On elliptic operators and non-rigid shapes

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On elliptic operators and non-rigid shapes

Research Thesis

Submitted in partial fulfillment of the requirements for the degree of Master of Science in Computer Science

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Submitted to the Senate of the Technion — Israel Institute of Technology Iyar 5777
Haifa May 2017
This research was carried out under the supervision of Prof. Ron Kimmel, in the Faculty of Computer Science.

Some results in this thesis have been published as articles by the author and research collaborators in conferences and journals during the course of the author’s MSc research period, the most up-to-date versions of which being:

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**ACKNOWLEDGEMENTS**

I would like to thank my advisor, collaborators and friends for helping me throughout this work. Especially, I would like to thank my family, and most my wife and son for their moral support and constant belief in me during my years of study.

The generous financial help of the Technion is gratefully acknowledged.
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Abstract

Many shape analysis methods treat the geometry of an object as a metric space captured by the Laplace-Beltrami operator. In this thesis we present an adaptation of a classical operator from quantum mechanics to shape analysis where we suggest to integrate a scalar function through a unified elliptical Hamiltonian operator. We study the addition of a potential function to the Laplacian as a generator for dual spaces in which shape processing is performed. After exploration of the decomposition of this operator, we evaluate the resulting spectral basis for different applications. First, we present a general optimization approach for solving variational problems involving the basis defined by the Hamiltonian using perturbation theory for eigenvectors. Then, we propose an iteratively-reweighted $L_2$ norm for sparsity promoting problems such as the compressed harmonics where solution is reduced to a sequence of simple eigendecomposition of the Hamiltonian. Physically understandable, they do not require non-convex optimization on Stiefel manifolds and produce faster, stable and more accurate results. We then suggest a new framework for mesh compression using a Hamiltonian based dictionary where regions of interest are enhanced through the proposed operator. By sparsely encoding the geometry of the shape using the proposed data-dependent basis, we improve compression performance compared to previous results that use the standard Laplacian and spectral graph wavelets. Finally, we propose to apply the Hamiltonian for shape matching where information such as anchor points, corresponding features, and consistent photometry or inconsistent regions can be considered through a potential function for improving the performance in finding correspondence between surfaces.
Glossary

\( \mathcal{M}, \mathcal{N} \)  
Riemannian manifolds

\( M, N \)  
Discrete representation of manifolds \( \mathcal{M} \) and \( \mathcal{N} \) as meshes

\( x, y \)  
Points on a manifold

\( m_i, n_i \)  
Vertex \( i \) on meshes \( M \) and \( N \) respectively

\( S(u) \)  
Global parametrization of the manifold

\( T_x(\mathcal{M}) \)  
Tangent space at point \( x \) on manifold \( \mathcal{M} \)

\( g \)  
Riemannian metric on manifold

\( f, h \)  
Functions defined on a manifold

\( \tau \)  
A correspondence function

\( d_M \)  
Distance measures on \( \mathcal{M} \)

\( \gamma(t) \)  
Curve on the manifold

\( \delta_{ij} \)  
Kronecker delta

\( \nabla_M \)  
Intrinsic gradient defined on manifold

\( \text{div}_M \)  
Intrinsic divergence defined on manifold

\( \Delta_M \)  
Laplace Beltrami operator defined on manifold according to the metric \( g \)

\( \phi_i, \lambda_i \)  
\( i^{th} \) eigenfunction, and corresponding eigenvalue, of the Laplace Beltrami operator

\( \psi_i, E_i \)  
\( i^{th} \) eigenfunction, and corresponding eigenvalue, of the Hamiltonian operator

\( \mathcal{N}(f) \)  
Nodal set of the function \( f \)

\( L \)  
Discrete Laplace Beltrami operator matrix

\( \alpha_{ij}, \beta_{ij} \)  
Angles belonging to triangles sharing an edge on a mesh

\( W \)  
A matrix consisting of cotangent weights

\( W_{ij} \)  
A weight in the discretized Laplace Beltrami operator

\( A \)  
Diagonal matrix of vertex area

\( V \)  
Potential function on a manifold

\( H \)  
Hamiltonian operator

\( \mathbf{H} \)  
Discrete Hamiltonian operator matrix
Chapter 1

Introduction

The field of shape analysis has been evolving rapidly during the last decades. The constant increase in computing power allowed image and shape understanding algorithms to efficiently handle difficult problems that could not have been practically addressed in the past. A large set of theoretical tools from metric geometry, differential geometry, and spectral analysis has been imported and translated into action within the shape understanding arena. Among the numerous ways of analyzing shapes, a common one is to embed them into a different space where they can be processed more efficiently.

[EK03] introduced a method for analyzing surfaces based on embedding the intrinsic geometry of a given shape into a Euclidean space, extending previous efforts of [SSW89, ZKK02, GKK02]. Their key idea was to consider a shape as a metric space, whose metric structure is defined by geodesic distances between pairs of points on the shape. Two non-rigid shapes are compared by first having their respective geometric structures mapped into a low-dimensional Euclidean space using multidimensional scaling (MDS) [CC00], and then comparing rigidly the resulting images, also called canonical forms.

[MS05] proposed a metric framework for non-rigid shape comparison based on the Gromov-Hausdorff distance that was suggested by Gromov as a theoretical tool to quantify dissimilarity between metric spaces. Using the Gromov-Hausdorff formalism, the distance between two shapes is defined by matching pairwise distances on the shapes. However, the Gromov-Hausdorff distance is difficult to compute when treated in a straightforward manner. To overcome this difficulty [BBK06a, BBK06b] proposed an efficient numerical solver based on a continuous optimization problem, known as Generalized MDS (GMDS). Recently, other relaxation schemes have been proposed, see for example [CK15, ADK16].

Among the operators recently explored, the Laplace-Beltrami operator (LBO) is ubiquitous. The LBO is an extension of the Laplacian to non-flat manifolds. Its properties have been well studied in differential geometry and it was used extensively in computer graphics. The LBO can be found in countless applications such as mesh filtering [VL08], mesh compression [KG00], shape retrieval [BBGO11], to name just a few. It has been widely used in shape matching where several approaches treat the correspondence problem by comparing isometric invariant pointwise descriptors between the two shapes. For example, the Global Point Signature (GPS) [Rus07],
the Heat Kernel Signature (HKS) [SOG09] and the Wave Kernel Signature (WKS) [ASC11], all use the eigenfunctions and eigenvalues of the LBO to compute local shape descriptors. Similarly, local descriptors based on the Laplace-Beltrami eigendecomposition were employed together with the pairwise distances into a unified penalty measure [DK10], while [RDK13] used a hierarchical matching scheme to obtain dense correspondence. Matching only signatures at a small set of points, the correspondence between the points on the two shapes can be found. These points can serve as anchors and interpolated for the entire shape [OMMG10] where refinement of the basis can be performed to produce dense correspondence [OBCS+12, PBB+13, SK14a].

Recently, learning based approaches [LB14, WHC+16, BMRB16] have also become highly popular in the shape matching arena.

The use of the basis defined by the LBO has been a natural choice for surfaces analysis. It was chosen in the functional map framework [OBCS+12] because of its compactness, stability, and invariance to isometries. Subsequently, it was proven to be optimal [ABK15a] for representing smooth functions on the surface. In an attempt to overcome the topological sensitivity of the LBO and the non-local support of its eigenfunctions, compressed eigenfunctions have been adapted from mathematical physics to shape analysis [NVT+14, BCKS16]. Here, we try to find a richer family of basis functions that are based on intrinsic properties that can go beyond the geometry of the shape. Exploring a similar goal, [KBBK11] combined geometric and photometric information within a unified metric for shape retrieval. [IK12] used artificial surface textures on shapes to define elliptic operators that give birth to a new family of diffusion distances. In a similar manner [HSvTP12] designed a new family of eigenvibrations using extrinsic curvatures and deformation energies.

We suggest to further explore this idea and construct from the intrinsic metric a so-called potential that is added to the Laplace Beltrami operator. Here, a designed perturbation of the Laplacian can permit a supervised control of the vibrational modes on the manifold.

1.1 Contributions

The main contribution of this thesis is the exploration of the Hamiltonian operator on manifolds. After a brief mathematical overview, we study spectral properties of the operator and the impact of an additional potential function to the Laplacian for shape analysis applications. The properties of the Hamiltonian allow it to be efficiently utilized by many spectral-based methods. The potential part can lead to a more descriptive operator when treated as a truncated basis generator. Modulated harmonics on the surface can also be obtained by treating different regions of interest as different values of the potential. We show that using the resulting basis as part of classical shape analysis methods could improve their performance.

The rest of the thesis is organized as follows. In Chapter 3, we propose to study the Hamiltonian on manifolds from a variational calculus point of view with motivation from quantum mechanics. We provide optimality properties of its eigenspace, characterize the associated diffusion process, the resulting nodal sets, introduce a discretization method and test the robustness of the proposed operator. In Chapter 4, we propose a global optimization
framework for variational problems involving the basis defined by the Hamiltonian. We provide an approach for computing derivative with respect to the potential based on perturbation theory for eigenvectors. We demonstrate the effectiveness of the framework on the task of data representation. In Chapter 5, we suggest to use the Hamiltonian for obtaining sparse harmonics on manifolds by using an iterative-reweighted least square norm through the potential. The compressed modes problem is reduced to a simple eigendecomposition of the Hamiltonian and a low rank matrix avoiding heavy non-convex optimization. Also we present an optimization approach for efficient eigendecomposition of general sparse and low rank matrices. In Chapter 6, we propose the Hamiltonian as a basis for problematic area enhancer in the mesh compression task. By using sparse approximation of the mesh coordinates through designed basis of the Hamiltonian, we focus on difficult regions for better reconstruction than the recently used spectral graph wavelets. Finally, in Chapter 7 we review several spectral-based shape matching methods such as spectral features and refinement methods. We then present properties of the proposed basis that make it a better choice for the task of shape correspondence.
Chapter 2

Mathematical background

Since the notion of shape is central to our discussion, in this chapter, we briefly overview the mathematical definitions of Riemannian geometry on which our research is based [dCV92] where shapes are modeled as two-dimensional Riemannian manifolds embedded into $\mathbb{R}^3$.

2.1 Riemannian manifolds

A manifold is defined as a topological space in which every point has a neighborhood homeomorphic to a topological (half-) disc. A homeomorphism from a neighborhood of a point on the manifold to the disc is called a chart while the manifold is called smooth if all the transitions between the charts composing it are smooth.

Let $\mathcal{M} \subseteq \mathbb{R}^n$ denote an $m$-dimensional compact manifold with or without boundaries. Denote by $S(u) = S(u_1, ..., u_m) : U \subseteq \mathbb{R}^m \to \mathcal{M} \subset \mathbb{R}^n$ the embedding (global parametrization) of the manifold and $U$ is a parametrization domain. Assuming that the parametrization is regular, the vectors $\frac{\partial S}{\partial u_i}$ span the $m$-dimensional tangent space $T_x \mathcal{M}$ at point $x$ that can be considered as a local Euclidean approximation of $\mathcal{M}$ at $x$. An illustration is presented in Figure 2.1.

Figure 2.1: Embedding of a two dimensional manifold $\mathcal{M}$ and the tangent plane $T_x \mathcal{M}$ defined by the map $S$. 

Consider an infinitesimal displacement on the chart $du$ from the point $u$. Considering first order expansion, the mapping displacement $dx$ from $x = S(u)$ on the surface is given by

$$ dx = S(u + du) - S(u) \approx \sum_{i} \frac{\partial S}{\partial u_i} du_i = Jdu, \quad (2.1) $$

with $J$ the $n \times m$ Jacobian matrix whose columns are the spanning vectors defined above. Then, the length of displacement on the Euclidean chart is defined as

$$ \|dx\|^2 = \langle Jdu, Jdu \rangle = du^T J^T J du = du^T G du = \langle du, du \rangle_g, \quad (2.2) $$

with $\langle \cdot, \cdot \rangle_g : T_xM \times T_xM \to \mathbb{R}$ an inner product on the tangent space smoothly depending on $x$ referred to as the Riemannian metric. Here, $G$ defines the first fundamental form, a symmetric positive definite $m \times m$ matrix with inner product elements

$$ g_{ij} = \left\langle \frac{\partial S}{\partial u_i}, \frac{\partial S}{\partial u_j} \right\rangle, \quad (2.3) $$

and $g = \det(G)$ is the induced metric.

A real smooth manifold $M$ equipped with an inner product $\langle \cdot, \cdot \rangle_g$ on the tangent space $T_xM \times T_xM$ at each point $x$ is called a Riemannian space or Riemannian manifold $(M, g)$. In the particular known setting $m = 2$, the manifold is a two-dimensional surface and the tangent space is called the tangent plane.

### 2.2 Geometric quantities

#### 2.2.1 Length

Given an $m$-dimensional Riemannian manifold $M$ let us be given a smooth curve on the chart $\gamma(t) : [a, b] \to U$ mapped to the surface by $\Gamma : S \circ \gamma$. Using the first fundamental form, displacement on the curve $d\gamma = \dot{\gamma}(t)dt$ induces a displacement on the surface $dl$ defined as

$$ dl = \sqrt{\dot{\gamma}(t)^T G(\gamma(t)) \dot{\gamma}(t)} dt, \quad (2.4) $$

as shown in Figure 2.2. The length of a curve on the manifold can be defined as

$$ L(\Gamma) = \int_{\Gamma} dl = \int_{a}^{b} \sqrt{\dot{\gamma}(t)^T G(\gamma(t)) \dot{\gamma}(t)} dt. \quad (2.5) $$

An intrinsic metric (invariant to isometries) can be induced from the first fundamental form. The length between two points $x_1 = S(u_1), x_2 = S(u_2)$ on the manifold is defined as

$$ d_M(x_1, x_2) = \min_{\Gamma} L(\Gamma) \quad \text{s.t.} \quad \Gamma(a) = x_1, \Gamma(b) = x_2. \quad (2.6) $$
The intrinsic geometry is then totally described by the first fundamental form where the formed curves generalize the notion of straight lines to manifolds and are called geodesics.

