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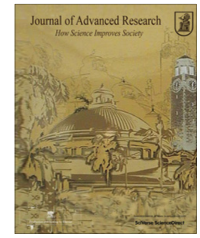

ORIGINAL ARTICLE

Diffusive smoothing of 3D segmented medical data

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A B S T R A C T

This paper proposes an accurate, computationally efficient, and spectrum-free formulation of the heat diffusion smoothing on 3D shapes, represented as triangle meshes. The idea behind our approach is to apply a (r, r)-degree Padé–Chebyshev rational approximation to the solution of the heat diffusion equation. The proposed formulation is equivalent to solve r sparse, symmetric linear systems, is free of user-defined parameters, and is robust to surface discretization. We also discuss a simple criterion to select the time parameter that provides the best compromise between approximation accuracy and smoothness of the solution. Finally, our experiments on anatomical data show that the spectrum-free approach greatly reduces the computational cost and guarantees a higher approximation accuracy than previous work.

Introduction

In medical applications, the heat kernel is central in diffusion filtering and smoothing of images [1–6], 3D shapes [7,8], and anatomical surfaces [9,10]. However, the computational cost for the evaluation of the heat kernel is the main bottleneck for processing both surfaces and volumetric data; in fact, it takes from $\mathcal{O}(n)$ to $\mathcal{O}(n^3)$ time on a data set sampled with n points, according to the sparsity of the Laplacian matrix. This aspect becomes more evident for medical data, which are nowadays acquired by PET, MRI systems and whose resolution is constantly increasing with the improvement of the underlying imaging protocols and hardware.

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To overcome the time-consuming computation of the Laplacian spectrum on large data sets (Section 'Previous work'), the heat kernel has been approximated by prolongating its values evaluated on a sub-sampling of the input surface [11–13]; applying multi-resolution decompositions [14] or a rational approximation of the exponential representation of the heat kernel [15]; and considering the contribution of the eigenvectors related to smaller eigenvalues. The heat equation has been solved through explicit [16] or backward [17,18] Euler methods, whose solution no more satisfies the diffusion problem. Further approaches apply a Krylov subspace projection [19], which becomes computationally expensive when the dimension of the Krylov space increases, still remaining much lower than n.

This paper proposes an accurate, computationally efficient, and spectrum-free evaluation of the diffusive smoothing on 3D shapes, represented as polygonal meshes. The idea behind our approach (Section 'Discrete heat diffusion smoothing') is to apply the (r, r)-degree Padé–Chebyshev rational polynomial approximation of the exponential map to the solution of the

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heat equation. This spectrum-free formulation converts the heat equation to a set of sparse, symmetric linear systems and the resulting computational scheme is independent of the evaluation of the Laplacian spectrum, the selection of a specific subset of eigenpairs, and multi-resolutive prolongation operators. Our approach has a linear computational cost, is free of user-defined parameters, and works with sparse, symmetric, well-conditioned matrices. Since the computation is mainly based on numerical linear algebra, our method can be applied to any class of Laplacian weights and any data representation (e.g., 3D shapes, multi-dimensional data), thus overcoming the ambiguous definition of multi-resolutive and prolongation operators on point-sampled or non-manifold surfaces. Bypassing the computation of the eigenvectors related to small eigenvalues, which are necessary to correctly recover local features of the input shape or signal, the spectrum-free computation is robust with respect to data discretization. As a result, it properly encodes local and global features of the input data in the heat diffusion kernel. For any data representation and Laplacian weights, the accuracy of the heat smoothing computed through the Padé–Chebyshev approximation is lower than 10^{-r}, where $r := 5,7$ is the degree of the rational polynomial, and can be further reduced by slightly increasing r. Finally (Section 'Results and Discussion'), our experiments on surfaces and volumes representing anatomical data show that the spectrum-free approach greatly reduces the computational cost (from 32 up to 164 times) and guarantees a higher approximation accuracy than previous work.

