eigenfunctions $\{\bar\psi_i\}_{i\in\mathbb{I}}$ satisfying (1.26). From $\mathcal{K} = \mathcal{Y}^\star\mathcal{Y}$ it follows that there is a sequence $\{\bar\phi_i\}_{i\in\mathbb{I}}$ such that

$$\mathcal{K}\bar\phi_i = \bar\lambda_i\bar\phi_i, \quad 1\ldots,\ell.$$

We set $\mathbb{R}_0^+ = \{s \in \mathbb{R} \,|\, s \ge 0\}$ and $\bar\sigma_i = \bar\lambda_i^{1/2}$. The sequence $\{\bar\sigma_i, \bar\phi_i, \bar\psi_i\}_{i\in\mathbb{I}}$ in $\mathbb{R}_0^+ \times L^2(0,T;\mathbb{R}^\wp)\times X$ can be interpreted as a singular value decomposition of the mapping $\mathcal{Y} : L^2(0,T;\mathbb{R}^\wp) \to X$ introduced in (1.25). In fact, we have

$$\mathcal{Y}\bar\phi_i = \bar\sigma_i\bar\psi_i, \quad \mathcal{Y}^\star\bar\psi_i = \bar\sigma_i\bar\phi_i, \quad i \in \mathbb{I}.$$

Since $\bar\sigma_i > 0$ holds for $1 = 1\ldots,d$, we have $\bar\psi_i = \mathcal{Y}\bar\phi_i/\sigma_i$ for $i = 1,\ldots,d$. ◊

1.3 Perturbation analysis for the POD basis

The eigenvalues $\{\bar\lambda_i^n\}_{i\in\mathbb{I}}$ satisfying (1.5) depend on the time grid $\{t_j\}_{j=1}^n$. In this section we investigate the sum $\sum_{i=\ell+1}^{d^n} \bar\lambda_i^n$, the value of the cost in $(\mathbf{P}_n^\ell)$ evaluated at the solution $\{\bar\psi_i^n\}_{i=1}^\ell$ for $n \to \infty$. Clearly, $n \to \infty$ is equivalent with $\Delta t = T/(n-1) \to 0$.

In general the spectrum $\sigma(\mathcal{T})$ of an operator $\mathcal{T} \in \mathcal{L}(X)$ does not depend continuously on $\mathcal{T}$. This is an essential difference to the finite dimensional case. For the compact and selfadjoint operator $\mathcal{R}$ we have $\sigma(\mathcal{R}) = \{\bar\lambda_i\}_{i\in\mathbb{I}}$. Suppose that for $\ell \in \mathbb{N}$ we have $\bar\lambda_\ell > \bar\lambda_{\ell+1}$ so that we can seperate the spectrum as follows: $\sigma(\mathcal{R}) = \mathcal{S}_\ell \cup \mathcal{S}_\ell'$ with $\mathcal{S}_\ell = \{\bar\lambda_1,\ldots,\bar\lambda_\ell\}$ and $\mathcal{S}_\ell' = \sigma(\mathcal{R})\setminus\mathcal{S}_\ell$. Then, $\mathcal{S}_\ell \cap \mathcal{S}_\ell' = \emptyset$. Moreover, setting $V^\ell = \operatorname{span}\{\bar\psi_1,\ldots,\bar\psi_\ell\}$ we have $X = V^\ell \oplus (V^\ell)^\perp$, where the linear space $(V^\ell)^\perp$ stands for the X-orthogonal complement of V^ℓ. Let us assume that

$$\lim_{n\to\infty} \|\mathcal{R}^n - \mathcal{R}\|_{\mathcal{L}(X)} = 0 \tag{1.30}$$

holds. Then it follows from the perturbation theory of the spectrum of linear operators [Kat80, pp. 212-214] that the space $V_n^\ell = \operatorname{span}\{\bar\psi_1^n, \ldots, \bar\psi_\ell^n\}$ is isomorphic to V^ℓ if n is sufficiently large. Furthermore, the change of a finite set of eigenvalues of $\mathcal{R}$ is small provided $\|\mathcal{R}^n - \mathcal{R}\|_{\mathcal{L}(X)}$ is sufficiently small. Summarizing, the behavior of the spectrum is much the same as in the finite dimensional case if we can ensure (1.30). Therefore, we start this section by investigating the convergence of $\mathcal{R}^n - \mathcal{R}$ in the operator norm.

Recall that the Sobolev space $H^1(0,T;X)$ is given by

$$H^1(0,T;X) = \big\{\varphi \in L^2(0,T;X) \,\big|\, \varphi_t \in L^2(0,T;X)\big\},$$

where φ_t denotes the weak derivative of φ. The space $H^1(0,T;X)$ is a Hilbert space with the inner product

$$\langle \varphi, \phi\rangle_{H^1(0,T;X)} = \int_0^T \langle \varphi(t), \phi(t)\rangle_X + \langle \varphi_t(t), \phi_t(t)\rangle_X \,\mathrm{d}t \text{ for } \varphi, \phi \in H^1(0,T;X)$$

and the induced norm $\|\varphi\|_{H^1(0,T;X)} = \langle \varphi, \varphi\rangle_{H^1(0,T;X)}^{1/2}$.

Let us choose the trapezoidal weights

$$\alpha_1^n = \frac{T}{2(n-1)},\ \alpha_j^n = \frac{T}{n-1} \text{ for } 2 \le j \le n-1,\ \alpha_n^n = \frac{T}{2(n-1)}. \tag{1.31}$$

For this choice we observe that for every $\psi \in X$ the element $\mathcal{R}^n\psi$ is a trapezoidal approximation for $\mathcal{R}\psi$. We will make use of the following lemma.

Lemma 1.18. *Suppose that X is a (separable) real Hilbert space and that the snapshot trajectories y^k belong to $H^1(0,T;X)$ for $1 \le k \le \wp$. Then, (1.30) holds true.*

Proof. For an arbitrary $\psi \in X$ with $\|\psi\|_X = 1$ we define $F : [0,T] \to X$ by

$$F(t) = \sum_{k=1}^{\wp} \langle y^k(t), \psi\rangle_X \, y^k(t) \quad \text{for } t \in [0,T].$$

It follows that

$$\begin{aligned}
\mathcal{R}\psi &= \int_0^T F(t)\,\mathrm{d}t = \sum_{j=1}^{n-1} \int_{t_j}^{t_{j+1}} F(t)\,\mathrm{d}t,\\
\mathcal{R}^n\psi &= \sum_{j=1}^{n} \alpha_j F(t_j) = \frac{\Delta t}{2} \sum_{j=1}^{n-1} \big(F(t_j) + F(t_{j+1})\big).
\end{aligned} \tag{1.32}$$

Then, we infer from $\|\psi\|_X = 1$ that

$$\|F(t)\|_X^2 \le \bigg(\sum_{k=1}^{\wp} \|y^k(t)\|_X^2\bigg)^2. \tag{1.33}$$

Now we show that F belongs to $H^1(0,T;X)$ and its norm is bounded independently of ψ. Recall that $y^k \in H^1(0,T;X)$ imply that $y^k \in C([0,T];X)$ holds for $1 \le k \le \wp$. Using (1.33) we have

$$\|F\|_{L^2(0,T;X)}^2 \le \int_0^T \bigg(\sum_{k=1}^{\wp} \|y^k\|_{C([0,T];X)}^2\bigg)^2 \mathrm{d}t \le C_1$$

with $C_1 = T(\sum_{k=1}^{\wp} \|y^k\|_{C([0,T];X)}^2)^2$. Moreover, $F \in H^1(0,T;X)$ with

$$F_t(t) = \sum_{k=1}^{\wp} \langle y_t^k(t), \psi\rangle_X \, y^k(t) + \langle y^k(t), \psi\rangle_X \, y_t^k(t) \quad \text{f.a.a. } t \in [0,T],$$

where 'f.a.a.' stands for 'for almost all'. Thus, we derive

$$\|F_t\|^2_{L^2(0,T;X)} \leq 4\int_0^T \Big(\sum_{k=1}^{\wp} \|y^k(t)\|_X \|y_t^k(t)\|_X\Big)^2 \mathrm{d}t \leq C_2$$

with $C_2 = 4\sum_{k=1}^{\wp} \|y^k\|^2_{C([0,T];X)} \sum_{l=1}^{\wp} \|y_t^l\|^2_{L^2(0,T;X)} < \infty$. Consequently,

$$\|F\|_{H^1(0,T;X)} = \Big(\int_0^T \|F(t)\|_X^2 + \|F_t(t)\|_X^2 \,\mathrm{d}t\Big)^{1/2} \leq C_3 \tag{1.34}$$

with the constant $C_3 = (C_1 + C_2)^{1/2}$, which is independent of ψ. To evaluate $\mathcal{R}^n\psi$ we notice that

$$\begin{aligned}\int_{t_j}^{t_{j+1}} F(t)\,\mathrm{d}t &= \frac{1}{2}\int_{t_j}^{t_{j+1}} \Big(F(t_j) + \int_{t_j}^{t} F_t(s)\,\mathrm{d}s\Big)\mathrm{d}t \\ &\quad + \frac{1}{2}\int_{t_j}^{t_{j+1}} \Big(F(t_{j+1}) + \int_{t_{j+1}}^{t} F_t(s)\,\mathrm{d}s\Big)\mathrm{d}t \\ &= \frac{\Delta t}{2}\big(F(t_j) + F(t_{j+1})\big) \\ &\quad + \frac{1}{2}\int_{t_j}^{t_{j+1}} \Big(\int_{t_{j+1}}^{t} F_t(s)\,\mathrm{d}s + \int_{t_{j+1}}^{t} F_t(s)\,\mathrm{d}s\Big)\mathrm{d}t.\end{aligned} \tag{1.35}$$

Utilizing (1.32) and (1.35) we obtain

$$\begin{aligned}\big\|\mathcal{R}^n\psi - \mathcal{R}\psi\big\|_X &= \Big\|\sum_{j=1}^{n-1}\Big(\frac{\Delta t}{2}\big(F(t_j) + F(t_{j+1})\big) - \int_{t_j}^{t_{j+1}} F(t)\,\mathrm{d}t\Big)\Big\|_X \\ &\leq \frac{1}{2}\sum_{j=1}^{n-1}\Big\|\int_{t_j}^{t_{j+1}}\int_{t_j}^{t} F_t(s)\,\mathrm{d}s\mathrm{d}t\Big\|_X + \frac{1}{2}\sum_{j=1}^{n-1}\Big\|\int_{t_j}^{t_{j+1}}\int_{t_{j+1}}^{t} F_t(s)\,\mathrm{d}s\mathrm{d}t\Big\|_X.\end{aligned}$$

From the Cauchy-Schwarz inequality [DR12, Satz 12.17] we deduce that

$$\begin{aligned}\sum_{j=1}^{n-1}\Big\|\int_{t_j}^{t_{j+1}}\int_{t_j}^{t} F_t(s)\,\mathrm{d}s\mathrm{d}t\Big\|_X &\leq \sum_{j=1}^{n-1}\int_{t_j}^{t_{j+1}}\Big\|\int_{t_j}^{t} F_t(s)\,\mathrm{d}s\Big\|_X\mathrm{d}t \\ &\leq \sqrt{\Delta t}\sum_{j=1}^{n-1}\Big(\int_{t_j}^{t_{j+1}}\Big\|\int_{t_j}^{t} F_t(s)\,\mathrm{d}s\Big\|_X^2\mathrm{d}t\Big)^{1/2} \\ &\leq \sqrt{\Delta t}\sum_{j=1}^{n-1}\Big(\int_{t_j}^{t_{j+1}}\Big(\int_{t_j}^{t}\|F_t(s)\|_X\,\mathrm{d}s\Big)^2\mathrm{d}t\Big)^{1/2} \\ &\leq \Delta t\sum_{j=1}^{n-1}\Big(\int_{t_j}^{t_{j+1}}\int_{t_j}^{t}\|F_t(s)\|_X^2\,\mathrm{d}s\mathrm{d}t\Big)^{1/2} \leq T\sqrt{\Delta t}\,\|F\|_{H^1(0,T;X)}.\end{aligned} \tag{1.36}$$

Analogously, we derive

$$\sum_{j=1}^{n-1}\Big\|\int_{t_j}^{t_{j+1}}\int_{t_{j+1}}^{t} F_t(s)\,\mathrm{d}s\mathrm{d}t\Big\|_X \leq T\sqrt{\Delta t}\,\|F\|_{H^1(0,T;X)}. \tag{1.37}$$

From (1.34), (1.36) and (1.37) it follows that

$$\big\|\mathcal{R}^n\psi - \mathcal{R}\psi\big\|_X \leq \frac{C_4}{\sqrt{n}},$$

where $C_4 = C_3 T^{3/2}$ is independent of n and ψ. Consequently,

$$\|\mathcal{R}^n - \mathcal{R}\|_{\mathcal{L}(X)} = \sup_{\|\psi\|_X = 1} \|\mathcal{R}^n\psi - \mathcal{R}\psi\|_X \stackrel{n\to\infty}{\longrightarrow} 0$$

which gives the claim. $\square$

Now we follow [KV02a, Section 3.2]. We suppose that $y^k \in H^1(0,T;X)$ for $1 \le k \le \wp$. Thus $y^k \in C([0,T];X)$ holds, which implies that

$$\sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j^n \|y^k(t_j)\|_X^2 \to \sum_{k=1}^{\wp}\int_0^T \|y^k(t)\|_X^2 \,\mathrm{d}t \quad \text{as } n\to\infty. \tag{1.38}$$

Combining (1.38) with (1.8) and (1.29) we find

$$\sum_{i=1}^{d^n} \bar\lambda_i^n \to \sum_{i=1}^{d} \bar\lambda_i \quad \text{as } n\to\infty. \tag{1.39}$$

Now choose and fix

$$\ell \quad \text{such that} \quad \bar\lambda_\ell \neq \bar\lambda_{\ell+1}. \tag{1.40}$$

Then, by spectral analysis of compact operators and Lemma 1.18 it follows that

$$\bar\lambda_i^n \to \bar\lambda_i \quad \text{for } 1 \le i \le \ell \text{ as } n\to\infty. \tag{1.41}$$

Combining (1.39) and (1.41) we derive

$$\sum_{i=\ell+1}^{d^n} \bar\lambda_i^n \to \sum_{i=\ell+1}^{d} \bar\lambda_i \quad \text{as } n\to\infty.$$

Especially, if $\lambda_1 > \lambda_2 > \cdots > \lambda_\ell$ is satisfied, we conclude from (1.40) and Lemma 1.18 that $\lim_{n\to\infty} \|\bar\psi_i^n - \bar\psi_i\|_X = 0$ for $i = 1,\dots,\ell$. Summarizing the following theorem has been shown.