2.2.2 Area

Consider a differential area element on the chart at point $u$ defined by $du_1 \times \ldots \times du_m$. The parametrization $S(u_1, \ldots, u_m)$ maps to a volume element $d\mu$ on the manifold defined as

$$
d\mu = \left| \frac{\partial S}{\partial u_1} \times \ldots \times \frac{\partial S}{\partial u_m} \right| du_1 \ldots du_m = \sqrt{g} du_1 \ldots du_m.
$$

If $M$ is a two-manifold, $d\mu$ is the area element of a surface denoted $da$.

2.2.3 Normal

The normal to $M$ at point $x$ is defined as the unit vector orthogonal to the tangent plane $T_x M$. With $v, w \in T_x M$ the normal may be expressed as $n(x) = \frac{v \times w}{\|v \times w\|}$, and can be represented uniquely by a point on a sphere (Gauss map).

2.3 Differential Operators

Let us consider a smooth scalar field $f : M \to \mathbb{R}$. The Riemannian metric on the manifold implies a new definition of the intrinsic gradient $\nabla_M f$ induced by $g$. Using Taylor expansion we have

$$
f(u + du) = f(u) + \langle \nabla_M f, du \rangle_g + O(||du||^2) = f(u) + \nabla_M f^T G du + O(||du||^2)
$$

$$
= f(u) + \nabla f^T du + O(||du||^2),
$$

(2.8)
when the equality is obtained because of the chart-manifold equivalence for infinitesimal
displacement. We readily have
\[ \nabla_M f = G^{-1} \nabla f. \]  
(2.9)
Using the Einstein summation the gradient is expressed in term of the local basis as [dCV92]
\[ \nabla_M f = g^{ij} \partial_j f, \]  
(2.10)
where \( g_{ij} = (G^{-1})_{i,j} \) and \( \partial_i f \) the derivative with respect to the \( i^{th} \) coordinate.
Given a smooth vector field \( V \), we can similarly define the intrinsic divergence operator
\[ \text{div}_M V(x) = \frac{1}{\sqrt{g}} \sum_i \frac{\partial}{\partial u_i} (\sqrt{g} V^i). \]  
(2.11)
Chapter 3

Hamiltonian operator

3.1 Laplace Beltrami Operator

Consider a parametrized surface \( M : \Omega \subset \mathbb{R}^2 \to \mathbb{R}^3 \) with a metric tensor \((g_{ij})\). The space of square-integrable functions on \( M \) is denoted by \( L^2(M) = \{ f : M \to \mathbb{R} | \int_M f^2 \, da < \infty \} \) with the standard inner product \( \langle f, g \rangle_M = \int_M fg \, da \), where \( da \) is an area element induced by the Riemannian metric \( \langle \cdot, \cdot \rangle_g \). The Laplace Beltrami Operator acting on a scalar function \( f \in L^2(M) \) is defined as

\[
\Delta_M f \equiv \text{div}_M(\nabla_M f) = \frac{1}{\sqrt{g}} \sum_{ij} \partial_i (\sqrt{g} g^{ij} \partial_j f),
\]

(3.1)

where \( g \) is the determinant of the metric matrix and \((g^{ij}) = (g_{ij})^{-1}\) is the inverse metric. If \( M \) is a domain in the Euclidean plane, the metric matrix is generally the identity matrix and the LBO reduces to the well-known Laplacian

\[
\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}.
\]

(3.2)

The LBO is self-adjoint and thus admits a spectral decomposition \( \{ \lambda_i, \phi_i \} \), where \( 0 = \lambda_1 \leq \lambda_2 \leq ... \uparrow \infty \) and \( \lambda_i \in \mathbb{R} \), such that,

\[
-\Delta_M \phi_i = \lambda_i \phi_i,
\]

(3.3)

with \( \delta_{ij} \) the Kronecker delta.

The LBO eigendecomposition can be extracted from the Euler Lagrange solution of the Dirichlet energy minimization

\[
\min_{\phi_i} \sum_i \int_M \| \nabla_M \phi_i \|_g^2 \, da,
\]

s.t. \( \langle \phi_i, \phi_j \rangle_M = \delta_{ij} \).

(3.4)
Here, each ordered eigenfunction composing the basis on the manifold corresponds to the function with the smallest possible energy that is orthogonal to all the previous. Therefore, the LBO eigenfunctions can be seen as an extension of the Fourier harmonics in Euclidean space to manifolds and are also referred to as *Manifold Harmonics*.

Figure 3.1: Influence of the potential on the harmonics in one dimension.

A Hamiltonian operator $H$ on a manifold $\mathcal{M}$ acting on a scalar function $f \in L^2(\mathcal{M})$, is an elliptic operator of the form

$$Hf = -\Delta_M f + Vf,$$

(3.5)

where $V : \mathcal{M} \rightarrow \mathbb{R}$ is a real-valued scalar function. It plays a fundamental role in the field of quantum mechanics via the famous Schrödinger equation that describes the wave motion of a particle with mass $m$ under potential $V$,

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi + V \Psi,$$

(3.6)

where $\hbar$ is the Planck’s constant. Here, $\Psi(x, t)$ represents the wave function of the particle such that $|\Psi(x, t)|^2$ is interpreted as the probability distribution of finding the particle at a given position $x$ at time $t$.

The Schrödinger equation can be analyzed via perturbation theory by solving the spectral decomposition $\{\psi_i, E_i\}_{i=0}^{\infty}$ of the Hamiltonian

$$H \psi_i = E_i \psi_i,$$

(3.7)

also known as the time-independent Schrödinger equation, where $E_i$ is the energy of a particle at the stationary eigenstate $\psi_i$. 

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Since the Hamiltonian is a symmetric operator, its eigenfunctions form a complete orthonormal basis on the manifold $\mathcal{M}$. As a generalization of the regular Laplacian, its spectral theory can be derived almost straightforwardly from that of the latter. We provide some examples of potential functions in the one dimensional Euclidean domain in Figure 3.1.

3.3 Variational principle

Let us consider the following functional

$$
\min_{\psi_i} \sum_i \int_{\mathcal{M}} \left( \| \nabla_{\mathcal{M}} \psi_i \|^2_g + V \psi_i^2 \right) \, da,
$$

s.t. $\langle \psi_i, \psi_j \rangle_\mathcal{M} = \delta_{ij}, \tag{3.8}$

for which the Euler-Lagrange equation defines the eigendecomposition of the Hamiltonian $H = -\Delta_{\mathcal{M}} + V$.

Thus, the basis defined by the Hamiltonian operator corresponds to the orthogonal harmonics regularized by the potential function. The potential defines the trade-off between the orientation and the compactness of the basis and its global support. Larger values of the potential will enforce smooth solutions that concentrate on the low potential regions, while smaller ones will give solutions that better minimize the total energy at the expense of more extended wave functions as shown in Figure 3.2.

3.4 Finite step potential

The time-independent Schrödinger equation can yield a rather complicated problem to solve analytically, even in one dimension. Let us consider a system with an ideal step potential in one dimension [Gri05]. We need to solve the differential equation $H \Psi = E \Psi$, with $E$ the energy of the particle and $V$ the Heaviside function with step of magnitude $V_0 > 0$, at point $x_0$, given by

$$
V(x) = \begin{cases} 
0, & x < x_0 \\
V_0, & \text{otherwise.}
\end{cases} \tag{3.9}
$$

The step divides the space in two parts where in each the potential is constant. At the zero potential region, the particle is free to move and the harmonic solutions are known. At the domain with high potential, for $E < V_0$, the solution is a decaying exponentially, meaning that the particle cannot pass the potential barrier and is reflected according to classical physics. If $E > V_0$, the solution is also harmonic, which means there is a probability for the particle to penetrate into the effective potential region with a different energy than that of particles in the zero potential region. We illustrate this effect by an numerical experiment of potential $V$ defined on human surface in Figure 3.3.

Therefore, the potential energy can be tuned to enforce localization of the basis at the expense of loss of smoothness. Given the eigenvalues of the LBO $\{\lambda_i\}_{i=0}^\infty$, we can estimate the
Figure 3.2: Absolute values of the first eigenfunctions \( \{\phi_i\} \) of the LBO on a sphere (top). Potential \( V \) with increasing magnitude (second, third and fourth rows) defined as constant in the red area and vanishing elsewhere. The resulting deviated first eigenfunctions \( \{\psi_i\} \) of the Hamiltonian operator. Red and blue colors represent high and low values, respectively. Quantum tunneling can be observed at the second row where the eigenenergy \( E_4 \) is inferior to the potential barrier value. Non-zero probability is obtained in this area in opposition to classical physics.
Figure 3.3: Absolute values of the $1^{\text{st}}$, $2^{\text{nd}}$, $5^{\text{th}}$, $7^{\text{th}}$, $8^{\text{th}}$ and $11^{\text{th}}$ eigenfunctions $\{\phi_i\}$ of the LBO (top). Absolute values of the corresponding eigenfunctions $\{\psi_i\}$ of the Hamiltonian with a step-function potential $V$ (bottom left), with step value $V_0$. For this potential, the first eigenstate $\psi_i$ with energy $E_i$ greater than $V_0$ is the eighth. As analyzed, the eigenfunctions corresponding to lower eigenvalues (energies) are restricted to the region with $V = 0$, while the higher ones can have effective values (and oscillate) at the $V = V_0 > 0$ region. Evanescent wave can be observed at the seventh eigenstate.
magnitude of the potential required in order to allow for oscillations outside the regions where the potential vanishes.

**Theorem 3.1.** Let \( \{ \phi_i, \lambda_i \}_{i=1}^{\infty} \) and \( \{ \psi_i, E_i \}_{i=1}^{\infty} \) be the spectral decompositions of the Laplacian, and the Hamiltonian, respectively, with \( \lambda_i \geq 0, \forall i \). Then, \( V \geq 0 \) everywhere on the manifold implies that \( \forall i \), the eigenvalues \( E_i \) satisfy

\[
\max_M(V) + \lambda_i \geq E_i \geq \min_M(V) + \lambda_i \geq 0.
\]

**Proof.** According to the Courant-Fischer min-max theorem, we have

\[
E_i = \max_{\Lambda \ codim \Lambda = i} \min_{\varphi_i \in \Lambda, \varphi_i \neq 0} \left\{ \frac{\int_M (\| \nabla_M \varphi_i \|^2_g + V \varphi_i^2) \, da}{\int_M \varphi_i^2 \, da} \right\}
\]

\[
\geq \max_{\Lambda \ codim \Lambda = i} \min_{\varphi_i \in \Lambda, \varphi_i \neq 0} \left\{ \frac{\int_M (\| \nabla_M \varphi_i \|^2_g + \min_M(V) \varphi_i^2) \, da}{\int_M \varphi_i^2 \, da} \right\}
\]

\[
= \lambda_i + \min_M(V). \quad (3.10)
\]

Similarly,

\[
E_i \leq \max_{\Lambda \ codim \Lambda = i} \min_{\varphi_i \in \Lambda, \varphi_i \neq 0} \left\{ \frac{\int_M (\| \nabla_M \varphi_i \|^2_g + \max_M(V) \varphi_i^2) \, da}{\int_M \varphi_i^2 \, da} \right\}
\]

\[
= \lambda_i + \max_M(V). \quad (3.11)
\]

Since the family of eigenvalues of the Helmholtz equation (3.3) consist of a diverging sequence, there exists an \( i \) such that \( E_i \geq \lambda_i + \min_M(V) \geq \max_M(V) \) and the trade-off between local-compact and global support of the basis elements can be controlled by the potential energy.

Given a scalar \( \mu \in \mathbb{R}^+ \) we can define the Hamiltonian as

\[
H_\mu = -\Delta_M + \mu V, \quad (3.12)
\]

where \( \mu \) controls the resistance to diffusion induced by the potential. Let \( \lambda_i \) and \( E_i \) be the \( i \)th eigenvalue of the LBO and Hamiltonian respectively, we seek for a constant \( \mu \) such that \( E_i > \max_M(\mu V) \) so the particle can penetrate the high potential region. Considering the potential as small perturbation of the Laplacian, up to first order, the eigenenergies are defined as \( E_i \approx \lambda_i + \mu \langle \phi_i, V \phi_i \rangle_M \). In order to contain the basis support at most until the \( i \)th eigenfunction, \( \mu \) must satisfy

\[
\mu < \frac{\lambda_i}{\max_M(V) - \langle \psi_i, V \psi_i \rangle_M}. \quad (3.13)
\]

According to its potential energy, the basis can then provide a supervised multiresolution analysis on the manifold.
3.5 Optimality of the Hamiltonian eigenspace

Among the numerous reasons that motivated the selection of the Laplacian for shape analysis, one ubiquitous is its efficiency in representing functions with bounded gradient magnitude. This property is defined by the following result. Consider a function $f \in L^2(\mathcal{M})$. We define the representation residual function as

$$
\|r_n\|^2_{\mathcal{M}} = \left\| f - \sum_{i=1}^{\infty} \langle f, \phi_i \rangle_{\mathcal{M}} \phi_i \right\|^2_{\mathcal{M}} = \left\| \sum_{i=n+1}^{\infty} \langle f, \phi_i \rangle_{\mathcal{M}} \phi_i \right\|^2_{\mathcal{M}} = \sum_{i=n+1}^{\infty} \langle f, \phi_i \rangle^2_{\mathcal{M}}. \tag{3.14}
$$

We know that

$$
\|\nabla g f\|^2_{\mathcal{M}} = \int_{\mathcal{M}} (-\Delta f) f \, da = \sum_{i=1}^{n} \int_{\mathcal{M}} (\langle f, \phi_i \rangle_{\mathcal{M}} \lambda_i \phi_i) f \, da = \sum_{i=1}^{\infty} \lambda_i \langle f, \phi_i \rangle^2_{\mathcal{M}} \geq \sum_{i=n+1}^{\infty} \lambda_i \langle f, \phi_i \rangle^2_{\mathcal{M}} \geq \lambda_{n+1} \sum_{i=n+1}^{\infty} \langle f, \phi_i \rangle^2_{\mathcal{M}}.
$$

Thus, from (3.14) and (3.15) we obtain

$$
\|r_n\|^2_{\mathcal{M}} = \left\| f - \sum_{i=1}^{n} \langle f, \phi_i \rangle_{\mathcal{M}} \phi_i \right\|^2_{\mathcal{M}} \leq \frac{\|\nabla g f\|^2_{\mathcal{M}}}{\lambda_{n+1}}, \tag{3.16}
$$

The representation error $r_n$ for a function $f$ using the eigenfunctions of the Laplacian $\{\phi_i\}_{i=1}^{\infty}$ is bounded by a factor of the squared magnitude of its gradient. This result was subsequently proved to be optimal for representing functions with bounded gradient magnitude over surfaces in [ABK15b], which says that there exists no other basis with better representation error for all possible $L^2(\mathcal{M})$ functions.

