Myself

 Laplacian Spectral Functions, Kernels, and Distances
 Group" (since 20

 Responsible of t

Theory & Applications to Geometry Processing & Shape Analysis

> Giuseppe Patanè CNR-IMATI, Genova - Italy patane@ge.imati.cnr.it





- Researcher at CNR-IMATI & Member of the "Shape and Semantics Modelling Group" (since 2001)
- Responsible of the research line "Numerical Geometry and Signal Processing"
- National Scientific Habilitation
 - Full Professor in Computer Science (INF01)
 - Full Professor in Systems for Information Processing (ENG-09/H1)
- My research and training interests lie at the intersection of
 - -Computer Science: Computer Graphics & Multimedia, Machine Learning
 - Engineering: Information & Signal Processing
 - Applied Mathematics: Numerical Analysis
- ERC Sector: PE6 Computer Science & Informatics









Introduction

 Target properties of the Laplacian spectral functions, kernels, and distances

-smoothness & orthonormality

- -intrinsic definition; ie., independent of data embedding/representation
- -multi-scale definition, in order to encode local and global shape features
- -invariance to shape transformations; eg., isometries for pose invariance
- -compact support & localisation at feature/ seed points for encoding local geometry properties & saving memory space
- –efficient, stable, and parameter-free computation





Introduction

- Working on the **space of scalar functions** defined on the input domain (eg., surface, volume), we can address
 - multi-scale signal representations and denoising, by projecting the input signals/data on a set of (*multi-scale*) basis functions
 - sparse representations, by choosing a low number of basis functions in order to achieve a target approximation accuracy
 - compression, by quantising the representation coefficients



Introduction

- Working on the space of scalar functions defined on the input domain (eg., surface, volume), we can address
 - shape deformations, by modifying the coefficients that express the *geometry* of the input surface in terms of **geometry-driven** or shape-intrinsic basis functions (eg., harmonic barycentric coordinates)



Introduction

- Working on the **space of scalar functions** defined on the input domain (eg., surface, volume), we can address
 - the definition of Laplacian spectral kernels and distances, as a filtered combination of the Laplacian spectral basis



Introduction

- Working on the space of scalar functions defined on the input domain (eg., surface, volume), we can address
 - shape correspondence and comparison, by expressing the problem with respect to a basis and converting it to a linear or least-squares problem





Goals

- Review of previous work on the definition, discretisation, and computation of Laplacian spectral kernels and distances (eg. commute time, biharmonic, wave kernel distances) by
 - filtering the Laplacian spectrum
 - generalising results on the heat diffusion kernels and distances.



Goals

- Review of previous work on the definition, discretisation, and computation of Laplacian & Hamiltonian spectral functions
 - harmonic functions
 - Laplacian/Hamiltonian eigenfunctions
 - diffusive functions, as solutions to the heat equation









Laplacian eigen-functions at different frequencies Diffusive functions a different scales

Goals

- Our review will be "independent" of
 - data dimensionality (surface, volume, nD data)
 - discretisation of the input domain (mesh, point set) and the Laplace-Beltrami operator



Goals

- Analysis of preview work on the computation of the Laplacian spectral functions, kernels, and distances in terms of
 - robustness with respect to the discretisation of the input domain: connectivity, sampling, and smoothness (eg. geometric/topological noise)



Goals

- Analysis of preview work on the computation of the Laplacian spectral functions, kernels, and distances in terms of
 - numerical accuracy/stability: convergence, Gibbs phen.
 - computational cost & storage overhead
 - selection of parameters & heuristics



Goals

- Analysis of preview work on the computation of the Laplacian spectral functions, kernels, and distances in terms of
 - numerical properties (eg., sparsity, conditioning number) of the Laplacian matrix and filter behaviour





- In the space of scalar functions defined on M, we represent
 - point-wise or piecewise linear scalar functions as vectors
 - linear operators as matrices
- Numerical linear algebra is the main tool for addressing applications in spectral geometry processing and shape analysis

Goals

- Focus & Novelty: unified review of the definition, discretisation, and computation of Laplacian spectral functions, kernels, and distances, independent of the data dimensionality and discretisation of both the input domain and the Laplace-Beltrami operator
- Applications to geometry processing & shape analysis
 - Geodesics & signal approximation
 - Diffusion smoothing, distances & descriptors
 - Laplacian spectral kernels & distances for shape comparison
- Previous STARs have addressed
 - the comparison of different discrete Laplacians^[Zhang07]
 - Laplacian spectral smoothing^[Taubin99]
 - surface coding & spectral partitioning[Karni00]
 - shape deformation based on differential coordinates[Sorkine06]
 - applications to shape modeling & geometry processing[Lèvy06]
 - diffusion shape analysis^[Bronstein12] & comparison^[Biasotti15]

Laplacian & Hamiltonian Operators





Outline

- Laplacian & Hamiltonian operators
 - Continuous & discrete differential operators
 - Harmonic functions
 - Laplacian & Hamiltonian eigenfunctions
 - Heat diffusion kernels
 - Properties & computation
- Applications
 - Geometry processing
 - Shape analysis
- Laplacian spectral kernels & distances

 Properties & computation
- Conclusions

Laplacian equations

Continuous case

 $\Delta := \operatorname{div}(\operatorname{grad})$

Harmonic equation

 $\Delta f = 0$

• Laplacian eigenvalue problem

 $\Delta f = \lambda f$

• Heat diffusion equation

 $(\partial_t + \Delta)F(\cdot, t) = 0$

Discrete Laplacians

- Aim: review of previous work on the discretisation of the Laplace-Beltrami operator through a unified representation of the discrete Laplacians that is independent of the
 - "dimensionality" of the input domain: surfaces, volumes, nD data
 - discretisation of the input domain: graphs, triangle/ polygonal/tetrahedral meshes, point sets
 - Laplacian weights, as entries of the Laplacian matrix.

