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Volumetric heat Kernel: Padé-Chebyshev approximation, convergence, and computation

Giuseppe Patané

CNR-IMATI - Italy

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ABSTRACT

This paper proposes an accurate and computationally efficient solver of the heat equation $(\partial_t+\Delta)F(\cdot,t)=0$, $F(\cdot,0)=f$, on a volumetric domain, through the (r,r)-degree Padé-Chebyshev rational approximation of the exponential representation $F(\cdot,t)=\exp(-t\Delta)f$ of the solution. To this end, the heat diffusion problem is converted to a set of r differential equations, which involve only the Laplace–Beltrami operator, and whose solution converges to $F(\cdot,t)$, as $r\to+\infty$. The discrete heat equation is equivalent to r sparse, symmetric linear systems and is independent of the volume discretization as a tetrahedral mesh or a regular grid, the evaluation of the Laplacian spectrum, and the selection of a subset of eigenpairs. Our approach has a super-linear computational cost, is free of user-defined parameters, and has an approximation accuracy lower than 10^{-r}. Finally, we propose a simple criterion to select the time value that provides the best compromise between approximation accuracy and smoothness of the solution.

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1. Introduction

The heat kernel plays a central role in several applications, such as surface [3,16] and image [34,40] smoothing, shape segmentation [12] and comparison [5,6,14,25,26,35]. Furthermore, the wavelet operator [17], the geodesic [11] and diffusion [4,10,27] distances have been recently rewritten in terms of the heat kernel. Among its main properties, we mention the intrinsic and multi-scale encoding of the input shape, the invariance to isometries, the shape-awareness, the robustness to noise and tessellation.

In several applications, volumetric representations and descriptors are more suited than a two-dimensional manifold to model the shape invariance under rigid and elastic transformations. Furthermore, tetrahedral meshes are efficiently generated from surfaces [2,33] and are a standard volumetric representation for the discretization of differential equations. Due to the high computational cost for the solution to the heat equation, previous work has been mainly focused on the diffusion kernel and distance on surfaces rather than on volumes.

Given the complexity of volumetric computation, several alternatives to the heat kernel were proposed in the literature. FEM discretizations [1] of the heat equation tessellate the volume with a voxel grid or cuboid voxels [30] and apply a 6-neighborhood stencil [23,29] or a geometry-driven approximation field [22,36]. These approximations provide a low accuracy of the solution in a neighbor of the volume boundary, which is generally represented as a triangle mesh. Even though multi-resolution prolongation operators [39] and Chebyshev polynomials [27,28] can be extended to volumes, they have not been applied to the computation of the volumetric heat kernel or to the selection of the optimal time value. Additionally, the multi-resolution simplification of the input volume is time-consuming and the selection of the volume resolution with respect to the expected approximation accuracy is generally guided by heuristics. Further approaches extend the solution to the heat equation computed on the input surface to its interior through barycentric coordinates or a non-linear approximation, as done for the Laplacian [31,32] and harmonic [21,24] maps. Note that these methods do not intend to approximate the heat kernel quantitatively, but provide alternative approaches that qualitatively behave like the heat kernel on volumes.

Overview and contribution. We propose an accurate and computationally efficient solver of the heat equation $(\partial_t+\Delta)F(\cdot,t)=0$, $F(\cdot,0)=f$, on a closed and connected manifold $\mathcal{M}$ of $\mathbb{R}^3$, such that its boundary $\partial\mathcal{M}$ is a smooth and closed two-dimensional manifold. We also introduce a simple criterion to select the time value (or scale) that provides the best compromise between approximation accuracy and smoothness of the solution.