In the Hamiltonian case, we obtain similarly

$$
\|\nabla g f\|^2_{\mathcal{M}} + \|\sqrt{V} f\|^2_{\mathcal{M}} = \int_{\mathcal{M}} (-\Delta f + V f) f \, da \geq E_{n+1} \sum_{i=n+1}^{\infty} \langle f, \psi_i \rangle^2_{\mathcal{M}}. \tag{3.17}
$$

Thus we can bound the representation error of the Hamiltonian basis by

$$
\|r_n\|^2_{\mathcal{M}} = \left\| f - \sum_{i=1}^{n} \langle f, \psi_i \rangle_{\mathcal{M}} \psi_i \right\|^2_{\mathcal{M}} \leq \frac{\|\nabla g f\|^2_{\mathcal{M}} + \|\sqrt{V} f\|^2_{\mathcal{M}}}{E_{n+1}}. \tag{3.18}
$$

To gain further insight, we simulate this result in a discrete setting by analyzing the gradient operators for a simple one dimension case. In the discrete case, since the Laplacian $L$ is a symmetric positive semi-definite matrix it admits a square-root decomposition $L = \Phi \Lambda \Phi^T = DD^T$ such that $D = \Phi \Lambda^{1/2}$. Then, the discrete equivalent of result 3.16 is:

$$
\|r_n\|^2 = \left\| f - \sum_{i=1}^{n} \langle f, \phi_i \rangle \phi_i \right\|^2 \leq \frac{\|\nabla g f\|^2_{\mathcal{M}}}{\lambda_{n+1}}, \tag{3.19}
$$
It is interesting to perform a similar analysis on the eigenfunctions of the Hamiltonian and Figure 3.4 shows a visualization of the gradient operator of the Laplacian and the induced gradient of the Hamiltonian. The result in equation (3.19) gets modified to account for the action of the potential.

\[
\|r_n\|_2^2 = \left\| f - \sum_{i=1}^{n} (f, \psi_i) \psi_i \right\|_2^2 \leq \frac{\|\mathcal{W}Df\|_2^2}{E_{n+1}},
\]

(3.20)

with \( \mathcal{W} = (I + D^{-1}VD^{-T})^{1/2} \) such that \( H = (\mathcal{W}D)^T\mathcal{W}D \). Here, since the kernel of \( L \) is not empty, we approximate \( D^{-1} \) as the pseudo inverse of \( D \). Thus the basis defined by the Hamiltonian can be considered as optimal for the representation of functions which have a bounded weighted gradient. The weights depend on the potential function and its action in different regions.

The gradient matrix \( D \) for the 1D case is the result of a simple finite difference scheme of one dimensional forward differentiation yielding a circulant populated with the kernel \([1, -1]\) circulated along the diagonal. The Hamiltonian has the effect of escalating the cost of a strong gradient exclusively in regions of high potential. This shows that coefficients of the induced gradient matrix are larger in the high potential regions as compared to anywhere else in the domain. The non-zero values of the off-diagonal elements suggest that the linear operation loses its shift invariance property and the effect of a derivative is no more an exclusive property of its local neighborhood but also depends on its global positioning imposed by the potential function. Thus the Hamiltonian operator advocates measuring smoothness differently for different regions of the domain and this is a useful property to exploit in a compression setup.

![Figure 3.4: Matrix visualizations of the potential function (left), the standard gradient matrix \( D \) (middle) and the weighted gradient matrix \( \mathcal{W}D = (I + D^{-1}VD^{-T})^{1/2}D \) (right) for Euclidean 1D example.](image)

Next, we show that the Hamiltonian is optimal in approximating functions with bounded weighted gradient.

**Theorem 3.2.** Let \( 0 \leq \alpha < 1 \). There is no integer \( n \) and no sequence \( \{\psi_i\}_{i=0}^{\infty} \) of linearly
independent functions in $L_2(M)$ such that

\[
\left\| f - \sum_{i=1}^{n} (f, \psi_i)_M \psi_i \right\|_M^2 \leq \alpha \left( \| \nabla_g f \|_M^2 + \| \sqrt{V} f \|_M^2 \right) \frac{E_{n+1}}{E_{n+1}} \forall f.
\] (3.21)

The proof of Theorem 3.2 is given in the appendix. The basis is then optimal for representing functions with bounded gradient in high potential areas.

In some cases, the potential $V$ can then be designed to localize the support of the eigenfunctions for better analysis of specific regions as shown in Figure 3.5. Using this result, we could restrict the first harmonics to desired specific regions as shown in Figure 3.2.

![Figure 3.5](image)

Figure 3.5: First eigenfunctions $\{\phi_i\}$ of the LBO on the hand (top). The potential $V$ is defined by the geodesic distances from six points selected with farthest point sampling (bottom left) and first eigenfunctions $\psi_i$ of the Hamiltonian with compact support (bottom right). Here, because of the compactness of the basis, most of the surface is blue indicating zero values. Functions on fingers extremities are better approximated by the Hamiltonian eigenfunctions.

### 3.6 Diffusion process

Let us be given a Riemannian manifold $M$. The heat equation governing the diffusion process on $M$ is defined as

\[
\begin{cases}
\partial_t u(x, t) = \Delta_M u(x, t), & \forall x \in M, \\
u(x, 0) = u_0(x),
\end{cases}
\] (3.22)

with appropriate boundary conditions. A natural extension to the new operator with a potential function $V$, can be written as

\[
\begin{cases}
\partial_t u(x, t) = Hu(x, t) = \Delta_M u(x, t) - V(x)u(x, t) \\
u(x, 0) = u_0(x).
\end{cases}
\] (3.23)
The solutions of (3.22) and (3.23) have the form [IK12]

\[ u(x, t) = \int_{\mathcal{M}} u_0(y) K(x, y, t) \, da(y), \]  

(3.24)

that represents the diffusion in time of heat on the manifold \( \mathcal{M} \) with potential \( V \), where

\[ K(x, y, t) = \sum_i e^{-E_i t} \psi_i(x) \psi_i(y). \]

We refer to \( K(x, y, t) \) as the heat kernel. A standard proof is given in the appendix.

According to the Feynman-Kac formula [Sim05], the solution of the diffusion process is expressed in terms of Wiener process,

\[ u(x, t) = \mathbb{E}\left( u_0(X_t) \exp\left( \int_0^t V(X_{\tau}) \, d\tau \right) \mid X_t = x \right). \]  

(3.25)

In the Laplacian case, the initial value \( u_0(x) \) is carried over random path in time, while the expected value of the stochastic process is equal to the solution \( u(x, t) \). For \( V > 0 \), the diffusion spreads according to the potential on the manifold, when the transported value is modulated exponentially by the potential \( V \), diffusing anisotropically to low potential regions, as shown in Figure 3.6.

Figure 3.6: Heat diffusion with a delta function at the centaur’s head as initial condition. The diffusion is derived from the LBO (top) and the Hamiltonian (bottom) for different values of \( t \). The potential \( V \) used in this example is the geodesic distance from the front left leg. A signature extracted from a diffusion process using the Hamiltonian is more descriptive and in this case allows to resolve symmetric ambiguities.
3.7 Nodal sets

An interesting property of the Laplacian is the relation between its eigenfunctions, the number of connected nodal (zero) sets, and the number of complementary regions they define. Given an eigenfunction $\psi_i : M \rightarrow \mathbb{R}$, a nodal set is defined as the set of points at which the eigenfunction values are zero. That is,

$$N(\psi_i) = \{ x \in M | \psi_i(x) = 0 \}. \quad (3.26)$$

The Nodal Theorem [CH66] states that the $i$-th eigenfunction of the LBO can split $M$ to at most $i$ connected sub-domains. In other words, the zero set of the $i$-th eigenfunction can separate the manifold into at most $i$ connected components.

**Proposition 1.** Given the self-adjoint Hamiltonian operator $H$ on $M$, with arbitrary boundary conditions; if its eigenfunctions are ordered according to increasing eigenvalues, then, the nodal set of the $i$-th eigenfunction divides the domain into no more than $i$ connected sub-domains.

The proof is essentially the same as that of the Laplacian case. See [CH66] Vol.1 Sec. VI.6 for a proof.

As shown in Figure 3.3, the Hamiltonian eigenfunctions are tuned by the potential. Thus, shape segmentation can be obtained by separating the surface according to the induced nodal sets as described in [Lev06]. Given a potential $V$ defined on the surface, meaningful segmentation can be induced by the nodal domains of the resulting eigenfunctions, as presented in Figure 3.7.
3.8 Discretization

In the discrete setting, we look at a triangular mesh $M$ in $\mathbb{R}^3$ and consider the space of functions that are continuous and linear in every triangle. According to the Finite Element Method (FEM) [Dzi88], the solution of the Hamiltonian eigenvalue problem (3.7) can be computed by imposing that the equation $Hf = \lambda f$ is satisfied in a weak sense, that is,

$$\langle Hf, \varphi_j \rangle_M = \lambda \langle f, \varphi_j \rangle_M, \quad \forall j.$$  (3.27)

$\varphi_j$ denotes the Lagrange basis of piecewiselinear hat-functions on $M$, that take the value one at vertex $m_j$ and vanishes at all the other vertices. In this section $\lambda$ represents the eigenenergies of the Hamiltonian. On the mesh, the bilinear form $\langle \cdot, \cdot \rangle_M$ is evaluated by splitting the integrals into a sum over the triangles $T$ of $M$ by

$$\langle u, v \rangle_M = \sum_{T \in M} \langle u, v \rangle_T = \sum_{T \in M} \int_T uvda.$$  (3.28)

Since the Hamiltonian is a linear operator we have

$$\langle Hf, \varphi_j \rangle_M = \langle -\Delta_M f, \varphi_j \rangle_M + \langle Vf, \varphi_j \rangle_M.$$  (3.29)

The matrix representation of $\langle -\Delta_M f, \varphi_j \rangle_M$ and $\lambda \langle f, \varphi_j \rangle_M$ with respect to the Lagrange basis are well known [PP93] and define the stiffness matrix $W$ and the mass matrix $A$ with the entries

$$A_{ij} = \langle \varphi_i, \varphi_j \rangle_M \quad \text{and} \quad W_{ij} = \langle \nabla \varphi_i, \nabla \varphi_j \rangle_M.$$  (3.30)

Thus,

$$\langle Vf, \varphi_j \rangle_M = \sum_{T \in M} \langle Vf, \varphi_j \rangle_T = \sum_{T \in M} \sum_i f_i \langle V\varphi_i, \varphi_j \rangle_T = AVf,$$  (3.31)

where the last equality is obtained by representing the potential function $V$ as a diagonal matrix $V$ according to the Lagrange basis functions. The discretization of the eigenvalue problem (3.7) is defined by finding all pairs $\{\lambda, \psi\}$ such that

$$H\psi = W\psi + AV\psi = (W + AV)\psi = \lambda A\psi.$$  (3.32)

Efficient solution methods can be found in [VL08]. Among the possible explicit representations of the matrices $A$ and $W$, we use here the cotangent formula [MDSB03, PP93] where the stiffness matrix is defined as

$$W_{ij} = \begin{cases} -\sum_{j \neq i} W_{ij}, & i = j, (i, j) \in N_i \\ \frac{\cot \alpha_{ij} + \cot \beta_{ij}}{2}, & i \neq j, (i, j) \in N_i \end{cases},$$  (3.33)

with $N_i = \{j : (i, j) \in \Gamma\}$, where $\Gamma$ is the set of edges of the triangulated surface interpreted as a graph and $\alpha_{ij}, \beta_{ij}$ denote the angles $\angle ikj$ and $\angle jhi$ of the triangles sharing the edge $ij$. The
mass matrix is replaced by a diagonal lumped mass matrix of the area of local mixed Voronoi cells about each vertex $m_i$. Since $V$ only modifies the diagonal of $W$, our operator remains a sparse matrix with the same effective entries, and thus, there is no increase in the computational cost of the generalized eigendecomposition compared to that of the LBO.

### 3.9 Robustness

As a generalization of the Laplacian, the Hamiltonian exhibits similar robustness to noise. Consider the Hamiltonian matrix $H = A^{-1}(W + AV)$ with $V$ the potential, then the perturbed Hamiltonian has the form $\tilde{H} = \tilde{A}^{-1}(\tilde{W} + \tilde{A}\tilde{V})$. Let us define $\delta_A = |A - \tilde{A}|$ and $\delta_W = |(W - \tilde{W}) + (AV - \tilde{A}\tilde{V})|$. Based on perturbation theory, and up to first order expansion, the $i$-th eigenfunction $\tilde{\psi}_i$ of $\tilde{H}$ has the form

$$\tilde{\psi}_i = \psi_i (1 - \frac{\psi_i^T \delta_A \psi_i}{2}) + \sum_{k \neq i} \frac{\psi_i^T (\delta_W - E_i \delta_A) \psi_k}{E_i - E_k} \psi_k,$$

(3.34)

with $\psi_j$ and $E_j$ respectively the $j$th eigenfunction and eigenvalue of the unperturbed Hamiltonian. Assuming uniformly distributed random noise on the mesh, the eigenfunctions of the regular Laplacian may present smaller distortion to noise than the Hamiltonian since the perturbation is amplified by area and potential distortions. Still, in case of potential with small values the distortion is insignificant. In Figure 3.8, we present the original surface and its noisy version in which vertex positions have been corrupted by additive Gaussian noise with $\sigma_x^2 = 20\%$ of the mean edge length. The potential is also modified by adding a Gaussian noise with $\sigma_V^2 = 20\%$ of the initial variance of the potential.

