DIFFUSION MAPS FOR MANIFOLDS WITH BOUNDARY

by

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Abstract

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Diffusion maps and other graph Laplacian based methods in machine learning have a long history of pointwise consistency results. This work provides rigorous formulation for diffusion maps for manifolds with boundary. We show that different normalizations of graph Laplacians are asymptotically unbiased for manifolds with boundary when viewed in a variational sense. A crucial component of this work is the introduction of semigeodesic coordinates, which allow for more systematic treatment of boundary points. In particular, we derive new pointwise expansions which relate first-order error to the mean curvature of the boundary of $\mathcal{M}$.

Chapter 1: Introduction

The analysis of large, high-dimensional data sets is an integral part of the modern sciences. While classical linear methods such as regression and principal component analysis are an indispensable tool in modern data analysis, these methods often lack the ability to analyze nonlinear features. Since data is often highly correlated, it can be reasonable to assume that data resides on a low-dimensional submanifold $\mathcal{M}$ of the sample space $\mathbb{R}^d$. Important properties of the data can then be inferred through estimating geometric properties of the underlying manifold.

One of the most successful methods for inferring geometric properties of $\mathcal{M}$ in practice is through estimation of the Laplace-Beltrami operator. The Laplace-Beltrami operator Δ is a linear operator acting on smooth functions of $\mathcal{M}$ and is a generalization of the familiar Laplacian on $\mathbb{R}^d$:

$$\Delta f = -\sum_{i=1}^{d} \frac{\partial^2 f}{\partial x_i^2}.$$

Many important properties of the geometry of a manifold can be expressed through the behavior of the Laplace-Beltrami operator. The Laplace-Beltrami operator can be estimated on data through means of a *graph Laplacian.*

Given a finite sample of data $\{x_i\}_{i=1}^N \subseteq M$, the *graph Laplacian* associated to the data is an $N \times N$ matrix which approximates the Laplace-Beltrami operator on the data set by interpreting input vectors $\overrightarrow{f}$ as the vector whose entrees are $f(x_i)$ for some smooth function f. That is,

$$L\overrightarrow{f} \approx \Delta f$$

on the data set $\{x_i\}_{i=1}^N$.

Graph Laplacians were originally used to study finite graphs in the area of *spectral graph theory* [12]. Their first use in machine learning was through *spectral clustering*[30][26] in which eigenvectors of graph Laplacians were used to cluster nonconvex data sets. Graph Laplacians were also used in dimensionality reduction through *Laplacian Eigenmaps*[3]. Initially, the connection between graph Laplacians and the Laplace-Beltrami operator was informal and intuitive. Through a series of ensuing *consistency results* this notion was formalized by showing that the graph Laplacian converges to the Laplace-Beltrami operator in the limit of large data. It was first shown in [4] that graph Laplacians on uniformly distributed data converged to the Laplace-Beltrami operator. This convergence was generalized in [22] and then extended to more general distributions through *Diffusion Maps* in [13]. These results were later improved upon and summarized in [21].

The present work is a generalization of pointwise consistency results for graph Laplacians on manifolds with boundary. Manifolds with boundary are a natural extension of the notion of a manifold, and have been considered in several previous works[13][21]. Although manifolds with boundary are a natural class of objects to study, several issues arise when generalizing consistency proofs to manifolds with boundary. In addition to various technical issues with known proofs, it has been observed in [13] that the pointwise consistency results blow up for points near the boundary. In the present work, we resolve several long-standing technical issues with known proofs of convergence, and show that the pointwise blow up can be resolved by viewing the Laplacian in a weak sense.

We show that the associated kernel averaging operators Δ_ϵ corresponding to the graph Laplacians converge in a weak sense to the Laplace-Beltrami operator with Neumann Boundary conditions. That is, for smooth functions f, ϕ on a compact Riemannian manifold $\mathcal{M}$:

$$\int_{\mathcal{M}} \phi \Delta_\epsilon f \; d \text{ Vol} = \int_M \phi \Delta f \; d \text{ Vol} + \mathcal{O}(\epsilon)$$

$$= \int_M \langle \text{grad } \phi, \text{grad } f \rangle_g \; d \text{ Vol} + \mathcal{O}(\epsilon).$$

We show that by interpreting the Laplace-Beltrami operator in this weak sense, one can generalize the proof of consistency to hold for manifolds with boundary. This generalization requires the use of a particularly appropriate class of coordinates on $\mathcal{M}$, which are well-adapted for points near the boundary of $\mathcal{M}$. These coordinates are also used to derive asymptotic estimates of boundary integrals on $\mathcal{M}$.

There are three main applications to the results of this thesis. First, the consistency results proven here prove pointwise consistency of a new mesh-free numerical scheme for numerically solving elliptic boundary value problems on Riemannian manifolds with boundary. Second, the convergence to Neumann Laplacian gives rigorous proof to the empirically observed phenomenon of the graph Laplacian returning Neumann functions in practice. Third, the use of weak convergence allows for a connection to Sobolev space treatment of Diffusion maps, which is the appropriate function space to solve PDEs.

The results of this thesis are ultimately about the connection between graph Laplacian estimators in machine learning and the Laplace-Beltrami operator on a Riemannian manifold. Therefore, we begin with a brief overview of both the Laplace-Beltrami operator as well as graph Laplacians in order to contextualize the significance of our findings.

1.1 The Laplacian on a Riemannian Manifold

Fundamentally, the results of this thesis are about estimating the Laplace-Beltrami operator on a Riemannian manifold. The Laplace-Beltrami operator $\Delta : C^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$ is a second order differential operator defined on a manifold $\mathcal{M}$ with Riemannian metric g. In local coordinates, the Laplacian is defined by:

$$\Delta f = -\text{div grad } f = -\frac{1}{\sqrt{\det g}}\frac{\partial}{\partial x^i}\left(g^{ij}\sqrt{\det g}\frac{\partial f}{\partial x^j}\right).$$

Much of the geometry defined by the Riemannian metric g can be determined by the properties of the Laplace-Beltrami operator. The eigenfunctions of Δ are a generalization of a Fourier basis in the sense that they are the unique orthonormal basis of smooth functions

$\{\phi_i\}_{i=1}^{\infty}$ which minimize the following energy functional:

$$E(f) = \int_{\mathcal{M}} \langle \text{grad } f, \text{grad } f \rangle_g \; d \text{ Vol}.$$

1.2 Graph Laplacians

Graph Laplacians are a type of discrete approximation to the Laplace-Beltrami operator. In the context of machine learning, they are examples of so-called *kernel methods*[29]. Given a finite sample of points $\{x_n\}_{n=1}^{N} \subseteq \mathbb{R}^d$ in some high dimensional data space $\mathbb{R}^d$, together with a *kernel function* $k : \mathbb{R}^+ \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, one can construct for each fixed $\epsilon \in \mathbb{R}^+$ the $N \times N$ *kernel matrix* or *gram matrix* K_ϵ whose entries correspond to:

$$(K_\epsilon)_{ij} = k(\epsilon, x_i, x_j).$$

One then may also construct for each fixed $\epsilon > 0$ the diagonal $N \times N$ *degree matrix* D_ϵ by:

$$(D_\epsilon)_{ii} = \sum_{j=1}^{N} k(\epsilon, x_i, x_j).$$

Using D_ϵ and K_ϵ, one then may form three different standard Graph Laplacians. The *unnormalized graph Laplacian* L_{un} is given by:

$$L_{\text{un}} = D_\epsilon - K_\epsilon.$$

The *normalized graph Laplacian* is given by:

$$L_{\text{norm}} = I - D_\epsilon^{-\frac{1}{2}} K_\epsilon D_\epsilon^{-\frac{1}{2}}.$$

And the *random walks graph Laplacian* is given by:

$$L_{\text{rw}} = I - D_\epsilon^{-1} K_\epsilon.$$

The variable ϵ is the so-called *bandwidth* of the kernel, and is empirically seen as a parameter which controls fitting. In general, smaller values of ϵ provide a more accurate output, but too small value of ϵ relative to the data causes overfitting.

Graph Laplacians were first successfully used in machine learning as a framework for *spectral clustering*[30][26] where they were empirically seen to be particularly effective in clustering nonconvex datasets. The intuitive justification behind these results is that the graph Laplacians approximate the Laplace-Beltrami operator Δ on a Riemannian manifold. This intuition was later made rigorous through a sequence of several papers in which it was shown that graph Laplacians "converge" to the Laplace-Beltrami operator in the limit of large data. In order to rigorously show that the finite dimensional matrix L converges to the infinite-dimensional operator Δ, we next discuss the notions of convergence in probability. This will be done through a discussion of the *bias* and *variance* of graph Laplacian estimators.

1.3 Bias and Variance of Graph Laplacians

In order to make the intuition of convergence of graph Laplacians rigorous, we now outline some key ideas from the treatment of the bias and variance of Graph Laplacians. Informally, the convergence results concerning the *variance* show how the discrete graph Laplacian L acting on finite data converges to a continuous averaging operator Δ_ϵ acting on functions on an infinite manifold. However, even in the limit of large data, the resulting continuous operator does not converge to the Laplacian, but is an approximation based on the bandwidth parameter ϵ. The Bias analysis then shows that in the limit as the bandwidth approaches zero, the kernel averaging operator Δ_ϵ approaches the Laplace-Beltrami operator.

In order to discuss these results, we assume that $k : \mathbb{R}^+ \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a smooth kernel function with bandwidth $\epsilon > 0$ and *exponential decay* in extrinsic distance. That is, there exists $\alpha, \beta > 0$ such that for all $x, y \in \mathbb{R}^d$,

$$k(\epsilon, x, y) \leq \alpha e^{\frac{-\beta \|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}}.$$

Since the new results of the thesis concern the bias of graph Laplacians, we will focus mostly on the bias analysis. However, we will first discuss some intuition behind the variance analysis to see the connection between discrete graph Laplacians and the continuous operators that will be studied in this work.

1.3.1 Variance

In order to discuss convergence of the discrete operator L to a continuous operator Δ_ϵ, we represent the data is identically and independently distributed (i.i.d) random variables. With the setup above, we let $\{X_i\}_{i=1}^N$ be i.i.d. random variables $X_i : \mathcal{M} \to \mathbb{R}$ supported on $\mathcal{M} \subseteq \mathbb{R}^d$. This use of random variables allows us to analyze the discrete estimator L in terms of the continuous object $\mathcal{M}$. We then may express the kernel matrix on N data point $K_{N,\epsilon}$ as a linear operator on the space of measurable functions on $\mathcal{M}$ by

$$K_{N,\epsilon} f(x) = \frac{1}{N} \sum_{i=1}^{N} k(\epsilon, X_i, x) f(X_i).$$

That is, we perform the same operation as in the graph Laplacian, except instead of considering points $x_i \in \mathcal{M} \subseteq \mathbb{R}^d$, we consider distribution functions X_i which correspond to the sampling distribution.

Similarly, the degree matrix on N data points now corresponds to a real-valued function on $\mathcal{M}$ by:

$$D_{N,\epsilon}(x) = \frac{1}{N}\sum_{i=1}^{N} k(\epsilon, X_i, x).$$

The estimator $K_{N,\epsilon}f$ can then be shown to converge in probability to the kernel averaging operator $\mathcal{K}_\epsilon : C^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$

$$\mathcal{K}_\epsilon f(x) = \int_{\mathcal{M}} k(\epsilon, x, y) f(y) q(y)\ d\ \mathrm{Vol}$$

where q is the sampling density on $\mathcal{M}$. More specifically, for each $\delta > 0$, the measure of the set of points of $\mathcal{M}$ on which $K_{N,\epsilon}f$ and $\mathcal{K}_\epsilon f$ differ by more than δ converges to zero as $N \to \infty$. In an identical sense, the operator $D_{N,\epsilon}$ converges in probability to the operator $\mathcal{K}_\epsilon 1$ on $\mathcal{M}$.

Using this correspondence, we now can associate kernel averaging operators on the dimension-m manifold $\mathcal{M}$ to each graph Laplacian:

$$\lim_{N\to\infty} \frac{1}{N\epsilon^{m+2}} L_{\mathrm{un}} \overrightarrow{f} = \lim_{N\to\infty} \frac{1}{\epsilon^{m+2}} (D - K)\overrightarrow{f} = f\mathcal{K}_\epsilon 1 - \mathcal{K}_\epsilon f.$$

$$\lim_{N\to\infty} \frac{1}{N\epsilon^{2}} L_{\mathrm{norm}} \overrightarrow{f} = \lim_{N\to\infty} \frac{1}{\epsilon^{2}} (I - D^{-\frac{1}{2}} K D^{-\frac{1}{2}})\overrightarrow{f} = \mathcal{K}_\epsilon 1 - \mathcal{K}_\epsilon f$$

$$\lim_{N\to\infty} \frac{1}{N\epsilon^{2}} L_{\mathrm{rw}} \overrightarrow{f} = \lim_{N\to\infty} \frac{1}{\epsilon^{2}} (I - D^{-1} K)\overrightarrow{f} = f - \mathcal{K}_\epsilon^{-\frac{1}{2}} 1 \left(\mathcal{K}_\epsilon \left(\mathcal{K}_\epsilon^{-\frac{1}{2}}(1) f\right)\right).$$

Each of these normalizations have been used in different contexts. In the case of the unnormalized graph Laplacian, we note that the presence of the term ϵ^{m+2} means that in order to have convergence, one needs to know the dimension m of $\mathcal{M}$ *a priori*.

One of the observations of the present work is that using this correspondence, the scalar quantity $\overrightarrow{\phi}^\top K_\epsilon \overrightarrow{f}$ corresponds to the integral

$$\overrightarrow{\phi}^\top K_\epsilon \overrightarrow{f} \Leftrightarrow \int_{x\in\mathcal{M}} \phi(x) \int_{y\in\mathcal{M}} k(\epsilon, x, y) f(y) q(y)\ d\ \mathrm{Vol}(y)\ d\ \mathrm{Vol}(x).$$

Through this correspondence, we then may observe that all the tools necessary for studying the weak behavior of the Laplace Beltrami operator can be estimated using the graph Laplacian.

Historical Context

We remark that the statements in the previous section are written for the purpose of developing intuition between the discrete objects used in machine learning and the continuous kernel averaging operators discussed in this work. The corresponding results appear differently in the literature in the form of *consistency* proofs which combine convergence in bias as well as variance. Historically, the rigorous treatment of bias and variance of the graph Laplacians began with [4] studying pointwise consistency of graph Laplacians with uniform sampling distribution. This work was later extended in [22] and [31] which improved the analysis of the variance term. The bias analysis of the random walks graph Laplacian was considered in [13], which developed a crucial analysis of the bias which held for more general sampling densities. In [21] the work was synthesized and extended, showing pointwise consistency of each graph Laplacian under a more general class of manifolds.

1.3.2 Bias

We now turn our attention to the analysis of the *bias* of the kernel averaging operators associated to the various graph Laplacians in the previous section. In other words, convergence results of this type show that the kernel averaging operator corresponding to the associated graph Laplacian is pointwise a first-order approximation to the Laplace-Beltrami operator on $\mathcal{M}$. In other words, for any $f \in C^\infty(\mathcal{M})$, and any $x \in \mathcal{M}$, we have:

$$\Delta_\epsilon f(x) = \Delta f(x) + \mathcal{O}(\epsilon).$$

In the discussion of variance, we saw that the kernel averaging operators corresponding to the kernel and degree matrix were constructed from the kernel averaging operator

$$\mathcal{K}_\epsilon f(x) = \int_{\mathcal{M}} k(\epsilon, x, y) f(y) q(y) \; d\,\mathrm{Vol}(y).$$

Therefore obtaining a first-order approximation to Δ is obtained through obtaining an asyptotic expansion of the kernel operator $\mathcal{K}_\epsilon$. One of the first examples of such a result is given in [13]:

Lemma 1.3.1. *[13] Let k be a radially symmetric, exponentially decaying kernel function on $\mathbb{R}^d$ and let $\mathcal{K}_\epsilon$ be the associated kernel integral operator acting on smooth functions of $\mathcal{M} \subseteq \mathbb{R}^d$, then:*

$$\mathcal{K}_\epsilon f(x) = m_0 f(x) q(x) + \epsilon^2 \frac{m_2}{2} \left(\omega(x) f(x) q(x) - \Delta f q(x) \right) + \mathcal{O}(\epsilon^3).$$

where m_0 and m_2 are constants and $\omega(x)$ is a function depending on curvature.

The crux of the argument of this result comes from the fact that $\mathcal{K}_\epsilon$ is an *asymptotically local operator*, that is, that the value of $\mathcal{K}_\epsilon$ at a point is determined up to order ϵ^2 by a small metric ball $B^{\mathcal{M}}_{\epsilon^\gamma}(x)$ in $\mathcal{M}$, where γ is a fixed constant. Next, one performs an asymptotic expansion of $\mathcal{K}_\epsilon$ inside of a special set of coordinates called *Riemannian normal coordinates.* Inside of these Riemannian normal coordinates, the metric ball $B^{\mathcal{M}}_{\epsilon^\gamma}(x)$ is a radially symmetric domain. This radial symmetry allows for significant cancellation of problematic terms in the expansion and allows us to extract the Laplacian. Another important aspect of this result is that it holds *uniformly* in the variable ϵ. That is, if ϵ is small enough, then the result holds for all $x \in \mathcal{M}$ simultaneously.