Theorem 1.19. *Let X be a separable real Hilbert space, the weighting parameters $\{\alpha_j^n\}_{j=1}^n$ be given by* (1.31) *and $y^k \in H^1(0,T;X)$ for $1 \le k \le \wp$. Let $\{(\bar\psi_i^n, \bar\lambda_i^n)\}_{i\in\mathbb{I}}$ and $\{(\bar\psi_i, \bar\lambda_i)\}_{i\in\mathbb{I}}$ be eigenvector-eigenvalue pairs satisfying* (1.5) *and* (1.26)*, respectively. Suppose that $\ell \in \mathbb{N}$ is fixed such that* (1.40) *holds. Then we have*

$$\lim_{n\to\infty} \left|\bar\lambda_i^n - \bar\lambda_i\right| = 0 \quad \textit{for } 1 \le i \le \ell,$$

and

$$\lim_{n\to\infty} \sum_{i=\ell+1}^{d^n} \bar\lambda_i^n = \sum_{i=\ell+1}^{d} \bar\lambda_i.$$

In particular, if $\lambda_1 > \lambda_2 > \cdots > \lambda_\ell$ holds, then we even have

$$\lim_{n\to\infty} \|\bar\psi_i^n - \bar\psi_i\|_X = 0 \quad \textit{for } 1 \le i \le \ell.$$

Remark 1.20. Theorem 1.19 gives an answer to the two questions posed at the beginning of Section 1.2: The time instances $\{t_j\}_{j=1}^n$ and the associated positive weights $\{\alpha_j^n\}_{j=1}^n$ should be chosen such that $\mathcal{R}^n$ is a quadrature approximation of $\mathcal{R}$ and $\|\mathcal{R}^n - \mathcal{R}\|_{\mathcal{L}(X)}$ is small (for reasonable n). A different strategy is applied in [KV10], where the time instances $\{t_j\}_{j=1}^n$ are chosen by an optimization approach. Clearly, other choices for the weights $\{\alpha_j^n\}_{j=1}^n$ are also possible provided (1.30) is guaranteed. For instance, we can choose the Simpson weights. $\Diamond$

2 Reduced-order modelling for evolution problems

In this section we utilize the POD method to derive low-dimensional models for evolution problems. For that purpose the POD basis of rank ℓ serves as test and ansatz functions in a POD Galerkin approximation. The a-priori error of the POD Galerkin scheme is investigated. It turns out that the resulting error bounds depend on the number of POD basis functions.

2.1 The abstract evolution problem

In this subsection we introduce our abstract evolution problem which will be under consideration in Sections 2 and 3. Let V and H be real, separable Hilbert spaces and suppose that V is dense in H with compact embedding. By $\langle\cdot\,,\cdot\rangle_H$ and $\langle\cdot\,,\cdot\rangle_V$ we denote the inner products in H and V, respectively. In particular, there exists an embedding constant $c_V > 0$ such that

$$\|\varphi\|_H \le c_V\,\|\varphi\|_V \quad \text{for all } \varphi \in V. \tag{2.1}$$

Let $T > 0$ the final time. For $t \in [0,T]$ we define a time-dependent symmetric bilinear form $a(t;\cdot\,,\cdot) : V \times V \to \mathbb{R}$ satisfying

$$\big|a(t;\varphi,\psi)\big| \le \gamma\,\|\varphi\|_V\|\psi\|_V \qquad \forall\varphi \in V \text{ a.e. in } [0,T], \tag{2.2a}$$

$$a(t;\varphi,\varphi) \ge \gamma_1\,\|\varphi\|_V^2 - \gamma_2\,\|\varphi\|_H^2 \qquad \forall\varphi \in V \text{ a.e. in } [0,T] \tag{2.2b}$$

for constants γ, $\gamma_1 > 0$ and $\gamma_2 \ge 0$ which do not depend on t. In (2.2), the abbreviation "a.e." stands for "almost everywhere". By identifying H with its dual H' it follows that $V \hookrightarrow H = H' \hookrightarrow V'$ each embedding being continuous and dense. Here, V' denotes the dual space of V. Recall that the function space (see [Tro09, §3.4.1], for instance)

$$W(0,T) = \big\{\varphi \in L^2(0,T;V)\,\big|\,\varphi_t \in L^2(0,T;V')\big\}$$

is a Hilbert space endowed with the inner product

$$\langle\varphi,\phi\rangle_{W(0,T)} = \int_0^T \langle\varphi(t),\phi(t)\rangle_V + \langle\varphi_t(t),\phi_t(t)\rangle_{V'}\,\mathrm{d}t \text{ for } \varphi,\phi \in W(0,T)$$

and the induced norm $\|\varphi\|_{W(0,T)} = \langle\varphi,\varphi\rangle_{W(0,T)}^{1/2}$. Furthermore, $W(0,T)$ is continuously embedded into the space $C([0,T];H)$. Hence, $\varphi(0)$ and $\varphi(T)$ are meaningful in H for an element $\varphi \in W(0,T)$. The integration by parts formula reads

$$\begin{aligned}\int_0^T \langle\varphi_t(t),\phi(t)\rangle_{V',V}\,\mathrm{d}t + \int_0^T \langle\phi_t(t),\varphi(t)\rangle_{V',V}\,\mathrm{d}t &= \frac{\mathrm{d}}{\mathrm{d}t}\int_0^T \langle\varphi(t),\psi(t)\rangle_H\,\mathrm{d}t\\ &= \varphi(T)\phi(T) - \varphi(0)\phi(0)\end{aligned}$$

for φ, $\phi \in W(0,T)$, where $\langle\cdot\,,\cdot\rangle_{V',V}$ stands for the dual pairing between V and its dual space V'. Moreover, we have the formula

$$\langle\varphi_t(t),\phi\rangle_{V',V} = \frac{\mathrm{d}}{\mathrm{d}t}\,\langle\varphi(t),\phi\rangle_H \quad \text{for } (\varphi,\phi) \in W(0,T) \times V \text{ and f.a.a. } t \in [0,T].$$

Since we will consider optimal control problems in Section 3, we already introduce the evolution problem with an input term. We suppose that for $N_u \in \mathbb{N}$ the input space $U = L^2(0,T;\mathbb{R}^{N_u})$ is chosen. In particular, we identify U with its dual space U'. For $u \in U$, $y_\circ \in H$ and $f \in L^2(0,T;V')$ we consider the linear evolution problem

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle y(t),\varphi\rangle_H + a(t;y(t),\varphi) &= \langle (f+\mathcal{B}u)(t),\varphi\rangle_{V',V} && \forall \varphi \in V \text{ a.e. in } (0,T], \\ \langle y(0),\varphi\rangle_H &= \langle y_\circ,\varphi\rangle_H && \forall \varphi \in H, \end{aligned} \tag{2.3}$$

where $\mathcal{B} : U \to L^2(0,T;V')$ is a continuous, linear (control or input) operator.

Remark 2.1. Notice that the techniques presented in this work can be adapted for problems, where the input space U is given by $L^2(0,T;L^2(\mathcal{D}))$ for some open and bounded domain $\mathcal{D} \subset \mathbb{R}^{\widetilde{N}_u}$ for an $\widetilde{N}_u \in \mathbb{N}$. ◊

Theorem 2.2. *For $t \in [0,T]$ let $a(t;\cdot\,,\cdot) : V \times V \to \mathbb{R}$ be a time-dependent symmetric bilinear form satisfying (2.2). Then, for every $u \in U$, $f \in L^2(0,T;V')$ and $y_\circ \in H$ there is a unique weak solution $y \in W(0,T)$ satisfying (2.3) and*

$$\|y\|_{W(0,T)} \le C\left(\|y_\circ\|_H + \|f\|_{L^2(0,T;V')} + \|u\|_U\right) \tag{2.4}$$

for a constant $C > 0$ which is independent of u, $y_\circ$ and f. If $f \in L^2(0,T;H)$, $a(t;\cdot\,,\cdot) = a(\cdot\,,\cdot)$ (independent of t) and $y_\circ \in V$ hold, we even have $y \in L^\infty(0,T;V) \cap H^1(0,T;H)$. Here, $L^\infty(0,T;V)$ stands for the Banach space of all measurable functions $\varphi : [0,T] \to V$ with $\operatorname{ess\,sup}_{t\in[0,T]} \|\varphi(t)\|_V < \infty$ (see [Tro09, §3.4.1]*, for instance).*

Proof. For a proof of the existence of a unique solution we refer to [DL00, pp. 512-520]. The a-priori error estimate follows from standard variational techniques and energy estimates. The regularity result follows from [DL00, pp. 532-533] and [Eva08, pp. 360-364]. ☐

Remark 2.3. We split the solution to (2.3) in one part, which depends on the fixed initial condition $y_\circ$ and right-hand f, and another part depending linearly on the input variable u. Let $\hat{y} \in W(0,T)$ be the unique solution to

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{y}(t),\varphi\rangle_H + a(t;\hat{y}(t),\varphi) &= \langle f(t),\varphi\rangle_{V',V} && \forall \varphi \in V \text{ a.e. in } (0,T], \\ \hat{y}(0) &= y_\circ && \text{in } H. \end{aligned}$$

We define the subspace

$$W_0(0,T) = \big\{\varphi \in W(0,T) \,\big|\, \varphi(0) = 0 \text{ in } H\big\}$$

endowed with the topology of $W(0,T)$. Let us now introduce the linear solution operator $\mathcal{S} : U \to W_0(0,T)$: for $u \in U$ the function $y = \mathcal{S}u \in W_0(0,T)$ is the unique solution to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle y(t),\varphi\rangle_H + a(t;y(t),\varphi) = \langle (\mathcal{B}u)(t),\varphi\rangle_{V',V} \quad \forall \varphi \in V \text{ a.e. in } (0,T].$$

From $y \in W_0(0,T)$ we infer $y(0) = 0$ in H. The boundedness of $\mathcal{S}$ follows from (2.4). Now, the solution to (2.3) can be expressed as $y = \hat{y} + \mathcal{S}u$. ◊

2.2 The POD method for the evolution problem

Let $u \in U$, $f \in L^2(0,T;V')$ and $y_\circ \in H$ be given and $y = \hat{y} + \mathcal{S}u$. To keep the notation simple we apply only a spatial discretization with POD basis functions, but no time integration by, e.g., the implicit Euler method. Therefore, we utilize the continuous version of the POD method introduced in Section 1.2. In this section we distinguish two choices for X: $X = H$ and $X = V$. It turns out that the choice for X leads to different rate of convergence results. We suppose that the snapshots y^k, $k = 1, \dots, \wp$, belong to $L^2(0, T; V)$. Later, we will present different rate of convergence results for appropriate choices of the y^k's. Let us introduce the following notations:

$$\mathcal{R}_V \psi = \sum_{k=1}^{\wp} \int_0^T \langle \psi, y^k(t) \rangle_V \, y^k(t) \, \mathrm{d}t \qquad \text{for } \psi \in V,$$
$$\mathcal{R}_H \psi = \sum_{k=1}^{\wp} \int_0^T \langle \psi, y^k(t) \rangle_H \, y^k(t) \, \mathrm{d}t \qquad \text{for } \psi \in H. \tag{2.5}$$

Moreover, we set $\mathcal{K}_V = \mathcal{R}_V^\star$ and $\mathcal{K}_H = \mathcal{R}_H^\star$. In Remark 1.17 we have introduced the singular value decomposition of the operator $\mathcal{Y}$ defined by (1.25). To distinguish the two choices for the Hilbert space X we denote by the sequence $\{(\sigma_i^V, \psi_i^V, \phi_i^V)\}_{i \in \mathbb{I}}^{\ell} \subset \mathbb{R}_0^+ \times V \times L^2(0, T; \mathbb{R}^{\wp})$ of triples the singular value decomposition for $X = V$, i.e., we have that

$$\mathcal{R}_V \psi_i^V = \lambda_i^V \psi_i^V, \quad \mathcal{K}_V \phi_i^V = \lambda_i^V \phi_i^V, \quad \sigma_i^V = \sqrt{\lambda_i^V}, \quad i \in \mathbb{I}.$$

Furthermore, let the sequence $\{(\sigma_i^H, \psi_i^H, \phi_i^H)\}_{i \in \mathbb{I}}^{\ell} \subset \mathbb{R}_0^+ \times H \times L^2(0, T; \mathbb{R}^{\wp})$ in satisfy

$$\mathcal{R}_H \psi_i^H = \lambda_i^H \psi_i^H, \quad \mathcal{K}_H \phi_i^H = \lambda_i^H \phi_i^H, \quad \sigma_i^H = \sqrt{\lambda_i^H}, \quad i \in \mathbb{I}. \tag{2.6}$$

The relationship between the singular values σ_i^H and σ_i^V is investigated in the next lemma, which is taken from [Sin14].

Lemma 2.4. *Suppose that the snapshots $y^k \in L^2(0, T; V)$, $k = 1, \dots, \wp$. Then we have:*

1) *For all $i \in \mathbb{I}$ with $\sigma_i^H > 0$ we have $\psi_i^H \in V$.*
2) *$\sigma_i^V = 0$ for all $i > d$ with some $d \in \mathbb{N}$ if and only if $\sigma_i^H = 0$ for all $i > d$, i.e., we have $d_H = d_V$ if the rank of $\mathcal{R}_V$ is finite.*
3) *$\sigma_i^V > 0$ for all $i \in \mathbb{I}$ if and only if $\sigma_i^H > 0$ for all $i \in \mathbb{I}$.*

Proof. We argue similarly as in the proof of Lemma 3.1 in [Sin14].

1) Let $\sigma_i^H > 0$ hold. Then, it follows that $\lambda_i^H > 0$. We infer from $y^k \in L^2(0, T; V)$ that $\mathcal{R}_H \psi \in V$ for any $\psi \in H$. Hence, we infer from (2.6) and that $\psi_i^H = \mathcal{R}_H \psi_i^H / \lambda_i^H \in V$.
2) Assume that $\sigma_i^V = 0$ for all $i > d$ with some $d \in \mathbb{N}$. Then, we deduce from (1.27) that

$$y^k(t) = \sum_{i=1}^{d} \langle y^k(t), \psi_i^V \rangle_V \, \psi_i^V \quad \text{for every } k = 1, \dots, \wp. \tag{2.7}$$

   From

$$\begin{aligned} \mathcal{R}_H \psi_j^H &= \sum_{k=1}^{\wp} \int_0^T \langle \psi_j^H, y^k(t) \rangle_H \, y^k(t) \, \mathrm{d}t \\ &= \sum_{i=1}^{d} \left(\sum_{k=1}^{\wp} \int_0^T \langle \psi_j^H, y^k(t) \rangle_H \langle y^k(t), \psi_i^V \rangle_V \, \mathrm{d}t \right) \psi_i^V, \quad j \in \mathbb{I}, \end{aligned}$$

   we conclude that that the range of $\mathcal{R}_H$ is at most d-dimensional, which implies that $\lambda_i^H = 0$ for all $i > d$. Analogously, we deduce from $\sigma_i^H = 0$ for all $i > d$ that the range of $\mathcal{R}_V$ is at most d.
3) The claim follows directly from part 2).

