The Average Mixing Kernel Signature: Supplementary Material

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1 Perturbation Analysis

In order to understand the advantage of the use of finite-time averages, we perform a perturbation analysis on the eigendecomposition of the Laplace-Beltrami operator, showing that first order perturbation introduces a mixing of the eigenspaces similar to what is obtained in finite-time averaging of the ensemble.

Let L be the Laplace-Beltrami operator and assume that we observe a noisy version $\hat{L} = L + \mathcal{E}$ with $\mathcal{E}$ being a suitable additive noise on the operator, and from that an interpolating function $\mathcal{L}(t) = L + t\mathcal{E}$ with $t \in [0, 1]$. Clearly, as $t = 0$ we obtain the noiseless Laplace-Beltrami operator $\mathcal{L}(0) = L$, while for $t = 1$ we have the noisy operator $\mathcal{L}(1) = \hat{L}$. Further, let $\mathcal{L}\Phi = \Phi\Lambda$ be the eigenvector equation for $\mathcal{L}$, where Λ is the diagonal matrix of eigenvalues such that $(\Lambda)_{ii} = \lambda_i$, while Φ is the matrix of eigenvectors, so that $\Phi_{\cdot i} = \phi_{\lambda_i}$.

Following [1], we can write the derivatives at $t = 0$ of the eigenvectors ϕ_{λ_i} of $\mathcal{L}(t)$ introducing a matrix $B = (b_{ij})$, such that $\Phi' = \Phi B$. Under this representation, we can write the eigenvectors of $\hat{L}$ as a first order approximation of the expansion of $\mathcal{L}$ at 0, obtaining

$$\Phi_{\hat{L}} = \Phi + \Phi' = \Phi(I + B)\,, \tag{1}$$

where $\Phi_{\hat{L}}$ is the eigenvector matrix of $\hat{L}$.

Moreover, solving for the perturbation equations for a self-adjoint operator, we have

$$b_{ij} = \begin{cases} 0 & \text{if } i = j; \\ \frac{\phi_{\lambda_i}^T \mathcal{E} \phi_{\lambda_j}}{\lambda_j - \lambda_i} & \text{otherwise.} \end{cases} \tag{2}$$

From this perturbation analysis we see that, at least to the first order, the effect of noise is a mixing into the eigenspace related to eigenvalue λ_i of a component linked to the eigenspace of λ_j at a rate proportional to the reciprocal

⋆ Equal contribution.

of the difference in eigenvalues $\frac{1}{\lambda_j-\lambda_i}$, rate that is asymptotically equivalent to the $\mathrm{sinc}(T(\lambda_j-\lambda_i))$ obtained through finite-time averaging, for T approaching infinity. Hence, we can see the additive mixing of the finite-time averaging to be equivalent to a random projection onto the same portion of subspace induced by the noise process, or equivalently, we can see the additive mixing noise process as a random projection onto the subspace spanned by the additional components in the finite-time averaging. The end result is a descriptor that already includes and takes into account part of the deformation introduced by the noise process.

2 Computation of the AMKS

Let us consider the discrete setting in which a shape $\mathcal{X}$ is sampled at n points. To compute the descriptor we consider only the first $k \ll n$ smallest eigenvalues and corresponding eigenvectors of the discretized Laplace-Beltrami operator. Higher eigenvalues encode finer geometric details of the shape which are mostly dominated by noise introduced by sampling.

We can rewrite the equation of AMKS in terms of matrix operations, thus exploiting linear algebra computation capabilities of modern hardware and GPU computing. We first notice that, since we are only interested in the diagonal entries of the matrix $AMM(E)$, we can expand it as

$$AMKS(E) = \frac{\sum_{\lambda_1}\sum_{\lambda_2}\phi^2_{\lambda_1}\circ\phi^2_{\lambda_2}\mathrm{sinc}(T(\lambda_2-\lambda_1))f_E(\lambda_1)f_E(\lambda_2)}{\sum_{\lambda_1,\lambda_2}f_E(\lambda_1)f_E(\lambda_2)}\,, \tag{3}$$

where the diagonal part of P_λ is equal to ϕ^2_λ.

Let us define the $k\times k$ matrices $B(E)=(b(E)_{uv})$ and $S=(s_{uv})$ such that

$$\begin{aligned} s_{uv} =& \mathrm{sinc}(T(\lambda_u-\lambda_v)) \\ b(E)_{uv} =& \frac{S_{uv}f_E(\lambda_u)f_E(\lambda_v)}{\sum_{\lambda_1,\lambda_2}f_E(\lambda_u)f_E(\lambda_v)}\,. \end{aligned}$$

We can see that $B(E)=(S\circ \boldsymbol{f_E}\boldsymbol{f_E}^\top)/sum(\boldsymbol{f_E}\boldsymbol{f_E}^\top)$, with $\boldsymbol{f_E}=[f_E(\lambda_1)\dots f_E(\lambda_k)]^\top$ being a column vector. The value of the descriptor at energy level E can thus be computed as

$$\begin{aligned} AMKS(E) =& \sum_{\lambda_1}\phi^2_{\lambda_1}\circ(\Phi^{\circ 2}B) \\ =& \langle(\Phi^{\circ 2})^\top,(\Phi^{\circ 2}B)^\top\rangle\,, \end{aligned}$$

where $^{\circ 2}$ denotes the element-wise square of a matrix.

References

1. Murthy, D.V., Haftka, R.T.: Derivatives of eigenvalues and eigenvectors of a general complex matrix. Intl. J. Numer. Met. Eng. **26**(2), 293–311 (1988)