Discrete Laplacians

 We represent the Laplacian matrix for graphs, meshes, and point sets in a "unified" way as

$$\tilde{\mathbf{L}} = \mathbf{B}^{-1}\mathbf{L}$$
L sparse, symm., positive semi-definite, L1=0
B sparse, symm., positive definite
B-scalar product B:=f^TBg
on the space of scalar functions

- Main properties
 - Positive semi-definiteness: $\langle \tilde{\mathbf{L}} \mathbf{f}, \mathbf{f} \rangle_{\mathbf{B}} = \mathbf{f}^{\top} \mathbf{L} \mathbf{f} \geq 0$
 - Null eigenvalue: $ilde{\mathbf{L}}\mathbf{1} = \mathbf{0}$

- **B**-self-adjointness:

 $\langle ilde{\mathbf{L}} \mathbf{f}, \mathbf{g}
angle_{\mathbf{B}} = \langle \mathbf{f}, ilde{\mathbf{L}} \mathbf{g}
angle_{\mathbf{B}}$

defined on the input domain

Discrete Laplacians

Linear FEM Laplacian matrix^[Reuter06] on triangle meshes

Stiffness matrix

$L(i,j) := \begin{cases} w(i,j) := -\frac{\cot \alpha_{ij} + \cot \beta_{ij}}{2} & j \in N(i) \\ -\sum_{k \in N(i)} w(i,j) & i = j \\ 0 & \text{else} \end{cases}$ Mass matrix $B(i,j) := \begin{cases} \frac{|t_r| + |t_s|}{2} & j \in N(i), \\ \frac{\sum_{k \in N(i)} |t_k|}{6} & i = j, \\ 0 & \text{else}, \end{cases}$ α_{ij} $\frac{t_r}{t_s} t_s$ β_{ij} $\tilde{\mathbf{L}} = \mathbf{B}^{-1} \mathbf{L}$

- Voronoi-cotg on triangle^[Desbrun99,Pinkall99] & polygonal meshes^[Alexa11,Herholz11], Curvature-based Laplacians^[Aflalo2013]
- Anisotropic Voronoi-cotg weights[Andreux14,Shi08,Kim13]

Discrete Laplacians

• According to^[Aflalo2013], we consider the curvature-based Laplacian

 $\tilde{\mathbf{L}} := \mathbf{K}^{-1} \mathbf{A}^{-1} \mathbf{L}$

- A is the diagonal matrix whose ith component is the sum of the areas of the triangles that contain the vertex i (area mass matrix)
- K is the diagonal matrix whose entries are the regularised Gaussian curvature at the vertices (curvature-based weight matrix)
- L is the stiffness matrix with cotangent weights.

Discrete Laplacians• Laplacian matrix on point sets[Belkin03-06-08,Liu12] $L(i,j) = \begin{cases} \frac{1}{4\pi t^2} \exp\left(-\frac{\|\mathbf{p}_i - \mathbf{p}_j\|_2^2}{4t}\right) & i \neq j \\ -\sum_{k \neq i} L(i,k) & i = j \end{cases}$ $B(i,i) = v_i$ Area of the approximated
Vornoi cell $\tilde{\mathbf{L}} = \mathbf{B}^{-1}\mathbf{L}$

Discrete Laplacians $L(i,j) = \begin{cases} \frac{1}{6} \sum_{k=1}^{n} l_k \cot \alpha_k & j \in N(i) \\ -\sum_{k \neq i} L(i,k) & i = j \end{cases}$ B encodes tetrahedral volumes $\tilde{\mathbf{L}} = \mathbf{B}^{-1} \mathbf{L}$

Discrete Laplacians





Laplace-Beltrami operator

The anisotropic Laplace-Beltrami operator is defined as

 $\Delta_{\mathbf{D}} := \operatorname{div}(\mathbf{D}\nabla f)$

where the tensor **D** is a 2x2 matrix that

- applies to vectors belonging to the tangent planes to the surface at its points
- controls the direction and strength of the derivation from the isotropic case (D:=I, Laplace-Beltrami operator).
- Tensor^[Shi08,Andreux14]

 $\mathbf{D} := \operatorname{diag}(\varphi_{\alpha}(\kappa_m), \varphi_{\alpha}(\kappa_M)), \qquad \varphi_{\alpha}(s) := (1 + \alpha |s|)^{-1}$

 $\kappa_m,\kappa_M\,$ minimum and maximum curvature



Laplacian eigenfunctions

- Properties of the Laplace-Beltrami operator
 - self-adjoint: $\langle \Delta f,g \rangle_2 = \langle f,\Delta g \rangle_2$, $\forall f,g$
 - positive semi-definite: (Δf,f)₂≥0, ∀f. In particular, the Laplacian eigenvalues are positive
 - locality: the value $\Delta f(\mathbf{p})$ does not depend on $f(\mathbf{q})$, for any couple of distinct points \mathbf{p} , \mathbf{q}
 - **null eigenvalue**: the smallest Laplacian eigenvalue is null and the corresponding eigenfunction ϕ , $\Delta\phi$ =0, is constant
- Laplacian eigenbasis



Laplacian spectrum - Computation

- The O(n²) computation time and storage overhead of the whole Laplacian spectrum are addressed by computing only k eigenpairs - k<<n: O(kn) comput. & storage cost^[Golub89]
 - shift method computes spectral bands centred around a given eigenvalue
 - inverse method computes k smaller/larger eigenvalues
 - power method improves the convergence speed of the computation, by considering a power of the input matrix
- Numerically unstable computations of the Laplacian eigenpairs are due to
 - multiple eigenvalues, associated with high dimensional eigenspaces
 - switched and/or numerically close eigenvalues with respect to the approximation accuracy of the solver of the Laplacian eigenproblem
 - and are independent of the quality of the discretisation of the input domain.