Previous work

Let us consider the heat equation $(\partial_t + \Delta)F(\cdot,t) = 0$, $F(\cdot,0) = f$, on a closed, connected manifold $\mathcal{N}$ of $\mathbb{R}^3$, where $f: \mathcal{N} \rightarrow \mathbb{R}$ defines the initial condition on $\mathcal{M}$. The solution to the *heat equation* $(\partial_t + \Delta)F(\mathbf{p},t) = 0$, $F(\cdot,0) = f$, is computed as the convolution $F(\mathbf{p},t) := K_t(\mathbf{p},\cdot)\star$ between the initial condition f and the *heat kernel* $K_t(\mathbf{p},\mathbf{q}) := \sum_{n=0}^{+\infty}\exp(-\lambda_n t)\phi_n(\mathbf{p})\phi_n(\mathbf{q})$. Here, $\{(\lambda_n,\phi_n)\}_{n=0}^{+\infty}$ is the Laplacian eigensystem $\Delta\phi_n = \lambda_n\phi_n$, $\lambda_n \leqslant \lambda_{n+1}$.

The heat equation is solved through its FEM formulation [20] on a discrete surface $\mathcal{M}$ (e.g., triangle mesh, point set) of $\mathcal{N}$. Indicating with $\widetilde{\mathbf{L}}$ the Laplacian matrix, which discretizes the Laplace–Beltrami operator on $\mathcal{M}$, the "power" method applies the identity $(\mathbf{K}_{t/m})^m = \mathbf{K}_t$, where m is chosen in such a way that t/m is sufficiently small to guarantee that the approximation $\mathbf{K}_{t/m} \approx (\mathbf{I} - \frac{t}{m}\widetilde{\mathbf{L}})$ is accurate. Here, $\mathbf{I}$ is the identity matrix. However, the selection of m and its effect on the approximation accuracy cannot be estimated a-priori. In [17,18], the solution to the heat equation is computed through the Euler backward method $(t\widetilde{\mathbf{L}} + \mathbf{I})\mathbf{F}_{k+1}(t) = \mathbf{F}_k(t)$, $\mathbf{F}_0 = \mathbf{f}$. The resulting functions are over-smoothed and converge to a constant map, as $k \rightarrow +\infty$. Krylov subspace projection [19], which replaces the Laplacian matrix with a full coefficient matrix of smaller size, has computational and memory bottlenecks when the dimension k of the Krylov space increases, still remaining much lower than n (e.g., $k \approx 5$ K).

Once the Laplacian matrix has been computed, we evaluate its spectrum and approximate the heat kernel by considering the contribution of the Laplacian eigenvectors related to smaller eigenvalues, which are computed in superlinear time [21]. Such an approximation is accurate only if the exponential filter decays fast (e.g., large values of time). Otherwise, a larger number of eigenpairs is needed and the resulting computational cost varies from $\mathcal{O}(kn^2)$ to $\mathcal{O}(n^3)$ time, according to the sparsity of the Laplacian matrix. Furthermore, the number of eigenpairs is heuristically selected and its effect on the resulting approximation accuracy cannot be estimated without computing the whole spectrum. Finally, we can apply multi-resolution prolongation operators [13] and numerical schemes based on the Padé–Chebyshev polynomial [22,15]. However, previous work has not addressed this extension, convergence results, and the selection of the optimal scale.

Discrete heat diffusion smoothing

Let us discretize the input shape as a triangle mesh $\mathcal{M}$, with vertices $\mathcal{P} := \{\mathbf{p}_i\}_{i=1}^n$, which is the output of a 3D scanning device or a segmentation of a MRI acquisition of an anatomical structure. Let $\widetilde{\mathbf{L}} := \mathbf{B}^{-1}\mathbf{L}$ be the Laplacian matrix, where $\mathbf{L}$ is a symmetric, positive semi-definite matrix and $\mathbf{B}$ is a symmetric and positive definite matrix. On triangle meshes, $\mathbf{L}$ is the Laplacian matrix with cotangent weights [23,24] or associated with the Gaussian kernel [25], and $\mathbf{B}$ is the mass matrix of the Voronoi [18] or triangle [26] areas. For any class of weights, the Laplacian matrix $\widetilde{\mathbf{L}}$ is uniquely defined by the couple $(\mathbf{L},\mathbf{B})$ and is associated to the generalized eigensystem $(\mathbf{X},\Lambda)$ such that

