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Infinite-dimensional Log-Determinant divergences between positive definite trace class operators

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ABSTRACT

This work presents a novel parametrized family of Log-Determinant (Log-Det) divergences between positive definite unitized trace class operators on a Hilbert space. This is a generalization of the Log-Det divergences between symmetric, positive definite matrices to the infinite-dimensional setting. For the Log-Det divergences between covariance operators on a Reproducing Kernel Hilbert Space (RKHS), we obtain closed form solutions via the corresponding Gram matrices. By employing the Log-Det divergences, we then generalize the Bhattacharyya and Hellinger distances and the Kullback–Leibler and Rényi divergences between multivariate normal distributions to Gaussian measures on an infinite-dimensional Hilbert space.

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1. Introduction

Symmetric Positive Definite (SPD) matrices abound in numerous areas of mathematics, statistics, and their applications in machine learning, optimization, computer vision,

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and related fields, see e.g. [1–9]. The set $\mathrm{Sym}^{++}(n)$ of $n\times n$ SPD matrices is an open convex cone and can be equipped with a Riemannian manifold structure and much work has been done to exploit these geometrical structures. The manifold structure of $\mathrm{Sym}^{++}(n)$ has been studied extensively in the literature, with two of the most common Riemannian metrics on $\mathrm{Sym}^{++}(n)$ being the affine-invariant metric [1–3,5,6] and the Log-Euclidean metric [4,10,9,11]. The convex cone structure of $\mathrm{Sym}^{++}(n)$, on the other hand, gives rise to distance-like functions such as the Log-Determinant divergences [12]. While not arising from Riemannian metrics, these divergences are fast to compute and have been shown to work very well in practice [7,13,8]. The present work aims to generalize these divergences to the infinite-dimensional setting.

We recall that for $A, B \in \mathrm{Sym}^{++}(n)$, the *Log-Determinant* (or Log-Det) *α-divergence* between A and B is a parametrized family of divergences defined by (see [12])

$$d^{\alpha}_{\mathrm{logdet}}(A,B) = \frac{4}{1-\alpha^2}\log\frac{\det(\frac{1-\alpha}{2}A + \frac{1+\alpha}{2}B)}{\det(A)^{\frac{1-\alpha}{2}}\det(B)^{\frac{1+\alpha}{2}}}, \quad -1<\alpha<1, \tag{1}$$

$$d^{1}_{\mathrm{logdet}}(A,B) = \mathrm{tr}(B^{-1}A - I) - \log\det(B^{-1}A), \tag{2}$$

$$d^{-1}_{\mathrm{logdet}}(A,B) = \mathrm{tr}(A^{-1}B - I) - \log\det(A^{-1}B). \tag{3}$$

In particular, for $\alpha = 0$, we obtain the symmetric function

$$d^{0}_{\mathrm{logdet}}(A,B) = 4\left[\log\det\left(\frac{A+B}{2}\right) - \frac{1}{2}\log\det(AB)\right] = 4d^2_{\mathrm{stein}}, \tag{4}$$

where d^2_{stein} denotes the symmetric Stein divergence of [13].

Our contributions. In this work, we generalize the above family of parametrized Log-Determinant divergences on $\mathrm{Sym}^{++}(n)$ to the infinite-dimensional setting. The new divergences measure distances between positive definite unitized trace class operators, which are scalar perturbations of positive trace class operators on a Hilbert space. This set of operators is a *strict subset* of the infinite-dimensional Riemannian manifold of positive definite unitized Hilbert–Schmidt operators recently studied in [14,15]. Instead of the manifold viewpoint, the Log-Det divergences are formulated using the convex cone structure of the set of positive definite operators. In particular, they are defined via the novel concept of *extended Fredholm determinant*, which we introduce in this work for these operators, generalizing the classical Fredholm determinant [16–18]. In the case of RKHS covariance operators, we obtain closed form expressions for the Log-Det divergences via the corresponding Gram matrices. As we demonstrate throughout the paper, as in the case of the Log-Hilbert–Schmidt distance studied in [15], the infinite-dimensional Log-Det formulation is significantly different from its finite-dimensional counterpart on $\mathrm{Sym}^{++}(n)$ and one *cannot* obtain the infinite-dimensional Log-Det formulas from those on $\mathrm{Sym}^{++}(n)$ by letting the dimension n approach infinity.

After introducing the infinite-dimensional Log-Det divergences between positive definite trace class operators, we use them to generalize to the infinite-dimensional setting

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