In summary, two significant properties of $\mathcal{M}$ and $\mathcal{K}_\epsilon$ are necessary to prove this result. First, one must localize $\mathcal{K}_\epsilon$ to a small metric ball in $\mathcal{M}$. Then, one must expand $\mathcal{K}_\epsilon$ on the small metric ball inside of a normal coordinate chart and use symmetry of the metric ball in coordinates. If $\mathcal{M}$ is a compact manifold without boundary, then the result holds uniformly in ϵ for all $x \in \mathcal{M}$.

1.4 Manifolds with Boundary

Although manifolds with boundary have long been considered in the bias analysis of kernel averaging operators, the pointwise proof of consistency is less straightforward. The first intuitive issue, which was addressed in [13], is that metric balls in $\mathcal{M}$ which intersect the boundary of $\mathcal{M}$ are no longer radially symmetric.

Several attempts have been made to resolve this lack of symmetry. In [13] and later [34], the authors attempted to prove the following claim:

Claim 1.4.1. *Let k be a radially symmetric, exponentially decaying kernel function on $\mathbb{R}^d$ and let $\mathcal{K}_\epsilon$ be the associated kernel integral operator acting on smooth functions of $\mathcal{M} \subseteq \mathbb{R}^d$, then for all points distance ϵ^γ or less from $\partial\mathcal{M}$:*

$$\frac{1}{\epsilon^m}\mathcal{K}_\epsilon f(x) = m_0^\epsilon(x) f(x_0) + \epsilon m_1^\epsilon(x)\frac{\partial f}{\partial \eta}(x_0) + \mathcal{O}(\epsilon^2)$$

where $\gamma \in (0,1)$, x_0 is the closest boundary point to x and where $\frac{\partial f}{\partial \eta}(x_0)$ is the inward facing normal derivative of f, $m_0^\epsilon(x)$ and $m_0^\epsilon(x)$ are bounded functions of x and ϵ.

The proof attempted to emulate the proof of Lemma 1.3.1 by reflecting the image of a metric ball in coordinates along all directions except the inward-facing direction. Intuitively, this would lead to cancellation of many terms except for the inward-facing direction. This attempted proof, while potentially correct in spirit, did not address several significant geometric technicalities.

One of the ways around this, which was observed in [21], is to weaken the result of 1.3.1 to hold nonuniformly across $\mathcal{M} \setminus \partial\mathcal{M}$. That is for each point $x \in M$, there is a small enough $\delta(x)$ such that the result holds, but $\delta(x)$ shrinks to zero as one approaches the boundary. As long as the ball centered at x does not contain any boundary points, the proof is the same as for the case when $\mathcal{M}$ has no boundary. While this result was sufficient for the purposes in [21], the nonuniformity of the result causes issues with a weak-sense analysis of the Laplacian.

1.4.1 Semigeodesic Coordinates

One of the main results of this thesis is the resolution of the previous issues through the introduction of *semigeodesic coordinates.* Semigeodesic coordinates are a well-known set of coordinates which are well-adapted for computation on Riemannian submanifolds and boundaries. We show that uniformly across $\mathcal{M}$, one can localize $\mathcal{K}_\epsilon$ in such a way that all points of $\mathcal{M}$ will be contained in either a normal coordinate chart or a semigeodesic coordinate chart whose size is parameterized by ϵ. In this manner, the results we obtain are uniform in the variable ϵ.

Intuitively, these semigeodesic coordinate charts are shaped like cylinders, which are radially symmetric in all regions except for the inward pointing direction. Thus, they allow for almost as much cancellation as in regular Riemannian normal coordinates. The tradeoff for using these coordinates is that the notion of area and volume is distorted by *mean curvature* of the boundary of ∂M in $\mathcal{M}$. In this work we are able to derive an explicit relationship between error and mean curvature of the boundary. In particular, we prove the following proposition:

Proposition 1.4.2. *Let x be a point sufficiently close to the boundary of $\mathcal{M}$. If ϵ is sufficiently small, then*

$$\frac{1}{\epsilon^m}\mathcal{K}_\epsilon f = m_0^\partial(x) f(x)$$

$$+ \epsilon m_1^{\partial}(x) \left(\langle \text{grad } f, \eta \rangle_g + \frac{m-1}{2} H(x) f(x) \right)$$

$$+ \mathcal{O}(\epsilon^2).$$

where $m_0^{\partial}(x)$ and $m_1^{\partial}(x)$ are bounded functions of x and $H(x)$ is the mean curvature at x of the hypersurface ∂M_{b_x} of points distance b_x from ∂M.

This result is similar to Claim 1.4.1 in [13]. However, we notice that there is an additional term which involves the mean curvature $H(x)$. Additionally, this expansion still contains terms of order ϵ, which cause the extracted kernel averaging operator Δ_ϵ to diverge pointwise for points near the boundary. We then resolve this issue by showing that although it diverges pointwise, it converges when interpreted in a weak sense. A crucial aspect of the result in the weak-sense analysis is that the result holds uniformly in the variable ϵ and resolves the technical issues of [13].

In addition to this new expansion, we also make use of semigeodesic coordinates to perform asymptotic estimations of boundary integrals. Since in general boundaries are of measure zero in $\mathcal{M}$, one can never expect to sample data from the boundary. The next lemma shows that through the use of a kernel function, we can relate boundary integrals to an integral over the entire manifold. This crucially allows us to analyze the behavior of the weak-sense integral for boundary points.

Theorem 1.4.3. *Let $\mathcal{M}$ be a compact submanifold of $\mathbb{R}^d$ and let $\epsilon > 0$ be sufficiently small. Let $k : \mathbb{R} \to \mathbb{R}$ be an exponentially decaying function, and let $b_x : M \to \mathbb{R}$ denote the distance of a point x to the boundary of $\mathcal{M}$. Then we have:*

$$\frac{1}{\epsilon} \int_{x \in \mathcal{M}} k\left(\frac{b_x^2}{\epsilon^2}\right) f(x) q(x) \; d \text{ Vol} = \overline{m}_0 \int_{x \in \partial\mathcal{M}} f(x) q(x) \; d \text{ Vol}_{\partial}$$

$$+ \epsilon \overline{m}_1 \int_{x \in \partial\mathcal{M}} f(x) q(x) H(x)$$

$$- \langle \text{grad } f, \eta \rangle_g \; d \text{ Vol}_{\partial\mathcal{M}} + \mathcal{O}(\epsilon^2)$$

where $\overline{m}_0 = \int_0^\infty k(u)\, du$ *and* $\overline{m}_1 = \int_0^\infty uk(u)\, du$ *and* $H(x)$ *is the mean curvature of* $\partial\mathcal{M}$ *at* $x \in \partial\mathcal{M}$*.*

Intuitively, this shows that boundary integrals can be approximated by taking the integral over a thin (but not measure zero) strip of points in $\mathcal{M}$ near the boundary. In doing so, each term picks up an addtional ϵ.

Putting these two results together, we prove the main result that shows the consistency of the bias term of the unnormalized Laplacian.

Theorem 1.4.4. *Let* $\mathcal{M}$ *be a compact Riemannian manifold with boundary isometrically embedded into* $\mathbb{R}^d$ *via* $\iota : \mathcal{M} \hookrightarrow \mathbb{R}^d$*. Let* $\mathcal{K}_\epsilon$ *be the kernel integral operator on* $C^\infty(\mathcal{M})$ *induced by a kernel* k *and uniform distribution* $q \equiv 1$ *on* $\mathcal{M}$ *satisfying the previous conditions. Then for* $f \in C^\infty(M)$ *and test function* $\phi \in C^\infty(M)$*, we have:*

$$\frac{2}{m_2 \epsilon^{d+2}} \int_{\mathcal{M}} \phi \left(\mathcal{K}_\epsilon f - f \mathcal{K}_\epsilon 1\right)\ d\ \mathrm{Vol} = \int_{\mathcal{M}} \langle \mathrm{grad}\ \phi, \mathrm{grad}\ f \rangle_g\ \ d\ \mathrm{Vol} + \mathcal{O}(\epsilon).$$

Of particular note is the lack of boundary term in the right hand side, suggesting that the kernel integral operator converges to a Laplacian with Neumann boundary conditions. From this, we may also prove consistency of the random walks Laplacian as a corollary.

The organization of this thesis is as follows. In Chapter 2, we present known results about the bias of $\mathcal{K}_\epsilon$ for manifolds without boundary. Our approach is most similar to that in [21], however we present the proof in a different manner so as to make it easier to generalize in the case of compact manifolds with boundary.

In Chapter 3, we generalize the treatment in 2 to manifolds with boundary. In this chapter, we introduce semigeodesic coordinates and derive various comparison lemmas which allow us to derive analogous asymptotic expansions for points near the boundary. In particular, we use a classical result called the *first variation of area* to derive a connection between mean curvature and first order error of the expansion. This is a new observation to the field of manifold learning.

In Chapter 4, we use semigeodesic coordinates to derive an asymptotic estimate of boundary integrals. This result differs from the results in the previous chapter in that the asymptotic estimate holds in a larger region than a single coordinate chart. In order to derive this result, we require the asymptotic expansions of the previous chapter to hold uniformly in ϵ, which gives additional justification to the need for semigeodesic coordinates.

In Chapter 5, we put all the results developed in previous chapters together and prove the main result of this work. In particular, we show that the kernel averaging operators corresponding to the unnormalized and random walks Laplacian weakly converge to the Laplacian with Neumann boundary conditions.

Chapter 2: Bias of Diffusion Maps

2.1 Summary

In this chapter, we will review the previous consistency results for the bias of the random walks Laplacian estimator on compact manifolds without boundary. The proofs in this section were first shown in [13] and later in [21]. We present these classical results in a new way that is more easily generalized to the case of manifolds with boundary. The crux of the argument in this chapter is showing that the kernel averaging operator $\mathcal{K}_\epsilon$ may be uniformly asymptotically expanded in Riemannian normal coordinates.

2.2 Notation, Definitions, and Assumptions

For this chapter, we assume that $(\mathcal{M}, g)$ is a dimension m, compact Riemannian manifold without boundary (sometimes referred to as a *closed* manifold.) We furthermore assume that $\mathcal{M}$ is isometrically embedded into $\mathbb{R}^d$ via the embedding $\iota : \mathcal{M} \to \mathbb{R}^d$. For simplicity, we will assume that $\mathcal{M}$ is a C^∞ manifold and ι is a C^∞ embedding of $\mathcal{M}$.

We let $d\,\mathrm{Vol}$ denote the Riemannian volume measure inherited from the metric g on $\mathcal{M}$. We assume that $q : \mathcal{M} \to \mathbb{R}$ is a C^∞ probability density function corresponding to a probability measure $d\mu$ which is absolutely continuous with respect to $d\,\mathrm{Vol}$ and nowhere zero on $\mathcal{M}$.

We let $k : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ be a C^∞ function which has *exponential decay*, that is, that there exists $\alpha, \beta > 0$ such that $k(x) \leq \alpha e^{-\beta x}$ for all $x \in \mathbb{R}_{\geq 0}$. Furthermore, we assume that the first two derivatives of k also have exponential decay.

We will slightly abuse notation with regards to points in $\mathcal{M}$ and their image in the embedding ι. We use $\|x - y\|_{\mathbb{R}^d}$ to denote the distance in $\mathbb{R}^d$ between $\iota(x)$ and $\iota(y)$.Since we will be mostly working inside of normal coordinates in $\mathcal{M}$, we also make a slight abuse of notation. For any point $x \in \mathcal{M}$ and any point y in a normal coordinate chart centered at x, we use $\|s\|_g$ to denote the coordinate norm of the coordinate representative s of y. This corresponds to geodesic distance between x and y. We let $B_\epsilon^{\mathbb{R}^d}(x)$ denote the preimage $\iota^{-1}(B_\epsilon^{\mathbb{R}^d}(\iota(x))$ which is the set of points in $\mathcal{M}$ which are of extrinsic distance ϵ or less from x. We denote $B_\epsilon^{\mathcal{M}}(x)$ as a metric ball in $\mathcal{M}$ of radius ϵ centered at x.

In addition, we adopt the convention of Einstein notation, so that any algebraic terms consisting of a subscript and superscript are implied to be summed over the sum/superscript index. Since we will often distinguish sums on $\mathcal{M}$ with sums on $\mathbb{R}^d$, we adopt the convention that roman indices such as i, j, or k are taken to be summed over $1, ..., m$, while greek indices such as α, β or μ are taken to be summed over $1, ..., d$.

2.3 Asymptotic Convergence of the Kernel Averaging Operator

The main result of this chapter is a theorem originally proven by Coifman and Lafon [13] which shows pointwise convergence of a kernel averaging operator Δ_ϵ to the Laplace-Beltrami operator Δ.

Theorem 2.3.1. *For each $f \in C^\infty(\mathcal{M})$ and each $x \in \mathcal{M}$,*

$$\lim_{\epsilon \to 0} \Delta_\epsilon f(x) = \Delta f(x).$$

The proof can be divided into roughly three parts. First, we define a kernel integral operator $\mathcal{K}_\epsilon$ on $\mathcal{M}$ and show that $\mathcal{K}_\epsilon$ can be localized to a Riemannian normal coordinate chart for small ϵ. This will be referred to as the *localization step.* Next, we asymptotically expand $\mathcal{K}_\epsilon$ inside normal coordinate chart and obtain a pointwise asymptotic estimate for $\mathcal{K}_\epsilon$. This step will be referred to as the *expansion step.* Finally, we construct a *normalized* *kernel operator* $\hat{\mathcal{K}}_\epsilon$ using these pointwise estimates. This step is the *normalization step.* The normalization step allows us to extract the Laplace-Beltrami operator for general density function q.

2.3.1 The Kernel Integral Operator $\mathcal{K}_\epsilon$

For each $\epsilon > 0$, let $\mathcal{K}_\epsilon : C^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$ be defined by:

$$\mathcal{K}_\epsilon f(x) = \int_{\mathcal{M}} k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) f(y)q(y)\ d\ \mathrm{Vol}(y).$$

The next few lemmas and propositions show that if ϵ is chosen to be small enough, the operator $\mathcal{K}_\epsilon$ can be asymptotically localized to a single coordinate chart. This allows us to asymptotically expand $\mathcal{K}_\epsilon$ in coordinates. We remark that $\mathcal{K}_\epsilon$ will be localized to a ball of radius ϵ^γ for any fixed $0 < \gamma < 1$. Therefore, for the following lemmas, we assume that γ is a fixed constant between 0 and 1.

This first lemma shows that if one chooses ϵ small enough, then the preimage of a small extrinsic ball is contained inside of a normal coordinate chart in $\mathcal{M}$. This shows that although the kernel averaging operator $\mathcal{K}_\epsilon$ is defined using extrinsic distance, it may be related to intrinsic distance at small scales.

Proposition 2.3.2. *There exists a* $r_\iota > 0$ *such that for any* $0 < \epsilon^\gamma < r_\iota$*, the set* $\iota^{-1}(B_\epsilon^{\mathbb{R}^d}(\iota(x)))$ *is contained inside of a normal coordinate chart.*

Proof. This follows directly from the fact that the inverse of the embedding ι onto its image is uniformly continuous. Since ι is an embedding, it is a homeomorphic onto its image and by compactness of $\mathcal{M}$, the inverse of ι is uniformly continuous. Therefore given $\mathrm{inj}(\mathcal{M}) > 0$, there exists a $r_\iota > 0$ such that for any $x, y \in \mathcal{M}$, $\|x-y\|_{\mathbb{R}^d} < r_\iota$ implies that $d_{\mathcal{M}}(\iota^{-1}(x), \iota^{-1}(y)) < \mathrm{inj}(\mathcal{M})$. □

Our goal in this section is to localize the operator $\mathcal{K}_\epsilon$ to a small intrinsic ball in $\mathcal{M}$. An obstacle to this goal is that the kernel function k is a function of extrinsic distance in

$\mathbb{R}^d$. The next Proposition shows that we can relate the intrinsic and extrinsic distance, allowing us to localize to an intrinsic ball. In order to prove the proposition, we first make use of a corollary of Theorem A and Proposition 2.3 [15] which gives global bounds on the components of the metric in normal coordinates for manifolds of bounded curvature.

Corollary 2.3.3. *If $\mathcal{M}$ is a Riemannian manifold with bounded Riemannian curvature, then there exists a $\tilde{C}_0, \tilde{C}_1 \geq 0$ such that for any normal coordinate chart of radius* inj($\mathcal{M}$) *or less,*

$$|g_{ij}| \leq \tilde{C}_0 \text{ and } |g^{ij}| \leq \tilde{C}_1.$$

We next use this corollary to show that locally the metric space structure on $\mathcal{M}$ and the metric in $\mathbb{R}^d$ are equivalent.

Proposition 2.3.4. *There exists a $C_0, C_1 > 0$ such that in any normal coordinate chart of radius* inj($\mathcal{M}$) *or less centered at x, and any point y in that chart,*

$$C_0 \|s\|_g^2 \leq \|x - y\|_{\mathbb{R}^d}^2 \leq C_1 \|s\|_g^2$$

where s is the coordinate representative of y in normal coordinates.

Proof. Let x be a point in $\mathcal{M}$, and choose a normal coordinate chart $s = (s^1, ..., s^m)$ in $\mathcal{M}$ centered at x. We then choose a normal coordinate chart in $\mathbb{R}^d$ centered at $\iota(x)$. Let $\iota(s) = (\iota^1(s), ..., \iota^d(s))$ represent the coordinate image of $\iota(y)$ in these coordinates.

