Problem 1: Optimality of the Proper Orthogonal Decomposition

The objective of this problem is to develop a proof for the first theorem of Chapter 4 of the lecture notes:

**Theorem.** Let $\hat{K} \in \mathbb{R}^{N \times N}$ be the real, symmetric, positive semi-definite matrix defined as

$$
\hat{K} = \int_0^T w(t)w^T(t) dt
$$

Let $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq \hat{\lambda}_N \geq 0$ denote the ordered eigenvalues of $\hat{K}$, and $\hat{\phi}_i \in \mathbb{R}^N$, $i = 1, \cdots, N$ their associated eigenvectors – that is,

$$
\hat{K}\hat{\phi}_i = \hat{\lambda}_i\hat{\phi}_i, \ i = 1, \cdots, N
$$

The subspace $\hat{V} = \text{range } (\hat{V})$ of dimension $k$ that minimizes $J(\Pi_{V, V})$ is the invariant subspace of $\hat{K}$ associated with the eigenvalues $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq \hat{\lambda}_k$.

1. Show that an orthogonal basis $\hat{V} \in \mathbb{R}^{N \times k}$ that minimizes $J(\Pi_{V, V})$ maximizes

$$
G(\Pi_{V, V}) = \int_0^T \|\Pi_{V, V}w(t)\|^2 dt
$$

2. Show that

$$
G(\Pi_{V, V}) = \int_0^T \|V^T w(t)\|^2 dt
$$

3. Define $q(t) = V^T w(t)$. Show that

$$
\|q(t)\|^2 = \text{trace } (q(t)q^T(t)) = \text{trace } (V^T w(t)w^T(t)V)
$$

4. Show that

$$
G(\Pi_{V, V}) = \text{trace } (V^T \hat{K}V) = \sum_{i=1}^k v_i^T \hat{K}v_i
$$
where \( \mathbf{V} = [\mathbf{v}_1, \cdots, \mathbf{v}_k] \), and conclude that \( \hat{\mathbf{V}} \) is solution of the maximization problem

\[
\max_{\mathbf{V} \in \mathbb{R}^{N \times k}} \text{trace} \left( \mathbf{V}^T \hat{\mathbf{K}} \mathbf{V} \right)
\]

(4)

under the constraint \( \mathbf{V}^T \mathbf{V} = \mathbf{I}_k \).

5. Conclude using the following generalization of Rayleigh’s theorem:

**Theorem.** Let \( \mathbf{A} \) denote a symmetric matrix with eigenvalues \( \mu_1 \geq \cdots \geq \mu_k > \mu_{k+1} \geq \cdots \).

A solution of the maximization problem

\[
\max_{\mathbf{V} \in \mathbb{R}^{N \times k}, \mathbf{V}^T \mathbf{V} = \mathbf{I}_k} \text{trace} \left( \mathbf{V}^T \mathbf{A} \mathbf{V} \right)
\]

(5)

is given by an orthogonal basis \( \mathbf{V} \) for the invariant subspace of \( \mathbf{A} \) associated with the \( k \) largest eigenvalues of \( \mathbf{A} \).

**Problem 2: POD in the Frequency Domain**

The goal of this problem is to demonstrate the equivalence between applying POD in the time domain, and applying POD in the frequency domain.

1. Let \( \mathcal{T} > 0 \). Assume that \( \mathbf{w}(t) = 0 \) for \( t < 0 \), and define the \( N \times N \) matrix \( \hat{\mathbf{K}} \) as

\[
\hat{\mathbf{K}} = \int_{-\mathcal{T}}^{\mathcal{T}} \mathbf{w}(t) \mathbf{w}^T(t) dt = \int_{-\mathcal{T}}^{\mathcal{T}} \mathbf{w}(t) \mathbf{w}^T(t) dt
\]

What is the \((i,j)\) entry in \( \hat{\mathbf{K}} \) for \( 1 \leq i, j \leq N \)?