The idea behind our approach (Section 2) is to apply the (r,r)-degree Padé-Chebyshev rational approximation to the exponential representation $F(\cdot,t)=\exp(-t\Delta)f$ of the solution to the heat equation. Then, the diffusion problem is converted to a set of r differential equations, which involve only the Laplace–Beltrami

E-mail address: patane@ge.imati.cnr.it

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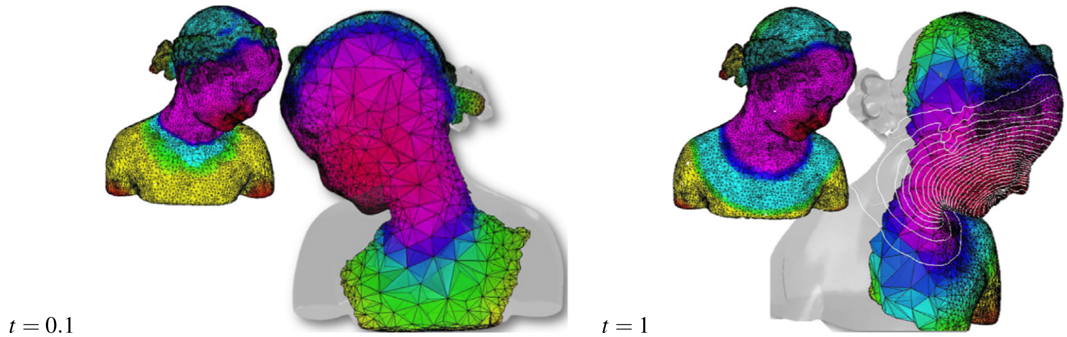

Fig. 1. Volumetric heat kernel. Color map of the solution to the volumetric heat equation at two time values and computed with the Padé-Chebyshev approximation of degree $r=7$; the initial condition takes value 1 at a point of the lips and 0 at the other vertices of the tetrahedralization. The color map varies the hue component of the hue-saturation-value color model; the colors begin with red, pass through yellow, green, cyan, blue, and magenta, and return to red. At scale $t=1$, the level-sets on the volume boundary correspond to iso-values uniformly sampled in the range of the solution restricted to the points of the volume boundary. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

operator, and the resulting solution converges to $F(\cdot,t)$, as $r\to+\infty$. Through the proposed approach, the solution to the heat equation is approximated in a low-dimensional space generated by $r+1$ functions, which are induced by the input volume, the initial condition f, and the selected time value. Furthermore, the approximation accuracy is lower than 10^{-r} (e.g., $r=5,7$). In comparison, the Laplacian eigenfunctions only encode the domain geometry and it is difficult to select the number of eigenpairs necessary to achieve a given approximation of $F(\cdot,t)$ with respect to t and f.

While a discretization of the heat kernel on a voxel grid is accurate enough for the evaluation of diffusion descriptors [23,29], which are quantized and clustered in bags-of-features, we focus on the computation of the heat kernel on tetrahedral meshes (Fig. 1). Our discretization (Section 3) is equivalent to a set of r sparse, symmetric linear systems and is applied to any representation of the input domain and of the Laplace–Beltrami operator. Furthermore, it properly encodes the local and global features in the heat kernel and bypasses the computation of the Laplacian spectrum. For a given time value, the overall computational cost of the r-degree Padé-Chebyshev rational polynomial is $\mathcal{O}(rn)$, where n is the number of volume vertices. Indeed, our approximation is competitive with respect to multi-resolutive simplification/prolongation operators, the Euler backward method, and the truncated spectral approximation.

As main novelties with respect to previous work [27], we apply the Padé-Chebyschev approximation to the more complex case of the heat kernel on volumes, also addressing the convergence of the approximation scheme and the selection of the time value.

For our experiments (Section 4), we consider volumetric diffusion smoothing, which is typically applied to thin film evolution [19], to the analysis of multi-material volume grids and their interfaces [20], and to volumetric shape deformation [22]. Other possible applications, which are not addressed in this paper, include volume-based approximation and the evaluation of volumetric descriptors.

2. Volumetric heat equation

Let us consider the heat equation $(\partial_t+\Delta)F(\cdot,t)=0$, $F(\cdot,0)=f$, on a closed, connected manifold $\mathcal{M}$ of $\mathbb{R}^3$, with $f:\mathcal{M}\to\mathbb{R}$ and $\partial\mathcal{M}$ smooth, closed two-dimensional boundary of $\mathcal{M}$. Then, the solution $F(\mathbf{p},t)=K_t(\mathbf{p},\cdot)\star f$ is the convolution between the heat kernel $K_t(\mathbf{p},\mathbf{q}):=(4\pi t)^{-3/2}\exp(-\|\mathbf{p}-\mathbf{q}\|_2^2/4t)$ and f.