Thus, Lemma 2.4 is proved. $\square$

Let us define the two POD subspaces

$$V^\ell = \text{span}\left\{\psi_1^V, \ldots, \psi_\ell^V\right\} \subset V, \quad H^\ell = \text{span}\left\{\psi_1^H, \ldots, \psi_\ell^H\right\} \subset V \subset H,$$

where $H^\ell \subset V$ follows from part 1) of Lemma 2.4. Moreover, we introduce the orthogonal projection operators $\mathcal{P}_H^\ell : V \to H^\ell \subset V$ and $\mathcal{P}_V^\ell : V \to V^\ell \subset V$ as follows:

$$\begin{aligned} v^\ell = \mathcal{P}_H^\ell \varphi \text{ for any } \varphi \in V \quad &\text{iff } v^\ell \text{ solves } \min_{w^\ell \in H^\ell} \|\varphi - w^\ell\|_V, \\ v^\ell = \mathcal{P}_V^\ell \varphi \text{ for any } \varphi \in V \quad &\text{iff } v^\ell \text{ solves } \min_{w^\ell \in V^\ell} \|\varphi - w^\ell\|_V. \end{aligned} \tag{2.8}$$

It follows from the first-order optimality conditions that $v^\ell = \mathcal{P}_H^\ell \varphi$ satisfies

$$\langle v^\ell, \psi_i^H \rangle_V = \langle \varphi, \psi_i^H \rangle_V, \quad 1 \le i \le \ell. \tag{2.9}$$

Writing $v^\ell \in H^\ell$ in the form $v^\ell = \sum_{j=1}^\ell \mathrm{v}_j^\ell \psi_j^H$ we derive from (2.9) that the vector $\mathrm{v}^\ell = (\mathrm{v}_1^\ell, \ldots, \mathrm{v}_\ell^\ell)^\top \in \mathbb{R}^\ell$ satisfies the linear system

$$\sum_{j=1}^\ell \langle \psi_j^H, \psi_i^H \rangle_V \, \mathrm{v}_j^\ell = \langle \varphi, \psi_i^H \rangle_V, \quad 1 \le i \le \ell.$$

For the operator $\mathcal{P}_V^\ell$ we have the explicit representation

$$\mathcal{P}_V^\ell \varphi = \sum_{i=1}^\ell \langle \varphi, \psi_i^V \rangle_V \, \psi_i^V \text{ for } \varphi \in V.$$

Since the linear operators $\mathcal{P}_V^\ell$ and $\mathcal{P}_H^\ell$ are orthogonal projections, we have $\|\mathcal{P}_V^\ell\|_{\mathcal{L}(V)} = \|\mathcal{P}_H^\ell\|_{\mathcal{L}(V)} = 1$. As $\{\psi_i^V\}_{i \in \mathbb{I}}$ is a complete orthonormal basis in V, we have

$$\lim_{\ell \to \infty} \int_0^T \|w(t) - \mathcal{P}_V^\ell w(t)\|_V^2 \, \mathrm{d}t = 0 \quad \text{for all } w \in L^2(0,T;V). \tag{2.10}$$

Next we review an essential result from [Sin14, Theorem 5.2], which we will use in our a-priori error analysis for the choice $X = H$. Recall that $\psi_i^H \in V$ holds for $1 \le i \le d_H$ and the image of $\mathcal{P}_H^\ell$ belongs to V. Consequently, $\|\psi_i^H - \mathcal{P}_H^\ell \psi_i^H\|_V$ is well-defined for $1 \le i \le d_H$.

Theorem 2.5. *Suppose that $y^k \in L^2(0,T;V)$ for $1 \le k \le \wp$. Then,*

$$\sum_{k=1}^\wp \int_0^T \|y^k(t) - \mathcal{P}_H^\ell y^k(t)\|_V^2 \, \mathrm{d}t = \sum_{i=\ell+1}^{d_H} \lambda_i^H \, \|\psi_i^H - \mathcal{P}_H^\ell \psi_i^H\|_V^2. \tag{2.11}$$

Here, d_H is the rank of the operator $\mathcal{R}_H$, which may be infinite. Moreover, $\mathcal{P}_H^\ell y^k$ converges to y^k in $L^2(0,T;V)$ as ℓ tends to ∞ for each $k \in \{1, \ldots, \wp\}$.

Proof. Suppose that $1 \le \ell \le d_H$ and $1 \le \ell_\circ < \infty$ hold. Then, $\lambda_i^H > 0$ for $1 \le i \le \ell$. Let $\mathcal{I} \in \mathcal{L}(V)$ denote the identity operator. As $\mathcal{I} - \mathcal{P}_H^\ell$ is an orthonormal projection on V, we conclude $\|\mathcal{I} - \mathcal{P}_H^\ell\|_{\mathcal{L}(V)} = 1$. Furthermore, $y^k \in L^2(0,T;V)$ holds for each $k \in \{1, \ldots \wp\}$. Thus, (2.10) implies that $\mathcal{P}_V^{\ell_\circ} y^k \to y^k$ in $L^2(0,T;V)$ as $\ell_\circ \to \infty$ for each k. The proof of (2.11) is essentially based on Hilbert-Schmidt theory and on the following result [Sin14, Lemma 5.1]:

$$\begin{aligned} &\sum_{k=1}^\wp \int_0^T \|(\mathcal{I} - \mathcal{P}_H^\ell)\mathcal{P}_V^{\ell_\circ} y^k(t))\|_V^2 \, \mathrm{d}t \\ &\quad = \sum_{i=1}^{\ell_\circ} \lambda_i^V \, \|\psi_i^V - \mathcal{P}_H^\ell \psi_i^V\|_V^2 \le \sum_{i:\lambda_i^V > 0} \lambda_i^V \, \|\psi_i^V - \mathcal{P}_H^\ell \psi_i^V\|_V^2 < \infty \end{aligned} \tag{2.12}$$

for any $\ell_\circ \in \mathbb{N}$. To prove that $\mathcal{P}_H^\ell y^k$ converges to y^k in $L^2(0,T;V)$ as ℓ tends to ∞ for each $k \in \{1,\dots,\wp\}$ we observe that

$$\begin{aligned}\sum_{i=\ell+1}^{d_H} \lambda_i^H \|\psi_i^H - \mathcal{P}_H^\ell \psi_i^H\|_V^2 &\le \sum_{i=\ell+1}^{d_H} \lambda_i^H \|\mathcal{I} - \mathcal{P}_H^\ell\|_{\mathcal{L}(V)} \|\psi_i^H\|_V^2 \\ &= \sum_{i=\ell+1}^{d_H} \lambda_i^H \|\psi_i^H\|_V^2\end{aligned}$$

By utilizing the singular value decomposition (see Remark 1.17) it is shown in [Sin14, Theorem 5.2] that $\sum_{i=\ell+1}^{d_H} \lambda_i^H \|\psi_i^H\|_V^2 < \infty$ holds. Therefore,

$$\lim_{\ell_\circ \to \infty} \sum_{k=1}^{\wp} \int_0^T \|(\mathcal{I} - \mathcal{P}_H^\ell)\mathcal{P}_V^{\ell_\circ} y^k(t))\|_V^2 \,\mathrm{d}t = 0$$

which gives the claim. $\square$

We will also need the following result, which follows from the continuous embedding $V \hookrightarrow H$. For a proof we refer to [Sin14, Proposition 5.5].

Lemma 2.6. *Let $y^k \in L^2(0,T;V)$ for each $k \in \{1,\dots,\wp\}$ and $\lambda_i^H > 0$ for all $i \in \mathbb{I}$. Then,*

$$\lim_{\ell \to \infty} \|\varphi - \mathcal{P}_H^\ell \varphi\|_V = 0 \quad \textit{for all } \varphi \in V.$$

2.3 The POD Galerkin approximation

After the computation of a POD basis of rank ℓ we are interested in deriving a low-dimensional approximation for the evolution problem (2.3). In the context of Section 1.2 we choose $\wp = 1$, $y^1 = \mathcal{S}u$ and compute a POD basis $\{\psi_i\}_{i=1}^\ell$ of rank ℓ by solving $(\mathbf{P}^\ell)$ with $\psi_i = \psi_i^V$ for $X = V$ and $\psi_i = \psi_i^H$ for $X = H$. Then, we define the subspace $X^\ell = \operatorname{span}\{\psi_1,\dots,\psi_\ell\}$, i.e., $X^\ell = V^\ell$ for $X = V$ and $X^\ell = H^\ell$ for $X = H$. Now we approximate the state variable y by the Galerkin expansion

$$y^\ell(t) = \hat{y}(t) + \sum_{i=1}^{\ell} \mathrm{y}_i^\ell(t)\psi_i \in V \quad \text{a.e. in } [0,T] \tag{2.13}$$

with coefficient functions $\mathrm{y}_i^\ell : [0,T] \to \mathbb{R}$. We introduce the vector-valued coefficient function

$$\mathrm{y}^\ell = \left(\mathrm{y}_1^\ell,\dots,\mathrm{y}_\ell^\ell\right) : [0,T] \to \mathbb{R}^\ell.$$

Since $\hat{y}(0) = y_\circ$ holds, we suppose that $\mathrm{y}^\ell(0) = 0$. Then, $y^\ell(0) = y_\circ$ is valid, i.e., the POD state matches exactly the initial condition. Inserting (2.13) into (2.3) and using the test space in V^ℓ for $1 \le i \le \ell$ we obtain the following POD Galerkin scheme for (2.3): $y^\ell \in W(0,T)$ solves

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\langle y^\ell(t),\psi\rangle_H + a(t;y^\ell(t),\psi) = \langle (f+\mathcal{B}u)(t),\psi\rangle_{V',V} \;\forall \psi \in X^\ell \text{ a.e.},\\ &\mathrm{y}^\ell(0) = 0.\end{aligned} \tag{2.14}$$

We call (2.14) a *low dimensional* or *reduced-order model* for (2.3).

Proposition 2.7. *Let all assumptions of Theorem 2.2 be satisfied and the POD basis of rank ℓ be computed as desribed at the beginning of Section 2.1. Then, there exists a unique solution $y^\ell \in H^1(0,T;V) \hookrightarrow W(0,T)$ solving (2.14).*

Proof. Choosing $\psi = \psi_i$, $1 \le i \le \ell$, and applying (2.13) we infer from (2.14) that the coefficient vector y^ℓ satisfies

$$\mathrm{M}^\ell \dot{\mathrm{y}}^\ell(t) + \mathrm{A}^\ell(t)\mathrm{y}(t) = \hat{\mathrm{F}}^\ell(t) \text{ a.e. in } [0,T], \quad \mathrm{y}^\ell(0) = 0, \tag{2.15}$$

where we have set

$$\begin{aligned} &\mathrm{M}^\ell = \big(\big(\langle \psi_i, \psi_j \rangle_H\big)\big) \in \mathbb{R}^{\ell \times \ell}, \quad \mathrm{A}^\ell(t) = \big(\big(a(t;\psi_i,\psi_j)\big)\big) \in \mathbb{R}^{\ell\times\ell}, \\ &\hat{\mathrm{F}}^\ell(t) = \big(\langle (f + \mathcal{B}u)(t) - \hat{y}_t(t), \psi_i \rangle_{V',V} - a(t;\hat{y}(t),\psi_i)\big) \in \mathbb{R}^\ell \end{aligned} \tag{2.16}$$

with $\psi_i = \psi_i^V$ for $X = V$ and $\psi_i = \psi_i^H$ for $X = H$. Since (2.15) is a linear ordinary differential equation system the existence of a unique $\mathrm{y}^\ell \in H^1(0,T;\mathbb{R}^\ell)$ follows by standard arguments. □

Remark 2.8. 1) Suppose $\hat{y} \ne 0$. Then, the POD approximation does admit values $y^\ell(t)$ in X, but $(y^\ell - \hat{y})(t) \in X^\ell$ holds. The benefit of this approach is that $y^\ell(0) = y_\circ$ – and not $y^\ell(0) = \mathcal{P}_H^\ell y_\circ$ or $y^\ell(0) = \mathcal{P}_V^\ell y_\circ$. This improves the approximation quality of the POD basis which is illustrated in our numerical tests.

2) We proceed analogously to Remark 2.3 and introduce the linear and bounded solution operator $\mathcal{S}^\ell : U \to W_0(0,T)$: for $u \in U$ the function $w^\ell = \mathcal{S}^\ell u \in W(0,T)$ satisfies $w^\ell(0) = 0$ and

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle w^\ell(t), \psi \rangle_H + a(t; w^\ell(t), \psi) = \langle (\mathcal{B}u)(t), \psi \rangle_{V',V} \quad \forall \psi \in X^\ell \text{ a.e.}$$

Then, the solution to (2.14) is given by $y^\ell = \hat{y} + \mathcal{S}^\ell u$. Analogous to the proof of (2.4) we derive that there exists a positive constant C_2 which does not depend on ℓ or u so that

$$\|\mathcal{S}^\ell u\|_{W(0,T)} \le C \, \|u\|_U.$$

Thus, $\mathcal{S}^\ell$ is bounded uniformly with respect to ℓ. ◊

To investigate the convergence of the error $y - y^\ell$ we make use of the following two inequalities:

1) *Gronwall's inequality* [DR11, Satz 16.6]: For $T > 0$ let $v : [0,T] \to \mathbb{R}$ be a nonnegative, differentiable function satisfying

$$v'(t) \le \varphi(t)v(t) + \chi(t) \quad \text{for all } t \in [0,T],$$

where φ and χ are real-valued, nonnegative, integrable functions on $[0,T]$. Then

$$v(t) \le \exp\left(\int_0^t \varphi(s)\,\mathrm{d}s\right)\left(v(0) + \int_0^t \chi(s)\,\mathrm{d}s\right) \quad \text{for all } t \in [0,T]. \tag{2.17}$$

In particular, if

$$v' \le \varphi v \text{ in } [0,T] \quad \text{and} \quad v(0) = 0$$

hold, then $v = 0$ in $[0,T]$.

2) *Young's inequality* [DR11, Satz 10.2-(iii)]: For every $a, b \in \mathbb{R}$ and for every $\varepsilon > 0$ we have

$$ab \le \frac{\varepsilon a^2}{2} + \frac{b^2}{2\varepsilon}.$$

Theorem 2.9. *Let $u \in U$ be chosen arbitrarily with $0 \ne \mathcal{S}u \in H^1(0,T;V)$.*

1) *To compute a POD basis $\{\psi_i\}_{i=1}^\ell$ of rank ℓ we choose $\wp = 1$ and $y^1 = \mathcal{S}u$. Then, $y = \hat{y} + \mathcal{S}u$ and $y^\ell = \hat{y} + \mathcal{S}^\ell u$ satisfies the a-priori error estimate*

$$\begin{aligned} &\|y^\ell - y\|^2_{W(0,T)} \\ &\le C_1 \cdot \begin{cases} \displaystyle\sum_{i=\ell+1}^{d_V} \lambda_i^V + \|y_t^1 - \mathcal{P}_V^\ell y_t^1\|^2_{L^2(0,T;V)} & \text{if } X = V, \\ \displaystyle\sum_{i=\ell+1}^{d_H} \lambda_i^H \, \|\psi_i^H - \mathcal{P}_H^\ell \psi_i^H\|_V^2 + \|y_t^1 - \mathcal{P}_H^\ell y_t^1\|^2_{L^2(0,T;V)} & \text{if } X = H, \end{cases} \end{aligned} \tag{2.18}$$

where the constant C_1 depends on the terminal time T and the constants γ, γ_1, γ_2 introduced in (2.2).

2) *Let $\mathcal{S}u \in H^1(0,T;V)$ holds true. If we set $\wp = 2$ and compute a POD basis of rank ℓ using the trajectories $y^1 = \mathcal{S}u$ and $y^2 = (\mathcal{S}u)_t$, it follows that*

$$\|y^\ell - y\|^2_{W(0,T)} \leq C_3 \cdot \begin{cases} \sum\limits_{i=\ell+1}^{d_V} \lambda_i^V & \text{for } X = V, \\ \sum\limits_{i=\ell+1}^{d_H} \lambda_i^H \|\psi_i^H - \mathcal{P}_H^\ell \psi_i^H\|_V^2 & \text{for } X = H \end{cases} \tag{2.19}$$

for a constant C_3 which depends on γ, γ_1, γ_2, and T.

Proof.

