Localized Manifold Harmonics for Spectral Shape Analysis

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Supplementary Material

These pages contain proofs for Theorems 1 and 2 appearing in the main paper [2].

Proof of Theorem 1. Let $\mathbf{W}$, $\mu_\perp \mathbf{A}\mathbf{P}_{k'}$ and $\mu_R \mathbf{A}\mathrm{diag}(\mathbf{v})$ be real symmetric positive semidefinite matrices of dimension $n \times n$, and define $\mathbf{Q}_{v,k'} = \mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'} + \mu_R \mathbf{A}\mathrm{diag}(\mathbf{v})$. Let $0 = \lambda_1(\mathbf{W}) \leq \ldots \leq \lambda_n(\mathbf{W})$ be the eigenvalues for the generalized eigenvalue problem of $\mathbf{W}$ and $\lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}) \leq \ldots \leq \lambda_n(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})$ and $\lambda_1(\mathbf{Q}_{v,k'}) \leq \ldots \leq \lambda_n(\mathbf{Q}_{v,k'})$ be the generalized eigenvalues of $\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}$ and $\mathbf{Q}_{v,k'}$ respectively. We aim to prove that

$$\lambda_{k'}(\mathbf{W}) \leq \lambda_1(\mathbf{Q}_{v,k'})\,, \tag{1}$$

for some $\mu_\perp, \mu_R \in \mathbb{R}$ and for every $k' \in \{0, \ldots, n-1\}$.

We start by observing that

$$\lambda_{k'}(\mathbf{W}) \leq \lambda_{k'+1}(\mathbf{W}) = \lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\,, \tag{2}$$

where the first inequality is given by the non-decreasing ordering of the eigenvalues, and the equality on the right follows from the fact that for some choice of $\mu_\perp > \lambda_{k'+1}(\mathbf{W})$, $\boldsymbol{\phi}_{k'+1}$ is the minimizer of $\mathbf{x}^\top(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x}$ under the orthogonality conditions $\langle \mathbf{x}, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 1$ and $\langle \boldsymbol{\phi}_l, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 0$, $\forall l \in \{1, \ldots, k'\}$, i.e., $(\mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \mathbf{0}$.

Invoking a special case of Corollary 4.3.4b in [1] and using the fact that $\mu_R \mathbf{A}\mathrm{diag}(\mathbf{v})$ only has non-negative eigenvalues (being a diagonal matrix with non-negative entries), we obtain the following inequality:

$$\lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}) \leq \lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}) + \mu_R \mathbf{A}\mathrm{diag}(\mathbf{v})) = \lambda_1(\mathbf{Q}_{v,k'})\,. \tag{3}$$

Furthermore, this inequality is an equality if and only if $\exists \mathbf{x} \in \mathbb{R}^n$ s.t. $\mathbf{x} \neq 0$ and the following three conditions are satisfied:

1. $(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x}$;
2. $(\mathbf{Q}_{v,k'})\mathbf{x} = \lambda_1(\mathbf{Q}_{v,k'})\mathbf{x}$;
3. $(\mu_R \mathbf{A}\mathrm{diag}(\mathbf{v}))\mathbf{x} = 0$.

Putting together (2) and (3) we can conclude that:

$$\lambda_{k'}(\mathbf{W}) \leq \lambda_{k'+1}(\mathbf{W}) \leq \lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}) \leq \lambda_1(\mathbf{Q}_{v,k'})\,. \tag{4}$$

Note that the existence of a gap is given either by the violation of any of the three conditions above, or in the presence of simple spectra, i.e., whenever $\lambda_{k'}(\mathbf{W}) \neq \lambda_{k'+1}(\mathbf{W})$.