In these coordinates, we have that

$$\|x - y\|_{\mathbb{R}^d}^2 = g_{\alpha\beta}^{\mathbb{R}^d}(0)\iota^\alpha(s)\iota^\beta(s). \tag{2.3.1}$$

where $\iota(s)$ is the coordinate representative of y in these coordinates.

We then perform an order-zero Taylor expansion of $\iota^\alpha(s)$ for each $\alpha \in \{1, ..., d\}$. Due to the remainder term, there exists a point $\tilde{s}$ in the domain such that

$$\iota^\alpha(s) = \iota^\alpha(0) + \frac{\partial \iota^\alpha(\tilde{s})}{\partial s^i} s^i.$$

Applying the above expansion to (2.3.1) and recalling that in these coordinates $\iota(0) = 0$, we have

$$\begin{aligned} g^{\mathbb{R}^d}_{\alpha\beta}(0)\iota^\alpha(s)\iota^\beta(s) &= g^{\mathbb{R}^d}_{\alpha\beta}(0)\left(\iota^\alpha(0) + \frac{\partial \iota^\alpha(\tilde{s})}{\partial s^i} s^i\right)\left(\iota^\beta(0) + \frac{\partial \iota^\beta(\tilde{s})}{\partial s^j} s^j\right) \\ &= g^{\mathbb{R}^d}_{\alpha\beta}(0)\frac{\partial \iota^\alpha(\tilde{s})}{\partial s^i}\frac{\partial \iota^\beta(\tilde{s})}{\partial s^j} s^i s^j. \end{aligned}$$

Since the $\mathbb{R}^d$ has no curvature, the components of the metric $g^{\mathbb{R}^d}_{\alpha\beta}$ are constant and equal to $\delta_{\alpha\beta}$. We therefore have that

$$g^{\mathbb{R}^d}_{\alpha\beta}(0) = g^{\mathbb{R}^d}_{\alpha\beta}(\iota(\tilde{s})) = \delta_{\alpha\beta}$$

and so therefore,

$$g^{\mathbb{R}^d}_{\alpha\beta}(0)\iota^\alpha(s)\iota^\beta(s) = g^{\mathbb{R}^d}_{\alpha\beta}(\iota(\tilde{s}))\frac{\partial \iota^\alpha(\tilde{s})}{\partial s^i}\frac{\partial \iota^\beta(\tilde{s})}{\partial s^j} s^i s^j.$$

The expression on the right hand side is exactly the expression for the pullback metric on $\mathcal{M}$ inherited from ι and thus,

$$\|x - y\|^2_{\mathbb{R}^d} = g^{\mathbb{R}^d}_{\alpha\beta}(0)\iota^\alpha(s)\iota^\beta(s) = g^{\mathcal{M}}_{ij}(\tilde{s}) s^i s^j. \tag{2.3.2}$$

We now note that the expression $g^{\mathcal{M}}_{ij}(\tilde{s}) s^i s^j$ is maximized by the maximum eigenvalue of the matrix with entries $g^{\mathcal{M}}_{ij}(\tilde{s})$ and minimized by the maximum eigenvalue of the matrix with entries $(g^{\mathcal{M}})^{ij}(\tilde{s})$. Since compactness of $\mathcal{M}$ implies bounded Riemannian curvature, Corollary 2.3.3 implies that there exists positive constants $\tilde{C}_0$ and $\tilde{C}_1$ such that in any normal coordinate chart of radius $\text{inj}(\mathcal{M})$ or less,

$$|g_{ij}| \leq \tilde{C}_0 \text{ and } |g^{ij}| \leq \tilde{C}_1.$$

Since the matrices with entries g_{ij} and g^{ij} are symmetric and positive definite, this implies that there exists positive bounds $\frac{1}{C_0}$ and C_1 on the largest eigenvalue of (g^{ij}) and (g_{ij}) respectively across all $\tilde{s}$ in our coordinate chart.

Hence, we have that

$$C_0 \delta_{ij} s^i s^j \leq g^{\mathcal{M}}_{ij}(\tilde{s}) s^i s^j \leq C_1 \delta_{ij} s^i s^j$$

and since $\delta_{ij} = g^{\mathcal{M}}_{ij}(0)$, we are left with

$$C_0 \|s\|_g^2 \leq g^{\mathcal{M}}_{\alpha\beta}(\tilde{s}) \iota^\alpha(s) \iota^\beta(s) \leq C_1 \|s\|_g^2 .$$

Combining these inequalities with (2.3.2), we obtain

$$C_0 \|s\|_g^2 \leq \|x - y\|_{\mathbb{R}^d}^2 \leq C_1 \|s\|_g^2 .$$

□

The following corollary shows that if ϵ^γ is chosen sufficiently small, then any point in $\mathcal{M}$ not contained in $B^{\mathcal{M}}_{\epsilon^\gamma}(x)$ has extrinsic distance greater than $C_0^{-1}\epsilon^\gamma$ from x.

Corollary 2.3.5. *If* $\epsilon^\gamma < \min\{\frac{r_\iota}{C_0}, \frac{\text{inj}(\mathcal{M})}{C_0}\}$ *then*

$$\iota^{-1}(B^{\mathbb{R}^d}_{C_0\epsilon^\gamma}(\iota(x))) \subseteq B^{\mathcal{M}}_{\epsilon^\gamma}(x).$$

and so

$$\left(\mathcal{M} \setminus B^{\mathcal{M}}_{\epsilon^\gamma}(x)\right) \subseteq \left(\mathcal{M} \setminus \iota^{-1}(B^{\mathbb{R}^d}_{C_0\epsilon^\gamma}(\iota(x)))\right).$$

Proof. Fix $x \in \mathcal{M}$ and let $\iota^{-1}(B^{\mathbb{R}^d}_{C_0\epsilon^\gamma}(\iota(x)))$ so that $d_{\mathbb{R}^d}(\iota(x), \iota(y)) < C_0\epsilon^\gamma$. Since $\epsilon^\gamma < C_0^{-1} r_\iota$, we have by Proposition 2.3.2 that $\iota^{-1}(B^{\mathbb{R}^d}_{C_0\epsilon^\gamma}(\iota(x)))$ is contained in a normal coordinate chart in $\mathcal{M}$ and thus we may apply Proposition 2.3.4 to yield:

$$C_0 \left\|s\right\|_g \leq d_{\mathbb{R}^d}(\iota(x), \iota(y)) \leq C_0\epsilon^\gamma.$$

division by C_0 yields that

$$\left\|s\right\|_g \leq \epsilon^\gamma.$$

and since the norm of s in coordinates corresponds to geodesic distance, we have that $d_{\mathcal{M}}(x, y) < \epsilon^\gamma$ and so $y \in B_{\epsilon^\gamma}(x)$. Hence $\iota^{-1}(B^{\mathbb{R}^d}_{C_0\epsilon^\gamma}(\iota(x))) \subseteq B^{\mathcal{M}}_{\epsilon^\gamma}(x)$. □

We now use Proposition 2.3.2 and Proposition 2.3.4 to show that $\mathcal{K}_\epsilon$ is asymtotically a local operator.

Proposition 2.3.6. *Let* $0 < \gamma < 1$ *and* $\epsilon^\gamma < \min\{\frac{r_\iota}{C_0}, \frac{\text{inj}(\mathcal{M})}{C_0}\}$. *For any* $z \in \mathbb{N}$,

$$\mathcal{K}_\epsilon f(x) = \int_{B^{\mathcal{M}}_{\epsilon^\gamma}(x)} k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) f(y)q(y)\ d\ \text{Vol}(y) + \mathcal{O}(\epsilon^z).$$

Proof. If $\epsilon^\gamma < \min\{\frac{r_\iota}{C_0}, \frac{\text{inj}(\mathcal{M})}{C_0}\}$, then we may apply Corollary 2.3.5 and we have that

$$\int_{\mathcal{M}\setminus B^{\mathcal{M}}_{\epsilon^\gamma}(x)} k^2\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) q(y)\, d\,\text{Vol}(y) \leq \int_{\mathcal{M}\setminus\iota^{-1}\left(B^{\mathbb{R}^d}_{C_0\epsilon^\gamma}(\iota(x))\right)} k^2\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) q(y)\, d\,\text{Vol}(y).$$

We then have that

$$\int_{\mathcal{M}\setminus\iota^{-1}\left(B^{\mathbb{R}^d}_{C_0\epsilon^\gamma}(\iota(x))\right)} k^2\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) q(y)\ d\ \mathrm{Vol}(y) \le \alpha e^{-2\beta\frac{(C_0\epsilon^\gamma)^2}{\epsilon^2}} \int_{\mathcal{M}\setminus B^{\mathcal{M}}_{\epsilon^\gamma}(x)} q(y)\ d\ \mathrm{Vol}(y)$$

$$\le \alpha e^{-2\beta\frac{C_0^2(\epsilon^\gamma)^2}{\epsilon^2}} \int_{\mathcal{M}} q(y)\ d\ \mathrm{Vol}(y)$$

$$= \alpha e^{-2\beta C_0^2 e^{2(\gamma-1)}}.$$

We then apply Cauchy-Schwarz inequality in q-weighted $L^2(\mathcal{M}\setminus B^g_{\epsilon^\gamma}(x))$ and use the above inequality:

$$\left\langle k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right), f\right\rangle^2 \le \left\langle k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right), k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right)\right\rangle^2 \langle f, f\rangle$$

$$= \langle f, f\rangle \alpha e^{-2\beta C_0^2 e^{2(\gamma-1)}}.$$

Hence, we are left with:

$$\int_{\mathcal{M}\setminus B^{\mathcal{M}}_{\epsilon^\gamma}(x)} k^2\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) q(y)\ d\ \mathrm{Vol}(y) \le \langle f, f\rangle \alpha e^{-2\beta C_0^2 e^{2(\gamma-1)}}.$$

We see that the term $\langle f, f\rangle \alpha e^{-2\beta C_0^2 \epsilon^{2(\gamma-1)}}$ is asymptotically bounded by any polynomial ϵ^z with $z \ge 1$ by making the substitution $\delta = \epsilon^{-1}$ and iterating L'Hôpital's rule z times. □

2.3.2 Asymptotic Expansion of $\mathcal{K}_\epsilon$

We begin by introducing asymtotic expansions of each of the terms in $\mathcal{K}_\epsilon$, which will then be combined to provide an asymptotic expansion of $\mathcal{K}_\epsilon$. We then show in the next section that after one applies the appropriate normalization of $\mathcal{K}_\epsilon$, one may extract an asymptotic estimator of the Laplace-Beltrami operator.

The following lemma of [35] provides an additional asymptotic comparison of extrinsic and intrinsic distance. It is proven in a similar manner to Proposition 2.3.4 except with a second order expansion. Significant cancellation also occurs through symmetries of the Riemannian curvature tensor.

Lemma 2.3.7 (Distance Comparison)**.** *In any normal coordinate chart* $s = (s^1, ..., s^m)$*, centered at* $x \in \mathcal{M}$*,*

$$\|x - y\|^2_{\mathbb{R}^d} = \|s\|^2_g - \frac{1}{12}\|\Pi(s,s)\|^2_g + \mathcal{O}(\|s\|^5_g), \tag{2.3.3}$$

where the vector s *in* $\Pi(s,s)$ *is the vector in* $T_x\mathcal{M}$ *corresponding to* s *through the exponential map.*

Proof. See [35]. □

The next useful result is the classical asymptotic expansion of the Riemannian metric in normal coordinates. It is a classical result from differential geometry first proven by Riemann.

Lemma 2.3.8 (Volume Comparison)**.** *In any normal coordinate chart* $s = (s^1, ..., s^m)$*, centered at* $x \in \mathcal{M}$*,*

$$\begin{aligned} d\ \mathrm{Vol} =& \sqrt{|\det g|}\ ds^1 \cdots ds^m \\ &= 1 - \frac{1}{6}\mathrm{Ric}(s,s) + \mathcal{O}(\|s\|^3_g) ds^1 \cdots ds^m. \end{aligned} \tag{2.3.4}$$

where, again, the vector s *in* $\mathrm{Ric}(s,s)$ *is the vector in* $T_x\mathcal{M}$ *which corresponds to* s *through the exponential map.*

Proof. See [25] □

The next lemma is an asymptotic expansion of the kernel function making use of Lemma 2.3.7.

Lemma 2.3.9. *Let $s = (s^1, ..., s^m)$ denote a system of normal coordinates in $\mathcal{M}$ centered about $x \in \mathcal{M}$. Then*

$$k\left(\frac{\|s\|_g^2 - \frac{1}{12}\|\Pi(s,s)\|_g^2 + \mathcal{O}(\|s\|_g^5)}{\epsilon^2}\right) = k\left(\frac{\|s\|_g^2}{\epsilon^2}\right)$$

$$+ k'\left(\frac{\|s\|_g^2}{\epsilon^2}\right)\frac{-\frac{1}{12}\|\Pi(s,s)\|_g^2}{\epsilon^2}$$

$$+ \mathcal{O}\left(k'\left(\frac{\|s\|_g^2}{\epsilon^2}\right)\|s\|_g^5, k''\left(\frac{\|\tilde{s}\|_g^2}{\epsilon^2}\right)\|s\|_g^8\right).$$

where $\|x-y\|_{\mathbb{R}^d} \leq \|\tilde{s}\|_g \leq \|s\|_g$.

Proof. For fixed $\epsilon > 0$, we first apply Taylor's theorem in the variable a centered about c of:

$$k\left(\frac{c+a}{\epsilon^2}\right) = k\left(\frac{c}{\epsilon^2}\right) + k'\left(\frac{c}{\epsilon^2}\right)\frac{a}{\epsilon^2} + k''\left(\frac{\tilde{c}}{\epsilon^2}\right)\frac{a^2}{\epsilon^2} \tag{2.3.5}$$

where $0 \leq \tilde{c} \leq c$.

Next, we apply Lemma 2.3.7 yielding

$$k\left(\frac{\|x-y\|_{\mathbb{R}^d}^2}{\epsilon^2}\right) = k\left(\frac{\|s\|_g^2 - \frac{1}{12}\|\Pi(s,s)\|_g^2 + \mathcal{O}(\|s\|_g^5)}{\epsilon^2}\right).$$

Substitution of $\|s\|_g^2$ in for c and $-\frac{1}{12}\|\Pi(s,s)\|_g^2 + \mathcal{O}(\|s\|_g^5)$ in for a yields:

$$k\left(\frac{\|s\|_g^2 - \frac{1}{12}\|\Pi(s,s)\|_g^2 + \mathcal{O}(\|s\|_g^5)}{\epsilon^2}\right) = k\left(\frac{\|s\|_g^2}{\epsilon^2}\right) + k'\left(\frac{\|s\|_g^2}{\epsilon^2}\right)\frac{-\frac{1}{12}\|\Pi(s,s)\|_g^2}{\epsilon^2}$$

$$+ \mathcal{O}\left(k'\left(\frac{\|s\|_g^2}{\epsilon^2}\right)\|s\|_g^5, k''\left(\frac{\|\tilde{s}\|_g^2}{\epsilon^2}\right)\|s\|_g^8\right).$$

□

The next technical lemma will also be used in the proof of the main proposition.

Lemma 2.3.10. *Suppose $k : \mathbb{R} \to \mathbb{R}$ has exponential decay, and ϵ^γ be as above. Then for any $\ell \in \mathbb{N} \cup 0$ and any $z \in \mathbb{N}$,*

$$\int_{\epsilon^{\gamma-1}}^{\infty} k(s^2)s^\ell ds \;\in\; \mathcal{O}(\epsilon^z). \tag{2.3.6}$$

Proof. We prove the first statement by induction on ℓ. If $\ell = 0$, then since k has exponential decay,

$$\left| \int_{\epsilon^\gamma}^{\infty} k(s^2)p(s)ds \right| \leq \alpha \int_{\epsilon^\gamma}^{\infty} e^{-\beta s^2} ds$$

for some $\alpha, \beta \geq 0$. Inequality (5) of [10], gives

$$\alpha \int_{\epsilon^\gamma}^{\infty} e^{-\beta s^2} ds \leq \alpha e^{-\beta \epsilon^{2(\gamma-1)}}.$$

Repeated application of L'hôpital's rule in the same manner as in the proof of Proposition 3.4.7 shows that $\alpha e^{-\beta\epsilon^{2(\gamma-1)}} \in \mathcal{O}(\epsilon^z)$. The case when $\ell = 1$ follows in a similar manner as the previous case by using u-substitution on the integral term. Suppose the statement holds for all $j < \ell$. We then have:

$$\begin{aligned} \left| \int_{\epsilon^{\gamma-1}}^{\infty} k(s^2)s^\ell ds \right| &\leq \alpha \int_{\epsilon^{\gamma-1}}^{\infty} e^{-\beta s^2} s^\ell ds \\ &= \alpha \left(e^{-\beta s^2} s^{\ell-1} \Big|_{\epsilon^{\gamma-1}}^{\infty} + \int_{\epsilon^{\gamma-1}}^{\infty} \frac{\ell-1}{2\beta} e^{-\beta s^2} s^{\ell-2} \right). \end{aligned}$$

Again, L'Hôpital's rule shows that the first term is of order $\mathcal{O}(\epsilon^z)$ and the second term is of order $\mathcal{O}(\epsilon^z)$ from the inductive hypothesis. Thus, equation (2.3.6) holds.