The construction of the Laplacian depends crucially on the mesh connectivity making it sensitive to topological noise such as holes and part removal that can be found in most scanning scenarios. The compact support of the basis elements of the Hamiltonian make it robust to noise compared to the basis elements that are generated by the Laplacian. We illustrate the robustness property in Figure 3.8 where $30\%$ of the surface area was removed due to topological noise in the form of small holes.
Figure 3.8: Robustness to noise of the Hamiltonian. First eigenfunctions $\psi_i$ of the Hamiltonian under potential $V$ (top). First eigenfunctions $\tilde{\psi}_i$ of the Hamiltonian subject to Gaussian noise in positions of the vertices and the potential (middle). First eigenfunctions $\tilde{\psi}_i$ of the Hamiltonian subject topological noise (bottom).
Chapter 4

Optimization involving the Hamiltonian operator

4.1 Problem statement

One natural problem emerging while working with the Hamiltonian is the ability to define an optimal potential function for enhanced performance. The choice of the potential is application dependent but can be represented through variational problems generically defined as

\[
\min_{V} D(X, V) \\
\text{s.t. } V \in \mathbb{R}^n,
\]

where \(D(X, V)\) denotes the data term depending on the data matrix \(X\) and the vector \(V\) defining the diagonal potential matrix. Also regularization terms can be added. If the analytical solution remains complex, a common approach is to minimize the goal function with an optimization algorithm involving the gradient of the goal function with respect to the potential. In this chapter we propose an optimization framework based on perturbation theory of the eigenvectors where (sub-)optimal potential is obtained. That is, our goal is to formulate \(\nabla_V D\) for a given objective \(D\).

4.2 Optimization framework

Here we will consider the problem of data representation using the discrete basis of the Hamiltonian referred to as \(\Psi_k(V) = \Psi_k \in \mathbb{R}^{n \times k}\) representing the \(k\) eigenvectors of the Hamiltonian. The discrete functional is defined as

\[
\min_{V} \| \Psi_k \Psi_k^T X - X \|_F^2 \\
\text{s.t. } V \in \mathbb{R}^n,
\]

(4.2)
with \( k < n \). It defines the representation error of the data \( X \) onto its projection on the basis \( \Psi_k \) and \( \| \cdot \|_F \) denotes the Frobenius norm. For general orthonormal matrix \( \Psi_k \), we return to the famous Principal Component Analysis (PCA) formulation. We can straightforwardly obtain that

\[
L = \| \Psi_k \Psi_k^T X - X \|_F^2 = \text{trace}\left( (\Psi_k \Psi_k^T X - X)^T (\Psi_k \Psi_k^T X - X) \right)
= \text{trace}(X^T X) + \text{trace}(X^T \Psi_k \Psi_k^T \Psi_k^T X) - 2\text{trace}(X^T \Psi_k \Psi_k^T X)
\]

(4.3)

Thus, the differential of the loss function \( L \) with respect to \( V \) is obtained by

\[
dL = -d\text{trace}(\Psi_k \Psi_k^T X X^T)
= -\text{trace}(d\Psi_k \Psi_k^T X X^T) - \text{trace}(\Psi_k d\Psi_k^T X X^T)
\]

(4.4)

The arising question is how to define differential of eigenvectors. Let us consider the full matrix of eigenvectors \( \Psi_n \in \mathbb{R}^{n \times n} \), the \( n \times n \) diagonal matrix of eigenenergies \( [\Lambda]_{ij} = \lambda_i \) and the discrete Hamiltonian operator \( H \). The eigenvalue decomposition problem is given by \( H \Psi_n = \Psi_n \Lambda \). Thus, the differential of the spectral decomposition problem is given by

\[
dH \Psi_n + H d\Psi_k = d\Psi_n \Lambda + \Psi_n d\Lambda.
\]

(4.5)

Multiplying by \( \Psi_n^T \) on the left side and denoting \( d\Psi_n = \Psi_n C \) with \( C \in \mathbb{R}^{n \times n} \), we have

\[
\Psi_n^T dH \Psi_n + \Psi_n^T H \Psi_n C = \Psi_n^T \Psi_n C \Lambda + \Psi_n^T \Psi_n d\Lambda
\]

(4.6)

since \( \Psi_n^T \Psi_n = I_n \). We readily obtain that the off diagonal elements of the matrix \( C \) can be defined by

\[
C_{ij} = \frac{(\Psi_i^j)^T dH \Psi_j}{\lambda_j - \lambda_i}, \forall i \neq j.
\]

(4.7)

Here \( \Psi_j \) represents the \( j \)th column of the matrix of eigenvectors. The diagonal elements of \( C \) are defined by the following

\[
(\Psi_n + d\Psi_n)^T (\Psi_n + d\Psi_n) = I
\]

\[
\Psi_n^T \Psi_n + \Psi_n^T d\Psi_n + d\Psi_n^T \Psi_n + d\Psi_n^T d\Psi_n = I
\]

\[
I + \Psi_n^T \Psi_n C + C^T \Psi_n^T \Psi_n C + C^T \Psi_n^T d\Psi_n C = I
\]

\[
C + C^T + C^T C = 0.
\]

(4.8)

The diagonal elements are then defined by \( 2C_{ii} + \sum_{k=1}^{n} C_{ki}^2 = 0 \). Since second order elements are negligible, we have \( 2C_{ii} = 0 \). We obtain that \( d\Psi_n = \Psi_n C = \Psi_n (\Psi_n^T dH \Psi_n) \odot B \), with \( \odot \).
the Hadamard product and the matrix $B$ defined as

$$
B_{ij} = \begin{cases} 
\frac{1}{\lambda_j - \lambda_i}, & i \neq j \\
0, & i = j.
\end{cases}
$$

(4.9)

The selection of the first $k$ eigenvectors $d\Psi_k$ are obtained by multiplying $d\Psi_n$ by the truncated identity matrix $Z = I_{n \times k}$. The differential now is known and can be inserted into the derivation framework of (4.4) in order to extract $dH$, that is:

$$
dL = -2\text{trace}(\Psi_k^TXX^Td\Psi_k)
= -2\text{trace}(\Psi_k^TXX^T\Psi_n CZ)
= -2\text{trace}(\Psi_k^TXX^T\Psi_n(\Psi_n^T dH \Psi_n \odot B) Z)
= -2\text{trace}(\Psi_n (Z\Psi_k^TXX^T\Psi_n) \odot B\Psi_n^T dH)
= \langle ( -2(\Psi_n (Z\Psi_k^TXX^T\Psi_n) \odot B\Psi_n^T )^T, dH \rangle.
$$

(4.10)

The fourth equation is obtained from the equivalence trace$(A (B \odot C)) = \text{trace}((A \odot C^T)B)$. Since $dH = d(L + \text{diag}(V)) = \text{diag}(dV)$, we obtain finally

$$
\nabla V L = \text{diag}( -2(\Psi_n (Z\Psi_k^TXX^T\Psi_n) \odot B\Psi_n^T )).
$$

(4.11)

### 4.3 Discussion

Two problems arise from the suggested scheme. First, the high computational cost of a full (sparse) matrix diagonalization. Second, the matrix $C$ remains undefined in case of multiplicity of the eigenvalues i.e. $\exists i \neq j$ such that $\lambda_i = \lambda_j$. The first problem can be relaxed by approximating the matrix $d\Psi$ with less eigenvectors. This is especially justified for distant indices, where the eigenenergies are well separated and the corresponding elements of matrix $B$ become negligible. Also, the data can be segmented and processed separately for better representation and efficiency. Even if the second problem has been treated in [VDATMM07], it seems that single non-derivable points are not critical for computation and convergence. Also a subgradient approach can be chosen. At any case, here we stabilize the matrix $B$ in order to avoid exploding gradient. We use the approximation

$$
B_{ij} \approx \frac{1}{(|\lambda_j - \lambda_i| + \epsilon)(\text{sign}(\lambda_j - \lambda_i))},
$$

(4.12)

where the sign function is not vanishing.

In its geometric setting, the solution remains similar and is obtained by defining a new basis $\tilde{\Psi}_k = A^{\frac{1}{2}} \Psi_k$, such that $\tilde{\Psi}_k^T \tilde{\Psi}_k = I_k$, coupled with a geometric Frobenius norm defined as $\|X\|_F^2 = \|A^{\frac{1}{2}} X\|_F^2$. In those experiments we allowed negative potential for performance consideration only, since the potential is defined over the whole codomain $\mathbb{R}$. Also, for physically
interpretable solutions we enforced positive potential by using quadratic function $V^2$. The extension of the derivation is straightforward but decreased the performance since it is more restrictive.

### 4.4 Experimental evaluation

As a toy experiment, we propose to find the best potential for the representation of function in the one dimensional euclidean domain. Given a function $f \in \mathbb{R}^n$, we seek for the best potential minimizing $\|\Psi_k \Psi_k^T f - f\|^2_2$. We present results for different functions in Figures 4.1,4.2 where we compare reconstruction performance with the Laplacian and the Hamiltonian built from the optimized potential. Finally, we propose to reconstruct the matrix of coordinates of a mesh.

![Figure 4.1: Reconstruction of a linear function using the Laplacian and the Hamiltonian constructed with the proposed framework. 15 eigenvectors were used in this experiment.](image)

so the data matrix is defined by $X = (x, y, z) \in \mathbb{R}^{n \times 3}$. Results are presented in Figure 4.3. The experiments were implemented in MATLAB using the quasi-Newton method with initial potential defined as the Fiedler vector (second eigenvector of the Laplacian).
Figure 4.2: Reconstruction of a step function using the Laplacian and the Hamiltonian constructed with the proposed framework. 15 eigenvectors were used in this experiment.

Figure 4.3: Potential function defined on the original mesh (left), reconstruction of the mesh coordinates using the LBO (middle) and the Hamiltonian constructed with the proposed method (right). Blue and red colors represent negative and positive values respectively. The Hamiltonian is able to focus on sharp regions of the mesh designated by the blue regions of the potential for a better reconstruction (fingers). The errors are 0.0015 and 0.00061 for the LBO and the Hamiltonian respectively, a reduction of nearly two orders of magnitude. 50 eigenvectors were used in this experiment.
Chapter 5

Hamiltonian for $L_1$ regularization of the Dirichlet energy

The $\ell_1$ norm plays a cardinal role in modern digital signal and image processing, mainly due to its sparsity-promoting properties and convexity. Robust PCA [ZHT06], compressed sensing, and inverse problem regularization using synthesis and analysis sparse models are just a few examples of applications of the $\ell_1$ norm. The $\ell_1$ norm constitutes a convex surrogate to the combinatorial $\ell_0$ norm counting the number of non-zero entries in a vector, and powerful theoretical results exist showing the equivalence of such convex relaxations of intractable $\ell_0$ minimization problems [Ela10].

A limited set of methods involving $L_1$-regularization have recently appeared for functions defined over discrete surfaces in a variety of tasks in geometry processing [DGP09, ASGCO10, DBD$^{+}$13, KBS00] and shape analysis [PBB$^{+}$13, CRA$^{+}$16, NVT$^{+}$14]. The compressed manifold modes (CMM) introduced in [NVT$^{+}$14] are an example of localized smooth truncated basis obtained via sparse regularization. Such bases enjoy most of the properties of the extensively used harmonic basis (the orthonormal basis diagonalizing the Laplacian operator), and can constitute an alternative thereof in many geometry processing and analysis tasks.

For optimization problems involving the proposed norm, we propose to translate the objective into a tractable weighted $\ell_2$ norm that is minimized by an iterative reweighing scheme. We demonstrate experimentally the advantages of the new scheme as a general framework for solving $\ell_1$ regularization problems on discrete surfaces. Using the compressed manifold modes problem, we show that it can be formulated as a sequence of Hamiltonian eigendecomposition problems, avoiding altogether non-convex optimization on Stiefel manifold originally used in [NVT$^{+}$14] and gaining orders of magnitude speedup in runtime. We show that the resulting bases are robust to different triangulation and isometries of a given shape.
5.1 \textit{L}_1 \textit{ norm minimization using iterative reweighted least squares}

One of the bold uses of the \textit{L}_1 \textit{ norm is its inclusion as a sparsity-promoting penalty or regularization term in optimization problems, giving rise to problems of the form

$$\min_{f} E(f) + \|f\|_1,$$

where \(E(f)\) is some objective. The lack of smoothness of the norm usually requires the utilization of non-smooth optimization techniques such as proximal [PB+14] or ADMM [BPC+11] algorithms.

Here we propose a generic approach to such problems combining the discretization presented above with the well-known iteratively-reweighted least squares (IRLS) method [HW77]. As we show in the following section, such a formulation appears to be beneficial in some problems.

We can formulate the minimization problem with a weighted \(\ell_2\) term of the form

$$\min_{f} E(f) + f^T V f$$  \hspace{1cm} (5.1)

with the diagonal matrix \(V = \text{diag}\{v_1, \ldots, v_n\}\) containing the weights. We would like the two problems to have the same minimizer. From first order optimality conditions, we require the gradients of \(|f|_1\) and \(f^T V f\) with respect to \(f\) to vanish at the same point, which yields

$$v_i = \frac{1}{2|f_i|} = \frac{1}{2\sqrt{f_i^2 + \epsilon}}.$$  \hspace{1cm} (5.2)

The minimization proceeds by solving a sequence of problems of the form (5.1), each time recalculating the weights according to (5.2).