1) For almost all $t \in [0,T]$ we make use of the decomposition

$$\begin{aligned} y^\ell(t) - y(t) &= \hat{y}(t) + (\mathcal{S}^\ell u)(t) - \hat{y}(t) - (\mathcal{S}u)(t) \\ &= (\mathcal{S}^\ell u)(t) - \mathcal{P}^\ell\big((\mathcal{S}u)(t)\big) + \mathcal{P}^\ell\big((\mathcal{S}u)(t)\big) - (\mathcal{S}u)(t) \\ &= \vartheta^\ell(t) + \varrho^\ell(t), \end{aligned} \tag{2.20}$$

where $\vartheta^\ell = \mathcal{S}^\ell u - \mathcal{P}^\ell(\mathcal{S}u) \in X^\ell$ and $\varrho^\ell = \mathcal{P}^\ell(\mathcal{S}u) - \mathcal{S}u$. In (2.20) we will consider the two choices $\mathcal{P}^\ell = \mathcal{P}_H^\ell$ for $X = H$ and $\mathcal{P}^\ell = \mathcal{P}_V^\ell$ for $X = V$. Since $H^1(0,T;V) \hookrightarrow W(0,T)$ holds, there exists an embedding constant $c_e > 0$ such that

$$\|\varphi\|_{W(0,T)} \leq c_e \|\varphi\|_{H^1(0,T;V)} \quad \text{for all } \varphi \in H^1(0,T;V). \tag{2.21}$$

From $y^1 = \mathcal{S}u$ and (1.27) we infer that

$$\|\varrho^\ell\|^2_{W(0,T)} \leq c_e^2 \|\varrho^\ell\|^2_{H^1(0,T;V)} = c_e^2 \sum_{i=\ell+1}^{d_V} \lambda_i^V + c_e^2 \|y_t^1 - \mathcal{P}_V^\ell y_t^1\|^2_{L^2(0,T;V)} \tag{2.22}$$

in case of $X = V$, where d_V stands for rank of $\mathcal{R}_V$. For the choice $X = H$ we derive from $y^1 = \mathcal{S}u$ and Theorem 2.5 that

$$\|\varrho^\ell\|^2_{W(0,T)} \leq c_e^2 \sum_{i=\ell+1}^{d_H} \lambda_i^H \|\psi_i^H - \mathcal{P}_H^\ell \psi_i^H\|_V^2 + c_e^2 \|y_t^1 - \mathcal{P}_H^\ell y_t^1\|^2_{L^2(0,T;V)}. \tag{2.23}$$

Here, d_H denotes for rank of $\mathcal{R}_H$. Using $\vartheta_t^\ell(t) \in H$ for almost all $t \in [0,T]$, (2.3), (2.14) and (2.2a) we derive that

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t} \langle \vartheta^\ell(t), \psi \rangle_H + a(t; \vartheta^\ell(t), \psi) \\ &\quad = \langle y_t^1(t) - \mathcal{P}^\ell y_t^1(t), \psi \rangle_H + a(t; y^1(t) - \mathcal{P}^\ell y^1(t), \psi) \\ &\quad \leq \|y_t^1(t) - \mathcal{P}^\ell y_t^1(t)\|_H \|\psi\|_H + \gamma \|y^1(t) - \mathcal{P}^\ell y^1(t)\|_V \|\psi\|_V \end{aligned} \tag{2.24}$$

for all $\psi \in X^\ell$ and for almost all $t \in [0,T]$. From choosing $\psi = \vartheta^\ell(t)$, (2.2b) and (2.24) we find

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t} \|\vartheta^\ell(t)\|_H^2 + \gamma_1 \|\vartheta^\ell(t)\|_V^2 - 3\gamma_2 \|\vartheta^\ell(t)\|_H^2 \\ &\qquad \leq \frac{1}{\gamma_2} \|y_t^1(t) - \mathcal{P}^\ell y_t^1(t)\|_H^2 + \frac{\gamma^2}{\gamma_1} \|y^1(t) - \mathcal{P}^\ell y^1(t)\|_V^2. \end{aligned}$$

From (2.17) – setting $v(t) = \|\vartheta^\ell(t)\|_H^2 \geq 0$,

$$\chi(t) = \frac{1}{\gamma_2} \|y_t^1(t) - \mathcal{P}^\ell y_t^1(t)\|_H^2 + \frac{\gamma^2}{\gamma_1} \|y^1(t) - \mathcal{P}^\ell y^1(t)\|_V^2 \geq 0,$$

$\varphi(t) = 3\gamma_2 > 0$ – and $\vartheta^\ell(0) = 0$ it follows that

$$\|\vartheta^\ell(t)\|_H^2 \leq c_1 \left(\|y_t^1 - \mathcal{P}^\ell y_t^1\|^2_{L^2(0,T;H)} + \|y^1 - \mathcal{P}^\ell y^1\|^2_{L^2(0,T;V)}\right)$$

for almost all $t \in [0, T]$ with the constants $c_1 = c_2 \exp(3\gamma_2 T)$ and $c_2 = \max(1/\gamma_2, \gamma^2/\gamma_1)$, so that we derive from (2.1)

$$\begin{aligned}
\|\vartheta^\ell\|^2_{L^2(0,T;V)} &\leq c_3\Big(\|\vartheta^\ell\|^2_{L^2(0,T;H)} + \|y_t^1 - \mathcal{P}^\ell y_t^1\|^2_{L^2(0,T;H)}\Big)\\
&\quad + c_3\,\|y^1 - \mathcal{P}^\ell y^1\|^2_{L^2(0,T;V)}\\
&\leq c_4\Big(\|y_t^1 - \mathcal{P}^\ell y_t^1\|^2_{L^2(0,T;H)} + \|\varrho^\ell(t)\|^2_{L^2(0,T;V)}\Big)\\
&\leq c_4\Big(c_V^2\,\|y_t^1 - \mathcal{P}^\ell y_t^1\|^2_{L^2(0,T;V)} + \|\varrho^\ell(t)\|^2_{L^2(0,T;V)}\Big)
\end{aligned} \tag{2.25}$$

with $c_3 = \max(3\gamma_2, c_2)/\gamma_1$ and $c_4 = c_3(1 + c_1 T)$. We conclude from (2.2a), (2.18), (2.25) and (2.1) that

$$\begin{aligned}
\|\vartheta_t^\ell\|_{L^2(0,T;(V^\ell)')} &= \sup\left\{\int_0^T \langle\vartheta_t^\ell(t), \psi(t)\rangle_{V',V}\,\Big|\,\|\psi\|_{L^2(0,T;V)} = 1,\ \psi(t) \in V^\ell\right\}\\
&\leq \gamma\,\|\vartheta^\ell\|_{L^2(0,T;V)} + \|y_t^1 - \mathcal{P}^\ell y_t^1\|_{L^2(0,T;H)}\\
&\leq c_5\Big(\|y_t^1 - \mathcal{P}^\ell y_t^1\|_{L^2(0,T;H)} + \|y^1 - \mathcal{P}^\ell y^1\|_{L^2(0,T;V)}\Big)\\
&\leq c_5\Big(c_V\,\|y_t^1 - \mathcal{P}^\ell y_t^1\|_{L^2(0,T;V)} + \|y^1 - \mathcal{P}^\ell y^1\|_{L^2(0,T;V)}\Big)
\end{aligned} \tag{2.26}$$

with $c_5 = 1 + c_4\gamma$. Consequently, (2.25) (2.26) and $c_4 \leq 2c_5^2$ imply

$$\begin{aligned}
\|\vartheta^\ell\|^2_{W(0,T)} &\leq \|\vartheta^\ell\|^2_{L^2(0,T;V)} + \|\vartheta_t^\ell\|^2_{L^2(0,T;V')}\\
&\leq 2c_5^2\,\|y^1 - \mathcal{P}^\ell y^1\|^2_{L^2(0,T;V)} + c_V^2\big(c_4 + 2c_5^2\big)\|y_t^1 - \mathcal{P}^\ell y_t^1\|^2_{L^2(0,T;V')}\\
&\quad + c_4\,\|\varrho^\ell(t)\|^2_{L^2(0,T;V)}\\
&\leq c_6\left(\|y^1 - \mathcal{P}^\ell y^1\|^2_{L^2(0,T;V)} + \|y_t^1 - \mathcal{P}^\ell y_t^1\|^2_{L^2(0,T;V')} + \|\varrho^\ell(t)\|^2_{L^2(0,T;V)}\right)
\end{aligned} \tag{2.27}$$

with $c_6 = \max(2c_5^2, c_V^2(c_4 + 2c_5^2))$. Utilizing (2.20)-(2.23) and (2.27) imply (2.18).

2) The claim follows directly from

$$\|y_t^1 - \mathcal{P}^\ell y_t^1\|^2_{L^2(0,T;V)} = \|y^2 - \mathcal{P}^\ell y^2\|^2_{L^2(0,T;V)},$$

(1.27) and Theorem 2.5. □

Remark 2.10. 1) Note that the a-priori error estimates (2.18) and (2.19) depend an the arbitrarily chosen, but fixed control $u \in U$, which is also utilized to compute the POD basis. Moreover, these a-priori estimates do not involve errors by the POD discretization of the initial condition $y_\circ$. Further, let us mention that the a-priori error analysis holds for $T < \infty$.

2) For the numerical realization we have to utilize also a time integration method like, e.g., the implicit Euler or the Crank-Nicolson method. ◊

Example 2.11. Accurate approximation results are achieved if the subspace spanned by the snapshots is (approximatively) of low dimension. Let $T > 0$, $\Omega = (0, 2) \subset \mathbb{R}$ and $Q = (0, T) \times \Omega$. We set $f(t, \boldsymbol{x}) = e^{-t}(\pi^2 - 1)\sin(\pi \boldsymbol{x})$ for $(t, \boldsymbol{x}) \in Q$ and $y_\circ(\boldsymbol{x}) = \sin(\pi \boldsymbol{x})$ for $\boldsymbol{x} \in \Omega$. Let $H = L^2(\Omega)$, $V = H_0^1(\Omega)$ and

$$a(t; \varphi, \phi) = \int_\Omega \varphi'(\boldsymbol{x})\phi'(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \quad \text{for } \varphi, \phi \in V,$$

i.e., the bilinear form a is independent of t. Finally, we choose $u = 0$. Then, the exact solution to (2.3) is given by $y(t, \boldsymbol{x}) = e^{-t}\sin(\pi \boldsymbol{x})$. Thus, the snapshot space $\mathcal{V}$ is the one-dimensional space $\{\alpha\psi \mid \alpha \in \mathbb{R}\}$ with $\psi(\boldsymbol{x}) = \sin(\pi\boldsymbol{x})$. Choosing the space $X = H$, this implies that all eigenvalues of the operator $\mathcal{R}_H$ introduced in (2.5) except of the first one are zero and $\psi_1 = \psi \in V$ is the single POD element corresponding to a nontrivial eigenvalue of $\mathcal{R}_H$. Further, the reduced order model of the rank-1 POD-Galerkin ansatz

$$\begin{aligned} \dot{\mathrm{y}}^1(t) + \|\psi_1'\|_H^2\, \mathrm{y}^1(t) &= \langle f(t), \psi_1\rangle_H \quad \text{for } t \in (0, T], \\ \mathrm{y}^1(0) &= \langle y_\circ, \psi_1\rangle_H \end{aligned}$$

has the solution $\mathrm{y}^1(t) = e^{-t}$, so both the projection

$$\big(\mathcal{P}^1 y\big)(t, \boldsymbol{x}) = \langle y(t), \psi_1\rangle_X \psi_1(\boldsymbol{x}), \quad (t, \boldsymbol{x}) \in \overline{Q},$$

of the state y on the POD-Galerkin space and the reduced-order solution $y^1(t) = \mathrm{y}^1(t)\psi_1$ coincide with the exact solution y. In the latter case, this is due to the fact that the data functions f and $y_\circ$ as well as all time derivative snapshots $\dot{y}(t)$ are already elements of $\mathrm{span}(\psi_1)$, so no projection error occurs here, cp. the a priori error bounds given in (2.19). In the case $X = V$, we get the same results with $\psi_1(\boldsymbol{x}) = \sin(\pi\boldsymbol{x})/\sqrt{1+\pi^2}$ and $\mathrm{y}^1(t) = \sqrt{1+\pi^2}e^{-t}$. $\Diamond$

Corollary 2.12. *Let $u, \tilde{u} \in U$ be chosen arbitrarily so that $0 \neq \mathcal{S}\tilde{u} \in H^1(0, T; V)$ and $u \neq \tilde{u}$ hold. To compute a POD basis $\{\psi_i\}_{i=1}^\ell$ of rank ℓ we choose $\wp = 1$ and $y^1 = \mathcal{S}\tilde{u}$. Moreover, let $\mathcal{P}^\ell = \mathcal{P}^\ell_V$. Then, $y = \hat{y} + \mathcal{S}u$ and $y^\ell = \hat{y} + \mathcal{S}^\ell u$ satisfies*

$$\lim_{\ell\to\infty} \|y^\ell - y\|_{W(0,T)} = 0. \tag{2.28}$$

Proof. We infer from (2.27), (2.20), (2.21) that

$$\begin{aligned} \|y^\ell - y\|^2_{W(0,T)} &= 2\Big(\|\vartheta^\ell\|^2_{W(0,T)} + \|\varrho^\ell\|^2_{W(0,T)}\Big) \\ &\leq 2c_6\left(\|\varrho^\ell\|^2_{L^2(0,T;V)} + \|\varrho^\ell_t\|^2_{L^2(0,T;V')} + \|\varrho^\ell\|^2_{L^2(0,T;V)}\right) + c_e^2\,\|\varrho^\ell\|^2_{H^1(0,T;V)} \\ &\leq 4c_6\,\|\varrho^\ell\|^2_{W(0,T)} + c_e^2\,\|\varrho^\ell\|^2_{H^1(0,T;V)} \leq c_7\,\|\varrho^\ell\|^2_{H^1(0,T;V)} \end{aligned}$$

with $c_7 = 4c_6c_e^2 + c_e^2$. From (2.10) and $y \in H^1(0, T; V)$ we infer that

$$\|\varrho^\ell\|^2_{H^1(0,T;V)} = \int_0^T \Big\|y(t) - \sum_{i=1}^\ell \langle y(t), \psi_i\rangle_V\,\psi_i\Big\|_V^2 + \Big\|y_t(t) - \sum_{i=1}^\ell \langle y_t(t), \psi_i\rangle_V\,\psi_i\Big\|_V^2\,\mathrm{d}t \stackrel{\ell\to\infty}{\longrightarrow} 0$$

which gives the claim. $\square$

Utilizing the techniques as in the proof of Theorem 6.5 in [Sin14] one can derive an a-priori error bound without including the time derivatives into the snapshot subspace. In the next proposition we formulate the a-priori error estimate.

Proposition 2.13. *Let $y_\circ \in V$ and $u \in U$ be chosen arbitrarily so that $\mathcal{S}u \neq 0$. To compute a POD basis $\{\psi_i\}_{i=1}^\ell$ of rank ℓ we choose $\wp = 1$ and $y^1 = \mathcal{S}u$. Then, $y = \hat{y} + \mathcal{S}u$ and $y^\ell = \hat{y} + \mathcal{S}^\ell u$ satisfies the a-priori error estimate*

$$\|y^\ell - y\|^2_{L^2(0,T;V)} \leq C \cdot \begin{cases} \displaystyle\sum_{i=\ell+1}^{d_V} \lambda_i^V\,\|\psi_i^V - \mathcal{P}^\ell_{H,V^\ell}\psi_i^V\|_V^2 & \text{if } X = V, \\ \displaystyle\sum_{i=\ell+1}^{d_H} \lambda_i^H\,\|\psi_i^H\|_V^2 & \text{if } X = H, \end{cases} \tag{2.29}$$

where the constant C depends on the terminal time T and the constants γ, γ_1, γ_2 introduced in (2.2). Moreover, $\mathcal{P}^\ell_{H,V^\ell} : H \to V^\ell$ is the H-orthogonal projection given as follows:

$$v^\ell = \mathcal{P}^\ell_{H,V^\ell}\varphi \text{ for any } \varphi \in H \text{ iff } v^\ell \text{ solves } \min_{w^\ell \in V^\ell} \|\varphi - w^\ell\|_H.$$

In particular, we have $y^\ell \to y$ in $L^2(0, T; V)$ as $\ell \to \infty$.