$$\begin{cases} \mathbf{L}\mathbf{X} = \mathbf{B}\mathbf{X}\Lambda, \quad \mathbf{X}^\top\mathbf{B}\mathbf{X} = \mathbf{I}, \\ \mathbf{X} := [\mathbf{x}_1,\ldots,\mathbf{x}_n], \quad \Lambda := \operatorname{diag}(\lambda_i)_{i=1}^n, \end{cases} \tag{1}$$

where $\mathbf{X}$ and Λ are the eigenvectors' and eigenvalues' matrices. From the relation (1), we get the identities $\mathbf{B}^{-1}\mathbf{L} = \mathbf{X}\Lambda\mathbf{X}^{-1} = \mathbf{X}\Lambda\mathbf{X}^\top\mathbf{B}$ and

$$\begin{aligned}(\mathbf{B}^{-1}\mathbf{L})^i &= (\mathbf{X}\Lambda\mathbf{X}^\top\mathbf{B})^i = \mathbf{X}\Lambda(\mathbf{X}^\top\mathbf{B}\mathbf{X})\ldots(\mathbf{X}^\top\mathbf{B}\mathbf{X})\Lambda\mathbf{X}^\top\mathbf{B} \\ &= \mathbf{X}\Lambda^i\mathbf{X}^\top\mathbf{B}, \quad i \in \mathbb{N}.\end{aligned} \tag{2}$$

Then, the *spectral representation* of the heat kernel is

$$\begin{cases} \mathbf{K}_t = \exp(-t\widetilde{\mathbf{L}}) = \sum_{i=0}^{+\infty}\frac{(-t\mathbf{B}^{-1}\mathbf{L})^i}{i!} =_{(2)} \mathbf{X}\mathbf{D}_t\mathbf{X}^\top\mathbf{B}, \\ \mathbf{D}_t := \operatorname{diag}(\exp(-\lambda_i t))_{i=1}^n. \end{cases} \tag{3}$$

For a signal $f: \mathcal{M} \rightarrow \mathbb{R}$, $\mathbf{f} := (f(\mathbf{p}_i))_{i=1}^n$, sampled at $\mathcal{P}$, the solution $\mathbf{F}(t) = \mathbf{K}_t\mathbf{f}$, $\mathbf{F}(t) := (F(\mathbf{p}_i,t))_{i=1}^n$, to the heat equation $(\partial_t + \widetilde{\mathbf{L}})\mathbf{F}(t) = \mathbf{0}$, $\mathbf{F}(0) = \mathbf{f}$, is achieved by multiplying the *heat kernel matrix* $\mathbf{K}_t := \exp(-t\widetilde{\mathbf{L}})$ with the initial condition $\mathbf{f}$. Applying the Padé–Chebyshev approximation to the exponential of the Laplacian matrix in Eq. (3), we get

$$\begin{cases} \exp(-t\widetilde{\mathbf{L}}) \approx \alpha_0\mathbf{I} + \sum_{i=1}^{r}\alpha_i(-t\widetilde{\mathbf{L}} - \theta_i\mathbf{I})^{-1}, \\ \mathbf{K}_t\mathbf{f} \approx \alpha_0\mathbf{f} + \sum_{i=1}^{r}\alpha_i(t\mathbf{L} + \theta_i\mathbf{B})^{-1}\mathbf{B}\mathbf{f} = \alpha_0\mathbf{f} + \sum_{i=1}^{r}\mathbf{g}_i, \end{cases} \tag{4}$$

and the vector $\mathbf{K}_t\mathbf{f}$ is the sum of the solutions of r sparse linear systems

$$(t\mathbf{L} + \theta_i\mathbf{B})\mathbf{g}_i = -\alpha_i\mathbf{B}\mathbf{f}, \quad i = 1,\ldots,r. \tag{5}$$

We briefly recall that the weights $(\alpha_i)_{i=1}^r$ and nodes $(\theta_i)_{i=1}^r$ of the Padé–Chebyshev approximation (4) are precomputed for any polynomial degree [27]. Each vector $\mathbf{g}_i$ is calculated as a mini-