Our approach applies the Padé-Chebyshev rational approximation to the exponential representation $F(\cdot,t)=\exp(-t\Delta)f$ of the solution to the heat equation. According to [15], on $\mathbb{R}^+$ the best (r,r)-degree rational polynomial approximation of $\exp(-x)$ with respect to the $\mathcal{L}_\infty$ norm is $c_{rr}(x)=\alpha_0+\sum_{i=1}^r\alpha_i(x-\theta_i)^{-1}$, with poles $\{\theta_i\}_{i=1}^r$ and coefficients $\{\alpha_i\}_{i=1}^r$. These values are precomputed for any degree through standard numerical routines; for more details, we refer the reader to [8]. Indicating with $\mathrm{id}(\cdot)$ the identity operator, the function

$$F(\cdot,t)=\exp(-t\Delta)f\approx\alpha_0 f-\sum_{i=1}^r\alpha_i(\Delta+\theta_i\mathrm{id})^{-1}f$$

$$=\alpha_0 f+\sum_{i=1}^r\alpha_i g_i,\quad (t\Delta+\theta_i\mathrm{id})g_i=-f, \tag{1}$$

is approximated by a linear combination of the solutions to r equations induced by the Laplace–Beltrami operator. The resulting approximation of $F(\cdot,t)$ belongs to the linear space $\mathcal{H}$ generated by f and $\{g_i\}_{i=1}^r$, which depend on the input volume, the initial condition f, and the selected time value t. In comparison, the Laplacian eigenfunctions $\{(\lambda_n,\phi_n)\}_{n=0}^{+\infty}$, $\Delta\phi_n=\lambda_n\phi_n$, encode only the domain geometry and it is difficult to select the number k of eigenpairs that are necessary to achieve an accurate approximation of $F(\cdot,t)$ through the truncated spectral representation $F(\cdot,t)\approx\sum_{n=1}^k\exp(-\lambda_n t)\langle f,\phi_n\rangle_2\phi_n$. Furthermore, a larger number of eigenpairs is necessary to accurately recover the solution at small time values.

Convergence of the approximation. Introducing the approximate solution $F_r(\cdot,t):=\sum_{n=0}^{+\infty}c_{rr}(\lambda_n)\langle f,\phi_n\rangle_2\phi_n$ to the (volumetric) heat equation induced by the r-degree Padé-Chebyshev polynomial c_{rr}, we show that the sequence $(F_r(\cdot,t))_{r=0}^{+\infty}$ converges to $F(\cdot,t)$. First of all, we notice that the approximation $F_r(\cdot,t)$ is well-posed; in fact, $\|c_{rr}\|_\infty\le 1$ and $\|F_r(\cdot,t)\|_2\le\|f\|_2$. According to [38], the $\mathcal{L}_\infty$ error between the exponential map and its rational polynomial approximation is bounded by the uniform rational Chebyshev constant σ_{rr}, which is independent of the evaluation point, and lower than 10^{-r}. Applying the upper bound

$$\|F_r(\cdot,t)-F(\cdot,t)\|_2^2\le\|c_{rr}(\cdot t)-\exp(-t\cdot)\|_\infty^2\sum_{n=0}^{+\infty}|\langle f,\phi_n\rangle_2|^2$$

$$\le\sigma_{rr}^2\sum_{n=0}^{+\infty}|\langle f,\phi_n\rangle_2|^2\le 10^{-2r}\|f\|_2^2,$$

we deduce that $\lim_{r\to+\infty}F_r(\cdot,t)=F(\cdot,t)$.

While the selection of a fixed number of eigenpairs does not allow us to estimate the resulting approximation accuracy, the projection of $F(\cdot,t)$ on the linear space generated by $\{f,g_1,\ldots,g_r\}$ guarantees an accuracy lower than 10^{-r}. Finally, this approximation is stable to a perturbation $f+e$ of the initial condition; in fact, the variation of the corresponding solutions $\tilde{F}_r(\cdot,t)$, $F_r(\cdot,t)$ is

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