3 The linear-quadratic optimal control problem

In this section we apply a POD Galerkin approximation to linear-quadratic optimal control problems. Linear-quadratic problems are interesting in several respects: In particular, they occur in each level of a sequential quadratic programming (SQP) methods; see, e.g., [NW06].

In this chapter we prove convergence and derive a-priori error estimates for the optimal control problem. The error estimates rely on the (unrealistic) assumption that the POD basis is computed from the (exact) optimal solution. However, these estimates are utilized to develop an a-posteriori error analysis for the POD Galerkin appproximation of the optimal control problem. We deduce how far the suboptimal control, computed by the POD Galerkin approximation, is from the (unknown) exact one.

3.1 Problem formulation

In this section we introduce our optimal control problem, which is an constrained optimization problem in a Hilbert space. The objective is a quadratic function. The evolution problem (2.3) serves as an equality constraint. Moreover, bilateral control bounds lead to inequality constraints in the minimization. For the readers' convenience we recall (2.3) here. Let $U = L^2(0, T; \mathbb{R}^{N_u})$ denote the control space with $N_u \in \mathbb{N}$. For $u \in U$, $y_\circ \in H$ and $f \in L^2(0, T; V')$ we consider the state equation

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle y(t), \varphi\rangle_H + a(t; y(t), \varphi) &= \langle (f + \mathcal{B}u)(t), \varphi\rangle_{V',V} && \forall \varphi \in V \text{ a.e. in } (0, T], \\ \langle y(0), \varphi\rangle_H &= \langle y_\circ, \varphi\rangle_H && \forall \varphi \in H, \end{aligned} \tag{3.1}$$

where $\mathcal{B} : U \to L^2(0, T; V')$ is a continuous, linear operator. Due to Theorem 2.2 there exists a unique solution $y \in W(0, T)$ to (3.1).

We introduce the Hilbert space

$$X = W(0, T) \times U$$

endowed with the natural product topology, i.e., with the inner product

$$\langle x, \tilde{x}\rangle_X = \langle y, \tilde{y}\rangle_{W(0,T)} + \langle u, \tilde{u}\rangle_U \quad \text{for } x = (y, u),\ \tilde{x} = (\tilde{y}, \tilde{u}) \in X$$

and the norm $\|x\|_X = (\|y\|^2_{W(0,T)} + \|u\|^2_U)^{1/2}$ for $x = (y, u) \in X$.

Assumption 1. *For $t \in [0, T]$ let $a(t; \cdot, \cdot) : V \times V \to \mathbb{R}$ be a time-dependent symmetric bilinear form satisfying* (2.2)*. Moreover, $f \in L^2(0, T; V')$, $y_\circ \in H$ and $\mathcal{B} \in \mathcal{L}(U, L^2(0, T; V'))$ holds.*

In Remark 2.3 we have introduced the particular solution $\hat{y} \in W(0, T)$ as well as the linear, bounded solution operator $\mathcal{S}$. Then, the solution to (3.1) can be expressed as $y = \hat{y} + \mathcal{S}u$. By X_{ad} we denote the closed, convex and bounded set of admissible solutions for the optimization problem as

$$X_{\mathsf{ad}} = \big\{(\hat{y} + \mathcal{S}u, u) \in X \,\big|\, u_a \le u \le u_b \text{ in } \mathbb{R}^{N_u} \text{ a.e. in } [0, T]\big\},$$

where $u_a = (u_{a,1}, \dots, u_{a,N_u}), u_b = (u_{b,1}, \dots, u_{b,N_u}) \in U$ satisfy $u_{a,i} \le u_{b,i}$ for $1 \le i \le N_u$ a.e. in $[0, T]$. Since $u_{a,i} \le u_{b,i}$ holds for $1 \le i \le N_u$, we infer from Theorem 2.2 that the set X_{ad} is nonempty.

The quadratic objective $J : X \to \mathbb{R}$ is given by

$$J(x) = \frac{\sigma_Q}{2} \int_0^T \|y(t) - y_Q(t)\|_H^2 \,\mathrm{d}t + \frac{\sigma_\Omega}{2} \|y(T) - y_\Omega\|_H^2 + \frac{\sigma}{2} \|u\|_U^2 \tag{3.2}$$

for $x = (y, u) \in X$, where $(y_Q, y_\Omega) \in L^2(0, T; H) \times H$ are given desired states. Furthermore, σ_Q, $\sigma_\Omega \geq 0$ and $\sigma > 0$. Of course, more general cost functionals can be treated analogously.

Now the quadratic programming problem is given by

$$\min J(x) \quad \text{subject to (s.t.)} \quad x \in X_{\mathbf{ad}}. \tag{$\mathbf{P}$}$$

From $x = (y, u) \in X_{\mathbf{ad}}$ we infer that $y = \hat{y} + \mathcal{S}u$ holds. Hence, y is a dependent variable. We call u the *control* and y the *state*. In this way, $(\mathbf{P})$ becomes an *optimal control problem*. Utilizing the relationship $y = \hat{y} + \mathcal{S}u$ we define a so-called *reduced cost functional* $\hat{J} : U \to \mathbb{R}$ by

$$\hat{J}(u) = J(\hat{y} + \mathcal{S}u, u) \quad \text{for } u \in U.$$

Moreover, the set of admissible controls is given as

$$U_{\mathbf{ad}} = \big\{ u \in U \,\big|\, u_a \leq u \leq u_b \text{ in } \mathbb{R}^{N_u} \text{ a.e. in } [0, T] \big\},$$

which is convex, closed and bounded in U. Then, we consider the reduced optimal control problem:

$$\min \hat{J}(u) \quad \text{s.t.} \quad u \in U_{\mathbf{ad}}. \tag{$\hat{\mathbf{P}}$}$$

Clearly, if $\bar{u}$ is the optimal solution to $(\hat{\mathbf{P}})$, then $\bar{x} = (\hat{y} + \mathcal{S}\bar{u}, \bar{u})$ is the optimal solution to $(\mathbf{P})$. On the other hand, if $\bar{x} = (\bar{y}, \bar{u})$ is the solution to $(\mathbf{P})$, then $\bar{u}$ solves $(\hat{\mathbf{P}})$.

Example 3.1. We introduce an example for $(\mathbf{P})$ and discuss the presented theory for this application. Let $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$, be an open and bounded domain with Lipschitz-continuous boundary $\Gamma = \partial\Omega$. For $T > 0$ we set $Q = (0, T) \times \Omega$ and $\Sigma = (0, T) \times \Gamma$. We choose $H = L^2(\Omega)$ and $V = H_0^1(\Omega)$ endowed with the usual inner products

$$\langle \varphi, \psi \rangle_H = \int_\Omega \varphi\psi \,\mathrm{d}\boldsymbol{x}, \quad \langle \varphi, \psi \rangle_V = \int_\Omega \varphi\psi + \nabla\varphi \cdot \nabla\psi \,\mathrm{d}\boldsymbol{x}$$

and their induced norms, respectively. Let $\chi_i \in H$, $1 \leq i \leq m$, denote given control shape functions. Then, for given control $u \in U$, initial condition $y_\circ \in H$ and inhomogeneity $f \in L^2(0, T; H)$ we consider the linear heat equation

$$\begin{aligned} y_t(t, \boldsymbol{x}) - \Delta y(t, \boldsymbol{x}) &= f(t, \boldsymbol{x}) + \sum_{i=1}^m u_i(t)\chi_i(\boldsymbol{x}), && \text{a.e. in } Q, \\ y(t, \boldsymbol{x}) &= 0, && \text{a.e. in } \Sigma, \\ y(0, \boldsymbol{x}) &= y_\circ(\boldsymbol{x}), && \text{a.e. in } \Omega. \end{aligned} \tag{3.3}$$

We introduce the time-independent, symmetric bilinear form

$$a(\varphi, \psi) = \int_\Omega \nabla\varphi \cdot \nabla\psi \,\mathrm{d}\boldsymbol{x} \quad \text{for } \varphi, \psi \in V$$

and the bounded, linear operator $\mathcal{B} : U \to L^2(0, T; H) \hookrightarrow L^2(0, T; V')$ as

$$(\mathcal{B}u)(t, \boldsymbol{x}) = \sum_{i=1}^m u_i(t)\chi_i(\boldsymbol{x}) \quad \text{for } (t, \boldsymbol{x}) \in Q \text{ a.e. and } u \in U.$$

Hence, we have $\gamma = \gamma_1 = \gamma_2 = 1$ in (2.2). It follows that the weak formulation of (3.3) can be expressed in the form (2.3). Moreover, the unique weak solution to (3.3) belongs to the space $L^\infty(0, T; V)$ provided $y_\circ \in V$ holds. $\Diamond$

3.2 Existence of a unique optimal solution

We suppose the following hypothesis for the objective.

Assumption 2. *In* (3.2) *the desired states* (y_Q, y_Ω) *belong to* $L^2(0,T;H) \times H$*. Furthermore,* $\sigma_Q\,, \sigma_\Omega \geq 0$ *and* $\sigma > 0$ *are satisfied.*

Let us review the following result for quadratic optimization problems in Hilbert spaces; see [Tro09, Satz 2.14].

Theorem 3.2. *Suppose that* $\mathcal{U}$ *and* $\mathcal{H}$ *are given Hilbert spaces with norms* $\|\cdot\|_{\mathcal{U}}$ *and* $\|\cdot\|_{\mathcal{H}}$*, respectively. Furthermore, let* $\mathcal{U}_{\mathsf{ad}} \subset \mathcal{U}$ *be non-empty, bounded, closed, convex and* $z_d \in \mathcal{H}$*,* $\kappa \geq 0$*. The mapping* $\mathcal{G} : \mathcal{U} \to \mathcal{H}$ *is assumed to be a linear and continuous operator. Then there exists an optimal control* $\bar{u}$ *solving*

$$\min_{u \in \mathcal{U}_{\mathsf{ad}}} \mathcal{J}(u) := \frac{1}{2}\,\|\mathcal{G}u - z_d\|_{\mathcal{H}}^2 + \frac{\kappa}{2}\,\|u\|_{\mathcal{U}}^2. \tag{3.4}$$

If $\kappa > 0$ *holds or if* $\mathcal{G}$ *is injective, then* $\bar{u}$ *is uniquely determined.*

Remark 3.3. In the proof of Theorem 3.2 it is only used that $\mathcal{J}$ is continuous and convex. Therefore, the existence of an optimal control follows for general convex, continuous cost functionals $\mathcal{J} : \mathcal{U} \to \mathbb{R}$ with a Hilbert space $\mathcal{U}$. ◊

Next we can use Theorem 3.2 to obtain an existence result for the optimal control problem $(\hat{\mathbf{P}})$, which imply the existence of an optimal solution to $(\mathbf{P})$.

Theorem 3.4. *Let Assumptions* 1 *and* 2 *be valid. Moreover, let the bilateral control constraints* $u_a, u_b \in U$ *satisfy* $u_a \leq u_b$ *componentwise in* $\mathbb{R}^{N_u}$ *a.e. in* $[0,T]$*. Then,* $(\hat{\mathbf{P}})$ *has a unique optimal solution* $\bar{u}$*.*

Proof. Let us choose the Hilbert spaces $\mathcal{H} = L^2(0,T;H) \times H$ and $\mathcal{U} = U$. Moreover, $\mathcal{E} : W(0,T) \to L^2(0,T;H)$ is the canonical embedding operator, which is linear and bounded. We define the operator $\mathcal{E}_2 : W(0,T) \to H$ by $\mathcal{E}_2\varphi = \varphi(T)$ for $\varphi \in W(0,T)$. Since $W(0,T)$ is continuously embedded into $C([0,T];H)$, the linear operator $\mathcal{E}_2$ is continuous. Finally, we set

$$\mathcal{G} = \begin{pmatrix} \sqrt{\sigma_Q}\,\mathcal{E}_1\mathcal{S} \\ \sqrt{\sigma_\Omega}\,\mathcal{E}_2\mathcal{S} \end{pmatrix} \in \mathcal{L}(\mathcal{U},\mathcal{H}), \quad z_d = \begin{pmatrix} \sqrt{\sigma_Q}\,(y_Q - \hat{y}) \\ \sqrt{\sigma_\Omega}\,\big(y_\Omega - \hat{y}(T)\big) \end{pmatrix} \in \mathcal{H} \tag{3.5}$$

and $\mathcal{U}_{\mathsf{ad}} = U_{\mathsf{ad}}$. Then, $(\hat{\mathbf{P}})$ and (3.4) coincide. Consequently, the claim follows from Theorem 3.2 and $\sigma > 0$. □

Next we consider the case that $u_a = -\infty$ or/and $u_b = +\infty$. In this case U_{ad} is not bounded. However, we have the following result [Tro09, Satz 2.17].

Theorem 3.5. *Let Assumptions* 1 *and* 2 *be satisfied. If* $u_a = -\infty$ *or/and* $u_b = +\infty$*, problem* $(\hat{\mathbf{P}})$ *admits a unique solution.*

Proof. We utilize the setting of the proof of Theorem 3.4. By assumption there exists an element $u_0 \in U_{\mathsf{ad}}$. For $u \in U$ with $\|u\|_U^2 > 2\hat{J}(u_0)/\sigma$ we have

$$\hat{J}(u) = \mathcal{J}(u) = \frac{1}{2}\,\|\mathcal{G}u - z_d\|_{\mathcal{H}}^2 + \frac{\sigma}{2}\,\|u\|_U^2 \geq \frac{\sigma}{2}\,\|u\|_U^2 > \hat{J}(u_0).$$

Thus, the minimization of $\hat{J}$ over U_{ad} is equivalent with the minimization of $\hat{J}$ over the bounded, convex and closed set

$$U_{\mathsf{ad}} \cap \left\{ u \in U \,\middle|\, \|u\|_U^2 \leq \frac{2\hat{J}(u_0)}{\sigma} \right\}.$$

Now the claim follows from Theorem 3.2. □

3.3 First-order necessary optimality conditions

In (3.4) we have introduced the quadratic programming problem

$$\min_{u\in\mathcal{U}_{\text{ad}}} \mathcal{J}(u) = \frac{1}{2}\,\|\mathcal{G}u - z_d\|^2_{\mathcal{H}} + \frac{\sigma}{2}\,\|u\|^2_{\mathcal{U}}. \tag{3.6}$$

Existence of a unique solution has been investigated in Section 3.2. In this section we characterize the solution to (3.6) by first-order optimality conditions, which are essential to prove convergence and rate of convergence results for the POD approximations in Section 3.4. To derive first-order conditions we require the notion of derivatives in function spaces. Therefore, we recall the following definition [Tro09, §2.6].

