An Introduction to Laplacian Spectral Distances and Kernels: Theory, Computation, and Applications

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CHAPTER 1

Introduction

In geometry processing and shape analysis, several applications have been addressed through the properties of the Laplacian spectral kernels and distances, such as commute-time, biharmonic, diffusion, and wave distances. Spectral distances are easily defined through a filtering of the Laplacian eigenpairs and include random walks [FPS05, RS13], heat diffusion [BBK$^+$10, BBOG11, CL06, GBAL09, LKC06, LSW09], biharmonic [LRF10, Rus11b], and wave kernel [BB11a, ASC11] distances. Biharmonic [LRF10, Rus11b] and diffusion [BBK$^+$10, BBOG11, CL06, GBAL09, LKC06, LSW09, PS13b] distances provide a trade-off between a nearly geodesic behavior for small distances and the encoding of global surface properties for large distances, thus guaranteeing an intrinsic and multi-scale characterisation of the input shape. The heat kernel [BBG94] is also central in diffusion geometry [BN03, CL06, GK06, Sin06], dimensionality reduction with spectral embeddings [BN03, XHW10], and data classification [SK03].

As main applications, we mention the multi-scale approximation of functions [PF10] and gradients [LSW09], shape segmentation and comparison through heat kernel shape descriptors, auto-diffusion functions, and diffusion distances. Laplacian spectral distances have been applied to shape segmentation [dGGV08] and comparison [BBOG11, GBAL09, Mem09, OMMG10, SOG09] with multi-scale and isometry-invariant signatures [DRW10, LKC06, MS05, Mem11, RBBK10, Rus07, MS09]. In fact, they are intrinsic to the input shape, invariant to isometries, multi-scale, and robust to noise and tessellation. Additional applications include image smoothing [ZH08], geometric characterisations [EH09] and embeddings [LWH03] of graphs, and shape analysis [BMR$^+$16, CRA$^+$16, RCB$^+$16]. The diffusion kernel and distance also play a central role in several applications, such as dimensionality reduction with spectral embeddings [BN03, XHW10]; data visualisation [BN03, HAvL05, RS00, TSL00], representation [CWS03, SK03, ZGL03], and classification [NJW01, SM00, ST07].

Our book is intended to provide a common background on the definition and computation of the Laplacian spectral kernels and distances for geometry processing and shape analysis. All the reviewed numerical schemes are discussed and compared in terms of robustness, approximation accuracy, and computational cost, thus supporting the reader in the selection of the most appropriate with respect to shape representation, computational resources, and target application. Indeed, our review is complementary to previous work, which has been focused mainly on specific applications, such as mesh filtering [Tau99], surface coding and spectral partitioning [KG00], 3D shape deformation based on differential coordinates [Sor06], spectral methods [ZvKD07, Pat16b] and Laplacian eigenfunctions [Lev06] for geometry processing and diffusion shape analysis [BCA12].

Firstly, we define a unified representation of the isotropic and anisotropic discrete Laplacian operator on surfaces and volumes (Sect. 2); then, we introduce the associated differential equations. For the harmonic equation and the Laplacian eigenproblem, we focus on the stability and accuracy of numerical solvers, also presenting their main applications. This discussion provides the background for a detailed analysis of the heat equation (Sect. 3) and allows us to identify the main limitations (e.g., computational cost, storage overhead, selection of user-defined parameters) of previous work on the approximation of the diffusion distances, which is based mainly on the evaluation of the Laplacian spectrum and on linear approximations of the exponential matrix. For the heat equation, we discuss the selection of the time scale and the main approaches for the computation of the solution to the heat equation, such as linear, polynomial, and rational approximations.

Filtering the Laplacian spectrum, we introduce the Laplacian spectral distances (Sect. 4), which generalise the commute-time, biharmonic, diffusion and wave distances, and their discretisation in terms of the Laplacian spectrum. The growing interest on these distances is motivated by their capability of encoding local geometric properties (e.g., Gaussian curvature, geodesic distance) of the input shape, their intrinsic and multi-scale definition with respect to the input shape, their invariance to isometries, shape-awareness, robustness to noise and tessellation. While previous work has been focused mainly on surfaces discretised as triangle meshes, we introduce a unified representation of the spectral distances and kernels, which is independent of the selected Laplacian weights, of the surface or volume representation as polygonal mesh, point set, tetrahedral or voxel grid. From this general representation, we show that the characteristic properties of the spectral distances are guided mainly by the filter that is applied to the Laplacian eigenpairs.

The expensive cost for the computation of the Laplacian spectrum and the sensitiveness of multiple Laplacian eigenvalues to surface discretisation generally preclude an accurate evaluation of the spectral kernels and distances on large data sets. To discuss these problems, we review and compare different methods for the numerical evaluation of the spectral distances and kernels (Sect. 5). In particular, we detail their spectrum-free computation, which is defined through a polynomial or rational approximation of the filter function. The resulting computational scheme only requires the solution of sparse linear systems, is not affected by the Gibbs phenomenon, is independent of the representation of the input domain, the selected Laplacian weights, and the evaluation of the Laplacian spectrum.

As main applications (Sect. 6), we will discuss the design of smooth functions, whose maxima, minima, and saddles are selected by the user or imported from a template function, and the Laplacian smoothing of noisy scalar functions, without and with constraints on the preservation of their critical points. Finally (Sect. 7), we conclude our review with a discussion of open questions and challenges.

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