□

Proposition 2.3.11. *Let* $0 < \gamma < 1$ *and* $\epsilon^\gamma < \min\{\frac{\mathrm{inj}(\mathcal{M})}{C_1}, C_{\mathcal{M}}\}$. *Then,*

$$\frac{1}{\epsilon^m}\mathcal{K}_\epsilon f(x) = m_0 f(x)q(x) + \frac{\epsilon^2 m_2}{2}\Big(f(x)q(x)S(x) - \Delta(fq)(x)\Big) + \mathcal{O}(\epsilon^3) \tag{2.3.7}$$

where S *is the scalar curvature of* $\mathcal{M}$, *and*

$$m_0 = \int_{\mathbb{R}^m} k(\|s\|^2_{\mathbb{R}^m})\ ds \text{ and } m_2 = \int_{\mathbb{R}^m} k(\|s\|^2_{\mathbb{R}^m})\,\|s\|^2_{\mathbb{R}^m}\ ds.$$

Proof. We begin by fixing a point $x \in \mathcal{M}$ and applying Proposition 3.4.7. From the proof of Proposition 3.4.7, we have that $B^g_{\epsilon^\gamma}(x)$ is contained in a normal coordinate neighborhood, so we proceed by expanding in coordinates and making the substitution $s \mapsto \epsilon s$. We obtain:

$$\begin{aligned}
&\frac{1}{\epsilon^m}\mathcal{K}_\epsilon f(x) = \\
&\int_{B^{\mathbb{R}^m}_{\epsilon^{\gamma-1}}(0)} \left(k\left(\|s\|^2_{\mathbb{R}^m}\right) - \frac{1}{12}\epsilon^2 k'\left(\|s\|^2_{\mathbb{R}^m}\right)\|\Pi(s,s)\|^2_{\mathbb{R}^m} + \epsilon^6 k''\left(\|\tilde{s}\|^2_g\right)\|s\|^8_g\right. \\
&\qquad \left. + \mathcal{O}\left(\epsilon^3 k'\left(\|s\|^2_{\mathbb{R}^m}\right)\|s\|^5_{\mathbb{R}^m}\right)\right) \\
&\qquad \times \left(fq(0) + \epsilon\frac{\partial fq(0)}{\partial s^i}s^i + \epsilon^2\frac{1}{2}\frac{\partial^2 fq(0)}{\partial s^i \partial s^j}s^i s^j + \mathcal{O}(\epsilon^3\|s\|^3_{\mathbb{R}^m})\right) \\
&\qquad \times \left(1 + \epsilon^2\frac{1}{6}\mathrm{Ric}(s,s) + \mathcal{O}(\epsilon^3\|s\|^3_{\mathbb{R}^m})\right) ds^1\cdots ds^m + \mathcal{O}(\epsilon^3).
\end{aligned}$$

Since k, k', and k'' all have exponential decay, we may apply Lemma 2.3.10 to extend each term to all of $\mathbb{R}^m$ by adding and subtracting terms of $\mathcal{O}(\epsilon^3)$. This allows us to express all asymptotic terms in terms of only ϵ.

The term of order zero is therefore given by:

$$\int_{\mathbb{R}^m} k(\|s\|^2_{\mathbb{R}^m})f(0)q(0)ds^1\cdots ds^m = m_0 f(x)q(x).$$

Since $\mathbb{R}^m$ is radially symmetric, all odd-order polynomials integrate to zero and thus there are no first-order terms. We next compute the second order terms:

$$\frac{\epsilon^2}{2}\int_{\mathbb{R}^m}\left(k(\|s\|^2_{\mathbb{R}^m})\frac{\partial^2 fq(0)}{\partial s^i \partial s^j}s^i s^j \right. \tag{2.3.8}$$

$$-\frac{1}{6}k'\left(\|s\|^2_{\mathbb{R}^m}\right)\|\Pi(s,s)\|^2_{\mathbb{R}^m} fq(0) \tag{2.3.9}$$

$$\left. + k(\|s\|^2_{\mathbb{R}^m})fq(0)\frac{1}{3}\mathrm{Ric}(s,s)\right) ds^1 \cdots ds^m. \tag{2.3.10}$$

Again, by symmetry of the domain of integration, odd-degree polynomials integrate to zero. More specifically, the integral of any symmetric 2-tensor over a unit ball is equal to the trace of the tensor. Since $g_{ij}(0) = \delta_{ij}$, the trace of the Hessian matrix in coordinates is the Laplace-Beltrami operator. Using this, we see that (2.3.8) becomes $m_2\Delta(x)$. The term $S(x)$ is obtained in a similar manner and an explicit form can be found in [21]. □

2.3.3 Normalization

In the normalization step, we show that by choosing a particular type of kernel, one can extract the Laplacian regardless of the underlying sampling distribution q. This was one of the main contributions of [13]. For notational convenience, we now define

$$q_\epsilon = \frac{1}{\epsilon^m}\mathcal{K}_\epsilon q(x)$$

as well as the *normalized kernel* $\hat{\mathcal{K}}_\epsilon$:

$$\hat{\mathcal{K}}_\epsilon f(x) = \int_{\mathcal{M}} \frac{k\left(\frac{\|x-y\|_{\mathbb{R}^d}}{\epsilon^2}\right)}{q_\epsilon(x)q_\epsilon(y)} f(y)q(y)dy.$$

The main result of this section shows that by appropriately normalizing $\hat{\mathcal{K}}$, one can extract the Laplace-Beltrami operator of $\mathcal{M}$.

Theorem 2.3.12. *With $\mathcal{M}$, k and f follow the assumptions listed above,*

$$\hat{\mathcal{K}}_\epsilon f(x) = f(x) - \epsilon^2 \frac{m_2}{2m_0}\Delta f(x) + \mathcal{O}(\epsilon^3)$$

Proof. By Proposition 2.3.11:

$$\frac{1}{\epsilon^m}\hat{\mathcal{K}}_\epsilon f(x) = q_\epsilon^{-1}(x)\left(m_0 \frac{fq}{q_\epsilon}(x) + \frac{\epsilon^2 m_2}{2}\left(\frac{fq}{q_\epsilon}(x)S(x) - \Delta(\frac{fq}{q_\epsilon})(x)\right)\right) + \mathcal{O}(\epsilon^3) \tag{2.3.11}$$

By applying Proposition 2.3.11 to the constant function 1, we see that

$$q_\epsilon(x) = m_0 q(x) + \epsilon^2 \frac{m_2}{2}(q(x)S(x) - \Delta q(x)) + \mathcal{O}(\epsilon^3) \tag{2.3.12}$$

If we let A, B, C, D, F, G be constants with $D \neq 0$, then by Taylor's theorem one may obtain:

$$\frac{A + B\epsilon^2 + C\epsilon^3}{D + F\epsilon^2 + G\epsilon^3} = \frac{A}{D} + \frac{DB - AF}{D^2}\epsilon^2 + \mathcal{O}(\epsilon^3). \tag{2.3.13}$$

Combining equations (2.3.12) and (2.3.13), we obtain:

$$\frac{fq}{q_\epsilon}(x) = \frac{f}{m_0} - \epsilon^2 \frac{m_2}{2m_0^3} f(x)\left(S(x) - \frac{\Delta q}{q}(x)\right) + \mathcal{O}(\epsilon^2)$$

so (2.3.11) becomes:

$$\frac{1}{\epsilon^m}\hat{\mathcal{K}}_\epsilon f(x) = q_\epsilon^{-1}(x)\left(f(x) + \epsilon^2 \frac{m_2}{2m_0}\left(f(x)S(x) - \Delta f(x) - \frac{f}{m_0^2}\right)\right) + \mathcal{O}(\epsilon^3). \tag{2.3.14}$$

For $f \equiv 1$, we obtain

$$\frac{1}{\epsilon^m}\hat{\mathcal{K}}_\epsilon 1(x) = q_\epsilon^{-1}(x)\left(1 + \epsilon^2 \frac{m_2}{2m_0}\left(S(x) - \frac{1}{m_0^2}\right)\right) + \mathcal{O}(\epsilon^3). \tag{2.3.15}$$

Taking the quotient of equations (2.3.14) and (2.3.15) and expanding using the identity in (2.3.13), we obtain:

$$\begin{aligned}\frac{\hat{\mathcal{K}}_\epsilon f(x)}{\hat{\mathcal{K}}_\epsilon 1(x)} &= \frac{f(x) + \epsilon^2 \frac{m_2}{2m_0}\left(f(x)S(x) - \Delta f(x) - \frac{f}{m_0^2}\right) + \mathcal{O}(\epsilon^3)}{1 + \epsilon^2 \frac{m_2}{2m_0}\left(S(x) - \frac{1}{m_0^2}\right) + \mathcal{O}(\epsilon^3)} \\ &= f(x) + \frac{m_2}{2m_0}\left(\left(f(x)S(x) - \Delta f(x) - \frac{f}{m_0^2}\right) - f(x)\left(S(x) - \frac{1}{m_0^2}\right)\right) + \mathcal{O}(\epsilon^3) \\ &= f(x) - \epsilon^2 \frac{m_2}{2m_0}\Delta f(x) + \mathcal{O}(\epsilon^3)\end{aligned}$$

□

We now define the kernel averaging operator $\Delta_\epsilon : C^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$ by:

$$\Delta_\epsilon f(x) = \frac{2m_0}{\epsilon^2 m_2}\left(f(x) - \hat{\mathcal{K}}_\epsilon f(x)\right).$$

From Theorem 2.3.12, one immediately derives the main result:

Corollary 2.3.13. *Let $\Delta_\epsilon : C^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$ be defined by:*

$$\Delta_\epsilon f(x) = \frac{2m_0}{\epsilon^2 m_2}\left(f(x) - \hat{K}_\epsilon f(x)\right).$$

Then for ϵ sufficiently small, $\mathcal{M}$, ι and $\|$ under the conditions above,

$$\Delta_\epsilon f(x) = \Delta f(x) + \mathcal{O}(\epsilon).$$

We have now recreated the classical proof of pointwise convergence [13] of the kernel integral operator corresponding to the random walks graph Laplacian. In addition to recreating this classical proof, we have adopted a number of important conventions which make the proof more easily generalizable to manifolds with boundary. In the next chapter, we will use this framework to generalize our approach to manifolds with boundary. We will derive an analogous asymptotic expansion for points near the boundary using *semigeodesic* coordinates instead of normal coordinates.

Chapter 3: Bias of Diffusion Maps on Manifolds with Boundary

3.1 Summary

We generalize the results of the previous chapter to compact manifolds with boundary. Our approach differs from previous attempts [13, 21, 34] in that we derive an asymptotic expansion similar to that in Proposition 2.3.11 which is *uniform* in the variable ϵ. Although this expansion does not converge in the limit as $\epsilon \to 0$, we will later use this uniformity to prove that the kernel operator $\hat{\mathcal{K}}_\epsilon$ does in fact converge *weakly* on manifolds with boundary.

3.2 Semigeodesic Coordinates

Our arguments in in this chapter will rely on a generalization of the argument in the previous chapter. More specifically, we will rely on the use of *semigeodesic coordinates* instead of Riemannian normal coordinates for points near the boundary. These coordinates are also sometimes referred to as *normal coordinates relative to a hypersurface.* As we will show, the use of these coordinates allows for a more systematic treatment of points near the boundary. Before going into more detail, we will begin with a simple example showing the inadequacy of normal coordinates for analysis of points close to the boundary.

In the proofs of the previous chapter, we first localized integral operator to a *metric ball* in $\mathcal{M}$ of radius ϵ^γ for some fixed $\gamma \in (0,1)$. Next, we performed a Taylor expansion of the operator $\mathcal{K}_\epsilon$ inside of a normal coordinate chart. In this example, we show that the maximum size of a normal coordinate chart decreases as one approaches the boundary and is thus independent of ϵ. This shows that the argument in the last chapter does not necessarily generalize to manifolds with boundary, since one can no longer guarantee that the localized integral can be represented in a single normal coordinate chart.

3.2.1 Motivating Example

In this example, we let $\mathcal{M} = \{x \in \mathbb{R}^2 : 1 \leq \|x\| \leq 3\}$ be the closed annulus with inner radius 1 and outer radius 3. We let $\mathcal{M}$ be naturally embedded into $\mathbb{R}^2$ via the inclusion map. By construction, this means that geodesic segments in the interior of $\mathcal{M}$ are straight lines in $\mathbb{R}^2$ and geodesic segments on the boundary correspond to segments along the inner circle $S^1(1)$ of radius 1 or the outer circle $S^1(3)$ of radius 3.

We now let $x(t) = t(0, 1)$ be a curve in $\mathcal{M}$ which corresponds to a straight line where $x(1)$ is an interior point and $x(0)$ is a boundary point. We will show that for any $\epsilon > 0$, there is a t' such that if $t \leq t'$, then $B_\epsilon(x(t))$ is not contained in a normal coordinate chart.

Using simple Euclidean geometry, one has that for each $t > 0$, there are two geodesics γ_1 and γ_2 which intersect the inner boundary tangentially. Furthermore, the distance from $x(t)$ to the point of tangency is $\sqrt{t(t+2)}$. We then observe that if one moves along the tangential geodesic γ_1 past the point of tangency, all points "below the horizon" no longer correspond uniquely to an initial velocity vector based at $x(t)$. Thus, a normal coordinate chart exists only until the point of tangency. Thus, since $\sqrt{t(t+2)}$ approaches zero as $t \to 0$, a metric ball of fixed radius ϵ is not contained in normal coordinates for all points of $x(t)$.

3.2.2 The Normal Collar

In order to generalize the argument of Chapter 2 for manifolds with boundary, we will subdivide the manifold into two regions whose size is dependent on the parameter $\epsilon^\gamma > 0$. The *interior region* $\mathcal{M}_{\epsilon^\gamma}$ is the set of points whose distance from $\partial\mathcal{M}$ is greater than ϵ^γ. The *boundary region*, which we will denote N_{ϵ^γ} is then the set of points whose distance from $\partial\mathcal{M}$ is less than or equal to ϵ^γ.

For small enough ϵ^γ, the boundary region N_{ϵ^γ} is contained inside the so-called *normal collar* of $\mathcal{M}$. This will be used to construct semigeodesic coordinates and perform a similar uniform expansion to that in Chapter 2.

Let $\mathcal{M}$ be a compact manifold with boundary, and let η denote the inward-facing normal vector field on $\partial\mathcal{M}$. Then there exists a $r_C > 0$ such that the mapping $\phi : \partial\mathcal{M} \times [0, r_C) \to \mathcal{M}$ defined by:

$$\phi(x, t) = \exp_x(-t\eta_x)$$

is a diffeomorphism onto its image. We call the image of ϕ the *normal collar* of $\mathcal{M}$ and the value r_C the *normal collar width*. Note that due to the fact that geodesics are locally minimizing, this implies that if $\epsilon^\gamma < r_C$, then the boundary region N_{ϵ^γ} is contained in the normal collar.

If we let $\mathcal{M}_t$ be as above for each $t < r_C$, the Gauss lemma for submanifolds [25] (Theorem 6.3.8) implies the inward-flowing geodesics $\gamma(t) = \exp_x(-t\eta_x)$ intersect the boundary $\partial\mathcal{M}_t$ orthogonally for each t. Therefore the boundaries of the interior region $\partial\mathcal{M}_{\epsilon^\gamma}$ are "parallel" in the sense that they do not overlap and intersect the inward-facing geodesics orthogonally.

Using this idea, for each point x in the normal collar, we let $b_x = d_g(x, \partial\mathcal{M})$ denote the distance from x to the boundary. We then see that the boundary of the interior region $\partial\mathcal{M}_{b_x}$ is then a hypersurface in $\mathcal{M}$ which intersects the inward-flowing geodesics orthogonally. We also may uniquely extend the inward-facing vector field η to be defined on each of the parallel hypersurfaces $\partial\mathcal{M}_t$ for each t so that η is defined on the entire normal collar.

3.2.3 Properties of Semigeodesic Coordinates

A semigeodesic coordinate chart centered at x is then constructed by first choosing normal coordinates $(u^1, ..., u^{m-1})$ on the hypersurface $\partial\mathcal{M}_{b_x}$, then "extending" these coordinates $(u^1, .., u^{m-1}, u^m)$ to a neighborhood in the normal collar so that u^m parameterizes the geodesic distance from $\partial\mathcal{M}_{b_x}$. Thus, a semigeodesic coordinate chart centered at x is like a "hypercylinder" in $\mathcal{M}$ whose height is parameterized by u^m and radius parameterizes geodesic distance in $\partial\mathcal{M}_{b_x}$ when $u^m = 0$.

For notational convenience, we will use the nonstandard term *semigeodesic cylinder* of radius and height ϵ^γ based at x to mean a semigeodesic coordinate chart $(u^1, ..., u^m)$ centered at x such that $\sum_{i=1}^{m-1} u^i \leq \epsilon^\gamma$ and $-b_x \leq u^m < \epsilon^\gamma$.

These coordinates naturally avoid the problems introduced in the motivating example and also are defined on the boundary. In addition, we see that they are radially symmetric in the first $m-1$ components, and so much of the cancellation that was present in the arguments of the previous chapter still apply in these coordinates. We now introduce some of the other useful properties of semigeodesic coordinates. A proof of existence of semigeodesic coordinates, as well as the proof of the following properties can be found in [25].