Definition 3.6. *Suppose that $\mathcal{B}_1$ and $\mathcal{B}_2$ are real Banach spaces, $\mathcal{U} \subset \mathcal{B}_1$ be an open subset and $\mathcal{F} : \mathcal{U} \supset \mathcal{B}_1 \to \mathcal{B}_2$ a given mapping. The* directional derivative *of $\mathcal{F}$ at a point $u \in \mathcal{U}$ in the direction $h \in \mathcal{B}_2$ is defined by*

$$D\mathcal{F}(u; h) := \lim_{\varepsilon\searrow 0} \frac{1}{\varepsilon}\big(\mathcal{F}(u + \varepsilon h) - \mathcal{F}(u)\big)$$

provided the limit exists in $\mathcal{B}_2$. Suppose that the directional derivative exists for all $h \in \mathcal{B}_1$ and there is a linear, continuous operator $\mathcal{T} : \mathcal{U} \to \mathcal{B}_2$ satisfying

$$D\mathcal{F}(u; h) = \mathcal{T}h \quad \text{for all } h \in \mathcal{U}.$$

Then, $\mathcal{F}$ is said to be Gâteaux-differentiable *at u and $\mathcal{T}$ is the* Gâteaux derivative *of $\mathcal{F}$ at u. We write $\mathcal{T} = \mathcal{F}'(u)$.*

Remark 3.7. Let $\mathcal{H}$ be a real Hilbert space and $\mathcal{F} : \mathcal{H} \to \mathbb{R}$ be *Gâteaux-differentiable* at $u \in \mathcal{H}$. Then, its Gâteaux derivative $\mathcal{F}'(u)$ at u belongs to $\mathcal{H}' = \mathcal{L}(\mathcal{H}, \mathbb{R})$. Due to Riesz theorem [DR12, Satz 12.24] there exists a unique element $\nabla\mathcal{F}(u) \in \mathcal{H}$ satisfying

$$\langle\nabla\mathcal{F}(u), v\rangle_{\mathcal{H}} = \langle\mathcal{F}'(u), v\rangle_{\mathcal{H}',\mathcal{H}} \quad \text{for all } v \in \mathcal{H}.$$

We call $\nabla\mathcal{F}(u)$ the *(Gâteaux) gradient* of $\mathcal{F}$ at u. $\Diamond$

Theorem 3.8. *Let $\mathcal{U}$ be a real Hilbert space and $\mathcal{U}_{\text{ad}}$ be convex subset. Suppose that $\bar{u} \in \mathcal{U}_{\text{ad}}$ is a solution to* (3.6)

$$\min_{u\in\mathcal{U}_{\text{ad}}} \mathcal{J}(u).$$

Then the following variational inequality holds

$$\langle\nabla\mathcal{J}(\bar{u}), u - \bar{u}\rangle_{\mathcal{U}} \geq 0 \quad \text{for all } u \in \mathcal{U}_{\text{ad}}, \tag{3.7}$$

where the gradient of $\mathcal{J}$ is given by

$$\nabla\mathcal{J}(\bar{u}) = \mathcal{G}^\star(\mathcal{G}u - z_d) + \sigma u \quad \text{for } u \in \mathcal{U}.$$

If $\bar{u} \in \mathcal{U}_{\text{ad}}$ solves (3.7)*, then $\bar{u}$ is a solution to* (3.6)*.*

Proof. Let $\bar{u} \in \mathcal{U}_{\text{ad}}$ be a solution to (3.6), $u \in \mathcal{U}_{\text{ad}}$ be arbitrarily chosen. Since $\mathcal{U}_{\text{ad}}$ is convex, we have $\bar{u} + t(u - \bar{u}) = tu + (1 - t)\bar{u} \in \mathcal{U}_{\text{ad}}$ for all $t \in [0, 1]$. In particular, for we find that

$$\mathcal{J}(\bar{u}) \leq \mathcal{J}(\bar{u} + t(u - \bar{u})) \quad \text{for all } t \in (0, 1].$$

Consequently,

$$\frac{1}{t}\big(\mathcal{J}(\bar{u} + t(u - \bar{u})) - \mathcal{J}(\bar{u})\big) \geq 0 \quad \text{for all } t \in (0, 1]$$

Since $\mathcal{J}$ is Gâteaux-differentiable, we get (3.7), which is a sufficient condition becaus $\mathcal{J}$ and $\mathcal{U}_{\mathbf{ad}}$ are convex. $\square$

Inequality (3.7) is a first-order necessary and sufficient condition for (3.6), which can be expressed as

$$\langle \mathcal{G}\bar{u} - z_d, \mathcal{G}u - \mathcal{G}\bar{u}\rangle_{\mathcal{H}} + \langle \sigma\bar{u}, u - \bar{u}\rangle_{\mathcal{U}} \geq 0 \quad \text{for all } u \in \mathcal{U}_{\mathbf{ad}}. \tag{3.8}$$

Next we study (3.8) for ($\hat{\mathbf{P}}$). Utilizing the setting from (3.5) we obtain

$$\begin{aligned}
&\langle \mathcal{G}\bar{u} - z_d, \mathcal{G}(u - \bar{u})\rangle_{\mathcal{H}}\\
&\quad = \sigma_Q \left\langle \mathcal{S}\bar{u} - (y_Q - \hat{y}), \mathcal{S}(u - \bar{u})\right\rangle_{L^2(0,T;H)}\\
&\qquad + \sigma_\Omega \left\langle (\mathcal{S}\bar{u})(T) - (y_\Omega - \hat{y}(T)), (\mathcal{S}(u - \bar{u}))(T)\right\rangle_H\\
&\quad = \sigma_Q \left\langle \mathcal{S}\bar{u}, \mathcal{S}(u - \bar{u})\right\rangle_{L^2(0,T;H)} + \sigma_\Omega \left\langle (\mathcal{S}\bar{u})(T), (\mathcal{S}(u - \bar{u}))(T)\right\rangle_H\\
&\qquad - \sigma_Q \left\langle y_Q - \hat{y}, \mathcal{S}(u - \bar{u})\right\rangle_{L^2(0,T;H)} - \sigma_\Omega \left\langle y_\Omega - \hat{y}(T), (\mathcal{S}(u - \bar{u}))(T)\right\rangle_H.
\end{aligned}$$

Let us define the two linear, bounded operators $\Theta : W_0(0,T) \to W_0(0,T)'$ and $\Xi : L^2(0,T;H) \times H \to W_0(0,T)'$ by

$$\begin{aligned}
\langle \Theta\varphi, \phi\rangle_{W_0(0,T)',W_0(0,T)} &= \int_0^T \langle \sigma_Q\varphi(t), \phi(t)\rangle_H \,\mathrm{d}t + \langle \sigma_\Omega\varphi(T), \phi(T)\rangle_H,\\
\langle \Xi z, \phi\rangle_{W_0(0,T)',W_0(0,T)} &= \int_0^T \langle \sigma_Q z_Q(t), \phi(t)\rangle_H \,\mathrm{d}t + \langle \sigma_\Omega z_\Omega, \phi(T)\rangle_H
\end{aligned} \tag{3.9}$$

for φ, $\phi \in W_0(0,T)$ and $z = (z_Q, z_\Omega) \in L^2(0,T;H) \times H$. Then, we find

$$\begin{aligned}
&\langle \mathcal{G}\bar{u} - z_d, \mathcal{G}(u - \bar{u})\rangle_{\mathcal{H}}\\
&\quad = \langle \Theta(\mathcal{S}\bar{u}) - \Xi(y_Q - \hat{y}, y_\Omega - \hat{y}(T)), \mathcal{S}(u - \bar{u})\rangle_{W_0(0,T)',W_0(0,T)}\\
&\quad = \langle \mathcal{S}'\Theta\mathcal{S}\bar{u}, u - \bar{u}\rangle_U - \langle \mathcal{S}'\Xi(y_Q - \hat{y}, y_\Omega - \hat{y}(T)), u - \bar{u}\rangle_U.
\end{aligned} \tag{3.10}$$

Let us define the linear $\mathcal{A} : U \to W(0,T)$ as follows: for given $u \in U$ the function $p = \mathcal{A}u \in W(0,T)$ is the unique solution to

$$\begin{aligned}
-\frac{\mathrm{d}}{\mathrm{d}t} \langle p(t), \varphi\rangle_H + a(t; p(t), \varphi) &= -\sigma_Q \left\langle (\mathcal{S}u)(t), \varphi\right\rangle_H \quad && \forall \varphi \in V \text{ a.e.},\\
p(T) &= -\sigma_\Omega\, (\mathcal{S}u)(T) && \text{in } H.
\end{aligned} \tag{3.11}$$

It follows from (2.2) and $\mathcal{S}u \in W(0,T)$ that the operator $\mathcal{A}$ is well-defined and bounded.

Lemma 3.9. *Let Assumption 1 be satisfied and $u, v \in U$. We set $y = \mathcal{S}u \in W_0(0,T)$, $w = \mathcal{S}v \in W_0(0,T)$, and $p = \mathcal{A}v \in W(0,T)$. Then,*

$$\int_0^T \langle (\mathcal{B}u)(t), p(t)\rangle_{V',V} \,\mathrm{d}t = -\int_0^T \sigma_Q \left\langle w(t), y(t)\right\rangle_H \mathrm{d}t - \sigma_\Omega \left\langle w(T), y(T)\right\rangle_H.$$

Proof. We derive from $y = \mathcal{S}u$, $p = \mathcal{A}u$, $y \in W_0(0,T)$ and integration by parts

$$\begin{aligned}
\int_0^T \langle (\mathcal{B}u)(t), p(t)\rangle_{V',V} \,\mathrm{d}t &= \int_0^T \langle y_t(t), p(t)\rangle_{V',V} + a(t; y(t), p(t)) \,\mathrm{d}t\\
&= \int_0^T -\langle p_t(t), y(t)\rangle_{V',V} + a(t; p(t), y(t)) \,\mathrm{d}t + \langle p(T), y(T)\rangle_H\\
&= -\int_0^T \sigma_Q \left\langle w(t), y(t)\right\rangle_H \mathrm{d}t - \sigma_\Omega \left\langle w(T), y(T)\right\rangle_H
\end{aligned}$$

which is the claim. $\square$

We define $\hat{p} \in W(0,T)$ as the unique solution to

$$
\begin{aligned}
-\frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{p}(t), \varphi \rangle_H + a(t; \hat{p}(t), \varphi) &= \sigma_Q \langle y_Q(t) - \hat{y}(t), \varphi \rangle_H && \forall \varphi \in V \text{ a.e.}, \\
p(T) &= \sigma_\Omega (y_\Omega - \hat{y}(T)) && \text{in } H.
\end{aligned}
\tag{3.12}
$$

Then, for every $u \in U$ the function $p = \hat{p} + \mathcal{A}u$ is the unique solution to

$$
\begin{aligned}
-\frac{\mathrm{d}}{\mathrm{d}t} \langle p(t), \varphi \rangle_H + a(t; p(t), \varphi) &= \sigma_Q \langle y_Q(t) - y(t), \varphi \rangle_H && \forall \varphi \in V \text{ a.e.}, \\
p(T) &= \sigma_\Omega (y_\Omega - y(T)) && \text{in } H
\end{aligned}
$$

with $y = \hat{y} + \mathcal{S}u$. Moreover, we have the following result.

Lemma 3.10. *Let Assumption* 1 *be satisfied. Then, $\mathcal{B}'\mathcal{A} = -\mathcal{S}'\Theta\mathcal{S} \in \mathcal{L}(U)$, where linear and bounded operator Θ has been defined in* (3.9)*. Moreover, $\mathcal{B}'\hat{p} = \mathcal{S}'\Xi(y_Q - \hat{y}, y_\Omega - \hat{y}(T))$, where $\hat{p}$ is the solution to* (3.12)*.*

Proof. Let $u, v \in \mathfrak{U}$ be chosen arbitrarily. We set $y = \mathcal{S}u \in W_0(0,T)$ and $w = \mathcal{S}v \in W_0(0,T)$. Recall that we identify U with its dual space U'. From the integration by parts formula and Lemma 3.9 we infer that

$$
\begin{aligned}
&\langle \mathcal{S}'\Theta\mathcal{S}v, u \rangle_U = \langle \Theta\mathcal{S}v, \mathcal{S}u \rangle_{W_0(0,T)', W_0(0,T)} = \langle \Theta w, y \rangle_{W_0(0,T)', W_0(0,T)} \\
&= \int_0^T \sigma_Q \langle w(t), y(t) \rangle_H \,\mathrm{d}t + \sigma_\Omega \langle w(T), y(T) \rangle_H \\
&= -\langle \mathcal{B}u, p \rangle_{L^2(0,T;V'), L^2(0,T;V)} = -\langle u, \mathcal{B}'p \rangle_U = -\langle \mathcal{B}'\mathcal{A}v, u \rangle_U.
\end{aligned}
$$

Since $u, v \in U$ are chosen arbitrarily, we have $\mathcal{B}'\mathcal{A} = \mathcal{S}'\Theta\mathcal{S}$. Further, we find

$$
\begin{aligned}
&\langle \mathcal{S}'\Xi(y_Q - \hat{y}, y_\Omega - \hat{y}(T)), u \rangle_U = \langle \Xi(y_Q - \hat{y}), y_\Omega - \hat{y}(T)), \mathcal{S}u \rangle_{W_0(0,T)', W_0(0,T)} \\
&= \int_0^T \sigma_Q \langle y_Q - \hat{y}(t), y(t) \rangle_H \,\mathrm{d}t + \sigma_\Omega \langle y_\Omega - \hat{y}(T), y(T) \rangle_H \\
&= \int_0^T -\langle \hat{p}_t(t), y(t) \rangle_H + a(t; \hat{p}(t), y(t)) \,\mathrm{d}t + \langle \hat{p}(T), y(T) \rangle_H \\
&= \int_0^T \langle y_t(t), \hat{p}(t) \rangle_H + a(t; y(t), \hat{p}(t)) \,\mathrm{d}t = \int_0^T \langle (\mathcal{B}u)(t), \hat{p}(t) \rangle_{V',V} \,\mathrm{d}t \\
&= \langle \mathcal{B}'\hat{p}, u \rangle_U.
\end{aligned}
$$

which gives the claim. □

We infer from (3.10) and Lemma 3.10 that

$$
\langle \mathcal{G}\bar{u} - z_d, \mathcal{G}\bar{v} \rangle_{\mathcal{H}} = -\langle \mathcal{B}'(\hat{p} + \mathcal{A}\bar{u}), u - \bar{u} \rangle_U.
$$

This implies the following variational inequality for $(\hat{\mathbf{P}})$

$$
\begin{aligned}
&\langle \mathcal{G}\bar{u} - z_d, \mathcal{G}u - \mathcal{G}\bar{u} \rangle_{\mathcal{H}} + \sigma \langle \bar{u}, u - \bar{u} \rangle_{\mathfrak{U}} \\
&\qquad = \langle \sigma\bar{u} - \mathcal{B}'(\hat{p} + \mathcal{A}\bar{u}), u - \bar{u} \rangle_U \geq 0 \quad \text{for all } u \in U_{\mathsf{ad}}.
\end{aligned}
$$

Summarizing we have proved the following result.