Choice of $\mu_\perp$. We aim to prove that for every $\mu_\perp > \gamma$ for some $\gamma \in \mathbb{R}^+$ we have:

$$\lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}) \geq \lambda_{k'+1}(\mathbf{W})\,. \tag{5}$$

We can rewrite the two terms of this inequality as:

$$\lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}) = \min_{\langle \mathbf{x},\mathbf{x}\rangle_{L^2(\mathcal{X})}=1} \mathbf{x}^\top(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} \tag{6}$$

$$\lambda_{k'+1}(\mathbf{W}) = \min_{\substack{\langle \mathbf{x},\mathbf{x}\rangle_{L^2(\mathcal{X})}=1 \\ \langle \boldsymbol{\phi}_i,\mathbf{x}\rangle_{L^2(\mathcal{X})}=0,\ \forall i=1,\ldots,k'}} \mathbf{x}^\top \mathbf{W}\mathbf{x}\,. \tag{7}$$

The objective in (6) can be rewritten as:

$$\mathbf{x}^\top(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \mathbf{x}^\top \mathbf{W}\mathbf{x} + \mathbf{x}^\top(\mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x}\,. \tag{8}$$

We now express our vectors as the Fourier series $\mathbf{x} = \sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i$, where $\alpha_i = \langle \boldsymbol{\phi}_i, \mathbf{x}\rangle_{L^2(\mathcal{X})}$. Noting that $\langle \mathbf{x}, \mathbf{x}\rangle_{L^2(\mathcal{X})} = 1$ implies $\sum_{i=1}^n \alpha_i^2 = 1$, we can write:

$$\mathbf{x}^\top \mathbf{W}\mathbf{x} = (\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i)^\top \mathbf{W}(\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i) = (\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i)^\top(\sum_{i=1}^n \lambda_i(\mathbf{W})\alpha_i \mathbf{A}\boldsymbol{\phi}_i) = \sum_{i=1}^n \lambda_i(\mathbf{W})\alpha_i^2\,. \tag{9}$$

Similarly, we can rewrite the second summand in (8) as:

$$\begin{aligned}
\mathbf{x}^\top(\mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} &= (\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i)^\top(\mu_\perp \mathbf{A}\mathbf{P}_{k'})(\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i) && (10)\\
&= \mu_\perp(\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i)^\top(\mathbf{A}\boldsymbol{\Phi}\boldsymbol{\Phi}^\top\mathbf{A})(\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i) && (11)\\
&= \mu_\perp\Big((\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i)^\top\mathbf{A}\boldsymbol{\Phi}\Big)\Big(\boldsymbol{\Phi}^\top\mathbf{A}(\sum_{i=1}^n \alpha_i \boldsymbol{\phi}_i)\Big) && (12)\\
&= \mu_\perp\,[\alpha_1,\ldots,\alpha_{k'}]\,[\alpha_1,\ldots,\alpha_{k'}]^\top && (13)\\
&= \mu_\perp \sum_{i=1}^{k'} \alpha_i^2\,. && (14)
\end{aligned}$$

From (9) and (14) we can conclude:

$$\mathbf{x}^\top(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \mathbf{x}^\top \mathbf{W}\mathbf{x} + \mathbf{x}^\top(\mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \sum_{i=1}^n \lambda_i(\mathbf{W})\alpha_i^2 + \mu_\perp \sum_{i=1}^{k'} \alpha_i^2\,. \tag{15}$$

At this point we split the proof in three different cases:

1. $\langle \boldsymbol{\phi}_i, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 0, \ \forall i = 1, \dots, k'$, that is equivalent to ask that $\mathbf{P}_{k'}\mathbf{x} = \mathbf{0}$. In this case we have:

$$\lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}) = \min_{\langle \mathbf{x}, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 1} \mathbf{x}^\top (\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} \tag{16}$$

$$= \min_{\substack{\langle \mathbf{x}, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 1 \\ \langle \boldsymbol{\phi}_i, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 0, \ \forall i = 1, \dots, k'}} (\mathbf{x}^\top (\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x}) \tag{17}$$

$$= \min_{\substack{\langle \mathbf{x}, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 1 \\ \langle \boldsymbol{\phi}_i, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 0, \ \forall i = 1, \dots, k'}} \mathbf{x}^\top \mathbf{W}\mathbf{x} = \lambda_{k'+1}(\mathbf{W})\,. \tag{18}$$