Laplacian eigenfunctions

• The generalised Laplacian eigensystem of (L,B)



defines a set of n linearly independent functions that

- can be used for the solution to discrete differential equations involving the Laplacian matrix (eg., heat equation)
- have a different behaviour: eigenfunctions associated with small/ large eigenvalues have a smooth/irregular behaviour



Laplacian spectrum - Stability

 $(\lambda(\epsilon), \mathbf{x}(\epsilon)):$ $(\tilde{\mathbf{L}} + \epsilon \mathbf{E})\mathbf{x}(\epsilon) = \lambda(\epsilon)\mathbf{x}(\epsilon), \qquad \lambda(0) = \lambda, \ \mathbf{x}(0) = \mathbf{x}$

- Perturb the input Laplacian matrix $\tilde{\mathbf{L}} + \epsilon \mathbf{E}$ and compute the eigenvalue of the new problem

whose initial conditions are the eigenpairs of (L,B).

- The size of the derivative $\lambda'(0)$ indicates the variation that a Laplacian eigenvalue undergoes when the Laplacian matrix is perturbed.
- For a single eigenvalue, the upper bound

 $|\lambda'(0)| \le \|\mathbf{E}\mathbf{x}\|_{\mathbf{B}} \le \|\mathbf{E}\|_{\mathbf{B}}$

shows that its computation is stable.

Laplacian spectrum - Stability

Considering an eigenvalue of multiplicity m, m>1, and the approximation

 $\left(\lambda(\delta) \approx \lambda^m + \mathcal{O}(\delta^{1/m})\right)$

a perturbation of order 10^{-m} induces a change of order 0.1.

For the perturbation of Laplacian eigenvectors^[Golub89],

$$\|\mathbf{x}_{i} - \mathbf{x}_{j}\|_{2} \leq \epsilon \sum_{j \neq i} \left| \frac{\mathbf{x}_{i}^{\top} \mathbf{E} \mathbf{x}_{j}}{\lambda_{i} - \lambda_{j}} \right| + \mathcal{O}(\epsilon^{2})$$

close eigenvalues generally induce numerical instabilities.

 Laplacian eigenspaces are generally stable to perturbations (—>projection operator)

Applications

- Spectral graph theory & Machine Learning
 - Graph partitioning^[Chung97,Fiedler93,Mohar93,Koren03]
 - Reduction of the bandwidth of sparse matrices^[Golub89,Alpert99,Diaz02]
 - Dimensionality reduction with spectral embeddings[Belkin03,Xiao10]
- Shape analysis
 - Shape segmentation^[Liu07,Zhang05]
 - Shape correspondence^[Jain07,Jain&ZhangK07]
 - Shape comparison[Marini11,Reuter05-06-07,Rustamov07,Wardetzky07,Jain06-07]
 - Spectral kernels and distances
 - bi-harmonic kernels/distances[Lipman10,Rustamov11]
 - diffusion kernels/ distances[Bronstein10-11,Coifman06,Gebal09,Lafon06,Luo09,Hammond11,Patanè10]
 - wave kernels/distances[Bronstein11,Aubry11]

Applications

- Geometry processing
 - Data reduction^[Belkin03-08] & compression^[Karni00]
 - Discrete differential forms^[Desbrun99-05,Gu03]
 - Design of low-pass filters & Implicit mesh fairing^[Taubin95,Desbrun99,Kim05,Pinkall93,Zhang03]
 - Mesh watermarking & Geometry compression^[Obuchi01-02,Karni00]
 - -Approximation and smoothing of scalar functions^[Patanè13]
 - -Surface deformation[Levy06,Sorkine04,Vallet08,Zhang07]
 - -Local/global parameterisation^[Floater,Patanè04-07,Zhang05]
 - -Surface quadrangulation^[Dong05]

Heat Equation & Kernel





Heat diffusion equation



Heat diffusion equation

- On surfaces, the diffusion kernel encodes local geometric properties: ie.,
 - for an **isometry** between 2 manifolds^[SOG09,Gri06]

$$\Phi: \mathcal{N} \to \mathcal{Q} \qquad K_t^{\mathcal{N}}(\mathbf{p}, \mathbf{q}) = K_t^{\mathcal{Q}}(\Phi(\mathbf{p}), \Phi(\mathbf{q}))$$

 at small scales^[SOG09, Var67], the auto-diffusive function encodes the Gaussian and total curvature

$$K_t(\mathbf{p}, \mathbf{p}) \approx \begin{cases} (4\pi t)^{-1} (1 + 1/3t\kappa(\mathbf{p})) + \mathcal{O}(t^2), \\ (4\pi t)^{3/2} (1 + 1/6s(\mathbf{p})), \end{cases} t \to 0,$$

Heat diffusion equation

- The solution to the heat equation can be expressed in terms of
 - the Laplacian spectrum $(\lambda_n, \phi_n)_{n=0}^{+\infty}$

$$F(\mathbf{p},t) = \langle K_t(\mathbf{p},\cdot), f \rangle_2, \quad K_t(\mathbf{p},\mathbf{q}) = \sum_{n=0}^{+\infty} \exp(-\lambda_n t) \phi_n(\mathbf{p}) \phi_n(\mathbf{q})$$

diffusion kernel

– the action of the diffusion operator $\Phi_t := \exp(-t\Delta)$

$$F(\cdot,t) = \exp(-t\Delta)f = \sum_{n=0}^{+\infty} \exp(-\lambda_n t) \langle f, \phi_n \rangle_2 \phi_n$$