Theorem 3.11. *Suppose that Assumptions* 1 *and* 2 *hold. Then, $(\bar{y}, \bar{u})$ is a solution to* $(\mathbf{P})$ *if and only if $(\bar{y}, \bar{u})$ satisfy together with the adjoint variable $\bar{p}$ the first-order optimality system*

$$
\bar{y} = \hat{y} + \mathcal{S}\bar{u}, \quad \bar{p} = \hat{p} + \mathcal{A}\bar{u}, \quad u_a \leq \bar{u} \leq u_b \tag{3.13a}
$$

$$
\langle \sigma\bar{u} - \mathcal{B}'\bar{p}, u - \bar{u} \rangle_U \geq 0 \quad \textit{for all } u \in U_{\mathsf{ad}}. \tag{3.13b}
$$

Remark 3.12. By using a Lagrangian framework it follows from Theorem 3.11 and [Tro09] that the variational inequality (3.13b) is equivalent to the existence of two Lagrange multiplier functions $\bar{\mu}_a, \bar{\mu}_b \in U$ satisfying $\bar{\mu}_a, \bar{\mu}_b \geq 0$,

$$\sigma \bar{u} - \mathcal{B}' \bar{p} + \bar{\mu}_b - \bar{\mu}_a = 0$$

and the complementarity condition

$$\bar{\mu}_a(t)^\top (u_a(t) - \bar{u}(t)) = \bar{\mu}_b(t)^\top (\bar{u}(t) - u_b(t)) = 0 \quad \text{f.a.a. } t \in [0, T].$$

Thus, (3.13) is equivalent to the system

$$\begin{aligned} &\bar{y} = \hat{y} + \mathcal{S}\bar{u}, \quad \bar{p} = \hat{p} + \mathcal{A}\bar{u}, \quad \sigma\bar{u} - \mathcal{B}'\bar{p} + \bar{\mu}_b - \bar{\mu}_a = 0, \\ &u_a \leq \bar{u} \leq u_b, \quad 0 \leq \bar{\mu}_a, \quad 0 \leq \bar{\mu}_b, \\ &\bar{\mu}_a(t)^\top (u_a(t) - \bar{u}(t)) = \bar{\mu}_b(t)^\top (\bar{u}(t) - u_b(t)) = 0 \text{ a.e. in } [0, T]. \end{aligned} \tag{3.14}$$

Utilizing a complementarity function it can be shown that (3.14) is equivalent with

$$\begin{aligned} &\bar{y} = \hat{y} + \mathcal{S}\bar{u}, \quad \bar{p} = \hat{p} + \mathcal{A}\bar{u}, \quad \sigma\bar{u} - \mathcal{B}'\bar{p} + \bar{\mu}_b - \bar{\mu}_a = 0, \quad u_a \leq \bar{u} \leq u_b, \\ &\bar{\mu}_a = \max\big(0, \bar{\mu}_a + \eta(\bar{u} - u_a)\big), \ \bar{\mu}_b = \max\big(0, \bar{\mu}_b + \eta(\bar{u} - u_b)\big), \end{aligned} \tag{3.15}$$

where $\eta > 0$ is an arbitrary real number. The max-and min-operations are interpreted componentwise in the pointwise everywhere sense. $\Diamond$

The gradient $\nabla \hat{J} : U \to U$ of the reduced cost functional $\hat{J}$ is given by

$$\nabla J(u) = \sigma u - \mathcal{B}^\star p, \quad u \in U,$$

where $p = \hat{p} + \mathcal{A}u$ holds true; see, e.g., [HPUU09]. Thus, a first-order sufficient optimality condition for ($\hat{\mathbf{P}}$) is given by the variational inequality

$$\langle \sigma\bar{u} - \mathcal{B}'\bar{p}, u - \bar{u} \rangle_U \geq 0 \quad \text{for all } u \in U_{\mathsf{ad}}, \tag{3.16}$$

with $\bar{p} = \hat{p} + \mathcal{A}\bar{u}$.

3.4 The POD Galerkin approximation for ($\hat{\mathbf{P}}$)

In this subsection we introduce the POD Galerkin schemes for the variational inequality (3.16) using a POD Galerkin approximation for the state and dual variables. Moreover, we study the convergence of the POD discretizations. In Section 2.3 we have introduced a POD Galerkin scheme for the state equation (3.1). Suppose that $\{\psi_i\}_{i=1}^\ell$ be a POD basis of rank ℓ computed from ($\mathbf{P}^\ell$) with $\psi_i = \psi_i^V$ in case of $X = V$ and $\psi_i = \psi_i^H$ in case of $X = H$. We set $X^\ell = \operatorname{span}\{\psi_1, \ldots, \psi_\ell\} \subset V$. Let the linear and bounded projection operator $\mathcal{P}^\ell$ denote $\mathcal{P}_V^\ell$ for $X = V$ and $\mathcal{P}_H^\ell$ for $X = H$; see (2.8).

Recall the POD Galerkin ansatz (2.13) for the state variable. Analogously, we approximate the adjoint variable $p = \hat{p} + \mathcal{A}u$ by the Galerkin expansion

$$p^\ell(t) = \hat{p}(t) + \sum_{i=1}^{\ell} \mathrm{p}_i^\ell(t)\psi_i \in V \quad \text{for } t \in [0, T] \tag{3.17}$$

with coefficient functions $\mathrm{p}_i^\ell : [0, T] \to \mathbb{R}$ and with $\hat{p}$ from (3.12). Let the vector-valued coefficient function given by

$$\mathrm{p}^\ell = \big(\mathrm{p}_1^\ell, \ldots, \mathrm{p}_\ell^\ell\big) : [0, T] \to \mathbb{R}^\ell$$

If we assume that $\mathrm{p}^\ell(T) = -\sigma_\Omega \mathrm{y}^\ell(T)$ holds, then we infer from $\hat p(T) = \sigma_\Omega(y_\Omega - \hat y(T))$ and (3.17) that

$$p^\ell(T) = \hat p(T) - \sigma_\Omega \sum_{i=1}^{\ell} \mathrm{y}_i^\ell(t)\psi_i = \sigma_\Omega\big(y_\Omega - y^\ell(T)\big).$$

This motivates the following POD scheme for the approximation of $p = \hat p + \mathcal{A}u$ is given as follows: $p^\ell \in W(0,T)$ satisfies

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\langle p^\ell(t),\psi\rangle_H + a(t;p^\ell(t),\psi) &= \sigma_Q \langle (y_Q - y^\ell)(t),\psi\rangle_H \quad \forall \psi \in X^\ell \text{ a.e.},\\ \mathrm{p}^\ell(T) &= -\sigma_\Omega \mathrm{y}^\ell(T). \end{aligned} \tag{3.18}$$

It follows by similar arguments as for (2.14) that there is a unique solution $p^\ell \in W(0,T)$.

Remark 3.13. Recall that we have introduced the linear and bounded solution operator $\mathcal{S}^\ell : U \to W(0,T)$ as an approximation for the state solution operator $\mathcal{S}$; see Remark 2.8-2). Analogously, we define an approximation of the adjoint solution operator $\mathcal{A}$ as follows: Let $\mathcal{A}^\ell : U \to W(0,T)$ denote the solution operator to

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\langle w^\ell(t),\psi\rangle_H + a(t;w^\ell(t),\psi) &= -\sigma_1 \langle (\mathcal{S}^\ell u)(t),\psi\rangle_H \qquad \forall \psi \in X^\ell \text{ a.e.},\\ w^\ell(T) &= -\sigma_2 (\mathcal{S}^\ell u)(T). \end{aligned}$$

Then $p^\ell = \hat p + \mathcal{A}^\ell u$ is the unique solution to (3.18). ◊

Lemma 3.14. *Let Assumption 1 on page 28 be satisfied and $u, v \in U$. We set $y^\ell = \mathcal{S}^\ell u \in W_0(0,T)$, $w^\ell = \mathcal{S}^\ell v \in W_0(0,T)$, and $p^\ell = \mathcal{A}^\ell v \in W(0,T)$. Then,*

$$\int_0^T \langle (\mathcal{B}u)(t), p^\ell(t)\rangle_{V',V}\,\mathrm{d}t = -\int_0^T \sigma_Q \langle w^\ell(t), y^\ell(t)\rangle_H\,\mathrm{d}t - \sigma_\Omega \langle w^\ell(T), y^\ell(T)\rangle_H.$$

Moreover, $\mathcal{B}'\mathcal{A}^\ell = -(\mathcal{S}^\ell)'\Theta\mathcal{S}^\ell \in \mathcal{L}(U)$, where linear and bounded operator Θ has been defined in (3.9).

Proof. Since the POD basis for the state and adjoint coincide, the claim follows by the same arguments used to prove Lemmas 3.9 and 3.10. □

Theorem 3.15. *Suppose that Assumptions 1 and 2 hold. Let $X = V$ and $u \in U$ be arbitrarily given so that $\mathcal{S}u$, $\mathcal{A}u \in H^1(0,T;V)\setminus\{0\}$. To compute a POD basis $\{\psi_i\}_{i=1}^\ell$ of rank ℓ we choose $\wp = 4$, $y^1 = \mathcal{S}u$, $y^2 = (\mathcal{S}u)_t$, $y^3 = \mathcal{A}u$ and $y^4 = (\mathcal{A}u)_t$. Then, $p = \hat p + \mathcal{A}u$ and $p^\ell = \hat p + \mathcal{A}^\ell u$ satisfies the a-priori error estimate*

$$\|p^\ell - p\|^2_{H^1(0,T;V)} \le \begin{cases} C \sum\limits_{i=\ell+1}^{d_V} \lambda_i^V & \text{if } X = V,\\ C \sum\limits_{i=\ell+1}^{d_H} \lambda_i^H \,\|\psi_i^H - \mathcal{P}_H^\ell \psi_i^H\|_V^2 & \text{if } X = H \end{cases} \tag{3.19}$$

for a constant C which depends on γ, γ_1, γ_2, T, σ_Ω and σ_Q.

Proof. Analogous to (2.20) we have $p^\ell(t) - p(t) = \theta^\ell(t) + \rho^\ell(t)$ for almost all $t \in [0,T]$ with $\theta^\ell = \mathcal{A}^\ell u - \mathcal{P}^\ell(\mathcal{A}u)$ and $\rho^\ell = \mathcal{P}^\ell(\mathcal{A}u) - \mathcal{A}u$. Here, $\mathcal{P}^\ell = \mathcal{P}_V^\ell$ for $X = V$ and $\mathcal{P}^\ell = \mathcal{P}_H^\ell$ for $X = H$. Now, the proof of the claims follows by similar arguments as the proofs of Theorem 2.9, Proposition 4.7 in [HV08], Proposition 4.6 in [TV09] and Theorem 6.3 in [Sin14]. To estimate the terminal term $\theta^\ell(T)$ we use observe that

$$\begin{aligned} \big\|\theta^\ell(T)\big\|_H &= \big\|\mathcal{P}^\ell((\mathcal{A}u)(T)) - (\mathcal{A}^\ell u)(T)\big\|_H\\ &\le \sigma_\Omega\Big(\big\|\mathcal{P}^\ell((\mathcal{S}u)(T)) - (\mathcal{S}u)(T)\big\|_H + \big\|(\mathcal{S}u)(T) - (\mathcal{S}^\ell u)(T)\big\|_H\Big)\\ &\le \sigma_\Omega\Big(\big\|\mathcal{P}^\ell(\mathcal{S}u) - \mathcal{S}u\big\|_{C([0,T];H)} + \big\|\mathcal{S}u - \mathcal{S}^\ell u\big\|_{C([0,T];H)}\Big)\\ &\le \sigma_\Omega c_E\Big(\big\|\mathcal{P}^\ell(\mathcal{S}u) - \mathcal{S}u\big\|_{H^1(0,T;V)} + \big\|\mathcal{S}u - \mathcal{S}^\ell u\big\|_{H^1(0,T;V)}\Big) \end{aligned}$$

with an embedding constant c_E. The first term on the right-hand side can be handled by (1.27), the second term is estimated in Theorem 2.9. $\square$

Remark 3.16. 1) Analogous to Remark 2.10-2) the a-priori estimate (3.19) holds for an arbitrarily chosen, but fixed control $u \in U$. Argueing as in the proof of Corollary 2.12 we find that

$$\lim_{\ell\to\infty} \big\|\hat p + \mathcal{A}^\ell \tilde u - \hat p - \mathcal{A}\tilde u\big\|_{W(0,T)} = 0$$

for any $\tilde u \in U$.

2) We can also extend the results in Proposition 2.13 for the adjoint equation and get an a-priori error estimate choosing $\wp = 2$, $y^1 = \mathcal{S}u$ and $y^2 = \mathcal{A}u$. $\Diamond$

The POD Galerkin approximation for $(\hat{\mathbf{P}})$ is as follows:

$$\min \hat{J}^\ell(u) \quad \text{s.t.} \quad u \in U_{\mathsf{ad}}, \qquad (\hat{\mathbf{P}}^\ell)$$

where the cost is defined by $\hat J^\ell(u) = J(\hat y + \mathcal{S}^\ell u, u)$ for $u \in U$. Let $\bar u^\ell$ be the solution to $(\hat{\mathbf{P}}^\ell)$. Then, a first-order sufficient optimality condition is given by the variational inequality

$$\langle \sigma \bar u^\ell - \mathcal{B}'\bar p^\ell, u - \bar u^\ell\rangle_U \ge 0 \quad \text{for all } u \in U_{\mathsf{ad}}, \tag{3.20}$$

where $\bar p^\ell = \hat p^\ell + \mathcal{A}^\ell \bar u^\ell$ holds.

Theorem 3.17. *Suppose that Assumptions* 1 *and* 2 *hold. Let $u \in U$ be arbitrarily given so that $\mathcal{S}u$, $\mathcal{A}u \in H^1(0,T;V)\setminus\{0\}$.*

1) *To compute a POD basis $\{\psi_i\}_{i=1}^\ell$ of rank ℓ we choose $\wp = 4$, $y^1 = \mathcal{S}u$, $y^2 = (\mathcal{S}u)_t$, $y^3 = \mathcal{A}u$ and $y^4 = (\mathcal{A}u)_t$. Then, the optimal solution $\bar u$ to $(\hat{\mathbf{P}})$ and the associated POD suboptimal solution $\bar u^\ell$ to $(\hat{\mathbf{P}}^\ell)$ satisfy*

$$\lim_{\ell\to\infty} \big\|\bar u^\ell - \bar u\big\|_U = 0 \tag{3.21}$$

for $X = V$ and $X = H$.

2) *If an optimal POD basis of rank is computed by choosing $\wp = 4$, $y^1 = \mathcal{S}\bar u$, $y^2 = (\mathcal{S}\bar u)_t$, $y^3 = \mathcal{A}\bar u$ and $y^4 = (\mathcal{A}\bar u)_t$, then we have*

$$\big\|\bar u^\ell - \bar u\big\|_U \le \begin{cases} \dfrac{C}{\sigma}\displaystyle\sum_{i=\ell+1}^{d_V} \lambda_i^V & \text{if } X = V,\\[2ex] \dfrac{C}{\sigma}\displaystyle\sum_{i=\ell+1}^{d_H} \lambda_i^H\,\|\psi_i^H - \mathcal{P}_H^\ell\psi_i^H\|_V^2 & \text{if } X = H,\end{cases} \tag{3.22}$$

where the constant C depends on γ, γ_1, γ_2, T, σ_Ω, σ_Q and the norm $\|\mathcal{B}'\|_{\mathcal{L}(L^2(0,T;V),U)}$.