5.2 \textit{Compressed manifold modes}

In what follows, we briefly overview the compressed manifold modes problem used as a case study for the proposed \textit{L}_1 \textit{ norm discretization. Ozoliņš et al. [OLCO13] proposed a general formalism for sparse solutions to a class of physical problems in Euclidean domains. To that end, they modified the construction of the standard harmonic basis that minimizes the Dirichlet energy among all orthonormal bases by adding an \textit{L}_1 \textit{ regularization term. The resulting quasi-harmonics were dubbed \textit{compressed modes} of the domain and were shown to be compactly supported [Bre74, BCO14]. Neumann et al. [NVT+14] extended this construction to manifolds, suggesting the following \textit{L}_1 \textit{ normalized problem

$$\min_{\phi} \sum_i \int_M \left( \langle \phi_i, \Delta_M \phi_i \rangle_M + \mu |\phi_i| \right) da,$$

s.t. \(\langle \phi_i, \phi_j \rangle_M = \delta_{ij},$$  \hspace{1cm} (5.3)
where $\Delta_M$ denotes the Laplace-Beltrami operator and $\langle \cdot, \cdot \rangle_M$ is the intrinsic inner product on $\mathcal{M}$. The non-negative parameter $\mu$ controls the relative importance of smoothness expressed as the Dirichlet energy (first term) and localization expressed as the $L_1$ norm (second term).

Neumann et al. discretized the problem using the naïve vector $l_1$ norm, obtaining

$$
\min_{\Phi} \text{trace}(\Phi^T W \Phi) + \mu \| \Phi \|_1 \\
\text{s.t. } \Phi^T A \Phi = I,
$$

where $W$ is the cotangent weight matrix used in the popular Laplacian discretization scheme [PP93, MDSB03]. The non-convex orthogonality constraint combined with the non-smooth objective required the use of non-trivial optimization technique based on ADMM [BPC+11, KGB16] and proximal operators, guaranteeing no global solution. The complexity of the compressed modes problem ($\mu > 0$) is strikingly higher than the computation of the regular harmonic basis ($\mu = 0$) obtained by the simple generalized eigendecomposition $W \Phi = A \Phi \Lambda$.

### 5.2.1 Iterative reweighting scheme

Using the proposed iteratively-reweighted $L_2$ formulation, we can rewrite the original variational problem (5.3) as

$$
\min_{\phi_i} \sum_i \int_M \langle \phi_i, (\Delta_M + \mu v_i) \phi_i \rangle_M da, \\
\text{s.t. } \langle \phi_i, \phi_j \rangle_M = \delta_{ij},
$$

where $v_i(x)$ can be interpreted as a potential function enforcing diffusion and localizing the support of $\phi_i$ in low-potential areas (Figure 5.1). Contrary to the original problem (5.3), the above problem has a meaningful physical interpretation from quantum mechanics and still looks like operator eigendecomposition.

Using the cotangent discretization of the Laplacian, we formulate the compressed manifold

Figure 5.1: Potential $v_i$ (left), and its corresponding eigenfunction $\phi_i$ (right) computed using the proposed framework. Hot and cold colors represent positive and negative values, respectively, while white values represent zero.
modes problem as the solution of the problem

$$\min_{\phi_i} \phi_i^T (W + \mu AV_i) \phi_i + \beta \sum_{j<i} \|\phi_j^T A \phi_i\|_2^2$$

s.t. \( \phi_i^T A \phi_i = 1 \), \hspace{1cm} (5.6)

where \( \beta \) is a sufficiently large constant such that the third term guarantees that the \( i \)-th mode \( \phi_i \) is \( A \)-orthogonal to the previously computed modes \( \phi_j, j < i \). Observe that albeit non-convex, the problem has a closed form global solution, that is the smallest generalized eigenvector \( \phi_i \) of

$$\phi_i (W + \mu AV_i + \beta Z_i) = \lambda_i A \phi_i$$

with \( Z_i = A \left( \sum_{j<i} \phi_j \phi_j^T \right) A \).

When only the few first compressed modes are required, \( Z_i \) is low rank and finding the smallest generalized eigenvector can be solved efficiently since the involved matrix is the sum of a sparse and a low-rank matrix.

Several numerical eigendecomposition implementations use the Arnoldi iteration algorithm to extract the eigenvector associated with the eigenvalue of largest magnitude. The main computationally demanding operation of this method is the multiplication of the matrix we aim at decomposing by a vector. Largest eigenvectors of sparse matrices can therefore be computed very efficiently. However, since we are seeking the smallest eigenvector, the core operation is the multiplication by the inverse of the matrix we want to decompose. Solved straightforwardly, the iterative solution can be computationally expensive.

For our configuration, let us consider the matrix \( B \) such that \( B = Q + U U^T \) with \( Q \) and \( U U^T \) being, respectively, the sparse and the low-rank matrix from (5.7). Arnoldi’s method for the computation of the smallest eigenvector of \( B \) proceeds by solving at each iteration \( B \phi^{k+1} = \phi^k \) for the next iterate \( \phi^{k+1} \) given the current iterate \( \phi^k \) and normalizing the result. The Woodbury identity

$$(Q + U U^T)^{-1} = Q^{-1} - Q^{-1} U (I + U^T Q^{-1} U)^{-1} U^T Q^{-1}$$

can be used to compute the inverse of the sum of an invertible matrix \( Q \) and the outer product of two matrices \( U \) and \( U^T \).

At \( k \)-th iteration, we first compute \( \psi^k = Q^{-1} \phi^k \) by solving the sparse system \( Q \psi^k = \phi^k \). Next, we compute \( \xi^k = Q^{-1} U (I + U^T Q^{-1} U)^{-1} U^T \) by solving another sparse system

$$Q \xi^k = U (I + U^T Q^{-1} U)^{-1} (U^T \psi^k).$$

Finally, substituting these two solutions into the Woodbury identity yields \( \phi^{k+1} = B^{-1} \phi^k = \psi^k - \xi^k \). Since \( Q \) is sparse, and \( U \) has only a few columns, the above computations can be
carried out efficiently.

5.2.2 Experimental evaluation

Figure (5.2) presents the CMM computed on different surfaces from the TOSCA dataset [BBK08] (low resolution) with the method [NVT+14] and the proposed IRLS approach. The results show spectral decomposition under different sampling, triangulation and deformation. The basis functions obtained by [NVT+14] are sorted according to the cost derived from (5.4). The eigenvectors obtained with the proposed method are naturally sorted by the corresponding eigenvalues. Superior stability under different sampling and nearly isometric deformation of the mesh can be observed.

For performance comparison we present in Figure (5.3) the runtimes for the different methods using the same sparse parameter $\mu$. The IRLS approach generally requires around 15 iterations to converge, while each iteration is computed efficiently using scheme detailed in Section 5.2.1. In other approaches [NVT+14, KGB16], high computational complexity make them impractical for dense meshes or when many eigenvectors are required. The system was implemented in MATLAB and all the experiments were executed on a 2.5 GHz Intel Core i7 machine with 16GB RAM. We provided a random initialization to the reference method [NVT+14] for the computation of the eigenvectors.
Figure 5.2: First eight compressed manifold modes computed for different sampling (upsampling by a factor of 5.5) and under nearly isometric deformation of the same mesh using the the proposed IRLS technique (three first rows) and the technique proposed by [NVT+14] (three bottom rows). Note the better stability of the proposed technique to different triangulation.
Figure 5.3: Runtimes of [NVT+14] and the proposed framework on meshes of varying size (number of vertices $n$) and number of eigenvectors $k$. Averages and standard deviations are presented over 10 runs. Same stopping criteria were applied to all methods.
Chapter 6

Hamiltonian operator for sparse approximation of shapes

6.1 Introduction

In most areas that involve representation of discrete virtual surfaces as 3D meshes, there has been an increasing trend in working with higher precision. This has lead to the generation of meshes which comprise of a large number of elements, for which the processing, visualization and storage of has become a challenge. The task of transmission of these geometric models over communication networks can lead to a large amount of storage space and put a considerable strain on network resources.

The research on mesh compression started in the direction of single-rate compression methods that constructed a compact representation of an input mesh as a whole. However, the need for transmission of large geometric models led to the development of algorithms based on progressive mesh compression where a mesh can be transmitted and reconstructed progressively, that is, with increasing levels of detail. This enables the rendering of the 3D model in progression where the finer details of the model can be processed in a cumulative fashion.

The information contained in a mesh is generally divided into two categories: the geometry information, which is the position of each vertex of the mesh in the 3D Euclidean space and the connectivity or topological information, which describes the incidence relations between the mesh vertices. Since the geometric information comprises a dominant part of the mesh, most recent algorithms focused on its efficient compression. Complete reviews, summarizing work on mesh compression can be found in [AG05, PKK05, MLDH15].

6.1.1 Related Results

Fourier analysis has been used extensively in many signal processing areas. By projecting the data into the frequency domain, one can retrieve a good approximation of the original signal with only a few Fourier coefficients. A very prominent application is the JPEG [Wal91] image compression method based on the closely related 2D Discrete Cosine Transform.
Karni and Gotsman [KG00] proposed a generalization of the Fourier basis on discrete graphs in order to compress mesh vertex positions. This is achieved by projecting the coordinate vectors onto the orthonormal basis obtained from the spectral decomposition of the combinatorial Laplacian of the shape. For smooth meshes, most of the signal energy is contained in the low frequencies of the mesh spectrum and hence, the coefficients corresponding to the lower frequencies are sufficient to build a good approximation of the original mesh. Ben-Chen and Gotsman [BCG05] proved that for certain geometric models, spectral compression is optimal and is equivalent to Principal Component Analysis.

The idea of using a representative basis for approximating a mesh has been explored in detail in multiple prior works. [KG01] proposed to use a fixed basis independent of the mesh connectivity. [SCOIT05] proposed a geometry-aware basis that considers both the connectivity and the geometry of the mesh for mesh compression. Mahadevan [Mah07] replaced the manifold harmonics by a diffusion wavelet bases and showed an improvement in compression performance. This was attributed to the rich multi-scale nature of the wavelet basis.

Given a basis, a plain spectral truncation of the signal in that basis is a fairly simplistic method for representation. Instead, sparse approximation techniques have been proposed and have become very popular. The basic idea is to estimate a given signal as a sparse linear combination of a large pool of constituent vectors - called a dictionary. These vectors, or atoms, are selected such that the coefficients of representation are sparse. The rationale is that high dimensional signals generally possess intrinsic structures that are better represented in a lower-dimensional linear subspace. Although these dictionaries have traditionally been populated with complete orthogonal bases, redundant or overcomplete dictionaries allow a greater flexibility in design by better capturing the intrinsic characteristics of a signal.

The main difficulty with sparse algorithms is the availability of a rich representative dictionary. This seems trivial for signals defined over regularly and consistently sampled domains, like images and speech, but it is not straightforward to extend the idea to non-flat domains like meshes of surfaces in 3D or general graphs. The use of redundant representations for mesh representation and compression have started to emerge in [PM05, TFV06, KAW13, ZQ14]. We extend the ideas discussed in these papers by choosing the eigenfunctions of a data-aware operator as the constituents of a large overcomplete dictionary to represent the mesh.

6.1.2 Contribution

In this chapter, we introduce a Schrödinger operator for spectral approximation of meshes representing surfaces in 3D. The operator is obtained by modifying the Laplacian with a potential function which defines the rate of oscillation of the harmonics on different regions of the surface. We design the potential using a vertex ordering scheme which modulates the Fourier basis of a 3D mesh to focus on crucial regions of the shape having high-frequency structures and employ a sparse approximation framework to maximize compression performance. The combination of the spectral geometry of the Hamiltonian in conjunction with a sparse approximation approach outperforms existing spectral compression schemes.
6.2 Background

6.2.1 Graph Laplacian

Let \( G = (\Pi, \Upsilon) \) be an undirected graph of \( n \) vertices \( \Pi = \{\pi_i\}_{i=1}^n \) representing a sampled version of a manifold \( M \). Let the graph edges be equipped with nonnegative weights \( \{w_{ij}\}_{i,j=1}^n \), defining the weighted adjacency matrix \( W \) of the graph as

\[
[W]_{ij} = \begin{cases} w_{ij}, & \text{if } (i, j) \in \Upsilon, \\ 0, & \text{otherwise}. \end{cases}
\]

(6.1)

The diagonal vertex degree matrix \( A \) is defined as

\[
[A]_{ii} = a_{ii} = \sum_j w_{ij}.
\]

(6.2)

The unnormalized graph Laplacian is defined as the \( n \times n \) matrix \( L = A - W \). For properties of the Laplacian, the reader is referred to [MACO91].

The combinatorial graph Laplacian is constructed by solely considering the connectivity of the mesh, where the edge weights are defined as \( w_{ij} = 1 \). Therefore, the degree matrix \( A \) is populated with the valence of each vertex. While other geometric discretizations of the Laplacian on graphs exist [PP93], the combinatorial Laplacian is used in this chapter, since the mesh topology can be efficiently encoded.

The discrete manifold harmonics are then obtained by solving the spectral decomposition of the combinatorial Laplacian

\[
L\Phi = \Phi\Lambda.
\]

(6.3)

Here, \( \Phi \in \mathbb{R}^{n \times n} \) is the matrix of eigenvectors where each column \( \phi_k \) is one eigenvector and \( \Lambda \) is the diagonal matrix of eigenvalues where each element \( \lambda_k \) is one eigenvalue.

6.2.2 Spectral Mesh Compression

Given a complete basis \( \{\varphi_i\}_{i=0}^\infty \) on \( M \), any function \( f \in L^2(M) \) can be expressed as

\[
f = \sum_{i=1}^\infty \langle f, \varphi_i \rangle_M \varphi_i = \sum_{i=1}^\infty \hat{f}_i \varphi_i,
\]

(6.4)

where \( \hat{f}_i \) is the \( i \)-th (manifold) Fourier coefficient of \( f \). Since the manifold harmonics form a complete basis, Karni and Gotsman [KG00] proposed to use them for spectral mesh compression. Considering the mesh coordinate functions \( X, Y, Z \) as functions defined on the vertices of the mesh, the basic idea of spectral mesh compression is to compute the Fourier transform of the coordinate functions and truncate the high-frequency coefficients. Thus, if \( u \) is a coordinate
function, it can be approximated using the graph Laplacian decomposition as
\[ u \approx \sum_{i=1}^{K} (u, \phi_i) G \phi_i \tag{6.5} \]

with \( K \ll n \) and \( (u, \phi_i) G = \phi_i^T u \). By using the graph connectivity information and constructing the manifold harmonics as a representative basis, the geometric information of the mesh can be encoded efficiently through the obtained coefficients. Figure 6.1 illustrates spectral reconstructions as applied to a toy example of a 2D curve.