Discrete heat kernel

• The solution to the discrete heat equation is

$$\mathbf{F}(t) = \mathbf{K}_t \mathbf{f}, \qquad \left(\mathbf{K}_t \equiv \exp(-t\tilde{\mathbf{L}}) \right)$$

• Considering the **spectral factorisation** of the Laplacian matrix (B area/volume-driven matrix)

$$ilde{\mathbf{L}} = \mathbf{X} \Gamma \mathbf{X}^{\top} \mathbf{B}$$
 $\Gamma := \operatorname{diag}(\lambda_i)_{i=1}^n$ Lapl. eig. val.
 $\mathbf{X} := [\mathbf{x}_1, \dots, \mathbf{x}_n]$ Lapl. eig. vec

the resulting discrete heat kernel \mathbf{K}_{t} admits the spectral representation

$$\left(\mathbf{K}_t = \mathbf{X} \Gamma_t \mathbf{X}^\top \mathbf{B}\right) \Gamma_t := \operatorname{diag}(\exp(-\lambda_i t))_{i=1}^n$$

Previous work

- Previous work for the computation of the heat kernel and the corresponding diffusion distances can be classified as
 - geometry-driven approach
 - multi-resolution prolongation operator
 - numerical approaches
 - truncated spectral approximation
 - theta-method method
 - power method
 - numerical approaches higher precision
 - Padè-Chebyshev approximation
 - polynomial approximation
 - Krylov subspace projection

Previous work

Spectrum-free

Truncated spectral approximation (k=200)



Previous work

• Truncated spectral approximation of the heat kernel considers the contribution of the Laplacian eigenvectors related to the k smaller eigenvalues

$$\mathbf{F}(t) = \sum_{i=1}^{\mathbf{I}} \exp(-\lambda_i t) \langle \mathbf{f}, \mathbf{x}_i \rangle_{\mathbf{B}} \mathbf{x}_i$$

Main motivations

- -exponential decay of the filter as the eigenvalues/time increase
- -the computation of the whole spectrum is not feasible for a large n
- –numerical instabilities due to close/multiple eigenvalues, associated with "high" dimensional eigenspaces (eg., symmetric shapes)
- **Remark:** for small scales, we must compute a large number of eigenpairs to achieve a good approximation accuracy

Previous work

- Approximate the heat kernel with multi-resolution prolongation operators^[Vaxman10]
 - using k eigenpairs on a specific level of a multi-resolutive shape representation
 - selecting k according to time and the shape resolution in the hierarchy
 - prolongating the heat kernel from a given resolution to the input shape



Previous work

 We discrete the temporal derivative as a finite difference and introduce a convex combination of the values of the solution at consecutive times: *θ*-method

$\begin{cases} (\partial_t + \Delta)F(\cdot, t) = g \\ F(\cdot, 0) = f \end{cases} \begin{pmatrix} \frac{1}{\delta t} \left[F(\mathbf{p}, t_{k+1}) - F(\mathbf{p}, t_k)\right] + \dots & \longrightarrow \\ + \theta \Delta F(\mathbf{p}, t_{k+1}) + (1 - \theta) \Delta F(\mathbf{p}, t_k) = \dots & \longrightarrow \\ = g(\mathbf{p}, t_{k+1}). & \longrightarrow & g \end{cases}$

- Special cases: Euler forward (theta=0) & backward method (theta=1)
- In geometry processing: Euler backward method for fairing^[Desbrun99]

Spectrum-free approximation



Previous work

- Limitations
 - Need to select/adapt parameters (eg., number of eigenpairs, iterations, resolution in the hierarchy) to shape/volume details and selected scales
 - No a-priori estimation of the approximation accuracy with respect to the selection of k Laplacian eigenpairs
- Goal: review of numerical approaches with a higher approximation accuracy achieved by applying a (rational) polynomial approximation to the exponential filter
 - No computation of the Laplacian spectrum
 - High approximation accuracy, adjusted through the selection of the polynomial degree
 - No selection of input parameters

Chebyshev approximation

- Idea 1D case^[Golub89]
 - Compute the best (r,r)-degree rational approximation $c_{rr}(x)$ of e^x with respect to the l_{∞}-norm

$$\exp(x) \approx \alpha_0 - \sum_{i=1}^r \alpha_i (x + \theta_i)^{-1}$$

- I_{∞} error between e^x and its rational approximation is lower than $\sigma_{rr} \approx 10^{-r}$ (*unif. rational Cheb. constant*)

Chebyshev approximation

 Apply the (r,r)-degree Padè-Chebyshev rational approximation to the exponential representation of the solution to the heat equation^[Hammond11,Patane14]

$$\begin{array}{c} \hline F(\cdot,t) = \exp(-t\Delta)f \\ \approx \alpha_0 f - \sum_{i=1}^r \alpha_i \left(t\Delta + \theta_i \mathrm{id}\right)^{-1} f \\ = \alpha_0 f + \sum_{i=1}^r \alpha_i g_i, & (t\Delta + \theta_i \mathrm{id}) g_i = -f \end{array}$$

• Convert the diffusion problem to a set of r differential equations that involve only the Laplace-Beltrami operator

Chebyshev approximation

• Applying the Chebyshev approximation to $\mathbf{K}_t = \exp(-t\tilde{\mathbf{L}})$, we get the spectrum-free computation of the solution to the heat equation

$$\mathbf{K}_t \mathbf{f} \approx \alpha_0 \mathbf{f} + \sum_{i=1}^r \alpha_i \mathbf{g}$$

that requires the solution to r sparse, symmetric linear systems

$$(t\mathbf{L}+\theta_i\mathbf{B})\mathbf{g}_i = -\mathbf{B}\mathbf{f}, \quad i = 1, \dots, r$$