2. Let \( \Omega > 0 \). Denote by \( \mathcal{W}(\omega) \in \mathbb{C}^N \) the Fourier transform of \( \mathbf{w}(t) \), and define the \( N \times N \) matrix \( \tilde{\mathbf{K}} \) as

\[
\tilde{\mathbf{K}} = \int_{-\Omega}^{\Omega} \mathcal{W}(\omega) \mathcal{W}(\omega)^* d\omega
\]

where \((\ )^*\) denotes the complex conjugate transpose operation. What is the \((i,j)\) entry in \( \tilde{\mathbf{K}} \) for \( 1 \leq i, j \leq N \)?

3. Recall Parseval’s theorem for real square-integrable functions \( a(t) \in \mathbb{R} \) and \( b(t) \in \mathbb{R} \) and their Fourier transforms \( \mathcal{A}(\omega) \in \mathbb{C} \) and \( \mathcal{B}(\omega) \in \mathbb{C} \):

\[
\lim_{\mathcal{T} \to \infty} \frac{1}{\mathcal{T}} \int_{-\mathcal{T}}^{\mathcal{T}} a(t)b(t) dt = \lim_{\mathcal{T}, \Omega \to \infty} \frac{1}{2\pi\mathcal{T}} \int_{-\Omega}^{\Omega} \mathcal{A}(\omega) \mathcal{B}(\omega) d\omega
\]

where \((\ )^*\) denotes the complex conjugate operation. Show that

\[
\lim_{\mathcal{T} \to \infty} \frac{1}{\mathcal{T}} \int_{-\mathcal{T}}^{\mathcal{T}} \mathbf{w}(t) \mathbf{w}^T(t) dt = \lim_{\mathcal{T}, \Omega \to \infty} \frac{1}{2\pi\mathcal{T}} \int_{-\Omega}^{\Omega} \mathcal{W}(\omega) \mathcal{W}(\omega)^* d\omega
\]

(Note that Parseval’s theorem cannot be applied directly as it is only stated for scalar valued functions \( a(t) \) and \( b(t) \).)
4. Show that for any $V \in \mathbb{R}^{N \times k}$,

$$V^T \left( \lim_{T \to \infty} \frac{1}{T} \int_{-T}^{T} w(t)w^T(t) dt \right) V = V^T \left( \lim_{T, \Omega \to \infty} \frac{1}{2\pi T} \int_{-\Omega}^{\Omega} W(\omega)W(\omega)^* d\omega \right) V$$

and conclude on the equivalence between applying POD in the time domain and applying POD in the frequency domain.

**Problem 3: Model Reduction by Residual Minimization**

Consider the parameterized, linear, steady-state, High-Dimensional Model (HDM)

$$A(\mu)w(\mu) = b(\mu) \quad (6)$$

where $\mu \in \mathbb{R}^d$ is the parameter vector, $w \in \mathbb{R}^N$ is the HDM solution, $A \in \mathbb{R}^{N \times N}$, and $b \in \mathbb{R}^N$. Let $V \in \mathbb{R}^{N \times k}$ be a Reduced-Order Basis (ROB), and

$$w(\mu) \approx Vq(\mu) \quad (7)$$

where $q \in \mathbb{R}^k$, denote the considered approximate solution of the above problem.

1. Let $q \in \mathbb{R}^k$ and $\mu \in \mathbb{R}^d$. What is the residual $r(q; \mu)$ associated with equation (6) and the approximation (7)?

2. Let $H \in \mathbb{R}^{N \times N}$ denote a Symmetric Positive Definite matrix (SPD). For a fixed $\mu \in \mathbb{R}^d$, one can determine the reduced state vector $q(\mu)$ as

$$q(\mu) = \arg\min_{z \in \mathbb{R}^k} \frac{1}{2} \|r(z; \mu)\|_H^2 \quad (8)$$

where

$$\|v\|_H = \sqrt{v^T Hv} \quad (9)$$

What is the linear system of equations corresponding to the first-order optimality conditions associated with the minimization problem (8)? (Hint: write the function to be minimized as a quadratic function of $z$.)

3. When $H = I_N$, what are the corresponding equations? What is the name of this system in the context of the least-squares method?

4. For a fixed $\mu \in \mathbb{R}^d$, is there a specific choice of $H$ that leads to a Galerkin projection? Are there any associated restrictions on $A(\mu)$?