Figure 6.1: Approximation of a planar curve by simple truncation of the LBO and the proposed basis (Hamiltonian). The potential function for the Hamiltonian is defined by the error between the curve and its LBO truncated approximation. By biasing the 1D harmonics with this potential, the reconstruction with the Hamiltonian can be seen to preserve finer details of the contour for the same number of coefficients.

Simple truncation as showed in eq. (6.5) uses a restrictive assumption of only focusing on the lower frequencies and is analogous to low-pass filtering of the signal. In general, the lower frequencies encapsulate most of signal energy and the reconstructed mesh tends to preserve the global features of the original. However, local geometry and fine details of the mesh corresponding to high frequencies are generally missing and require a much larger support for their preservation if a truncation approach is followed.

In the next section we promote a more pragmatic approach of sparsity where the data itself searches for its best constituents (frequencies) with the objective of attaining sparsity in a certain basis of representation. This leads to an improved compression strategy.

**6.2.3 Sparse Approximation of Mesh Coordinates**

As motivated in the last section, classical methods are based on the premise that signals are best represented using only the first few components of a rich orthonormal basis. The concept of sparsity provides an alternative perspective for representation.
Let consider a graph $G$ and $D \in \mathbb{R}^{n \times m}$ a normalized overcomplete ($m \gg n$) dictionary containing $m$ atoms $d_i \in \mathbb{R}^n$. We aim to approximate any given signal $u$ on $G$ by

$$u = D\alpha = \sum_{i=1}^{m} d_i \alpha_i,$$

(6.6)

with $\alpha = [\alpha_1, \ldots, \alpha_m]^T$ the coefficient representation of the input signal $u$ with respect to the dictionary $D$. In order to achieve significant reduction in storage we should assume that the number of non-zero elements of the coefficient vector $\alpha$ should satisfy $\|\alpha\|_0 = k \ll n$. Thus, the sparse approximation of the signal can be obtained by solving the sparse coding problem

$$\min_{\alpha} \|u - D\alpha\|_2^2$$

s.t. $\|\alpha\|_0 = k$.

(6.7)

Let us be given a multiple channels signals $U \in \mathbb{R}^{n \times c}$, the new coefficient matrix is designated by $\Gamma = [\alpha_1, \ldots, \alpha_c]^T$ with $U = D\Gamma$. The new sparse approximation is obtained by solving the simultaneous sparse approximation

$$\min_{\Gamma} \|U - D\Gamma\|_F^2$$

s.t. $\|\alpha_1\|_0 = \ldots = \|\alpha_c\|_0 = k$;

(6.8)

where $\| \cdot \|_F$ denotes the Frobenius norm. In our mesh compression configuration, the input signal is defined by the mesh coordinates such that $U = [X, Y, Z]$.

Since sparse coding solution is a combinatorial NP-hard problem, well known relaxations are generally used [MZ93, PRK93]. In this chapter Simultaneous Orthogonal Matching Pursuit algorithm [TGS06] is used for sparse approximation of the mesh geometry. Pursuit algorithms are based on a greedy approach of solving for the optimization in (6.8) by incrementally selecting atoms from the dictionary $D$ that minimize the residual error. The orthogonal matching pursuit is one such way of picking the atoms where at each stage of the selection, the residual error vector is orthogonal to the atoms already selected in the support and hence will not be chosen again. Simultaneous OMP is a scheme of atom selection such that multiple signals have the same support in the dictionary $D$, i.e. simultaneously solving three sparse problems by imposing a strict similar support constraint.

The success of a sparsity based algorithm depends on the availability of a representative dictionary. However, developing dictionaries for the representation of functions defined over graphs is a non-trivial task, since they do not possess a fixed structure as in Euclidean domains. As a result, elements composed from fixed spectral bases have been used for populating the atoms of the dictionary [KAW13].

The manifold harmonics can be used because of their stability and compactness, that is, low frequencies contain most of the signal energy. However, fine local structures are not well represented using this basis due to the global nature of their support. In [ZQ14], it is shown
that a dictionary constructed from spectral graph wavelets [HVG11] show better compression performance as compared to the standard Laplacian, since it encapsulates fine details and some dominant high-frequency structures of the mesh. However, since the locality of the basis cannot be controlled, the wavelet dictionaries are highly redundant, yielding large dictionaries which enforce higher compression rates. These shortcomings motivate the need for finding a basis which can be modulated in a data-dependent manner. This will lead to an optimal local-global structure trade-off, thereby requiring a smaller cardinality of representation. In the next section we borrow an operator from quantum mechanics which has precisely the aforementioned properties.

### 6.3 Schrödinger Operator for Spectral Mesh Compression

#### 6.3.1 Definition

We will refer here to the Hamiltonian operator $H$ acting on a scalar function $f \in L^2(\mathcal{M})$ as

$$ Hf = -\Delta_M f + \mu V f, \quad (6.9) $$

where $V : \mathcal{M} \rightarrow \mathbb{R}$ is a potential function and $\mu \in \mathbb{R}$.

In this discrete setting, the basis defined by the Hamiltonian is obtained by solving

$$ H\psi_i = (L + \mu V)\psi_i = E_i \psi_i \quad (6.10) $$

with $\{\psi_i\}_{i=1}^n \in \mathbb{R}^n$. Here $L$ denotes the previously described graph Laplacian, and $V$ a diagonal matrix that is defined by the potential scalar function values at vertex $\pi_i \in \Pi$. Since $V$ only modifies the diagonal of the sparse Laplacian, the Hamiltonian is also a sparse matrix with the same non-zero entries. Thus, there is no increase in the computational cost of the decomposition compared to that of the Laplacian.

The Hamiltonian operator can improve the compression performance by modifying the harmonics in order to emphasize designated regions of interest. We propose a method for choosing a potential function which does not require any additional encoding. We construct a dictionary based on the eigendecomposition of both the Laplacian and the Hamiltonian that can focus on difficult reconstruction areas of the harmonics. Thus, by designing high vibrations in selected regions of the shape, our dictionary is much less redundant than the wavelets proposed in [Mah07], has a better ability to encode high frequency details and achieves better compression performance.

#### 6.3.2 Potential design

Consider a mesh (graph) $M = \{\Pi, \mathcal{V}\}$ with $|\Pi| = n$ and the coordinates matrix $U$. Given the Laplacian eigenvectors matrix $\Phi \in \mathbb{R}^{n \times n}$, one can design a fixed dictionary $D_L$ composed of the full harmonics basis matrix $D_L = \Phi$ and solve the simultaneous sparse coding problem of
\[ \tilde{U} = D_L \Gamma \approx U. \]

Then, a \( L_2 \) norm reconstruction error \( \epsilon(\pi_i) = \| \pi_i - \tilde{\pi}_i \|_2 \) can be obtained at each vertex of the mesh. This vertex error profile over the mesh provides an indication of difficult regions that can be enhanced through the potential.

Since a fixed potential must be used to avoid additional encoding, we permute the arbitrary indexing of the mesh according to this error. The vertices are sorted in ascending order such that vertices having small indexes correspond to points with a small error while vertices with the larger index correspond to regions with higher distortion in approximation. It can be done trivially in \( O(Y) \) complexity and has no influence on the mesh itself since the ordering has no physical meaning.

Given the Hamiltonian \( H = L + \mu V \), we propose to use a fixed potential matrix defined as

\[ V = \text{diag}(1, \ldots, n), \tag{6.11} \]

normalized such that \( \| V \|_F^2 = \sum_i^n V_{ii}^2 = 1 \). We illustrate the influence of a linear potential in one dimension in figure 6.2. Since we sorted the indexes according to the error, a designed hierarchical energy of the potential is defined over the shape while the potential encoding itself is avoided. At the decoder side, the Hamiltonian can be built using the mesh connectivity (Laplacian) and the encoded scalar \( \mu \) coupled with the fixed linear potential \( V \) described above.

![Figure 6.2: Zero potential (left up) and its corresponding harmonics (right up). Linear potential for different parameter \( \mu \) (left middle and bottom) and their corresponding first eigenfunctions (right middle and bottom). The Hamiltonian eigenfunctions focus on the low potential areas without neglecting other regions for higher energies.](image)

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6.3.3 Dictionary Construction

We construct a dictionary built from the eigendecomposition of both the Laplacian and the Hamiltonian to benefit from their global and local properties. The potential is defined according to the representation error of the basis obtained from the Laplacian as described in the previous section. We encode multiple constants \( \mu \) in order to obtain a multi-resolution of the basis. The regularization constants are found via a direct search on a given domain.

Thus, our dictionary can be obtained as:

\[
D_S = [\Phi, \Psi_{\mu_1}, \ldots, \Psi_{\mu_S}], \tag{6.12}
\]

where the sub-dictionary \( \Psi_{\mu_i} \in \mathbb{R}^{n \times n} \) is the matrix of eigenvectors of the Hamiltonian \( L + \mu_i V \) and \( \Phi = \Psi_0 \). The constant \( \mu_i \) is obtained by solving

\[
\min_{\mu_i} \min_{\Gamma} \| U - D_i \Gamma \|_F^2 \quad \text{s.t.} \quad \| \alpha_1 \|_0 = \ldots = \| \alpha_c \|_0 = k, \tag{6.13}
\]

The algorithm is summarized in Algorithm 6.1. Given a compression ratio requirement, the number of atoms is calculated according to the formulas elucidated in Section 6.4.2.

**Algorithm 6.1 Algorithm for sparse approximation**

**Input**: Mesh connectivity \( \Upsilon \), mesh coordinates \( U \) and compression ratio \( k \)

**Output**: Sparse coding \( \{ \alpha_i \}_i \) and coefficients \( \{ \mu_j \}_j \)

1. Compute the pointwise error \( \epsilon(\pi_i) = \| \tilde{U}(\pi_i) - U(\pi_i) \|_2 \) where \( \tilde{U} = \Phi \Gamma \) is obtained from (6.8);
   Permute the vertices according to the sorting of the error \( \epsilon \);
   Build constant potential \( V \) as in (6.11) and set \( j = 0 \);

2. do
   3. \( j = j + 1 \);
      Find \( \mu_j \) minimizing (6.13) using \( D_j = [\Phi, \Psi_{\mu_1}, \ldots, \Psi_{\mu_j}] \);

4. while Decrease in representation error > \( \epsilon \);

6.3.4 Discussion

Algorithm 6.1 is designed to take advantage of the two principle components of our contribution: sparsity and data-dependent basis. The potential design enumerated in section 6.3.2 alters the Laplacian eigenfunctions to focus on error-prone regions of the shape. The extent to which such an alteration must be enforced is encoded in the coefficients: \( \{ \mu_j \}_{j=1}^K \) which are again sequentially optimized in algorithm 6.1. The final dictionary obtained comprises of the regular Laplacian appended with these optimized Hamiltonians. The results in section 6.4 demonstrate that this provides a distinct improvement in shape-reconstruction errors.

Another advantage of our approach is that the potential design is based on mesh connectivity information alone. The vertex re-ordering enables us to encode information about the error-
prone regions of the shape, which are encoded in the eigenvectors of the Hamiltonian. This re-ordering scheme avoids any secondary encoding of information and hence provides a distinct gain in saving of information units for compression.

6.4 Experimental Results

6.4.1 Evaluation Metric

In order to measure the loss resulting from an estimated approximation, Karni and Gotsman [KG00] used a visual metric that captures well the visual difference between the original mesh \( M = \{ \Pi, \Upsilon \} \) and its reconstruction \( \tilde{M} = \{ \tilde{\Pi}, \tilde{\Upsilon} \} \). The measure is a linear combination of the RMS geometric distance between corresponding vertices in both models and a visual metric capturing the smoothness of the reconstruction. The error \( \epsilon \in \mathbb{R}^n \) at each vertex is defined as

\[
\epsilon_M(\tilde{\pi}_i) = \frac{1}{2n} \left( \| \pi_i - \tilde{\pi}_i \|_2 + \| GL(\pi_i) - GL(\tilde{\pi}_i) \|_2 \right). \tag{6.14}
\]

The visual metric \( GL \) is defined as

\[
GL(\pi_i) = \pi_i - \sum_{j \in \mathcal{N}(i)} l_{ij}^{-1} \pi_j \sum_{j \in \mathcal{N}(i)} l_{ij}^{-1} \tag{6.15}
\]

with \( \mathcal{N}(i) \) is the set of indexes of the neighbors of vertex \( i \), and \( l_{ij} \) is the geometric distance between vertices \( i \) and \( j \). A global representation error is obtained by summing \( \epsilon_M \) over the mesh vertices.

6.4.2 Compression Ratio

The compression ratio calculation is obtained as a ratio of the net information before and after the dictionary encoding [ZQ14]. If each coordinate takes up to \( k \) bits, then for a mesh of \( n \) vertices, the total uncompressed information is \( 3nk \). Now, assuming that the dictionary \( D \in \mathbb{R}^{m \times n} \) is known in advance, or can be constructed from the connectivity information of the mesh, on both the encoder and decoder sides, let \( n_d \) be the total number of atoms each taking \( k_d \) bits to encode each coordinate function, making the total information equal to \( 3n_d k_d \). The information required to store the indexes of the coefficients which is given by \( \min(m, n_d \lceil \log_2 m \rceil) \). The compression ratio is given as

\[
C.R. = \frac{3n_d k_d + \min(m, n_d \lceil \log_2 m \rceil)}{3nk}. \tag{6.16}
\]

The \( \min \) function is used since it can be more efficient to represent the selected atoms with a bit vector of size \( m \) instead of the indexes themselves. The compression ratio in the coefficient truncation scheme is given by

\[
C.R. = \frac{n_d}{n}, \tag{6.17}
\]
since only the ordered coefficients must be encoded. The compression ratio of the Hamiltonian dictionary can be easily extended by adding $n_{\mu}k_{\mu}$ to the numerator of (6.16), with $n_{\mu}$ the number of regulation coefficients and $k_{\mu}$ the number of bits required to encode each one of them.