- No input parameters (degree r is fixed)
- Numerical solver
 - apply an iterative solver for linear systems (e.g., minres):
 O(rn)-O(rnlog(n)), according to the sparsity of (L,B)
 - pre-factorise the matrix B (if not diagonal); only for several values of t or several initial conditions F(.,0)=f (eg., diffusion distances)

Chebyshev approximation

• The solution is approximated in a low dimensional space generated by (r+1) functions, which are induced by the input domain, the initial condition f, and the selected scale t.

$$F(\cdot,t) = \sum_{n=0}^{+\infty} \exp(-\lambda_n t) \langle f, \phi_n \rangle_2 \phi_n \qquad \underbrace{ \begin{pmatrix} (\lambda_n, \phi_n)_{n=0}^{+\infty} \\ \Delta \phi_n = \lambda_n \phi_n \end{pmatrix} }_{\Delta \phi_n = \lambda_n \phi_n}$$

• **Convergence.** The resulting Padè-Chebyshev approximation converges to the solution as the polynomial degree increases

$$\begin{split} \|F_r(\cdot,t) - F(\cdot,t)\|_2 &\leq \|c_{rr}(\cdot,t) - \exp(\cdot,t)\|_{\infty} \|f\|_2 \\ &\leq \sigma_{rr} \|f\|_2 \\ &\leq 10^{-r} \|f\|_2 \to 0, \quad r \to +\infty \end{split}$$

e seed point P.C. approx, r = 7

Chebyshev approximation



Chebyshev approximation



Isotropic diffusion

Voronoi-cotg Laplacian weights^[Desbrun99,Pinkial199]



Anisotropic Laplacian weights^[Andreux14]



Numerical stability

- The Cheb./polyn. approx. of exp(-t**C**) is unstable if ||t**C**||₂ is too large.
- From the upper bound $||t\mathbf{B}^{-1}\mathbf{L}||_2 \leq t\lambda_{\max}(\mathbf{L})\lambda_{\min}^{-1}(\mathbf{B})$ a well-conditioned matrix **B** guarantees that $||t\mathbf{B}^{-1}\mathbf{L}||_2$ is low.
- If the Laplacian matrix is ill-conditioned, then we can apply specialized Laplacian pre-conditioners^[Krishnan13].







Robustness



Robustness

Holes

Robustness

SHREC'16: Matching of Deformable Shapes with Topological Noise -[Lahner16]

Topological noise

Polynomial approximation

- **Rational polynomial approximation**[Pusa11] of the exponential filter based on quadrature formulas derived from complex contour integrals.
- Polynomial approximation^[Golub89]
 - applies the Taylor power series to the exponential matrix (first r terms)

- has an accuracy lower than the Padè-Chebyshev method (point-wise instead of uniform convergence)
- generalises the $1^{\mbox{\scriptsize st}}$ order Taylor approximation applied by the power method

Polynomial approximation

• The discrete spectral kernel is approximated as

$$\begin{aligned} \underbrace{\mathbf{K}_{i}\mathbf{f} \approx \sum_{i=0}^{r} \alpha_{i}\tilde{\mathbf{L}}^{i}\mathbf{f}}_{= \alpha_{0}\mathbf{f}_{0} + \sum_{i=1}^{r} \alpha_{i}\mathbf{g}_{i}, \qquad \mathbf{g}_{i} := \tilde{\mathbf{L}}^{i}\mathbf{f} = (\mathbf{B}^{-1}\mathbf{L})^{i}\mathbf{f} \end{aligned}$$

• If **B** is not diagonal (eg., linear/cubic FEM weights), then each vector **g**_i is computed through the recursive relation

$$\mathbf{g}_i := \tilde{\mathbf{L}}^i \mathbf{f} = (\mathbf{B}^{-1} \mathbf{L})^i \mathbf{f} \qquad \begin{cases} \mathbf{B} \mathbf{g}_1 = \mathbf{L} \mathbf{f} \\ \mathbf{B} \mathbf{g}_i = \mathbf{L} \mathbf{g}_{i-1} \end{cases} i = 2, \dots, r$$

and we solve r sparse and symmetric linear systems.

Summary

Method	Numerical scheme	Scales	Comput. cost
Linear approximation			
Trunc. spec. approx.	$\mathbf{F}_{k}(t) = \sum_{i=1}^{k} \exp(-\lambda_{i} t) \langle \mathbf{f}, \mathbf{x}_{i} \rangle_{\mathbf{B}} \mathbf{x}_{i}$	Any	$\mathcal{O}(kn)$
Euler backw. approx.	$(t\tilde{\mathbf{L}}+\mathbf{I})\mathbf{F}_{k+1}(t) = \mathbf{F}_k(t)$	Small	$\mathcal{O}(\mathfrak{r}(n))$
I order Taylor approx.	$\mathbf{BF}(t) = (\mathbf{B} - t\mathbf{L})\mathbf{f}$	Small	$\mathcal{O}(\mathfrak{r}(n))$
Krylov/Schur approx.	Projection on	Any	$\mathcal{O}(m\tau(n)), \mathbf{B} \neq \mathbf{I}$
	$\{\mathbf{g}_i := (\mathbf{B}^{-1}\mathbf{L})^i \mathbf{f}\}_{i=1}^m$		$\mathcal{O}(n), \mathbf{B} = \mathbf{I}$
Polynomial approximation			
Power approx.	$\mathbf{F}(t) = \sum_{i=0}^{m} \mathbf{g}_i / i!$	Any	$\mathcal{O}(m\tau(n)), \mathbf{B} \neq \mathbf{I}$
	$\mathbf{g}_i := ilde{\mathbf{L}}^i \mathbf{f}$		$\mathcal{O}(n), \mathbf{B} = \mathbf{I}$
Rational approximation			
Padé-Cheb. approx.	$\mathbf{F}(t) = \boldsymbol{\alpha}_0 \mathbf{f} + \sum_{i=1}^r \mathbf{g}_i$	Any	$\mathcal{O}(r\tau(n))$
	$(t\mathbf{L}+\mathbf{\theta}_i\mathbf{B})\mathbf{g}_i=-\alpha_i\mathbf{B}\mathbf{f}$		
Contour integral approx.	$\mathbf{F}(t) = \sum_{i=1}^{r} \alpha_i \mathbf{g}_i$	Any	$\mathcal{O}(r\tau(n))$
	$(\alpha_i)_{i=1}^r$ quadr. coeff.		