Proposition 3.2.1. *Let x be a point in the normal collar and let $(u^1, .., u^m)$ denote a system of semigeodesic coordinates centered at x. Then*

(a) The coordinates of x are $(0, .., 0)$.

(b) The components of the metric at x are $g_{ij}(x) = \delta_{ij}$.

(c) The n-th coordinate vector field $\partial_n = \text{grad } b_x = \eta$ on each parallel hypersurface.

(d) For every vector $v = v^i\partial_i$ at x, the radial geodesic in $\partial\mathcal{M}_{b_x}$ with initial velocity $\sum_{i=1}^{m-1} v^i$ is represented in coordinates by:

$$\gamma(t) = t(v^1, ..., v^{m-1}, 0).$$

The geodesic in $\mathcal{M}$ starting at x with initial velocity $v^m\eta_x$ is represented in coordinates as:

$$\gamma(t) = t(0, ..., 0, v^m).$$

3.3 Notation, Definitions, and Assumptions

We again assume that $(\mathcal{M}, g)$ is a C^∞, dimension m compact Riemannian manifold. We now assume that $\mathcal{M}$ is a manifold with boundary and that $\iota : \mathcal{M} \to \mathbb{R}^d$ is an isometric embedding of $\mathcal{M}$ into $\mathbb{R}^d$. We further assume that ι is a proper embedding so that in particular, the topological boundary of $\iota(\mathcal{M})$ in $\mathbb{R}^d$ is equal to $\iota(\partial\mathcal{M})$.

We let $d\,\mathrm{Vol}$ denote the Riemannian volume measure inherited from the metric g on $\mathcal{M}$. We assume that $q : \mathcal{M} \to \mathbb{R}$ is a C^∞ probability density function corresponding to a probability measure $d\mu$ which is absolutely continuous with respect to $d\,\mathrm{Vol}$ and nowhere zero on $\mathcal{M}$.

We again assume $k : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ is a C^∞ function which has exponential decay, so that $k(x) \leq \alpha e^{-\beta x}$ for all $x \in \mathbb{R}_{\geq 0}$. We again assume that the first two derivatives of k also have exponential decay.

We will again use $\|x - y\|_{\mathbb{R}^d}$ to denote the so-called extrinsic distance in $\mathbb{R}^d$ between $\iota(x)$ and $\iota(y)$. However, we will now use $\|u\|_{\mathrm{sem}}$ to denote the euclidean norm of the coordinate representative u of y in semigeodesic coordinates. In contrast to the previous chapter, this norm no longer corresponds to geodesic distance between x and y. However, the norm of the first $m-1$ coordinates does correspond to geodesic distance in $\partial\mathcal{M}_{b_x}$. Furthermore, the magnitude of u^m corresponds to geodesic distance in $\mathcal{M}$ of the inward-flowing geodesic.

We again let $B_\epsilon^{\mathbb{R}^d}(x)$ denote the preimage $\iota^{-1}(B_\epsilon^{\mathbb{R}^d}(\iota(x))$ which is the set of points in $\mathcal{M}$ which are of extrinsic distance ϵ or less from x. We fix a value of $\gamma \in (0,1)$, since all localization results are phrased in terms of a ball of radius ϵ^γ. Whereas in the previous chapter, the value ϵ^γ was used to parameterize radial distance, in this chapter, ϵ^γ will parameterize the height and radius of a semigeodesic cylinder. We abuse notation and denote a semigeodesic cylinder with height and radius ϵ^γ in $\mathcal{M}$ as $B_{\epsilon^\gamma}^{\mathrm{sem}}(x)$. This convention is an abuse of notation since semigeodesic cylinders are not metric balls in $\mathcal{M}$.

It will sometimes be the case that our arguments will be simultaneously true for both semigeodesic cylinders near the boundary as well as geodesic balls near the interior. In that case, we will let $\tilde{B}_{\epsilon^\gamma}(x)$ denote either a semigeodesic cylinder if x is in the boundary region, or a geodesic ball if x is in the interior region.

We again, adopt the convention of Einstein notation, so that roman indices such as i, j, or k are taken to be summed over $1, ..., m$, while greek indices such as α, β or μ are taken to be summed over $1, ..., d$.

3.4 Asymptotic Convergence of the Kernel Averaging Operator

As in the previous chapter, we will now provide a pointwise expansion of the kernel integral operator

$$\mathcal{K}_\epsilon f(x) = \int_{\mathcal{M}} k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) f(y)q(y)\ d\ \mathrm{Vol}(y).$$

In this case will carry out the asymptotic expansion in both normal and semigeodesic coordinates. We will follow the same general framework as in the previous chapter. First, we will show that one can localize the kernel integral operator $\mathcal{K}_\epsilon$ to a coordinate neighborhood of $\mathcal{M}$. Using these coordinates, we will then asymptotically expand $\mathcal{K}_\epsilon$. Finally we will normalize $\mathcal{K}_\epsilon$ to a kernel integral operator that is independent of the density function.

3.4.1 Localization

In contrast to the previous chapter, we will now break up the localization step into two cases. If $x \in \mathcal{M}_{\epsilon^\gamma}$, then $\mathcal{K}_\epsilon$ can be localized to a geodesic ball of radius ϵ^γ. If $x \in N_{\epsilon^\gamma}$, we will show that $\mathcal{K}_\epsilon$ can be localized to a semigeodesic cylinder of radius and height ϵ^γ. After proving a small technical lemma, the expansion and normalization steps on the interior region follow as in the previous chapter. Therefore, we will focus mostly on the expansion and normalization steps for points inside the boundary region N_{ϵ^γ}

We will first show that if ϵ is chosen small enough, each point in $\mathcal{M}_{\epsilon^\gamma}$ is contained in a geodesic ball of radius ϵ^γ and each point in N_{ϵ^γ} is contained in a semigeodesic cylinder of height and radius ϵ^γ. For points on the interior region $\mathcal{M}_{\epsilon^\gamma}$, the expansion will be exactly the same as in Chapter 2. We will therefore derive the expansion in semigeodesic coordinates for points in N_{ϵ^γ}.

The main difference between the expansion for manifolds without boundary and the expansion for points in $\mathcal{M}_{\epsilon^\gamma}$ is that $\mathcal{M}_{\epsilon^\gamma}$ grows larger as $\epsilon \to 0$. Hence, it is possible for the injectivity radius of $\mathcal{M}_{\epsilon^\gamma}$ to change as $\epsilon \to 0$. The following lemma is a new result which shows that for small enough ϵ, the injectivity radius of $\mathcal{M}_{\epsilon^\gamma}$ is at least ϵ^γ.

Lemma 3.4.1. *Let $\mathcal{M}_{\epsilon^\gamma}$ be the set of points in $\mathcal{M}$ whose geodesic distance from the boundary is greater than ϵ^γ. Then there exists an $r_\mathcal{M} > 0$ such that if $\epsilon^\gamma < r_\mathcal{M}$ then $\mathrm{inj}(x) > \epsilon^\gamma$ for all $x \in \mathcal{M}_{\epsilon^\gamma}$.*

Proof. Since $\mathcal{M}$ is compact, its double $D(\mathcal{M}) = (\mathcal{M} \coprod \mathcal{M})/\partial\mathcal{M}$ is a compact manifold without boundary. Endow $D(\mathcal{M})$ with a Riemannian metric by smoothly extending the metric inherited by the natural embedding $\iota : \mathcal{M} \hookrightarrow D(\mathcal{M})$. Then $D(\mathcal{M})$ has a positive injectivity radius $r > 0$. Since the natural embedding ι is by definition a Riemannian isometry on the image of $\mathcal{M}$, it is an isometry for any $\mathcal{M}_{\epsilon^\gamma}$. Hence, for any $\epsilon < r$, and any $x \in \mathcal{M}_{\epsilon^\gamma}$, we have $\mathrm{inj}(x) = \mathrm{inj}(\iota(x)) > r \geq \epsilon^\gamma$. □

We now turn our attention to the boundary region. The next lemma is an application of a classical result in differential geometry to show that the injectivity radius of the parallel hypersurfaces $\partial\mathcal{M}_t$ does not shrink to zero for $t \in [0, \frac{r_C}{2}]$. This shows that for small enough ϵ^γ, one can construct semigeodesic coordinates of radius and height ϵ^γ centered at any point in N_{ϵ^γ}.

Lemma 3.4.2. *There exists a $r_{C'} > 0$ such that for any $\partial\mathcal{M}_t$ with $t \in [0, \frac{r_C}{2}]$, the injectivity radius of $\partial\mathcal{M}_t$ is bounded below by $r_{C'}$.*

Proof. A property of the normal collar is that for each $t \in [0, r_C)$, the hypersurface $\partial\mathcal{M}_t$ is diffeomorphic to $\partial\mathcal{M}$. In this way, we can express the metric on $\partial\mathcal{M}_t$ as a metric on $\partial\mathcal{M}$ by pulling back via the diffeomorphism. This induces a continuous family of metrics g_t on

$\partial\mathcal{M}$. The main theorem of [14] shows that the mapping $t \mapsto \text{inj}((\partial\mathcal{M}, g_t))$ is continous. Since $(\mathcal{M}, g_t)$ each have nonzero injectivity radius, the continuity of this mapping together with compactness of $[0, \frac{r_C}{2}]$ implies that the mapping attains its minimum and is thus nonzero. Hence, there exists a nonzero lower bound $r_{C'}$ on the injectivity radii of $\partial\mathcal{M}_t$ for $t \in [0, \frac{r_C}{2}]$. □

Next, we show a generalization of Proposition 2.3.2 that there exists a constant r_ι such that small enough ϵ, $\iota^{-1}(B_\epsilon^{\mathbb{R}^d}(\iota(x))$ is contained inside of a normal coordinate or semigeodesic coordinate chart in $\mathcal{M}$. This proposition is crucial since it allows us to use Taylor's theorem to relate the extrinsic distance in $\mathbb{R}^d$ to the norm in either normal or semigeodesic coordinates.

Proposition 3.4.3. *There exists a $r_\iota > 0$ such that for any $0 < \epsilon^\gamma < r_\iota$, the set $\iota^{-1}(B_\epsilon^{\mathbb{R}^d}(\iota(x))$ is contained inside of a semigeodesic coordinate chart if $x \in N_{\epsilon^\gamma}$ and contained in a normal coordinate chart if $x \in \mathcal{M}_\epsilon^\gamma$.*

Proof. Let $r = \min\{r_C, r_{C'}, r_\mathcal{M}\}$. Then semigeodesic cylinders of radius and height r exist for any point x in N_r and normal coordinates For each $x \in \mathcal{M}$, let $\tilde{B}_r(x)$ denote a geodesic ball of radius r or semigeodesic cylinder of height and radius r. We then consider the following two sets $\mathcal{B}_1$ and $\mathcal{B}_2$:

$$\mathcal{B}_1 = \bigcup_{x\in\mathcal{M}} \tilde{B}_r(x) \times \tilde{B}_r(x).$$

$$\mathcal{B}_2 = \left(\bigcup_{x\in\mathcal{M}\setminus\partial\mathcal{M}} B_r(x) \times B_r(x)\right) \cup \left(\bigcup_{x\in\partial\mathcal{M}} \tilde{B}_r(x) \times \tilde{B}_r(x)\right).$$

We remark that if (x, y) are in $\mathcal{B}_1$, then x and y are contained in a common coordinate chart, which is either normal or semigeodesic. If (x, y) are in $\mathcal{B}_2$, then any metric ball centered at x which contains y and does not contain boundary points is contained in a normal coordinate chart centered at x if x is not a boundary point.

We remark that the sets $\mathcal{B}_1$ and $\mathcal{B}_2$ are open, and thus their complements $\mathcal{B}_1^c$ and $\mathcal{B}_2^c$ in $\mathcal{M} \times \mathcal{M}$ are compact sets which do not contain any point of the form (x, x) for $x \in \mathcal{M}$. Thus by metric space properties, the function $d_{\mathbb{R}^d}$ is nowhere zero on $\mathcal{B}_1^c$ or $\mathcal{B}_2^c$.

The restriction of the function $d_{\mathbb{R}^d}$ to $\mathcal{B}$ is continuous, and nowhere zero. Since $\mathcal{B}$ is compact, $d_{\mathbb{R}^d}$ attains its minimum value on $\mathcal{B}_1^c$ and $\mathcal{B}_2^c$. If we let r_ι be the minimum of these two values, then we have that if $\|x - y\|_{\mathbb{R}^d} < r_\iota$ then y is inside of a chart centered at x. □

With these two results, we have shown that if $\epsilon^\gamma < \min\{r, r_\iota\}$, then each point in $\mathcal{M}_{\epsilon^\gamma}$ is contained in a normal coordinate chart. We briefly remark that in contrast to the analogous Proposition 2.3.2 of the previous chapter, we require the use of compactness for this proposition.

By using [15] as in the previous chapter, bounded curvature of $\mathcal{M}_{\epsilon^\gamma}$ implies that there exists uniform bounds on the components of the metric g_{ij} and g^{ij} in normal coordinate charts of radius ϵ in the region $\mathcal{M}_\epsilon$.

The following theorem is a simplified version of Theorem 2.5 in [28] which is a generalization of [15] for manifolds with boundary. In particular, we use the fact that compact manifolds with boundary have bounded curvature and the second fundamental form of $\partial\mathcal{M}$ in $\mathcal{M}$ is also bounded.

Corollary 3.4.4. *Let $\mathcal{M}$ be a compact manifold with boundary. Then there exists a $\tilde{C}_0, \tilde{C}_1 \geq 0$ and $r > 0$ such that in any semigeodesic cylinder or any geodesic ball of radius less than r,*

$$|g_{ij}| \leq \tilde{C}_0 \text{ and } |g^{ij}| \leq \tilde{C}_1$$

in either semigeodesic or normal coordinate charts.

We remark that our situation is slightly different than that of [28] in that we are constructing semigeodesic coordinates not just about $\partial\mathcal{M}$, but $\partial\mathcal{M}_{\epsilon^\gamma}$. Using the Riccati Equation for submanifolds (Corollary 3.3 in [20]):

$$S'(t) = S(t)^2 + R(t)$$

one can then bound the shape operator $S(t)$ using compactness of $\partial\mathcal{M}_t$ and Gronwall's inequality. By then raising an index, we obtain a bound on the second fundamental forms of $\partial\mathcal{M}_t$. From here, the assumptions of the paper [28] are satisfied, and so we can follow the same method as in Theorem 2.5 in [28].

We next relate the norm inside a semigeodesic chart to the extrinsic distance in $\mathbb{R}^d$. This is in direct analogy to Proposition 2.3.4 in Chapter 2.

Proposition 3.4.5. *Let* $r = \min\{\frac{r_C}{2}, r_{C'}, r_{\mathcal{M}}\}$. *There exists a* $C_0, C_1 > 0$ *such that in any semigeodesic cylinder of radius and height less than* r*, or any geodesic ball of radius less than* r*,*

$$C_0 \left\|u\right\|_g^2 \leq \left\|x - y\right\|_{\mathbb{R}^d}^2 \leq C_1 \left\|u\right\|_g^2$$

or

$$C_0 \left\|u\right\|_{\text{sem}}^2 \leq \left\|x - y\right\|_{\mathbb{R}^d}^2 \leq C_1 \left\|u\right\|_{\text{sem}}^2$$

where u *is the coordinate representative of* y *in either normal or semigeodesic coordinates.*

Proof. Due to the similarities between semigeodesic coordinates and normal coordinates, our proof is identical to that of Proposition 2.3.4. We focus here on the proof for semigeodesic cylinders, but note that Proposition 2.3.4 still holds for normal coordinate charts.

Let x be a point in N_r, and choose a semigeodesic coordinate chart $u = (u^1, ..., u^m)$ in $\mathcal{M}$ centered at x. We then choose a normal coordinate chart centered at $\iota(x)$. Let $\iota(s) = (\iota^1(s), ..., \iota^d(s))$ represent the coordinate image of $\iota(y)$ in these coordinates.

In these coordinates, we have that

$$\|x-y\|_{\mathbb{R}^d}^2 = g_{\alpha\beta}^{\mathbb{R}^d}(0)\iota^\alpha(s)\iota^\beta(s). \tag{3.4.1}$$

where $\iota(s)$ is the coordinate representative of y in these coordinates.