### 6.4.3 Shape partition

Spectral methods, including the one proposed in this chapter are hinged on the eigendecomposition of a large matrix. This $O(n^3)$ time complexity operation can be computationally demanding especially when the number of points is large. Therefore, as motivated in [KG00], we resort to mesh partitioning, where we segment a mesh into smaller constituents and compress each segment independently. We use the METIS [KK98] package for fast graph partitioning and segmentation. Therefore, the time complexity can be seen as linear in the number of partitions.

### 6.4.4 Results

Figures 6.3, 6.5 and 6.4 show a visual comparison of the shape approximation results. We propose two visualizations. The first row present a regular reconstruction with the three different methods for a fixed compression ratio. The second row shows a profile of the error plot over the original mesh to highlight regions of erroneous representation. Clearly the MHB has a fairly large error profile over the surface. The results with the spectral graph wavelets show an improvement as compared to the manifold harmonics. However, the sparse approximation with the basis obtained from the Hamiltonian shows a distinct positive difference as compared to the other two methods both in the reconstruction and error profiles. Figures 6.6, 6.7 and 6.8 show...
Figure 6.4: Horse model (boxed mesh) composed of 19248 vertices. (Top) Shape reconstruction for a compression ratio of $4 : 10$ using dictionaries composed of the MHB, MHB+SGW and MHB+Hamiltonian (from left to right). (Bottom) Reconstruction error using the proposed spectral bases.

Figure 6.5: “The devil lies in the details.” The boxed frame on the left is the original shape. The center and right figures show sparse approximations obtained using the eigenfunctions of the standard Laplacian and the Hamiltonian operators respectively, using a compression ratio of 1:10. The global Laplacian eigenfunctions, also called manifold harmonics fail to capture the structure in the fine details. The approximation using the proposed framework Hamiltonian (figure on the right) preserves this significant fine structure for the same compression ratio.
compression results of our method compared with other spectral techniques on different shapes. We present results according to three methods. First with plain truncation of the Manifold Harmonic Basis (MHB) as suggested in [KG00]. Then MHB with sparse coding i.e. using the S-OMP algorithm (MHB-SOMP) on the manifold harmonics dictionary. Third, Spectral graph wavelets with sparse coding (MHB+SGW-SOMP) using dictionaries defined with the harmonics and the graph wavelets as presented in [ZQ14]. Finally, the method presented in this chapter (MHB+H-SOMP). We can see that our algorithm shows a considerable improvement in compression performance by generating smaller errors over the entire span of compression requirements for different shapes. We used 32 bits as for single bit-precision in the computation of compression ratio.

Figure 6.6: Reconstruction error as a function of the compression ratio for the seahorse model (2194 vertices).
Figure 6.7: Reconstruction error as a function of the compression ratio for the wolf model (4344 vertices).

Figure 6.8: Reconstruction error as a function of the compression ratio for the centaur model (15768 vertices).
Chapter 7

Hamiltonian for shape matching

The task of matching pairs of shapes lies at the core of many shape analysis tasks and plays a central role in operations such as 3D alignment and shape reconstruction. While rigid shape matching has been well studied in the literature, non-rigid correspondence remains a difficult task even for nearly isometric surfaces. When dealing with rigid objects, it is sufficient to find the rotation and translation that aligns one shape to the other [CM91]. Therefore, the rigid matching problem amounts to determining only six degrees of freedom. At the other end, matching when non-rigid deformations are involved often requires dealing with more degrees of freedom.

In order to perform matching between shapes we propose here to review some common spectral methods for establishing correspondence based on the eigendecomposition of the LBO and explore Hamiltonian properties for performance enhancement.

7.1 Spectral signatures

Signatures based on the eigendecomposition of the LBO are widely used for shape matching. The general idea is to embed two shapes one would like to compare into an Euclidean space by computing their point-wise signatures and then finding the correspondences by a nearest neighbor approach.

Manifold Harmonics Signature

[Rus07] proposed the global point signature, a dense shape descriptor constructed from the spectral decomposition of the LBO $\{\phi_i(x), \lambda_i\}_{i=0}^\infty$ by using eigenfunctions scaled by the eigenvalues

$$GPS(x) = \left(\frac{\phi_1(x)}{\sqrt{\lambda_1}}, \frac{\phi_2(x)}{\sqrt{\lambda_2}}, \ldots, \frac{\phi_Q(x)}{\sqrt{\lambda_Q}}\right),$$

at each point $x$ on the manifold. In this case, sign ambiguity, the possible multiplicity of the spectrum, and non-isometric deformations make this descriptor sensitive for shape matching tasks. Next, we will try to use the empirical observation that only the first few eigenfunctions of the Laplacian are similar, up to a sign, to those computed for a nearly isometrically deformed shape, a property we will refer to as stable eigenfunctions. Thus, one can try to match shapes by minimizing the distances defined between the first eigenfunctions. Given a sign sequence
\( s_i \in \{ \pm 1 \} \) for each eigenfunction, the signature \( J(x) \) has the form

\[
J(x) = (s_1 \phi_1(x), s_2 \phi_2(x), \ldots, s_N \phi_N(x)).
\] (7.2)

Similar signatures were used, for example, in [SK15, DK11].

**Heat and Wave Kernel Signature**

There are descriptors that are constructed by considering diffusion kernel at each point adding a virtual time \( t \), for example,

\[
K_t(x, x) = \sum_{i=1}^{\infty} e^{-\lambda_i^t} \phi_i^2(x).
\] (7.3)

The HKS descriptor [SOG09] at each point on the surface is defined by sampling \( K_t \) at different times. It can be interpreted as the amount of heat at a surface point \( x \in M \) after a diffusion of a delta profile at time \( t \). There are two drawbacks for the HKS. The first is that it is acting as a low-pass filter on the surface, rendering only macroscopic properties of the shape that are not suitable for high precision matching tasks. The second is that despite the fact that sign ambiguity of the LBO eigenfunctions is solved, symmetries cannot be resolved by this signature.

Instead of considering at the diffusion of a particle on the manifold, a different physical model of a quantum particle whose behavior is governed by the Schrödinger equation was considered in [ASC11]. The solution is derived from a particular setting of the diffusion kernel of (7.3) where a band pass filter is applied. Then, a high dimensional vector can be constructed in a similar way and is referred to as the Wave Kernel Signature or WKS. Typically, WKS exhibits oscillatory behavior and has better localization properties compared to HKS, but at the same token it tends to produce noisy matches and symmetries are still indistinguishable.

### 7.2 Functional correspondence

In many scenarios, the matching results obtained by applying spectral signatures require some refinement. This is due to non-isometric transformations and noise that make the LBO basis incompatible when computed independently for two different surfaces. [OBCS+12] proposed a way to avoid direct representation of correspondences as maps between shapes using a functional representation.

Let the map \( \tau : M \rightarrow N \) be a bijection between two surfaces \( M \) and \( N \). Then, for any function \( f : M \rightarrow \mathbb{R} \), we can reconstruct the function \( h : N \rightarrow \mathbb{R} \) as \( h = f \circ \tau^{-1} \). Given bases on the two surfaces, we can represent \( f \) as a row vector \( a \) with coefficients \( a_i \), and equivalently, \( h \) as a row vector \( b \) with coefficients \( b_i \). There exists a linear mapping between the two eigenspaces where the functional correspondence can be written as \( a = bC \). Here, \( C \) is independent of \( f \) and \( h \) and is completely determined by the bases and the map \( \tau \). The transformation matrix \( C = c_{ij} \) can be interpreted as the orthonormal rigid alignment matrix between the representation of the shapes in their basis spaces.

Given a set of \( n \) corresponding constraint functions, we can stack their respective corresponding coefficients and obtain the relation \( B = CA \), where constraints can be defined as
invariant descriptors, distance functions or indicator functions. Using rank-$k$ approximation of the matrix $C$, if $k \leq n$ a resulting linear problem can be solved using simple least squares method that is then projected onto an orthonormal space.

For isometric shapes, if the bases have a simple spectrum, we would have $c_{ij} = \pm \delta_{ij}$. In more realistic scenarios, shapes of the same object in different poses are usually nearly isometric and $C$ would be sparse and have a funnel-shaped structure [PBB+13].

### 7.3 Hamiltonian properties for shape matching

In order to obtain efficient and meaningful spectral signatures and corresponding refinement algorithms, we need to ensure the compactness, stability and descriptiveness of the isometric invariant basis we use.

**Invariance.** The Laplace-Beltrami Operator is defined in terms of the metric tensor which is invariant to isometries. For intrinsic potential function $V$, the resulting Hamiltonian would also be isometric invariant.

**Compactness.** Compactness means that scalar functions on a shape should be well approximated by using only a small number of basis elements. From Theorem 3.2 and as a generalization of the Laplacian, the global support and compactness hold for a bounded (low) potential.

**Descriptiveness.** The LBO eigenvalues can be related to frequency. Similarly, energies of the Hamiltonian eigen-system relate to the number of oscillations on the manifold. Theorem 3.1 demonstrates that the modes corresponding to small eigenvalues of the Hamiltonian defined with a positive potential, encapsulate higher frequencies, even when localized, compared to the modes of the regular LBO. At the other end, highly oscillating eigenfunctions can be used to represent fine details of the shape that can be crucial for shape matching. The Hamiltonian enforces different oscillations in designated regions, allowing for better matching of those regions as shown in Figure 7.1. The eigenfunctions will tend to oscillate more in regions with low potential compared to regions with high potential. Hence, it will be more descriptive than the LBO.

**Discriminativeness.** The quality of a signature and the convergence quality of the different refinement frameworks depend on the descriptiveness of the kernel on the manifold. The LBO heat kernel is analog to a Gaussian kernel on the manifold. Therefore, it sometimes fails to express fine details of the shape’s structure and delicate attributes and is sensitive to intrinsic symmetries. Intuitively, one can see that the diffusion kernel derived from the Hamiltonian seems to diffuse according to the potential that could remove possible ambiguities such as symmetries. For example, given an asymmetric potential, a diffusion kernel has the ability to remove symmetric ambiguities that are present in the LBO as shown in Figure 7.2.

**Stability.** Deformations of non-rigid shapes and articulated objects can stretch the surface. In such cases, the LBO eigendecomposition of the two shapes will be different. We could compensate for such local metric distortions by carefully designing a potential. High potential at high distortion regions would lead to lower values of the eigenfunctions those areas (3.8). Such a potential will reduce the discrepancy between corresponding eigenfunctions at least for
Figure 7.1: Left to right: The geodesic distance from the left knee (white sphere) defines the potential. The first figure shows the distance map in the descriptor space defined by the six first signed eigenfunctions as in (7.2). A point on the left toe (white sphere) is compared to all other points on the same shape using the LBO (center) and the Hamiltonian (right). Since the eigenvectors of the Hamiltonian are more descriptive in this region, they lead to better matching precision.

Figure 7.2: Left to right: Potential on the shape, GPS Kernel at every point derived from the regular Laplacian and one derived from the Hamiltonian. It is obvious that the symmetric ambiguity between the paws is resolved.
the low frequencies ones, as shown in Figure 7.3 where the potential $V$ at vertex $m_i = \tau^{-1}(n_i)$ is defined as

$$V(m_i) = \max \left\{ \frac{A_M(m_i)}{A_N(n_i)}, \frac{A_N(n_i)}{A_M(m_i)} \right\} \quad (7.4)$$

with $A_M(m_i)$ and $A_N(n_i)$, the area at vertex $m_i$ on mesh $M$ and $n_i$ on the second mesh $N$ respectively. Also, by removing possible multiplicities in the spectrum, asymmetric potentials increase stability since rotation ambiguities in sub-spaces of the spectral domain could be resolved.

Figure 7.3: Two nearly isometric meshes with high potential (hot colors) in large distortion regions (a), functional maps matrix $C$ of the LBO (b) and the Hamiltonian (c).

The choice of a potential is application dependent. While high potential values are required for focusing the basis to designated regions, global analysis of the shape would call upon lower potential energy. For the shape matching task, since the distortion of the surface is unknown, stability cannot be handled straightforwardly. However, two main spectral shape correspondence problems can still be addressed. Intrinsic symmetry ambiguities can be easily solved with asymmetric potentials. Highly descriptive potential enforces rapid oscillations and allows better distinction of similar and close areas on the surface.
Among the few stable intrinsic invariants that can be extracted from the geometry, we will use the stable first eigenfunctions of the LBO and geodesic distances. Other extrinsic information such as photometry can also be integrated into the Hamiltonian through its potential.

7.4 Experimental evaluation

We tested the proposed basis and compared its matching performances to that of the LBO basis as applied to pairs of triangulated meshes of shapes from the TOSCA dataset [BBK08] and the SCAPE dataset [DAPKST05]. The TOSCA data set contains densely sampled synthetic human and animal surfaces, divided into several classes with given ground-truth point-to-point correspondences between the shapes within each class. The SCAPE data set contains scans of real human bodies in different poses. The evaluation method used is described in [KLF11] where the distortion curves describe the percentage of surface points falling within a relative geodesic distance from what is assumed to be their true locations. The potential energy was fixed using (3.13). Symmetries were not allowed in all evaluations. Note that we assume that the sign ambiguity of the first eigenfunctions generating the potential is resolved [SK14b].

Figure 7.4 compares the two operators by matching diffusion kernel descriptors derived from the corresponding eigenfunctions. The diffusion on the shape using the Hamiltonian as the diffusion operator is more descriptive than regular diffusion that cannot resolve the symmetries. Also, it would be natural to compute the WKS signature when the Schrödinger equation is governed by a given effective potential. As intrinsic positive potential we use the normalized sum of the four first nontrivial eigenfunctions of the LBO on each shape, adding a constant of minimal value in order to obtain a non-negative potential. This way only the intrinsic geometry of the shape is involved in defining the Hamiltonian operator.