Applications

Signal Smoothing

Applications

- Applications of the heat diffusion kernel and distance include
 - multi-scale representations of functions [Rosenberg97,Patanè10-13]
 - shape comparison with heat kernel shape signatures [Bronstein11,Gebal09,Memoli09,Ovsjanikov10,Sun09]
 - intrinsic to the input shape
 - isometry-invariant
 - multi-scale (local vs. global details)
 - diffusion distances & descriptors
 - [Aubry11,Belkin03,Coifman06,Gine06,Litman14,Singer06,Smola03]
 - data matching [Lafon06]
 - gradient [Wang09], critical points computation [Luo09]
 - data representation and classification [Smola03]
 - shape segmentation [DeGoes08,Gebal08]
 - dimensionality reduction [Belkin03,Roweis00,Xiaoa10,Tenenbaum00]
 - clustering [Chapelle03]

- ...

Geodesics approx. via heat kernel

- Geodesic distances can be expressed in terms of the heat kernel as
 - $d_G(\mathbf{p},\mathbf{q}) = -\lim_{t\to 0} (4t\log K_t(\mathbf{p},\mathbf{q})) \quad \text{[Varadhan's formula[Varadhan67]]}$
 - Otherwise [Crane13],
 - Integrate the heat flow $\partial_t F(\cdot, t) = \Delta F(\cdot, t)$ (for a fixed t)
 - Evaluate the vector field $\mathbf{X} := \nabla F(\cdot, t) / \| \nabla F(\cdot, t) \|_2$
 - Solve the Poisson eq. $\Delta \phi = \operatorname{div} \mathbf{X}$
- **Optimal transportation distances** are approximated through the solution of two sparse linear systems that involve the heat kernel^[Solomon15].
- In both cases, we can apply the spectrum-free approach to guarantee an accurate approximation of the heat kernel.

Heat diffusion distance

- Idea: associate a shape M with the functional space
 - F(M):={f:M->R, f scalar function on M}

• eg., Laplacian eigenproblem, heat equation, etc and define the **metric space (M,d_M)**, equipped with **diffusion distances derived from K**t **on F(M)** (*diffusion geometry*).

Heat diffusion distance

Heat diffusion distance

 Apply the Padè-Chebyshev of the heat kernel to approximate diffusion distances.

Approximation accuracy Approximation accuracy error $t = 10^{-1}$ ℓ_{∞} error $t = 10^{-3}$ Padè-Chebyshev approximation versus truncated spectral • approximation of the diffusion distances (r=5) 10 -0.001 err. $\ell_{\infty}_{t=1}$ err. \sim t = 0.1t = 0.01t = 0.001t = 0.1t = 0.0110 10⁻⁵ 10 ℓ_{∞} error $t = 10^{-2}$ Comparison of the accuracy of 10 t = 1the diffusion distances at k10 different scales. 10 10° 0 10[°] 101 10^{2} 10^{2} 101 10³ 10³ Padè-Chebyshev approximation error: for all t, lower than 8.9*10⁻⁶ **Robustness Robustness**

Computational cost

- Truncated spectral approximation: O(kn)
- Padè-Chebyshev approximation: $\mathcal{O}(r\tau(n))$
 - solution to the heat equation or evaluation of the diffusion distance between 2 points

 $\begin{cases} \mathcal{O}(\tau(n)) \text{ lin. syst. solver} \\ \tau(n) \approx n, n \log n \end{cases}$

- one-to-all distance (no pre-factorisation): $O(rn\tau(n))$
- one-to-all distance (pre-factorisation of **B**): $\mathcal{O}(n \log n + rn)$
 - if **B** is not diagonal

Diffusion signatures & descriptors

- The heat kernel matrix K_t^[Bronstein10,Patanè14] is
 - self-adjoint with respect to the B-scalar product
 - intrinsically scale-covariant (ie., with no a-posteriori normalisation)

$$\left(K_t(\alpha \mathcal{M}) = K_{\alpha^2 t}(\mathcal{M})\right)$$

- scale-invariant through a normalisation of the Laplacian eigenvalues U(z, A, A) = V(A, A)

$$K_t(\alpha \mathcal{M}) = K_t(\mathcal{M})$$

 stable to noise and irregular sampling, thus improving the robustness of matching based on heat kernel descriptors^[SHREC10]

Diffusion signatures & descriptors

Heat kernel signature

$$HKS(\mathbf{p}) := \sum_{n=0}^{+\infty} \exp(-\lambda_n t) |\phi_n(\mathbf{p})|^2$$

• Diffusion embegging

$$DE(\mathbf{p}) := (\exp(-\lambda_n)\phi_n(\mathbf{p}))_{n=0}^{+\infty}$$

Wave kernel signature

$$WKS(\mathbf{p}) = \sum_{n=0}^{+\infty} \exp(-i\lambda_n t)\phi_n^2(\mathbf{p})$$

Heat kernel & shape comparison

• Diffusion descriptors for shape comparison have been extensively analysed in SHREC contexts.