We then perform an order-zero Taylor expansion of $\iota^\alpha(u)$ for each $\alpha \in \{1, ..., d\}$. Due to the remainder term, there exists a point $\tilde{u}$ in the domain such that

$$\iota^\alpha(s) = \iota^\alpha(0) + \frac{\partial \iota^\alpha(\tilde{u})}{\partial u^i}u^i.$$

Applying the above expansion to (3.4.1) and recalling that in these coordinates $\iota(0) = 0$, we have

$$\begin{aligned} g_{\alpha\beta}^{\mathbb{R}^d}(0)\iota^\alpha(u)\iota^\beta(u) &= g_{\alpha\beta}^{\mathbb{R}^d}(0)\left(\iota^\alpha(0) + \frac{\partial \iota^\alpha(\tilde{u})}{\partial u^i}u^i\right)\left(\iota^\beta(0) + \frac{\partial \iota^\beta(\tilde{u})}{\partial u^j}u^j\right) \\ &= g_{\alpha\beta}^{\mathbb{R}^d}(0)\frac{\partial \iota^\alpha(\tilde{u})}{\partial u^i}\frac{\partial \iota^\beta(\tilde{u})}{\partial u^j}u^i u^j. \end{aligned}$$

Since the $\mathbb{R}^d$ has no curvature, the components of the metric $g_{\alpha\beta}^{\mathbb{R}^d}$ are constant and equal to $\delta_{\alpha\beta}$. We therefore have that

$$g_{\alpha\beta}^{\mathbb{R}^d}(0) = g_{\alpha\beta}^{\mathbb{R}^d}(\iota(\tilde{u})) = \delta_{\alpha\beta}$$

and so therefore,

$$g_{\alpha\beta}^{\mathbb{R}^d}(0)\iota^\alpha(u)\iota^\beta(u) = g_{\alpha\beta}^{\mathbb{R}^d}(\iota(\tilde{u}))\frac{\partial \iota^\alpha(\tilde{u})}{\partial u^i}\frac{\partial \iota^\beta(\tilde{u})}{\partial u^j}u^i u^j.$$

The expression on the right hand side is exactly the expression for the pullback metric on $\mathcal{M}$ inherited from ι and thus,

$$\|x-y\|_{\mathbb{R}^d}^2 = g_{\alpha\beta}^{\mathbb{R}^d}(0)\iota^\alpha(u)\iota^\beta(u) = g_{ij}^{\mathcal{M}}(\tilde{u})u^i u^j. \tag{3.4.2}$$

We now note that the expression $g_{ij}^{\mathcal{M}}(\tilde{u})u^i u^j$ is maximized by the maximum eigenvalue of the matrix with entries $g_{ij}^{\mathcal{M}}(\tilde{u})$ and minimized by the maximum eigenvalue of the matrix with entries $(g^{\mathcal{M}})^{ij}(\tilde{u})$. Since compactness of $\mathcal{M}$ implies bounded Riemannian curvature, Corollary 3.4.4 implies that there exists positive constants $\tilde{C}_0$ and $\tilde{C}_1$ such that in any normal coordinate chart of radius $\text{inj}(\mathcal{M})$ or less,

$$|g_{ij}| \leq \tilde{C}_0 \text{ and } |g^{ij}| \leq \tilde{C}_1.$$

Since the matrices with entries g_{ij} and g^{ij} are symmetric and positive definite, this implies that there exists positive bounds $\frac{1}{C_0}$ and C_1 on the largest eigenvalue of (g^{ij}) and (g_{ij}) respectively across all $\tilde{u}$ in our coordinate chart.

Hence, we have that

$$C_0\delta_{ij}u^i u^j \leq g_{ij}^{\mathcal{M}}(\tilde{u})u^i u^j \leq C_1\delta_{ij}u^i u^j$$

and since $\delta_{ij} = g_{ij}^{\mathcal{M}}(0)$, we are left with

$$C_0 \|u\|_{\text{sem}}^2 \leq g_{\alpha\beta}^{\mathcal{M}}(\tilde{u})\iota^\alpha(u)\iota^\beta(u) \leq C_1 \|u\|_{\text{sem}}^2.$$

Combining these inequalities with (3.4.2), we obtain

$$C_0 \|u\|_{\text{sem}}^2 \leq \|x-y\|_{\mathbb{R}^d}^2 \leq C_1 \|u\|_{\text{sem}}^2.$$

□

Corollary 3.4.6. *Let* $r = \min\{r_C, r_{C'}, r_{\mathcal{M}}\}$. *Then if* $\epsilon^\gamma < \min\{r_\iota, \frac{r}{C_0}\}$ *then*

$$B^{\mathbb{R}^d}_{C_0^{-1}\epsilon^\gamma}(\iota(x)) \subseteq \tilde{B}\epsilon^\gamma(x).$$

where $\tilde{B}\epsilon^\gamma(x)$ *denotes either a geodesic ball if* $x \in \mathcal{M}_{\epsilon^\gamma}$ *or a semigeodesic ball if* $x \in N_{\epsilon^\gamma}$.

Proof. Suppose that $\epsilon^\gamma < \min\{r_\iota, \frac{\text{inj}(\mathcal{M})}{C_0}\}$ and let $x, y \in \mathcal{M}$ be such that $C_0^{-1} d_{\mathbb{R}^d}(\iota(x), \iota(y)) < \epsilon^\gamma$. Then by Proposition 3.4.3, since $\epsilon^\gamma < r_\iota$, we have that $C_0^{-1} d_{\mathcal{M}}(x, y) < \text{inj}(\mathcal{M})$. Applying Proposition 3.4.5, we have that

$$C_0(C_0^{-1} d_{\mathcal{M}}(x, y)) \leq C_0^{-1} d_{\mathbb{R}^d}(x, y) < \epsilon^\gamma.$$

Hence, $d_{\mathcal{M}}(x, y) < C_0^{-1}\epsilon^\gamma$ so $y \in B^{\mathcal{M}}_{C_0^{-1}\epsilon^\gamma}(x)$. □

We now use Proposition 3.4.3 and Proposition 3.4.5 to show that $\mathcal{K}_\epsilon$ is asymtotically a local operator.

Proposition 3.4.7. *Let* $0 < \gamma \leq 1$ *and* $\epsilon^\gamma < \min\{r_\iota, \frac{\text{inj}(\mathcal{M})}{C_0}\}$. *For any* $z \in \mathbb{N}$,

$$\mathcal{K}_\epsilon f(x) = \int_{B^{\mathcal{M}}_{\epsilon^\gamma}(x)} k\left(\frac{\|x - y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) f(y) q(y) \ d \ \text{Vol}(y) + \mathcal{O}(\epsilon^z).$$

Proof. By applying Corollary 3.4.6, we have that $B^{\mathbb{R}^d}_{C_0^{-1}\epsilon^\gamma}(\iota(x)) \subseteq B^{\mathcal{M}}_{\epsilon^\gamma}(x)$. Hence, if $y \notin B^{\mathcal{M}}_{\epsilon^\gamma}(x)$, then $\|x - y\|_{\mathbb{R}^d} > C_0^{-1}\epsilon^\gamma$. Using the fact that $\alpha e^{-\beta x^2}$ is monotone decreasing, we have that:

$$\int_{\mathcal{M}\setminus B^{\mathcal{M}}_{\epsilon^\gamma}(x)} k^2\left(\frac{\|x - y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) q(y) \ d \ \text{Vol}(y) \leq \int_{\mathcal{M}\setminus B^{\mathcal{M}}_{\epsilon^\gamma}(x)} \alpha e^{-2\beta \frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}} q(y) \ d \ \text{Vol}(y)$$

$$\leq \alpha e^{-2\beta \frac{(C_0^{-1}\epsilon^\gamma)^2}{\epsilon^2}} \int_{\mathcal{M}\setminus B^{\mathcal{M}}_{\epsilon^\gamma}(x)} q(y) \ d \ \text{Vol}(y)$$

$$\leq \alpha e^{-2\beta \frac{C_0^{-2}(\epsilon^\gamma)^2}{\epsilon^2}} \int_{\mathcal{M}} q(y)\ d\ \mathrm{Vol}(y)$$

$$= \alpha e^{-2\frac{\beta}{C_0^2}\epsilon^{2(\gamma-1)}}$$

We then apply Cauchy-Schwarz inequality in q-weighted $L^2(\mathcal{M} \setminus B^g_{\epsilon^\gamma}(x))$ and use the above inequality:

$$\left\langle k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right), f\right\rangle^2 \leq \left\langle k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right), k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right)\right\rangle^2 \langle f, f\rangle$$

$$= \langle f, f\rangle \alpha e^{-2\frac{\beta}{C_0^2}e^{2(\gamma-1)}}$$

We see that the term $\langle f, f\rangle \alpha e^{-2\frac{\beta}{C_0^2}\epsilon^{2(\gamma-1)}}$ is asymptotically bounded by any polynomial ϵ^z with $z \geq 1$ by making the substitution $\delta = \epsilon^{-1}$ and applying L'Hôpital's rule z-times. $\square$

We now have the necessary results to show that one can uniformly localize $\mathcal{K}_\epsilon$ to either geodesic ball or semigeodesic cylinder.

Proposition 3.4.8 (Localization to a Geodesic Neighborhood)**.** *Let* $0 < \gamma < 1$*. For any* $\epsilon > 0$ *such that* $\epsilon^\gamma < \min\{\frac{r}{C_1}, r_\iota\}$ *and for any* $z \in \mathbb{N}$*,*

$$\left| \int_{\mathcal{M}\setminus \tilde{B}_{\epsilon^\gamma}(x)} k\left(\frac{d_{\mathbb{R}^d}(\iota(x), \iota(y))}{\epsilon^2}\right) f(y) q(y)\ d\ \mathrm{Vol} \right| \in \mathcal{O}(\epsilon^z)$$

where $\tilde{B}_{\epsilon^\gamma}(x)$ *is a semigeodesic cylinder if* $x \in N_{\epsilon^\gamma}$ *and is a geodesic ball if* $x \in \mathcal{M}_{\epsilon^\gamma}$*.*

Proof. If $\epsilon^\gamma < r_\iota$, we have that the preimage of an ϵ^γ ball in $\mathbb{R}^d$ centered about $\iota(x)$ is contained in either a normal or semigeodesic coordinate chart centered at x by Proposition 3.4.3. If $\epsilon^\gamma < \frac{r}{C_1}$, then $\tilde{B}_{C_1\epsilon^\gamma}(x)$ contains this preimage by Proposition 3.4.5. Hence, any point in $\mathcal{M}$ outside of $\tilde{B}_{C_1\epsilon^\gamma}(x)$ has extrinsic distance no less than ϵ^γ from x.

From here, the argument of the previous chapter is the same. Using exponential decay of the kernel, this implies that

$$\int_{\tilde{B}_{C_1\epsilon^\gamma}(x)} k\left(\frac{d_{\mathbb{R}^d}(\iota(x),\iota(y))}{\epsilon^2}\right) q \; d \text{ Vol} \leq \int_{\tilde{B}^{\mathcal{M}}_{C_1\epsilon^\gamma}(x)} \alpha e^{-\beta \frac{d^2_{\mathbb{R}^d}(\iota(x),\iota(y))}{\epsilon^2}} q \; d \text{ Vol}$$

$$\leq \alpha e^{-\beta \frac{\epsilon^{2\gamma}}{\epsilon^2}}$$

$$= \alpha e^{-\beta e^{2(\gamma-1)}}$$

We then apply Cauchy-Schwarz inequality in q-weighted $L^2(\mathcal{M})$:

$$\left\langle k\left(\frac{d_{\mathbb{R}^d}(\iota(x),\iota(y))}{\epsilon^2}\right), f\right\rangle^2 \leq \left\langle k\left(\frac{d_{\mathbb{R}^d}(\iota(x),\iota(y))}{\epsilon^2}\right), k\left(\frac{d_{\mathbb{R}^d}(\iota(x),\iota(y))}{\epsilon^2}\right)\right\rangle^2 \langle f,f\rangle$$

$$\leq \langle f,f\rangle \alpha e^{-2\beta\epsilon^{2(\gamma-1)}} \int_{\mathcal{M}\setminus\tilde{B}^{\mathcal{M}}_{C_1\epsilon^\gamma}(x)} q \; d \text{ Vol}$$

$$\leq \langle f,f\rangle \alpha e^{-2\beta\epsilon^{2(\gamma-1)}} \int_{\mathcal{M}} q \; d \text{ Vol}$$

$$= \langle f,f\rangle \alpha e^{-2\beta\epsilon^{2(\gamma-1)}}$$

We see that the term $\langle f,f\rangle \alpha e^{-2\beta\epsilon^{2(\gamma-1)}}$ is asymptotically bounded by any polynomial ϵ^z with $z \geq 1$ by making the substitution $\delta = \epsilon^{-1}$ and applying L'Hôpital's rule z-times. □

3.4.2 Expansion

Since we have now shown that one can uniformly localize to a Riemannian normal coordinate ball of radius ϵ^γ or to a semigeodesic cylinder of height and raidus ϵ^γ, we now work out the asymptotic expansion for this chapter. We remark that on $\mathcal{M}_{\epsilon^\gamma}$, the asymptotic expansion follows exactly as in the previous chapter. We therefore now derive the asymptotic expansion on the boundary region N_{ϵ^γ}. We will find in the later chapter that we need only expand to order ϵ in contrast to order ϵ^2 in the previous chapter.

The proof again breaks down into several steps. W first must compute the Taylor expansion of the kernel k, function f, and volume form $d\,\mathrm{Vol}$ in these new coordinates. We will then use the radial symmetry of the coordinates in the first $m-1$ terms in a similar fashion to the previous chapter.

Preliminaries

In order to derive new expansions of the distance comparison and Riemannian volume form, it will be necessary to introduce some additional classical properties from differential geometry.

Since the hypersurfaces $\partial\mathcal{M}_t$ are codimension 1, the second fundamental form of $\partial\mathcal{M}_t$ can be regarded as real-valued function. Formally, this can be described by defining the *scalar second fundamental form* h of $\partial\mathcal{M}_t$ as:

$$h(X,Y) = \langle \Pi(X,Y), \eta \rangle_g .$$

We define the *shape operator* $s_\eta : \mathfrak{X}(\partial\mathcal{M}) \to \mathfrak{X}(\partial\mathcal{M})$ as

$$s_\eta(X) = \nabla^{\mathcal{M}}_X \eta$$

for any smooth extension of η to an open subset of $\mathcal{M}$. The shape operator can be expressed in terms of the second fundamental form as

$$\langle s_\eta(X), Y \rangle_g = \langle \eta, \Pi(X,Y) \rangle_g .$$

and we see that the shape operator is obtained by raising an index of the scalar second fundamental form.

The *mean curvature* $H : \partial\mathcal{M}_t \to \mathbb{R}$ of $\partial\mathcal{M}_t$ is the trace of the shape operator, computed by taking the trace of any matrix representation of the shape operator for each point in $\partial\mathcal{M}_t$. In particular, we will be interested in the representation of the shape operator in terms of the semigeodesic coordinate basis.

Lemma 3.4.9. *The matrix representation of the shape operator with respect to the semigeodesic coordinate frame is the $m-1 \times m-1$ matrix of Christoffel symbols*

$$s_\eta(X) = \left(\Gamma^\beta_{\alpha m}\right)(X_\alpha).$$

Proof. We express the shape operator in terms of the coordinate frame:

$$\begin{aligned} s_\eta(X) &= \nabla^{\mathcal{M}}_{X^i\partial_i}\partial_m = X^\alpha \nabla^{\mathcal{M}}_{\partial_\alpha}\partial_m \\ &= X^\alpha \partial_\alpha(1)\partial_m + X^\alpha \Gamma^j_{\alpha m}\partial_j \\ &= X^\alpha \Gamma^\beta_{\alpha m}\partial_\beta + X^\alpha \Gamma^m_{\alpha m}\partial_m \\ &= X^\alpha \Gamma^\beta_{\alpha m}\partial_\beta. \end{aligned}$$

Written as a matrix, this is precisely $\left(\Gamma^\beta_{\alpha m}\right)(X_\alpha)$. □

Expansion of the Riemannian Volume Form

We next will show that the Taylor expansion of the Riemannian volume form in terms of the geodesic distance from the boundary is precisely $H\ d\,\mathrm{Vol}$. This is a classical result called the *first variation of area.*

Lemma 3.4.10. *Let I denote an open, half open, or closed interval and let $A(t) : I \to GL(n, \mathbb{R})$ be a smooth family of matrices. Then*

$$\frac{d}{dt}\det(A)^{\frac{1}{2}} = \frac{1}{2}\mathrm{Tr}\left(A^{-1}(t)\frac{d}{dt}A(t)\right)\det(A)^{\frac{1}{2}}$$

Proposition 3.4.11 (First Variation of Area)**.** *In semigeodesic coordinates $(u^1, ..., u^m)$*

based at x,

$$d\ \mathrm{Vol}(u) = 1 + H(x)u^m + \mathcal{O}(\|u\|^2_{\mathrm{sem}})$$

where $H(x)$ is the mean curvature of the parallel hypersurface $\partial\mathcal{M}_{b_x}$ intersecting x.

Proof. Let $(u^1, ..., u^m)$ denote semigeodesic coordinates centered at x so that the coordinate u^m parameterizes the inward-flowing geodesic $\gamma(u^n) = (0, ..., 0, u^n)$. We first compute the first-order derivative of the volume form in the u^m-direction. Applying Lemma 3.4.10, we have:

$$\begin{aligned}\frac{d}{du^m}\ d\ \mathrm{Vol}(0, ..., 0, u^m) &= \frac{d}{du^m}\sqrt{|\det g(0, ..., 0, u^m)|} \\ &= \mathrm{Tr}\left(g^{ik}\frac{\partial g_{kj}}{\partial u^m}(0, ..., 0, u^m)\right)|\det(g(0, ..., 0, u^m))|^{\frac{1}{2}}\end{aligned}$$

Since by definition the m-th coordinate vector field ∂_m is orthogonal to each other coordinate vector field ∂_α for $\alpha \in \{1, .., m-1\}$, we have that

$$\frac{\partial g_{\alpha m}}{\partial u^m} = \frac{\partial g_{\alpha m}}{\partial u^\beta} = \frac{\partial g_{mm}}{\partial u^m} = 0 \tag{3.4.3}$$

for all $\alpha, \beta \in \{1, .., m-1\}$. Plugging this into the formula for Christoffel symbols

$$\Gamma^k_{ij} = \frac{1}{2}g^{kl}\left(\frac{\partial g_{jl}}{\partial x^i} + \frac{\partial g_{il}}{\partial x^j} - \frac{\partial g_{ij}}{\partial x^l}\right)$$

yields that

$$g^{ik}\frac{\partial g_{kj}}{\partial u^m} = \Gamma^j_{im}.$$

Furthermore, we also have that

$$\Gamma^m_{mm} = \Gamma^m_{im} = \Gamma^m_{mi} = \Gamma^i_{mm} = 0$$

for all $i \in \{1, ..., m-1\}$.