2. $\mathbf{x} \in span(\boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_{k'})$, implying that $\alpha_i = 0 \ \forall i > k'$ and hence $\mathbf{x} = \sum_{i=1}^{k'} \alpha_i \boldsymbol{\phi}_i$. We get:

$$\mathbf{x}^\top (\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \sum_{i=1}^{k'} \lambda_i(\mathbf{W})\alpha_i^2 + \mu_\perp \sum_{i=1}^{k'} \alpha_i^2\,. \tag{19}$$

   Since we take the minimum over the $\mathbf{x}$ s.t. $\langle \mathbf{x}, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 1$ we have $\sum_{i=1}^{k'} \alpha_i^2 = 1$ and:

$$\mathbf{x}^\top (\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \sum_{i=1}^{k'} \lambda_i(\mathbf{W})\alpha_i^2 + \mu_\perp \geq \mu_\perp\,, \tag{20}$$

   where the equality is realized for $\mathbf{x} = \boldsymbol{\phi}_1$ since $\lambda_1(\mathbf{W}) = 0$, and all other cases yield $\mu_\perp$ plus some non-negative quantity. We get to:

$$\lambda_1(\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'}) = \min_{\langle \mathbf{x}, \mathbf{x} \rangle_{L^2(\mathcal{X})} = 1} \mathbf{x}^\top (\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \mu_\perp\,. \tag{21}$$

3. For the last case we have $\langle \boldsymbol{\phi}_i, \mathbf{x} \rangle_{L^2(\mathcal{X})} \neq 0$ for at least one $i = 1, \dots, k'$ and for at least one $i > k'$ at the same time.

$$\mathbf{x}^\top (\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \sum_{i=1}^{n} \lambda_i(\mathbf{W})\alpha_i^2 + \mu_\perp \sum_{i=1}^{k'} \alpha_i^2 \tag{22}$$

$$= \sum_{i=1}^{k'} \lambda_i(\mathbf{W})\alpha_i^2 + \sum_{i=k'+1}^{n} \lambda_i(\mathbf{W})\alpha_i^2 + \mu_\perp \sum_{i=1}^{k'} \alpha_i^2 \tag{23}$$

$$= \sum_{i=1}^{k'} (\lambda_i(\mathbf{W}) + \mu_\perp)\alpha_i^2 + \sum_{i=k'+1}^{n} \lambda_i(\mathbf{W})\alpha_i^2\,. \tag{24}$$

   Since $\lambda_i(\mathbf{W}) \geq \lambda_{k'+1}(\mathbf{W}), \ \forall i \geq k'+1$ we can write:

$$\mathbf{x}^\top (\mathbf{W} + \mu_\perp \mathbf{A}\mathbf{P}_{k'})\mathbf{x} = \sum_{i=1}^{k'} (\lambda_i(\mathbf{W}) + \mu_\perp)\alpha_i^2 + \sum_{i=k'+1}^{n} \lambda_i(\mathbf{W})\alpha_i^2 \tag{25}$$

$$\geq \sum_{i=1}^{k'} (\lambda_i(\mathbf{W}) + \mu_\perp)\alpha_i^2 + \lambda_{k'+1}(\mathbf{W}) \sum_{i=k'+1}^{n} \alpha_i^2 \tag{26}$$

$$\geq \sum_{i=1}^{k'} \mu_\perp \alpha_i^2 + \lambda_{k'+1}(\mathbf{W}) \sum_{i=k'+1}^{n} \alpha_i^2\,. \tag{27}$$