Laplacian Spectral Kernels and Distances

Spectral distances

- **Aim:** review of previous work on the definition and computation of
 - the commute-time, bi-harmonic, diffusion, wave kernel distances
 - the corresponding embeddings and shape descriptors

in a unified way by

- introducing the spectral distances, which are defined by filtering the Laplacian spectrum
- interpreting the main properties of the spectral distances in terms of the properties of the corresponding filter function

Distances on 3D shapes

- **Geometry-driven approaches:** define the distance on the input shape; eg., geodesics[Mitchell87,Surazhsky05,Kimmel98,Lipman10]
- **Functional approaches:** define the distance in the space of functions on the input surface
 - diffusion distances[Bronstein10-11,Coifman06,Gebal09,Lafon06,Luo09,Hammond11,Patanè10]
 - commute-time & bi-harmomic distances[Lipman10,Rustamov11]
 - wave kernel distances[Bronstein11,Aubry11]
 - random walks^[Fouss05,Ramani13], Mexican hat wavelets & distances^[Hou12]
- **Mixed approaches:** geodesic distances & optimal transportation distances are approximated in the geometric and function space
 - approximation through the heat kernel^[Crane13]
 - multi-dimensional scaling^[Bronstein06,Panozzo13]

Spectral distances

• Idea: define spectral distances^[Bronstein11,Patane14-16] by filtering the Laplacian spectrum

Spectral distances $s^2 \exp(-s)$ $\rho^{2}(\mathbf{p}, \mathbf{q}) = \sum \varphi^{2}(\lambda_{n})|\phi_{n}(\mathbf{p}) - \phi_{n}(\mathbf{q})|$ Bi-harmonic dist. Diffusion dist. Mexican hat dist. $\varphi^{2}(s) = s^{-2}$ $\varphi_t^2(s) = \exp(-st)$ $\varphi_t^2(s) = s^{-1} \exp(-st)$ Distance Comm.-time Diffusion distances[Bronstein10-11,Coifman06,Gebal09,Lafon06,Luo09,Hammond11,Patanè10] s-2 Biharm. Polv-harm. - Commute-time & bi-harmomic distances [Lipman10, Rustamov11] e-st Heat diff. - Wave kernel distances[Bronstein11,Aubry11]

Random walks^[Fouss05,Ramani13], Mexican hat wavelets & distances^[Hou12]

Spectral distances

e-ist

Wave ker.

Bi-harmonic distances

Spectral distances

- Commute-time distance^[Bronstein11] are defined the integral of the diffusion distance with respect to scale $\varphi(s) := s^{-1/2}$

$$d^{2}(\mathbf{p}, \mathbf{q}) = \frac{1}{2} \int_{0}^{+\infty} d_{t}^{2}(\mathbf{p}, \mathbf{q}) dt$$
$$= \sum_{n=0}^{+\infty} \lambda_{n}^{-1} |\phi_{n}(\mathbf{p}) - \phi_{n}(\mathbf{q})|^{2}$$

- Bi-harmonic distances[Ovsjanikov12,Lipman10,Rustamov11] $arphi(s):=s^{-1}$
 - for small distances, they have a nearly geodesic behavior
 - for large distances, they encode global shape properties

Spectral distances

- The filters are defined
 - analytically and analogously to Laplacian signal smoothing[Desbrun99,Kim05,Taubin95-96,Zhang03]
 - by applying supervised learning^[Aflalo11,Litman14] on a data set of 3D shapes
 - optimal spectral signature^[Litman14]: linear combination of B-splines by minimising a task-specific loss function
 - $-\operatorname{by}$ controlling their behaviour
 - decay to zero, periodicity
 - normalisation with respect to geometric properties of the domain
 - in such a way that the corresponding distances are
 - multi-scale and/or invariant to isometric transformations
 - smooth and/or localised in both time and frequency^[Hammond11].

Spectral distances

- The **smoothness**, **locality**, and **encoding of local/global shape properties** depend on the convergence of the filtered Laplacian eigenvalues to zero
 - increasing the filter decay to zero
 - global shape properties are encoded by the spectral distances, by reducing the influence of eigenfunctions associated with small eigenvalues in the spectral distances
 - reducing the filter decay to zero
 - local shape properties are encoded by the spectral distances.

Spectral distances

- Given a strictly positive, square-integrable filter that admits the power series' representation $_{+\infty}$

$$\varphi(s) = \sum_{n=0}^{+\infty} \alpha_n s^n$$

we define the spectral operator $^{n=0}$

$$\Phi(f) := \varphi(\Delta)f = \sum_{n=0}^{+\infty} \varphi(\lambda_n) \langle f, \phi_n \rangle_2 \phi_n$$

which is well-defined, linear, continuous, and

$$\Phi(f) = \langle K_{arphi}, f
angle_2 \qquad \left(K_{arphi}(\mathbf{p}, \mathbf{q}) = \sum_{n=0}^{+\infty} arphi(\lambda_n) \phi_n(\mathbf{p}) \phi_n(\mathbf{q})
ight)$$

where
$$K_{\varphi}$$
 is the spectral kernel

Spectral distances

 Analogously to the diffusion distances, previous work has defined the equivalent representations of the spectral distances

$$d^{2}(\mathbf{p}, \mathbf{q}) = \|\Phi(\delta_{\mathbf{p}}) - \Phi(\delta_{\mathbf{q}})\|_{2}^{2} \qquad \text{Spectral operator}$$
$$= \sum_{n=0}^{+\infty} \varphi^{2}(\lambda_{n}) |\phi_{n}(\mathbf{p}) - \phi_{n}(\mathbf{q})|^{2} \text{ Lapl. spectrum}$$
$$= \|K_{\varphi}(\mathbf{p}, \cdot) - K_{\varphi}(\mathbf{q}, \cdot)\|_{2}^{2} \qquad \text{Spectral kernel}$$
$$= \|\phi(\mathbf{p}) - \phi(\mathbf{q})\|_{2}^{2} \qquad \text{Spectral embed.}$$
$$\phi : \mathcal{M} \to \ell_{2}, \phi(\mathbf{p}) = (\varphi(\lambda_{n})\phi_{n}(\mathbf{p}))_{n=0}^{+\infty}$$