This implies that m-th row and column of the matrix product

$$(g^{ij}) \left(\frac{\partial g_{ij}}{\partial u^m} \right)$$

are zero. We then have that for $\alpha, \beta, \mu \in \{1, ..., m-1\}$.

$$\mathrm{Tr}\left(g^{ij} \frac{\partial g_{ij}}{\partial u^m} \right) = \mathrm{Tr}\left(g^{\alpha\mu} \frac{\partial g_{\mu\beta}}{\partial u^m} \right)$$
$$= \mathrm{Tr}\left(\Gamma^\beta_{\alpha m} \right).$$

From Proposition 3.4.9 we see that this is the trace of the shape operator in semigeodesic coordinates, and thus equal to the mean curvature of the parallel hypersurface $\partial \mathcal{M}_{b_x}$ at x.

□

Distance Comparison

We now derive the comparison between extrinsic distance in $\mathbb{R}^d$ and the norm in semigeodesic coordinates. This is a new result which is a generalization of Lemma 2.3.7 which was first proven in [35]. The proof is obtained by performing a Taylor expansion of the embedding ι in semigdeodesic coordinates.

For clarity, we begin with a few lemmas which will show that terms in the Taylor expansion are coordinate expressions for the Levi-Civita connection in $\mathcal{M}$. A minor technical detail for these results is the fact that the Levi-Civita connection ∇ is not a pointwise operator. More specfically, when evaluating $\nabla_X Y$ at a point $x \in \mathcal{M}$, Y must be a vector field defined on a neighborhood of $\mathcal{M}$.

This motivates the following setup. For each of the next lemmas, we let $x \in \mathcal{M}$ be fixed, and let $u = (u^1, ..., u^m)$ be the coordinate representative of a point $y \in \mathcal{M}$ in semigeodesic coordinates constructed in the manner above. In this case, we have that u can be identified with a tangent vector in $T_x\mathcal{M}$ by

$$\exp^{\mathcal{M}}_{\exp^{\partial\mathcal{M}}_x(\sum_{i=1}^{m-1} u^i\partial_i)}(-u^m\eta).$$

In other words, u may be represented by the tangent vector in $T_x\mathcal{M}$ defined by $u^i\partial_i$. For each fixed u, we then extend this representation to a vector field $U = u^i\partial_i$ on the chart where u^i are constant functions. We then have that the vector field U is equal to u at the point $x \in \mathcal{M}$.

Lemma 3.4.12. *Let $x \in \mathcal{M}$ be fixed and suppose we choose semigeodesic coordinates centered at x in the manner illustrated above. If we then let u be the coordinate representative of the point y in semigeodesic coordinates, then u can be identified with a tangent vector in $T_x\mathcal{M}$ through the exponential map.*

(a) $U_p \in T_p\mathcal{M}$ maps to the point u in semigeodesic coordinates centered at p.

(b) The coordinate representation $U = u^i\partial_i$ has constant component functions u^i.

Then at the point x:

$$2\left\langle \nabla_U U, U\right\rangle_g = \delta_{\alpha\beta}\left(\frac{\partial^2\iota^\alpha}{\partial u^i\partial u^k}\frac{\partial\iota^\beta}{\partial u^j} + \frac{\partial\iota^\beta}{\partial u^i}\frac{\partial^2\iota^\alpha}{\partial u^j\partial u^k}\right).$$

Proof. Since $\iota : \mathcal{M} \to \mathbb{R}^d$ is an isometric embedding, we may relate the components of the metric in $\mathcal{M}$ to those in $\mathbb{R}^d$ via:

$$g^{\mathcal{M}}_{ab}(0) = g^{\mathbb{R}^d}_{\alpha\beta}(0)\frac{\partial\iota^\alpha}{\partial u^a}\frac{\partial\iota^\beta}{\partial u^b} = \delta_{\alpha\beta}\frac{\partial\iota^\alpha}{\partial u^a}\frac{\partial\iota^\beta}{\partial u^b}$$

We then take the partial derivative of both sides, noting that we are in normal coordinates in $\mathbb{R}^d$ and therefore all partial derivatives of the metric components vanish at 0. This yields:

$$\frac{\partial g_{ab}^{\mathcal{M}}(0)}{\partial u^c} = \frac{\partial g_{\alpha\beta}^{\mathbb{R}^d}(0)}{\partial u^c} \frac{\partial \iota^\alpha}{\partial u^\rho} \frac{\partial \iota^\rho}{\partial u^c} \frac{\partial \iota^\alpha}{\partial u^a} \frac{\partial \iota^\beta}{\partial u^b} + g_{\alpha\beta}^{\mathbb{R}^d}(0) \frac{\partial}{\partial u^c} \left(\frac{\partial \iota^\alpha}{\partial u^a} \frac{\partial \iota^\alpha}{\partial u^b} \right)$$

$$= \delta_{\alpha\beta} \left(\frac{\partial^2 \iota^\alpha}{\partial u^a \partial u^c} \frac{\partial \iota^\beta}{\partial u^b} + \frac{\partial \iota^\beta}{\partial u^a} \frac{\partial^2 \iota^\alpha}{\partial u^b \partial u^c} \right).$$

Given any $u \in T_p\mathcal{M}$, we can extend u to the vector field $U = u^i \partial_i$ on the coordinate chart where u^i are constant functions and ∂_i are the coordinate vector fields. Using that the Levi-Civita connection is compatible with the metric, we obtain:

$$\frac{\partial g_{ab}^{\mathcal{M}}(0)}{\partial u^c} u^a u^b u^c = U \langle U, U \rangle_g = 2 \langle \nabla_U U, U \rangle_g$$

as desired. □

Next we relate the Levi-Civita connection to the second fundamental form $\Pi_{\partial \mathcal{M}_t}$ of the hypersurfaces $\partial \mathcal{M}_t$ as a submanifolds of $\mathcal{M}$.

Lemma 3.4.13. *With u and U having the same conditions as above, decompose U into the vector field $U^\top = \sum_{i=1}^{m-1} u^i \partial_i$ tangential to the hypersurface $\partial \mathcal{M}_{b_x}$ and the normal vector field $U^\perp = u^m \partial_m = -u^m \eta_x$. Then we have:*

$$\langle \nabla_U U, U \rangle_g = -\left\langle \Pi_{\partial \mathcal{M}_{b_x}}(U^\top, U^\top), U^\perp \right\rangle_g$$

$$= -h(U^\top, U^\top) u^n$$

Proof. We decompose $\langle \nabla_U U, U \rangle_g$ into

$$\langle \nabla_U U, U \rangle_g = \left\langle \nabla_{(U^\top + U^\perp)} (U^\top + U^\perp), (U^\top + U^\perp) \right\rangle_g.$$

Since the connection is linear in both components over $\mathbb{R}$, and the component functions of U are constant, we may simply bilinearly expand the above term. We also note that

$$\nabla_{u^j \partial_j} u^i \partial_i = u^i u^j \nabla_{\partial_j} \partial_i = u^i u^j \Gamma^k_{ij} \partial_k.$$

Since many of the Christoffel symbols in semigeodesic coordinates are zero, we are left with:

$$\langle \nabla_U U, U \rangle_g = \left\langle \nabla_{U^\top} U^\top, U^\top \right\rangle_g + \left\langle \nabla_{U^\top} U^\top, U^\perp \right\rangle_g + \left\langle \nabla_{U^\top} U^\perp, U^\top \right\rangle_g + \left\langle \nabla_{U^\perp} U^\top, U^\top \right\rangle_g$$

Using the Gauss equation for the hypersurface embedded in $\mathcal{M}$, we get that $\nabla_{U^\top} U^\top = \Pi(U^\top, U^\top)$. This implies that the first term is zero since the second fundamental form is orthogonal to $\partial \mathcal{M}_{b_x}$ and the second term is $\left\langle \Pi_{\partial \mathcal{M}_{b_x}}(U^\top, U^\top), U^\perp \right\rangle_g$.

For the next two terms, we first note that since ∇ is a symmetric connection,

$$\nabla_{u^j \partial_j} u^i \partial_i = u^i u^j \Gamma^k_{ij} \partial_k = u^i u^j \Gamma^k_{ji} \partial_k = \nabla_{u^i \partial_i} u^j \partial_j$$

and so ∇ is a symmetric tensor over $\mathbb{R}$. Thus, both of the remaining terms are equal. The Weingarten equation implies that:

$$\left\langle \nabla_{U^\top} U^\perp, U^\top \right\rangle_g = - \left\langle \Pi(U^\top, U^\top), U^\perp \right\rangle_g.$$

Putting this all together, we are left with:

$$\langle \nabla_U U, U \rangle_g = \left\langle \Pi_{\partial \mathcal{M}^t}(U^\top, U^\top), U^\perp \right\rangle_g - 2 \left\langle \Pi(U^\top, U^\top), U^\perp \right\rangle_g = - \left\langle \Pi(U^\top, U^\top), U^\perp \right\rangle_g$$

□

We now are ready to perform the asymptotic expansion. This result is analogous to Proposition 6 of [35] except for semigeodesic coordinates instead of normal coordinates.

Lemma 3.4.14. *In semigeodesic coordinates we have the following distance comparison,*

$$\lim_{|u|^3 \to 0} \frac{\|x-y\|^2_{\mathbb{R}^d} - \|u\|^2_{\text{sem}}}{\|u\|^3_{\text{sem}}} = -\left\langle \Pi_{\partial \mathcal{M}_{b_x}}(u^\top, u^\top), u^\perp \right\rangle_g$$

and so

$$\|x-y\|^2_{\mathbb{R}^d} = \|u\|^2_{\text{sem}} - \left\langle \Pi_{\partial \mathcal{M}_{b_x}}(u^\top, u^\top), u^\perp \right\rangle_g + \mathcal{O}|(\|u\|^4_{\text{sem}}).$$

Proof. Fix $x \in \mathcal{M}$ and let $u = (u^1, ..., u^m)$ denote a system of semigeodesic coordinates centered at x. Construct a set of normal coordinates about $\iota(x)$ by orthonormally extending the pushforward of the orthonormal basis at x. The coordinate representation of $d\iota$ at x is then an $m \times n$ identity matrix.

We then Taylor expand ι:

$$\begin{aligned}
\|\iota(u)\|^2_{\mathbb{R}^d} &= g^{\mathbb{R}^d}_{\alpha\beta}(0)\iota^\alpha(0)\iota^\beta(0) \\
&= g^{\mathbb{R}^d}_{\alpha\beta}(0)\left(\iota^\alpha(0) + \frac{\partial \iota^\alpha(0)}{\partial u^i}u^i + \frac{\partial^2 \iota^\alpha(0)}{\partial u^i u^j}u^i u^j + \mathcal{O}(\|u^i\|^3_{\text{sem}})\right) \\
&\qquad \left(\iota^\beta(0) + \frac{\partial \iota^\beta(0)}{\partial u^i}u^i + \frac{\partial^2 \iota^\beta(0)}{\partial u^i u^j}u^i u^j + \mathcal{O}(\|u^i\|^3_{\text{sem}})\right)
\end{aligned}$$

Since $\iota(0) = 0$, many terms simplify and we have:

$$\begin{aligned}
\|\iota(u)\|^2_{\mathbb{R}^d} &= g_{\alpha\beta}(0)\frac{\partial \iota^\alpha}{\partial u^i}\frac{\partial \iota^\beta}{\partial u^j}u^i u^j + \frac{1}{2}g_{\alpha\beta}(0)\frac{\partial^2 \iota^\alpha}{\partial u^i u^k}\frac{\partial \iota^\beta}{\partial u^j}u^i u^j u^k \\
&\quad + \frac{1}{2}g_{\alpha\beta}(0)\frac{\partial \iota^\beta}{\partial u^i}\frac{\partial^2 \iota^\alpha}{\partial u^j u^k}u^i u^j u^k + \mathcal{O}(|u|^4) \\
&= \|u\|^2_{\text{sem}} + \frac{1}{2}g_{\alpha\beta}(0)\frac{\partial^2 \iota^\alpha}{\partial u^i u^k}\frac{\partial \iota^\beta}{\partial u^j}u^i u^j u^k \\
&\quad + \frac{1}{2}g_{\alpha\beta}(0)\frac{\partial \iota^\beta}{\partial u^i}\frac{\partial^2 \iota^\alpha}{\partial u^j u^k}u^i u^j u^k + \mathcal{O}(|u|^4)
\end{aligned}$$

We then apply Lemma 3.4.13 to obtain:

$$\begin{aligned}\|\iota(u)\|^2_{\mathbb{R}^d} &= \|u\|^2_{\text{sem}} + \frac{1}{2}\frac{\partial g^{\mathcal{M}}_{ij}(0)}{\partial u^k} u^i u^j u^k + \mathcal{O}(\|u\|^4) \\ &= \|u\|^2_{\text{sem}} + \langle \nabla_U U, U\rangle_g + \mathcal{O}(\|u\|^4) \\ &= \|u\|^2_{\text{sem}} - \left\langle \Pi_{\partial \mathcal{M}_{b_x}}(U^\top, U^\top), U^\perp \right\rangle_g + \mathcal{O}(\|u\|^4).\end{aligned}$$

□

Lemma 3.4.15. *Integrating over a cylinder* $B = \{u \mid \sum_{i=1}^{m-1}(u^i)^2 < \epsilon^2, u^m \in [-b_x/\epsilon, \epsilon]\}$ *which is symmetric in coordinates* u^i *for* $1 \leq i \leq m-1$ *we have*

$$\begin{aligned}\int_B k'(|u|^2) \left\langle \Pi_{\partial \mathcal{M}^t}(U^\top, U^\top), U^\perp \right\rangle_g du &= -\frac{(m-1)}{2} H(x) \int_B k(|u|^2) u^m \, du \\ &= \frac{(m-1)}{2} m_1^\partial(x) H(x) + \mathcal{O}(\epsilon^z) \qquad (3.4.4)\end{aligned}$$

for any $z \geq 1$*, where* $H(x)$ *is the mean curvature.*

Proof. Linear expansion of $\left\langle \Pi_{\partial \mathcal{M}^t}(U^\top, U^\top), U^\perp \right\rangle_g$ in terms of the coordinate basis at x yields:

$$\left\langle \Pi_{\partial \mathcal{M}^t}(U^\top, U^\top), U^\perp \right\rangle_g = \langle \Pi_{\partial \mathcal{M}}(\partial_i, \partial_j), \partial_m \rangle_g u^i u^j u^m.$$

since the domain B is symmetric in the coordinates u^i for $1 \leq i \leq m-1$, all of the terms $u^i u^j$ with $i \neq j$ will integrate to zero. Thus, we have

$$\int_B k'(|u|^2) \left\langle \Pi_{\partial \mathcal{M}^t}(U^\top, U^\top), U^\perp \right\rangle_g du = \langle \Pi_{\partial \mathcal{M}}(\partial_i, \partial_i), \partial_m \rangle_g \int_B k'(|u|^2) u^i u^i u^m du$$

and by the symmetry of the kernel, the integrals are equal for all $1 \leq i \leq m-1$, so we only need to compute

$$\int_B k'(|u|^2)u^1u^1u^m ds = \int_B \frac{1}{2}\left(\frac{\partial}{\partial u^1}k(|u|^2)\right)u^1u^m du^1du^2\cdots du^m = -\frac{1}{2}\int_B k(|u|^2)u^m du$$

where the last equality follows from integration by parts with respect to u^1. Finally, pulling the integral out of the sum, we have,

$$\int_B k'(|u|^2)\left\langle \Pi_{\partial\mathcal{M}^t}(U^\top,U^\top),U^\perp\right\rangle_g du = -\frac{1}{2}\int_B k(|u|^2)u^m du \sum_{i=1}^{m-1}\left\langle \Pi_{\partial\mathcal{M}}(\partial_i,\partial_i),\partial_m\right\rangle_g$$

and since the mean curvature is defined as $H(x) = \frac{1}{m-1}\sum_{i=1}^{m-1}\left\langle \Pi_{\partial\mathcal{M}}(\partial_i,\partial_i),\partial_m\right\rangle_g$ the first equality in (3.4.4) follows. Finally, substituting $u^m = -u\cdot\eta_x$ and extending the integral to all of $\{u \,|\, u^m > -b_x\} = \{u \,|\, u\cdot\eta_x < b_x\}$ by Lemma 3.4.8 we obtain the second equality of (3.4.4). □

Proposition 3.4.16. *Let x be a point in the normal collar of width $\frac{r_C}{2}$, $\gamma\in(0,1)$ and for ϵ sufficiently small, then we have*

$$\begin{aligned}\frac{1}{\epsilon^m}\int_{y\in\mathcal{M}} k\left(\frac{|x-y|^2}{\epsilon^2}\right) f(y)q(y)\; d\text{ Vol} = {} & m_0^\partial(x)f(x)q(x)\\ & + \epsilon m_1^\partial(x)\left(d(fq)_x(\eta) + \frac{m-1}{2}H(x)f(x)q(x)\right)\\ & + \mathcal{O}(\epsilon^2). \end{aligned} \tag{3.4.5}$$

where

$$m_0^\partial(x) = \int_B k(\|u\|^2_{\mathbb{R}^m})\; du \text{ and } m_2^\partial(x) = \int_B k(\|u\|^2_{\mathbb{R}^m})u^m\; du.$$

and $H(x)$ is the mean curvature of $\partial\mathcal{M}_{b_x}$ at x.