Proof. Choosing $u = \bar u^\ell$ in (3.16) and $u = \bar u$ in (3.20) we get the variational inequality

$$0 \le \langle \sigma(\bar u - \bar u^\ell) - \mathcal{B}'(\bar p - \bar p^\ell), \bar u^\ell - \bar u\rangle_U. \tag{3.23}$$

Utilizing Lemma 3.14 and $\langle \Theta\varphi,\varphi\rangle_{W_0(0,T)',W_0(0,T)} \ge 0$ for all $\varphi \in W_0(0,T)$ we infer from (3.23) that

$$\begin{aligned}
0 &\le \langle \mathcal{B}'\mathcal{A}^\ell \bar u^\ell - \mathcal{B}'\mathcal{A}\bar u, \bar u^\ell - \bar u\rangle_U - \sigma\,\|\bar u - \bar u^\ell\|_U^2\\
&= \langle \mathcal{B}'\mathcal{A}^\ell(\bar u^\ell - \bar u) + \mathcal{B}'(\mathcal{A}^\ell - \mathcal{A})\bar u, \bar u^\ell - \bar u\rangle_U - \sigma\,\|\bar u - \bar u^\ell\|_U^2\\
&\le \langle \Theta\mathcal{S}^\ell(\bar u - \bar u^\ell), \mathcal{S}^\ell(\bar u^\ell - \bar u)\rangle_U + \|\mathcal{B}'(\mathcal{A}^\ell - \mathcal{A})\bar u\|_U \|\bar u^\ell - \bar u\|_U - \sigma\,\|\bar u - \bar u^\ell\|_U^2\\
&\le \|\mathcal{B}'(\mathcal{A}^\ell - \mathcal{A})\bar u\|_U \|\bar u^\ell - \bar u\|_U - \sigma\,\|\bar u - \bar u^\ell\|_U^2.
\end{aligned}$$

Consequently,

$$\|\bar u - \bar u^\ell\|_U \le \frac{1}{\sigma}\,\|\mathcal{B}'(\mathcal{A}^\ell - \mathcal{A})\bar u\|_U.$$

Now (3.21) and (3.22) follow from Remark 3.16-1) and (3.19), respectively. $\square$

3.5 POD a-posteriori error analysis

In [TV09] a POD a-posteriori error estimates are presented which can be applied to our optimal control problem as well. It is deduced how far the suboptimal control $\bar{u}^\ell$ is from the (unknown) exact optimal control $\bar{u}$. Thus, our goal is to estimate the norm $\|\bar{u}-\bar{u}^\ell\|_U$ without the knowledge of the optimal solution $\bar{u}$. In general, $\bar{u}^\ell \neq \bar{u}$ holds, so that $\bar{u}^\ell$ does not satisfy the variational inequality (3.16). However, there exists a function $\zeta^\ell \in U$ such that

$$\langle \sigma\bar{u}^\ell - \mathcal{B}'\tilde{p}^\ell + \zeta^\ell, u - \bar{u}^\ell\rangle_U \geq 0 \quad \forall v \in U_{\mathrm{ad}}, \tag{3.24}$$

with $\tilde{p}^\ell = \hat{p} + \mathcal{A}\bar{u}^\ell$. Therefore, $\bar{u}^\ell$ satisfies the optimality condition of the perturbed parabolic optimal control problem

$$\min_{u\in U_{\mathrm{ad}}} \tilde{J}(u) = J(\hat{y}+\mathcal{S}u, u) + \langle \zeta^\ell, u\rangle_U$$

with "perturbation" ζ^ℓ. The smaller ζ^ℓ is, the closer $\bar{u}^\ell$ is to $\bar{u}$. Next we estimate $\|\bar{u}-\bar{u}^\ell\|_U$ in terms of $\|\zeta^\ell\|_U$. By Lemma 3.10 we have

$$\mathcal{B}'\big(\bar{p}-\tilde{p}^\ell\big) = \mathcal{B}'\mathcal{A}\big(\bar{u}-\bar{u}^\ell\big) = -\mathcal{S}'\Theta\mathcal{S}\big(\bar{u}-\bar{u}^\ell\big) = \mathcal{S}'\Theta\big(\tilde{y}^\ell - \bar{y}\big) \tag{3.25}$$

with $\tilde{y}^\ell = \hat{y} + \mathcal{S}\bar{u}^\ell$. Choosing $u = \bar{u}^\ell$ in (3.16), $u = \bar{u}$ in (3.24) and using (3.25) we obtain

$$\begin{aligned}
0 &\leq \langle -\sigma(\bar{u}-\bar{u}^\ell) + \mathcal{B}'(\bar{p}-\tilde{p}^\ell) + \zeta^\ell, \bar{u}-\bar{u}^\ell\rangle_U \\
&= -\sigma\,\|\bar{u}-\bar{u}^\ell\|_U^2 + \langle \mathcal{S}'\Theta(\tilde{y}^\ell-\bar{y}), \bar{u}-\bar{u}^\ell\rangle_U + \langle \zeta^\ell, \bar{u}-\bar{u}^\ell\rangle_U \\
&= -\sigma\,\|\bar{u}-u_p\|_U^2 - \langle \Theta(\bar{y}-\tilde{y}^\ell), \bar{y}-\tilde{y}^\ell\rangle_{W_0(0,T)',W_0(0,T)} + \langle \zeta^\ell, \bar{u}-\bar{u}^\ell\rangle_U \\
&= -\sigma\,\|\bar{u}-\bar{u}^\ell\|_U^2 + \langle \zeta^\ell, \bar{u}^\ell-\bar{u}^\ell\rangle_U \leq -\sigma\,\|\bar{u}-\bar{u}^\ell\|_U^2 + \|\zeta^\ell\|_U\|\bar{u}-\bar{u}^\ell\|_U.
\end{aligned}$$

Hence, we get the a-posteriori error estimation

$$\|\bar{u}-\bar{u}^\ell\|_U \leq \frac{1}{\sigma}\,\|\zeta^\ell\|_U.$$

Theorem 3.18. *Suppose that Assumptions* 1 *and* 2 *hold. Let $u \in U$ be arbitrarily given so that $\mathcal{S}u$, $\mathcal{A}u \in H^1(0,T;V)\setminus\{0\}$. To compute a POD basis $\{\psi_i\}_{i=1}^\ell$ of rank ℓ we choose $\wp = 4$, $y^1 = \mathcal{S}u$, $y^2 = (\mathcal{S}u)_t$, $y^3 = \mathcal{A}u$ and $y^4 = (\mathcal{A}u)_t$. Define the function $\zeta^\ell \in U$ by*

$$\zeta_i^\ell(t) = \begin{cases} -\min(0, \xi_i^\ell(t)) & \text{a.e. in } \mathcal{A}_{ai}^\ell = \big\{t\in[0,T]\,|\,\bar{u}_i^\ell(t) = u_{ai}(t)\big\}, \\ -\max(0,\xi_i^\ell(t)) & \text{a.e. in } \mathcal{A}_{bi}^\ell = \big\{t\in[0,T]\,|\,\bar{u}_i^\ell(t) = u_{bi}(t)\big\}, \\ -\xi_i^\ell(t) & \text{a.e. in } [0,T]\setminus\big(\mathcal{A}_{ai}^\ell\cup\mathcal{A}_{bi}^\ell\big), \end{cases}$$

where $\xi^\ell = \sigma\bar{u}^\ell - \mathcal{B}'(\hat{p}+\mathcal{A}\bar{u}^\ell)$ in U. Then, the a-posteriori error estimate

$$\|\bar{u}-\bar{u}^\ell\|_U \leq \frac{1}{\sigma}\,\|\zeta^\ell\|_U. \tag{3.26}$$

In particular, $\lim\limits_{\ell\to\infty}\big\|\zeta^\ell\big\|_U = 0$.

Proof. Estimate (3.26) has already be shown. We proceed by constructing the function ζ^ℓ. Here we adapt the lines of the proof of Proposition 3.2 in [TV09] to our optimal control problem. Suppose that we know $\bar{u}^\ell$ and $\tilde{p}^\ell = \hat{p} + \mathcal{A}\bar{u}^\ell$. The goal is to determine $\zeta^\ell \in U$ satisfying (3.24). We distinguish three different cases.

- Case $\bar{u}_i^\ell(t) = u_{ai}(t)$ for fixed $t\in[0,T]$ and $i \in \{1,\ldots,N_u\}$: Then, $u_i(t) - \bar{u}_i^\ell(t) = u_i(t) - u_{ai}(t) \geq 0$ for all $u \in U_{ad}$. Hence, $\zeta_i^\ell(t)$ has to satisfy

$$\big(\sigma\bar{u}^\ell - \mathcal{B}'\tilde{p}^\ell\big)_i(t) + \zeta_i^\ell(t) \geq 0. \tag{3.27}$$

  Setting $\zeta_i^\ell(t) = -\min(0, (\sigma\bar{u}^\ell - \mathcal{B}'\tilde{p}^\ell)_i(t))$ the value $\zeta_i^\ell(t)$ satisfies (3.27).

- Case $\bar{u}_i^\ell(t) = u_{bi}(t)$ for fixed $t \in [0,T]$ and $i \in \{1,\dots,N_u\}$: Now, $u_i(t) - \bar{u}_i^\ell(t) = u(t) - u_{bi}(t) \leq 0$ for all $u \in U_{ad}$. Analogously to the first case we define $\zeta_i^\ell(t) = -\max(0,(\sigma\bar{u}^\ell - \mathcal{B}'\tilde{p}^\ell)_i(t))$ to ensure (3.27).
- Case $u_{ai}(t) < \bar{u}_i^\ell(t) < u_{bi}(t)$ for fixed $t \in [0,T]$ and $i \in \{1,\dots,N_u\}$: Consequently, $(\sigma\bar{u}^\ell - \mathcal{B}'\tilde{p}^\ell)_i(t) + \zeta_i^\ell(t) = 0$ holds so that $\zeta_i^\ell(t) = -(\sigma\bar{u}^\ell - \mathcal{B}'\tilde{p}^\ell)_i(t)$ guarantees (3.27).

It remains to prove that ζ^ℓ tends to zero for $\ell \to \infty$. Here we adapt the proof of Theorem 4.11 in [TV09]. By Theorem 3.17-1), the sequence $\{\bar{u}^\ell\}_{\ell\in\mathbb{N}}$ converges to $\bar{u}$ in U. Since the linear operator $\mathcal{B}'\mathcal{A}$ is bounded and $\tilde{p}^\ell = \hat{p} + \mathcal{A}\bar{u}^\ell$ holds, $\{\mathcal{B}'\tilde{p}^\ell\}_{\ell\in\mathbb{N}}$ tends to $\mathcal{B}'\bar{p} = \mathcal{B}'\mathcal{A}\bar{u}$ as well. Hence, there exist subsequences $\{\bar{u}^{\ell_k}\}_{k\in\mathbb{N}}$ and $\{\mathcal{B}'\tilde{p}^{\ell_k}\}_{k\in\mathbb{N}}$ satisfying

$$\lim_{k\to\infty} \bar{u}_i^{\ell_k}(t) = \bar{u}_i(t) \quad \text{and} \quad \lim_{k\to\infty} (\mathcal{B}'\tilde{p}^{\ell_k})_i(t) = (\mathcal{B}'\bar{p})_i(t)$$

f.a.a. $t \in [0,T]$ and for $1 \leq i \leq N_u$. Next we consider the active and inactive sets for $\bar{u}$.

- Let $t \in \mathfrak{J}_i = \{t \in [0,T] \,|\, u_{ai}(t) < \bar{u}_i(t) < u_{bi}(t)\}$ for $i \in \{1,\dots,N_u\}$. For $k_\circ = k_\circ(t) \in \mathbb{N}$ sufficiently large, $\bar{u}_i^{\ell_k}(t) \in (u_{ai}(t), u_{bi}(t))$ for all $k \geq k_\circ$ and f.a.a. $t \in \mathfrak{J}_i$. Thus, $(\sigma\bar{u}^{\ell_k} - \mathcal{B}'\tilde{p}^{\ell_k})_i(t) = 0$ for all $k \geq k_\circ(t)$ in $\mathfrak{J}_i$ a.e. This implies

$$\zeta_i^{\ell_k}(t) = 0 \quad \forall k \geq k_\circ(t) \text{ and f.a.a. } t \in \mathfrak{J}_i. \tag{3.28}$$

- Suppose that $t \in \mathcal{A}_{ai} = \{t \in [0,T] \,|\, u_{ai}(t) = \bar{u}_i(t)\}$ for $i \in \{1,\dots,N_u\}$. From $(\sigma\bar{u}_i - \mathcal{B}'\bar{p})_i(t) \geq 0$ in $\mathcal{A}_{ai}$ a.e. we deduce

$$\lim_{k\to\infty} \zeta_i^{\ell_k}(t) = -\lim_{k\to\infty} \min(0,(\sigma\bar{u}^{\ell_k} - \mathcal{B}'\tilde{p}^{\ell_k})_i(t)) = 0 \quad \text{f.a.a. } t \in \mathcal{A}_{ai}.$$

- Suppose that $t \in \mathcal{A}_{bi} = \{t \in [0,T] \,|\, u_{bi}(t) = \bar{u}_i(t)\}$. Analogously to the second case we find

$$\lim_{k\to\infty} \zeta_i^{\ell_k}(t) = -\lim_{k\to\infty} \max(0,(\sigma\bar{u}^{\ell_k} - \mathcal{B}'\tilde{p}^{\ell_k})_i(t)) = 0 \quad \text{f.a.a. } t \in \mathcal{A}_{bi}. \tag{3.29}$$

Combining (3.28)-(3.29) we conclude that $\lim_{k\to\infty} \zeta_i^{\ell_k} = 0$ a.e. in $[0,T]$ and for $1 \leq i \leq N_u$. Moreover, the sequence $\{\|\zeta^{\ell_k}(\cdot)\|_{\mathbb{R}^{N_u}}\}_{k\in\mathbb{N}} \subset L^2(0,T)$ is bounded. Utilizing the dominated convergence theorem [DR11, Satz 13.28] we have

$$\lim_{k\to\infty} \big\|\zeta^{\ell_k}\big\|_U = 0.$$

Since all subsequences contain a subsequence converging to zero, the claim follows from a standard argument. $\square$

Remark 3.19. 1) Theorem 3.18 shows that $\|\zeta^\ell\|_U$ tends to zero as ℓ goes to infinity. Thus, $\|\zeta^\ell\|_U$ is smaller than any tolerance $\epsilon > 0$ provided that ℓ is taken sufficiently large. Motivated by this result we set up Algorithm 1. Note that the approximation quality of the POD Galerkin scheme is improved by only increasing the number of POD basis elements: A rank-ℓ POD basis can be extended to a rank-$(\ell+1)$ POD basis by adding a new eigenfunction and keeping all the old ones. Especially, the system matrices and projected data functions can be extended by the new element, they do not have to be reconstructed in all components.

2) We infer from Proposition 2.13 and Remark 3.16-3) that Theorem 3.18 holds still true if we take $\wp = 2$, $y^1 = \mathcal{S}u$ and $y^2 = \mathcal{A}u$. $\Diamond$

Algorithm 1 POD reduced-order method with a-posteriori estimator

Require: Initial control $u^{0\ell} \in U$, initial number ℓ for the POD ansatz functions, a maximal number $\ell_{\mathsf{max}} > \ell$ of POD ansatz functions, and a stopping tolerance $\epsilon > 0$.

```
Determine ŷ, p̂, y¹ = 𝒮u^{0ℓ}, y² = 𝒜u^{0ℓ}.
Compute a POD basis {ψ_i}_{i=1}^{ℓ_max} choosing y¹ and y². Set ℓ = 1.
repeat
    Establish the POD Galerkin discretization using {ψ_i}_{i=1}^{ℓ}.
    Compute suboptimal control ū^ℓ.
    Determine ζ^ℓ according to Theorem 3.15 and compute ϵ_ape = ‖ζ^ℓ‖_U/σ.
    if ϵ_ape < ϵ or ℓ = ℓ_max then
        Return ℓ and suboptimal control ū^ℓ and STOP.
    end if
    Set ℓ = ℓ + 1.
until ℓ > ℓ_max
```

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