![Figure 7.4: Evaluation of the diffusion kernels signatures matches on the TOSCA and SCAPE datasets.](image)

In case we know which regions are prone to elastic distortions, like joints and stretchable skin in articulated objects, we could suppress the effect of those regions in our matching procedures by using an appropriate potential as a selective mask. Figure 7.5, compares the operator
with and without potential by matching the spectral signatures computed by the framework of [SK15]. The potential we used is the local area distortion when comparing the meshes of two corresponding objects, as seen in Figure 7.3. The descriptiveness of the potential and the localization of the harmonics lead to more accurate matching results.

![Geodesic Error](image)

Figure 7.5: Evaluation of the spectral signature matches on the TOSCA and SCAPE data-sets.

To investigate the performances of the Hamiltonian with photometric textures used as potential, we present in Figure 7.6 the results of different signatures matching with a dalmatian texture defined for the “Dogs” shapes from the TOSCA data set.

![Photometric data](image)

Figure 7.6: Evaluation of the descriptors matches on the “Dogs” benchmark from the TOSCA dataset with dalmatian texture.

The Iterative Closest Spectral Kernel Maps (ICSKM) [SK14a] is a refinement algorithm similar in spirit to the iterative refinement process of [OBCS+12], which given an initial partial or dense map tries to recover dense and accurate matching between two given shapes. Based on LBO basis, it presents state of the art results for axiomatic shape matching. Figure 7.7 compares the regular ICSKM algorithm working with the Laplacian eigenspace and the Hamiltonian method when we provided one, two, or three landmark points, that were randomly selected from the ground-truth mapping. The texture used in these examples is the geodesic distance from

![Geodesic Error](image)

Figure 7.7: Comparing the regular ICSKM algorithm working with the Laplacian eigenspace and the Hamiltonian method when we provided one, two, or three landmark points.
the landmark points. Note that again we use only the geometry of the shapes in order to refine
the match between them using the new basis. Observe that with just three landmark points, the
algorithm outperforms previous state of the art methods.

Figure 7.7: Evaluation of the ICSKM algorithm with different landmark initialization matches
on the TOSCA dataset. We used geodesic distances from given landmark points as intrinsic
geometric texture on the shapes.
Chapter 8

Conclusion

A classical operator was adopted from the field of quantum mechanics and adapted to manifolds and shape analysis problems. Functional and spectral properties of the Hamiltonian operator were presented and compared to the popular Laplacian operator often used in spectral shape analysis procedures. Features and texture properties can be incorporated into the new operator to obtain a descriptive and stable basis that provides a powerful domain of operation for shape analysis. Spectral properties of the operator such as basis conduct according to the potential, optimality in functional representations, diffusion process, nodal sets and robustness were explored as long as its discretization.

We demonstrated the effectiveness of methods constructed from the decomposition of the Hamiltonian on several shape analysis tasks. First we proposed a general optimization method for solving variational problems involving the Hamiltonian operator. Based on perturbation of eigenvectors theory, gradient with respect to the potential is obtained allowing its integration to common optimization solvers. The technique was tested on the data representation problem where we showed that important improvement are possible compared to the Laplacian counterpart.

The Hamiltonian can also be used for a reweighted least squares variant of the $\ell_1$ regularization of the Dirichlet energy giving a physical flavor to the compressed modes basis. Also, we presented a general efficient optimization framework for eigendecomposition of matrices composed from sparse and low rank matrices using the Sherman–Morrison–Woodbury formula. We showed that our techniques lead to a significantly more efficient and stable numerical solver.

We also introduced the Schrödinger operator for spectral mesh compression. We use this operator to modify the standard manifold harmonics of the 3D surface by emphasizing the role of regions with errors that emerge as a result of compression with classical harmonics. We maximize compression performance by constructing meaningful dictionaries from this basis in a sparse approximation framework and show a distinct improvement from previous spectral techniques.

Last but not least, the operator has been adapted to the shape matching problem where prior data such as anchor points, photometry and perturbed areas were taken in account through the potential. The Hamiltonian ICSKM present considerable a improvement over its LBO
counterpart in shape correspondence refinement by using geodesic distances from scarce seed points obtained on the mesh.

Various directions for future research include exploration of the operator on other shape analysis tasks such as partial shape matching where occluded areas could be refined via the potential. Also general weakly supervised manifold learning problems could be solved using the presented operator. The use of the Schrödinger operator for generic graph structures or discrete manifolds is an uncharted territory that can lead to interesting spectral embedding.
Appendix A

Appendix

A.1 Proof of Theorem 2.

Let us be given the Hamiltonian operator $H = -\Delta + V$.

Recall the Courant–Fischer min-max principle; see also [ABK15a] and [Bre10] Problems 37 and 49. We have for every $i \geq 0$,

$$E_{i+1} = \max_{\operatorname{codim} \Lambda = i} \min_{f \neq 0} \left\{ \frac{\|\nabla f\|_2^2 + \|\sqrt{V}f\|_2^2}{\|f\|_2^2} \right\}, \quad (A.1)$$

That is, the min is taken over a linear subspace $\Lambda \subset H^1(S)$ with $H^1(S)$ is the Sobolev space $\{ f \in L^2, \nabla f \in L^2 \}$ of co-dimension $i$ and the max is taken over all such subspaces.

Set $\Lambda_0 = \{ f \in H^1(S); \langle f, \psi_k \rangle = 0, k = 1, 2, ..., i \}$, so that $\Lambda_0$ is a subspace of co-dimension $i$.

By A.1 we have that for all $f \neq 0, f \in \Lambda_0$

$$\frac{\|\nabla f\|_2^2 + \|\sqrt{V}f\|_2^2}{\|f\|_2^2} \geq \frac{E_{i+1}}{\alpha}, \quad (A.2)$$

and thus

$$X_0 = \min_{f \neq 0} \frac{\|\nabla f\|_2^2 + \|\sqrt{V}f\|_2^2}{\|f\|_2^2} \geq \frac{E_{i+1}}{\alpha}. \quad (A.3)$$

On the other hand, by A.1,

$$E_{i+1} \geq X_0. \quad (A.4)$$

Combining A.3 and A.4 yields $\alpha \geq 1$. \hfill \Box
A.2 Diffusion kernel of the Hamiltonian

In order to solve the diffusion equation, we first need to find the fundamental solution kernel $K(x, y, t)$ to the Dirichlet problem that yields the heat equation

$$
\begin{cases}
\partial_t K(x, y, t) = H(K(x, y, t)) \\
\lim_{t \to 0} K(x, y, t) = \delta_y(x).
\end{cases}
$$

(A.5)

Recall that for $V = 0$ we return to the regular LBO diffusion case.

Suppose that $H$ has a eigendecomposition $\{\psi_i, E_i\}_{i=1}^\infty$. In that case, we can write

$$
K(x, y, t) = \sum_i \langle K(x, y, t), \psi_i(x) \rangle_M \psi_i(x) = \sum_i \alpha_i(t) \psi_i(x),
$$

(A.6)

and from the linearity of $H$ we have

$$
\begin{cases}
H(K(x, y, t)) = \sum_i \alpha_i(t) H(\psi_i) = \sum_i -E_i \alpha_i(t) \psi_i \\
\partial_t K(x, y, t) = \sum_i \partial_t \alpha_i(t) \psi_i.
\end{cases}
$$

(A.7)

Since $\langle \psi_i, \psi_j \rangle_M = \delta_{ij}$, we have from (A.5) and (A.7)

$$
\partial_t \alpha_i(t) = -E_i \alpha_i(t),
$$

(A.8)

that leads to

$$
\alpha_i(t) = \alpha_i(0) e^{-E_i t}.
$$

(A.9)

As $\delta_y(x) = \sum_i \psi_i(y) \psi_i(x)$, from the initial condition $K(x, y, 0) = \delta_y(x)$, we obtain

$$
K(x, y, 0) = \sum_i \alpha_i(0) \psi_i(x) = \sum_i \psi_i(y) \psi_i(x) = \delta_y(x)
$$

$\Leftrightarrow \alpha_i(0) = \psi_i(y) \quad \Rightarrow K(x, y, t) = \sum_i e^{-E_i t} \psi_i(x) \psi_i(y).
$$

(A.10)

The solutions have the form

$$
u(x, t) = \int_\mathcal{M} u_0(y) K(x, y, t) da(y).
$$

(A.11)
Bibliography


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המוטב התאמה לפוטנציאל, ומחלקת התהליך דיפוזיה המתקבל על ידי דיפוזיה המשוואת החום עם אופרטור מוצע. בנוסף, אנא הוכיחים שהבסיס הנובע מפרוקה המילטוני להמילטוניאן אופטימלי ייצוג פונקציות עם גרדינט חוסם באזורים עם פוטנציאל גבוהי יותר מאשר התرمز הכורח. לבהל התלות בפונטציאלים האופרטור אורגנמי למצבجرائم תיר פרפורציות ניתן על בזירות הווה לשפוטציאלים עצמים. יסקטריפיציה של פונטציאלים מתחבצל בזירות פיתוח.

בלאלאנטימי סופי.

ה씬 והו מתניע ב_measure של האופרטור לתחילה את קסם يعد פונקציה פוטנציאלית פלרטור ביון יאצטניון ועיבור את האופרטור ההמילטוני. ואנו הוריות 是否 רגרדינט של פונקציה המוגדרת על ידי פונקציה המוגדרת על ידי דיפוזיה השונות בין הלפיטריה של פוטנציאל הפרפורציות של פוטנציאל הפסוה.

לפי סימון של מספרים של האופרטור. בתחילה השיטה האופטימיזציה לפתור בעיות וריאציות העולמות את האופרטור ההמילטוני. אנא הוכיחים חישוב גרדינט של פונקציית מטרהל הפוטנציאל בעזרת התורה הפרפורציות של פונקציה עצまいים.

בגללהתלות בפוטנציאל, האופרטור גם מפגין רגישות לפרפורציות על המתרבים והן לפוטנציאל עצמו. דיסקרטיזציה של הפוטנציאל מתקבלת בעזרת פיתוח לאלמנטים סופיים.

בתחילה השיטה אופטימיזציה לפתור בעיות וריאציות העולמות את האופרטור ההמילטוני. אנא הוכיחים חישוב גרדינט של פונקציית מטרהל הפוטנציאל בעזרת התורה הפרפורציות של פונקציה עצまいים.

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לפי סימון של מספרים של האופרטור. בתחילה השיטה האופטימיזציה לפתור בעיות וריאציות העולמות את האופרטור ההמילטוני. אנא הוכיחים חישוב גרדינט של פונקציית מטרהל הפוטנציאל בעזרת התורה הפרפורציות של פונקציה עצ십시ים.

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הקומבינטורית הלא פורמלית של מציאת התאמות שנקלעת לבעיה של מיפויפונקציות במדים קטנים. עלפניו, אופרטור לפלס בלטרמינרא Coinbase בחירת טבעית לניתוח צורה. הוא נבחר בשיטה של אי-קומבינטוריות וتأكد שהאסטרים משני והאינווארינטיים. בבסיס הופיעה האופרטור מוגדר, ולא ניתן לעיין ב.IsNullOrאויות. האופרטור בהרבה שיטות בהופעה של הפרוצדור סופטיים "מדוייקים" וapiaが出 שעה במדים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיין בмедицин סופטיים, וחישון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיין ב.weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה בweather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטор מגדיר, ולא ניתן לעיינה בweather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים סחופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיينة ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיينة ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיينة ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוצדור שהאופרטור מגדיר, ולא ניתן לעיינה ב(weather לחיסון מדוייקים ספופטיים."שבט במדים" ושתי וחיסונאיבועים בשיטה של הפרוכ
תקציר

תחום ניתוח צורות התפתח באופן מהיר בדרכים רבות. השיפור הרב והanmarית ייחודה מתבצע באמצעות פתרונות פרקטיים בעיבוד התוכןorado הצורות. המכניקות המאובנות הדרגת אחר מהלאישה ספקטרליות וממשיכות ל谁 גם הוא. השלוחת של צורות מגדירה יותר, כשנתקלים עם צורות שונות, ניתן להשתמש בתפקידים מתמטיים של גאומטריה דפרנציאלית ואנליזה ספקטרלית%A

כתוצאה מכך, כלים מתקifestyles ממגדירים את תהליך אלו במתמטיקה של צורות. ניתן להשתמש בתוכן של צורות, גם בטיעון של צורות, כדי להבין את התוכן של צורות באופן יותר התוכן של צורות. ניתן להשתמש בתוכן של צורות, גם בטיעון של צורות, כדי להבין את התוכן של צורות באופן יותר התוכן של צורות. ניתן להשתמש בתוכן של צורות, גם בטיעון של צורות, כדי להבין את התוכן של צורות.

דרד את המ.requireות על עקרון זה כדי להתייחס ולราชการ ולהNSError עקרונות העקביים של צורות. עקרון העקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של יישום, וتكلم עקביים של צורות עקביים זה עניין של 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טכניון - מדעי McA - מ.ס. תזה - 2017


תודות

אני רוצה להודות למנהלה של ברויס ולשותפיי על העזרה והדרכה بالمחלקה העובדה.

א. אני רוצה להודות למנהלה,zheimer, בונים ולאשחיות בין שיל על התמיכות והאמון התמידי.

אני מודה לסטודנטים על התמיכת בכיספף עדות בرشתמי.
על אופרטורים אליפטיים וэрוהת לא
כשייחות

תיעוד על מחקר

לשם מילוי החלק של הדרישות לעזרת התאר
מגיסטר לתמישים ימיים מכדיי המвшейב

יוני שוקרן

הווש לטנני הכנינו --- מרכז טכנולוגיה לישראל
אביר התuttle'ה היפע, מאי 2017
על אופרטורים אליפטיים וזורות לא קשיחות

יוני شוקרוב