Discrete spectral distances

 Applying the generalised eigendecomposition of the Laplacian matrix, the discrete spectral kernel is

$$\tilde{\mathbf{L}} = \mathbf{X} \Gamma \mathbf{X}^{\top} \mathbf{B}$$
 $(\mathbf{K}_{\varphi} = \varphi(\tilde{\mathbf{L}})) = \mathbf{X} \varphi(\Gamma) \mathbf{X}^{\top} \mathbf{B}$

and the resulting discrete spectral distance is

$$\begin{split} d^2(\mathbf{p}_i, \mathbf{p}_j) &= \|\mathbf{K}_{\varphi}(\mathbf{e}_i - \mathbf{e}_j)\|_{\mathbf{B}}^2 & \text{[spectrum-free approx.]} \\ &= \sum_{l=1}^n \varphi^2(\lambda_l) |\langle \mathbf{x}_l, \mathbf{e}_i - \mathbf{e}_j \rangle_{\mathbf{B}}|^2 & \text{[truncated spectral approx.]} \end{split}$$

Discrete spectral distances

- We generalise previous work on the computation of the diffusion kernels/distances to the case of spectral distances
 - spectrum-free approximation: considers the representation of the distance in terms of the spectral kernel and apply the
 - polynomial approximation of the filter
 - Padè-Chebyshev approximation of the filter
 - Krylov sub-space projection
 - truncated spectral approximation: applies the representation of the distances in terms of the Laplacian spectrum.

Spectrum-free computation

- Recalling that
 - the **spectral distances** are defined in terms of the spectral kernel as $d(\mathbf{p}_i, \mathbf{p}_j) = \|\mathbf{K}_{\varphi}(\mathbf{e}_i \mathbf{e}_j)\|_{\mathbf{B}}$
 - the **spectral kernel** is achieved by applying filtering the Laplacian matrix as $\mathbf{K}_{\varphi}=\varphi(\tilde{\mathbf{L}})$

we compute and apply the **best r-degree polynomial approximation of the selected filter** to the Laplacian matrix

Spectrum-free computation

Truncated spectral approximation

• The spectral distances can be approximated by considering the contribution of the Laplacian eigenvectors related to the smaller eigenvalues

$$d^{2}(\mathbf{p}_{i},\mathbf{p}_{j}) \approx \sum_{l=1}^{k} \varphi^{2}(\lambda_{l}) \left| \langle \mathbf{x}_{l},\mathbf{e}_{i}-\mathbf{e}_{j} \rangle_{\mathbf{B}} \right|^{2}$$

- accurate approximation for filters with a fast decay (periodic filter: eg., wave kernel?)
- the number of selected eigenpairs must be adapted to local shape details, target approximation accuracy, parameters (eg., time for wave kernel distances): *not a trivial task*

Approximation accuracy

Approximation of spectral distances

- Truncated spectral approximation: l∞ error between the ground-truth spectral distances induced by different filters and their approximation with k Laplacian eigenpairs
- Spectrum-free approximation: r:=8 degree polynomial and l_∞ error lower than 10⁻⁴

Discrete spectral distances

- Truncated spectral approximation
 - computes k Laplacian eigenpairs in O(kn) time
 - uses the Laplacian eigenpairs to quickly evaluate distances induced by different filters on the same surface
 - generally has an accuracy lower than the spectrum-free approach.
- Spectrum-free approximation
 - Distance evaluation between two points is reduced to solve r sparse, symmetric, linear systems: $\mathcal{O}(r\tau(n))$
 - Evaluation of the one-to-all distance
 - no factorisation of **B**: $\mathcal{O}(rn\tau(n))$
 - with factorisation **B**: $O(n \log n + rn)$

Conclusions

Conclusions

- Review of previous work on
 - the Laplacian spectral functions, kernels, and distances, defined by filtering the Laplacian spectrum and as a generalisation of the commute-time, bi-harmonic, diffusion, and wave kernel and distances
 - their discretisation according to a unified representation of the Laplace-Beltrami operator, which is "independent" of
 - the data dimensionality (surface, volume, nD data) and discretisation (mesh, point set) of the input domain
 - the selected Laplacian weights
 - the computational aspects behind their evaluation
 - approximation accuracy & stability
 - computational cost & storage overhead
 - use of input parameters & heuristics
 - their main applications to geometry processing and shape analysis

Conclusions

- Future work & possible collaborations
 - Definition of shape-aware functions for time-varying & multidimensional data (eg., graphs, videos);
 - Analysis of the constraints on the filter in order to define "optimal" spectral kernels and distances for applications in geometry processing and shape analysis
 - Application/specialisation of the spectral basis functions to
 - shape analysis
 - definition of shape-aware functional spaces where we approximate signal or solve PDEs
- Course material & Papers
 - http://pers.ge.imati.cnr.it/patane/SGP2019/Course.html
 - http://pers.ge.imati.cnr.it/patane/Home.html

References

Acknowledgments

- People •
 - SGP2019 Conference & Graduate School Chairs: Marcel Campen & Sylvain Lefebvre
 - Shape and Semantics Modelling Group, CNR-IMATI, Italy
- Projects ٠
 - H2020 ERC-AdG CHANGE
 - IMAGE-FUSION, Biannual Project funded by Regione Liguria & EU FESR
- ٠ Shapes
 - AIM@SHAPE Repository
 - SHREC2010/2016 data sets
- **Contact:** patane@ge.imati.cnr.it •

erc Research

Council