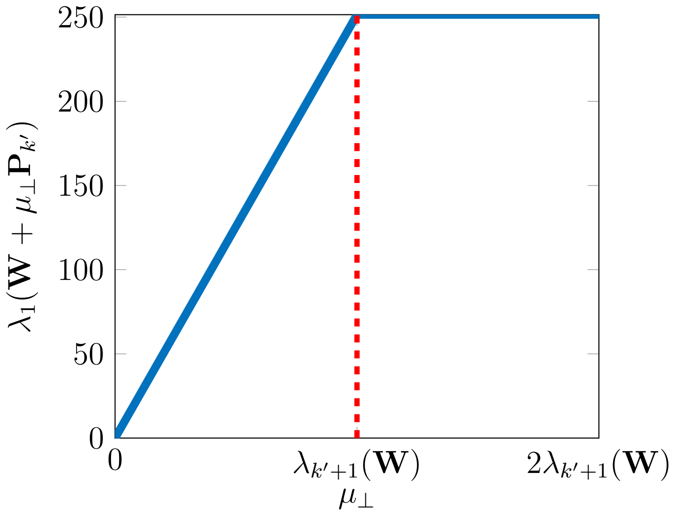

Figure 1: Plot of $\lambda_1(\mathbf{W} + \mu_\perp \mathbf{AP}_{k'})$ at increasing $\mu_\perp$. Note how for every $\mu_\perp \leq \lambda_{k'+1}(\mathbf{W})$ the frequency (y-axis) increases, converging at $\mu_\perp > \lambda_{k'+1}(\mathbf{W})$. At convergence, the orthogonality constraint (encoded in the penalty term $\mathcal{E}_\perp(\psi)$ in the LMH formulation) is satisfied.

If we take $\mu_\perp > \lambda_{k'+1}(\mathbf{W})$ in order to satisfy the condition imposed by case 2, we get:

$$\begin{aligned}
\mathbf{x}^\top(\mathbf{W} + \mu_\perp \mathbf{AP}_{k'})\mathbf{x} &\geq \sum_{i=1}^{k'} \mu_\perp \alpha_i^2 + \lambda_{k'+1}(\mathbf{W}) \sum_{i=k'+1}^{n} \alpha_i^2 && (28)\\
&> \lambda_{k'+1}(\mathbf{W}) \sum_{i=1}^{k'} \alpha_i^2 + \lambda_{k'+1}(\mathbf{W}) \sum_{i=k'+1}^{n} \alpha_i^2 && (29)\\
&= \lambda_{k'+1}(\mathbf{W}) \sum_{i=1}^{n} \alpha_i^2 && (30)\\
&= \lambda_{k'+1}(\mathbf{W})\,. && (31)
\end{aligned}$$

We can therefore conclude that

$$\lambda_1(\mathbf{W} + \mu_\perp \mathbf{AP}_{k'}) = \min_{\langle \mathbf{x},\mathbf{x}\rangle_{L^2(\mathcal{X})}=1} \mathbf{x}^\top(\mathbf{W} + \mu_\perp \mathbf{AP}_{k'})\mathbf{x} > \lambda_{k'+1}(\mathbf{W}) \textit{ if } \mu_\perp > \lambda_{k'+1}(\mathbf{W})\,. \tag{32}$$

In Figure 1 we show an empirical evaluation across several choices of $\mu_\perp$.

Proof of Theorem 2. We want to show that $\forall k \in \{1, 2, \ldots, n\}$ we have the following upper bound:

$$\lambda_i(\mathbf{Q}_{v,k'}) \leq \lambda_{i+k'}(\mathbf{W}^R)\ .$$

Similarly to Theorem 1, the proof follows directly from Corollary 4.3.4b in [1], which specialized to our case reads:

$$\lambda_i(\mathbf{W}^R + \mu_\perp \mathbf{AP}_{k'}) \leq \lambda_{i+\pi}(\mathbf{W}^R)\,, \tag{33}$$

where π is the number of positive eigenvalues of $\mu_\perp \mathbf{AP}_{k'}$. Since $\mathbf{Q}_{v,k'} = \mathbf{W}^R + \mu_\perp \mathbf{AP}_{k'}$ and using the fact that $\mu_\perp \mathbf{AP}_{k'}$ is a positive semidefinite matrix with rank k', we have $\pi = k'$, leading to:

$$\lambda_i(\mathbf{Q}_{v,k'}) = \lambda_i(\mathbf{W}^R + \mu_\perp \mathbf{AP}_{k'}) \leq \lambda_{i+\pi}(\mathbf{W}^R) = \lambda_{i+k'}(\mathbf{W}^R)\,. \tag{34}$$

References

[1] R. A. Horn and C. R. Johnson. *Matrix analysis*. Cambridge university press, 2012.

[2] S. Melzi, E. Rodolà, U. Castellani, and M. M. Bronstein. Localized manifold harmonics for spectral shape analysis. *Computer Graphics Forum*.