Proof. We first apply Proposition 3.4.8 to localize the integral to a semigeodesic cylinder of radius and height ϵ^γ. Then, following the same proof as in Lemma 2.3.9, we obtain:

$$k\left(\frac{\|x-y\|^2_{\mathbb{R}^d}}{\epsilon^2}\right) = k\left(\frac{\|u\|^2_{\text{sem}} - h(u^\top, u^\top)u^n + \mathcal{O}\left(\frac{\|u\|^4_{\text{sem}}}{\epsilon^2}\right)}{\epsilon^2}\right)$$

$$= k\left(\frac{\|u\|^2_{\text{sem}}}{\epsilon^2}\right) - k'\left(\frac{\|u\|^2_{\text{sem}}}{\epsilon^2}\right)\frac{1}{\epsilon^2}h(u^\top, u^\top)u^n + \mathcal{O}\left(\frac{\|u\|^5_{\text{sem}}}{\epsilon^2}\right)$$

Second, the Taylor expansion of f,

$$f(y) = f(x) + \frac{\partial f}{\partial u^i}u_i + \frac{1}{2}\frac{\partial^2 f}{\partial u^i \partial u^j}u^i u^j + \mathcal{O}(\|u\|^3_{\text{sem}})$$

and finally, by Lemma 3.4.11

$$d\ \text{Vol}(y) = 1 - (m-1)H(x)u^m + \mathcal{O}(\|u\|^2_{\text{sem}}).$$

The product of these three terms appears inside the integral, so multiplying the three expansions and making the change of variables $u \mapsto \epsilon u$, we find the order-ϵ^0 term is $k\left(\|u\|^2_{\text{sem}}\right) f(x)$ which integrates to $m_0^\partial(x) f(x)$. The order-ϵ^1 term is,

$$\epsilon \int_B k\left(\|u\|^2\right)\left(\frac{\partial f}{\partial u^i}u^i - f(x)(m-1)H(x)u^m\right)$$

$$- k'\left(\|u\|^2_{\text{sem}}\right)\left\langle \Pi_{\partial \mathcal{M}^t}(U^\top, U^\top), U^\perp \right\rangle_g f(x)\ du$$

$$= \epsilon m_1^\partial(x)\left\langle \text{grad } f, \eta\right\rangle_g + \epsilon m_1^\partial(x)(m-1)H(x)f(x) - \epsilon m_1^\partial(x)\frac{m-1}{2}H(x)f(x)$$

$$= \epsilon m_1^\partial(x)\left(\left\langle \text{grad } f, \eta\right\rangle_g + \frac{m-1}{2}H(x)f(x)\right)$$

where the first equality comes from noting that u^i integrates to zero by symmetry for $1 \le i \le m-1$ and then applying Lemma 3.4.15. □

We have now derived a pointwise asymptotic expansion of the kernel integral operator $\mathcal{K}_\epsilon$ in an analogous fashion to the expansion in Chapter 2. We show that using semigeodesic coordinates, one can derive that the first-order term in the expansion is related to the mean curvature of the boundary $\partial\mathcal{M}$ in $\mathcal{M}$. We have also shown that the expansion holds uniformly in the variable ϵ across all of M, so that one can simultaneously expand $\mathcal{K}_\epsilon$ for all points of $\mathcal{M}$ assuming small enough ϵ. Due to the first-order term in the expansion in semigeodesic coordinates, we cannot show the same pointwise convergence in the same way as the previous chapter. Instead, we will later show that the notion of weak convergence is a more suitable notion of convergence. In order to demonstrate this, we must derive asymptotics which allow us to estimate boundary integrals in $\mathcal{M}$. In the next chapter, we make use of semigeodesic coordinates to derive such an estimate.

Chapter 4: Asymptotic Estimation of Boundary Integrals

4.1 Summary

In this chapter, we use the properties of semigeodesic coordinates developed in the previous chapter to obtain an asymptotic estimate of boundary integrals on $\mathcal{M}$. We will show that integrating over the boundary region N_{ϵ^γ} is asymptotically equivalent to integrating over the boundary.

4.2 Notation, Definitions, and Assumptions

We again assume that (M, g) is a C^∞, dimension m compact Riemannian manifold. We now assume that M is a manifold with boundary and that $\iota : M \to \mathbb{R}^d$ is an isometric embedding of M into $\mathbb{R}^d$. We further assume that ι is a proper embedding so that in particular, the topological boundary of $\iota(M)$ in $\mathbb{R}^d$ is equal to $\iota(\partial M)$.

We let $d\,\mathrm{Vol}$ denote the Riemannian volume measure inherited from the metric g on $\mathcal{M}$. We assume that $q : \mathcal{M} \to \mathbb{R}$ is a C^∞ probability density function corresponding to a probability measure $d\mu$ which is absolutely continuous with respect to $d\,\mathrm{Vol}$ and nowhere zero on $\mathcal{M}$.

We again assume $k : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ is a C^∞ function which has exponential decay, so that $k(x) \leq \alpha e^{-\beta x}$ for all $x \in \mathbb{R}_{\geq 0}$. We again assume that the first two derivatives of k also have exponential decay.

In this chapter, we will be concerned with a special case of semigeodesic coordinates, constructed on the boundary. These are referred to as *boundary normal coordinates*.

4.3 Estimation of Boundary Integrals

We now prove the main result of the section:

Theorem 4.3.1. *Let $\mathcal{M}$ be a compact manifold with boundary isometrically and properly embedded into $\mathbb{R}^d$. Let $k : \mathbb{R}_{\geq 0} \to \mathbb{R}^{\geq 0}$ be a kernel function with exponential decay and whose first two derivatives have exponential decay. Then for $\gamma \in (0,1)$ and $\epsilon > 0$ such that $\epsilon^\gamma < \frac{R_C}{2}$,*

$$\frac{1}{\epsilon}\int_{x \in N_{\epsilon^\gamma}} k\left(\frac{b_x^2}{\epsilon^2}\right) f(x)q(x)\ d\ \mathrm{Vol} = \overline{m}_0 \int_{x \in \partial\mathcal{M}} f(x)q(x)\ d\ \mathrm{Vol}_\partial \tag{4.3.1}$$

$$+ \epsilon \overline{m}_1 \int_{x \in \partial\mathcal{M}} f(x)q(x)H(x) \tag{4.3.2}$$

$$- \langle \mathrm{grad}\ f, \eta \rangle_g\ d\ \mathrm{Vol}_{\partial M} + \mathcal{O}(\epsilon^2) \tag{4.3.3}$$

where $\overline{m}_0 = \int_0^\infty k(u)\, du$ and $\overline{m}_1 = \int_0^\infty uk(u)\, du$ and $H(x)$ is the mean curvature of ∂M at $x \in \partial M$.

Proof. Let $0 < \gamma < 1$ and $\epsilon > 0$ be such that ϵ^γ is less than $\frac{R_C}{2}$ so that the boundary region N_{ϵ^γ} is within the normal collar. Since k is assumed to have exponential decay, we can localize the integral to N_{ϵ^γ} by using the same argument as previously used in Lemmas 3.4.7 and 3.4.8. We then have:

$$\frac{1}{\epsilon}\int_{\mathcal{M}} k\left(\frac{b_x^2}{\epsilon^2}\right) f(x)q(x) d\mathrm{vol} = \frac{1}{\epsilon}\int_{N_{\epsilon^\gamma}} k\left(\frac{b_x^2}{\epsilon^2}\right) f(x)q(x) d\mathrm{vol} + \mathcal{O}(\epsilon^z)$$

for any choice of $z \in \mathbb{N}$.

In contrast to previous localization arguments, we are not localized to a single coordinate chart, but rather the boundary region N_{ϵ^γ}. We now compute the expansion by parameterizing the integral in boundary normal coordintes, which are simply semigeodesic coordinates constructed on ∂M. More specifically, We first generate a covering of N_{ϵ^γ} by measurable subsets, each of which are contained in a single boundary normal coordinate chart. Given such a covering, we can then perform an expansion in coordinates and use parameterizations to compute the integral.

Let $\mathcal{U} = \{U_i\}_{i\in I}$ be a covering of $\partial\mathcal{M}$ in boundary normal coordinate coordinate charts. By taking intersections and complements, we can then generate a covering of M by measurable sets $\{V_j\}_{j\in J}$ of ∂M such that V_j are disjoint, and each contained in a single U_i. We then extend each V_j to a measurable subset of M by letting $\tilde{V}_j = \phi(V_j \times [0, \epsilon^\gamma))$. Therefore each V_j can be extended to a measurable set $\tilde{V}_j$ of M which is contained in a boundary normal coordinate chart map ϕ_{U_i}.

Hence, the integral over N_{ϵ^γ} can be broken up into the sum of disjoint integrals over $\tilde{V}_j$, each of which are contained in a single boundary normal coordinate chart. We will then expand the expression inside of each coordinate chart, then sum each of the expansions to obtain an expansion of the integral over the entire boundary region N_{ϵ^γ}.

The integral over the boundary region can then be parameterized as:

$$\int_{N_{\epsilon^\gamma}} k\left(\frac{b_y^2}{\epsilon^2}\right) f(y)q(y)\ d\ \mathrm{Vol} = \sum_{j\in J}\int_{\tilde{V}_j} k\left(\frac{b_y^2}{\epsilon^2}\right) f(y)q(y)\ d\ \mathrm{Vol}. \tag{4.3.4}$$

In each of these charts $u^n = b_x$. We then Taylor expand in the u^n variable about $u^n = 0$ of fq. Using the first variation of area, we may also expand d Vol in the same manner, with the first term corresponding to mean curvature.

$$\begin{aligned}
\frac{1}{\epsilon}\int_{V_j} k\left(\frac{b_x}{\epsilon^2}\right) f(x)q(x)d\mathrm{vol} &= \frac{1}{\epsilon}\int_{V_j} k\left(\frac{(u^n)^2}{\epsilon^2}\right) f(u^\top, u^n)q(u^\top, u^n)\ d\ \mathrm{Vol}(u^\top, u^n) \\
&= \frac{1}{\epsilon}\Big(\int_{\phi_{U_i}(\tilde{V}_j)} k\left(\frac{(u^n)^2}{\epsilon^2}\right) f(u^\top, 0)q(u^\top, 0)\ d\ \mathrm{Vol}(u^\top, 0) \\
&+ \int_{V_j} k\left(\frac{(u^n)^2}{\epsilon^2}\right) fq(u^\top, 0)H(u^\top, 0)u^n\ d\ \mathrm{Vol}(u^\top, 0)
\end{aligned}$$

$$+\int_{V_j} k\left(\frac{(u^n)^2}{\epsilon^2}\right)\frac{\partial fq}{\partial u^n}(u^\top,0)u^n \ d\ \mathrm{Vol}(u^\top,0)$$

$$+\int_{V_j} k\left(\frac{(u^n)^2}{\epsilon^2}\right)\frac{\partial fq}{\partial u^n}(u^\top,0)H(u^\top,0)(u^n)^2 \ d\ \mathrm{Vol}(u^\top,0)$$

$$+\int_{V_j} k\left(\frac{(u^n)^2}{\epsilon^2}\right)\omega(u^\top,\tilde{u}^n))(u^n)^2 \ d\ \mathrm{Vol}(u^\top,\tilde{u}^n)\Big)$$

where $\omega(u^\top,\tilde{u}^n)$ is the sum of the second-order terms in both expansions with $0 \le \tilde{u}^n < \epsilon^\gamma$. Since $d\ \mathrm{Vol} = \sqrt{|g|}$ in coordinates, and the n-th coordinate vector field $\partial_n = -\eta_y$ is orthogonal to each of the other coordinate vector fields, cofactor expansion of $\sqrt{|g|}$ implies that $d\ \mathrm{Vol}(u^\top,0) = d\ \mathrm{Vol}_\partial(u^\top)$. We can then separate terms involving u^n to obtain:

$$\frac{1}{\epsilon}\int_{\tilde{V}_j} k\left(\frac{b_y^2}{\epsilon^2}\right) f(y)q(y)d\mathrm{vol} = \frac{1}{\epsilon}\int_{u^n=0}^{u^n=\epsilon^\gamma} k\left(\frac{u^n}{\epsilon}\right)du^n \int_{y\in V_j} f(y)q(y)\ d\ \mathrm{Vol}_\partial$$

$$+\frac{1}{\epsilon}\int_{u^n=0}^{u^n=\epsilon^\gamma} k\left(\frac{u^n}{\epsilon}\right)u^n du^n \int_{V_j} f(y)q(y)H(y)\ d\ \mathrm{Vol}_\partial$$

$$+\frac{1}{\epsilon}\int_{u^n=0}^{u^n=\epsilon^\gamma} k\left(\frac{u^n}{\epsilon}\right)u^n du^n \int_{V_j} -\langle \eta_y, \mathrm{grad}\ fq(y)\rangle_g\ d\ \mathrm{Vol}_\partial$$

$$+\frac{1}{\epsilon}\int_{u^n=0}^{u^n=\epsilon^\gamma} k\left(\frac{(u^n)^2}{\epsilon^2}\right)(u^n)^2du^n \int_{y\in V_j} -gdot\eta_y, \mathrm{grad}\ fqH(y)\ d\ \mathrm{Vol}_\partial$$

$$+\frac{1}{\epsilon}\int_{u^n=0}^{u^n=\epsilon^\gamma} k\left(\frac{(u^n)^2}{\epsilon^2}\right)(u^n)^2du^n \int_{y\in W_j} \omega(u^\top,\tilde{u}^n)\ d\ \mathrm{Vol}_{\partial M_{\tilde{u}^n}}$$

Where W_j is the coordinate image of $\partial M_{\tilde{u}^n}$ in these coordinates (recall that ∂M_t indicates the hypersurface of points distance t away from ∂M.)

Since the integral over V_j does not depend on ϵ, we may use exponential decay of the kernel to extend the integral over u^n to infinity. By then making a substitution $u^n \mapsto \epsilon u$, and letting $\overline{m}_0 = \int_0^\infty k(u)\,du$ and $\overline{m}_1 = \int_0^\infty k(u)u\,du$ we are left with:

$$\frac{1}{\epsilon}\int_{\tilde{V}_j} k\left(\frac{b_y}{\epsilon}\right) f(y)q(y)d\text{vol} = \overline{m}_0 \int_{\phi_{U_i}(V_j)} f(y)q(y)\ d\ \text{Vol}_\partial$$

$$+ \epsilon\overline{m}_1 \int_{\phi_{U_i}(V_j)} f(y)q(y)H(y) - \langle \eta_y, \text{grad}\ fq(y)\rangle_g\ d\ \text{Vol}_\partial$$

$$+ \mathcal{O}(\epsilon^2)$$

We remark that To compute the integral over the entire normal collar, we return to the parameterization of the integral in (4.3.4):

$$\int_{N_{\epsilon\gamma}} k\left(\frac{b_y^2}{\epsilon^2}\right) f(y)q(y)\ d\ \text{Vol} = \sum_{j\in J}\int_{\tilde{V}_j} k\left(\frac{b_y^2}{\epsilon^2}\right) f(y)q(y)\ d\ \text{Vol}.$$

Summation over all $\tilde{V}_j$ in the manner above, we are left with:

$$\frac{1}{\epsilon}\int_{N_{\epsilon\gamma}} k\left(\frac{b_y^2}{\epsilon^2}\right) f(y)q(y)d\text{vol} = \overline{m}_0 \int_{\partial\mathcal{M}} f(y)q(y)\ d\ \text{Vol}_\partial$$

$$+ \epsilon\overline{m}_1 \int_{\partial\mathcal{M}} f(y)q(y)H(y) - \langle \eta_y, \text{grad}\ fq(y)\rangle_g\ d\ \text{Vol}_\partial + \mathcal{O}(\epsilon^2)$$

from which the result follows. □

Chapter 5: Proof of Consistency

5.1 Summary

In this chapter, we put together the results of the previous chapters to prove the consistency of the Diffusion maps estimator in the weak sense. For simplicity, we begin with the case of the unnormalized Laplacian with uniform distribution.

5.2 Result for Unnormalized Laplacian with Uniform Distribution

We will now use the results developed in the previous chapter to prove asymptotic consistency of the unnormalized graph Laplacian. In addition to our standard assumptions, we assume that the density q on $\mathcal{M}$ is uniform, that is, $q \equiv 1$.

Theorem 5.2.1. *1.4.4 Let $\mathcal{M}$ be a compact Riemannian manifold with boundary isometrically embedded into $\mathbb{R}^d$ via $\iota : \mathcal{M} \hookrightarrow \mathbb{R}^d$. Let $\mathcal{K}_\epsilon$ be the kernel integral operator on $C^\infty(\mathcal{M})$ induced by a kernel k and uniform distribution $q \equiv 1$ on $\mathcal{M}$ satisfying the previous conditions. Then for $f \in C^\infty(M)$ and test function $\phi \in C^\infty(M)$, we have:*

$$\frac{2}{m_2 \epsilon^{d+2}} \int_{\mathcal{M}} \phi \left(\mathcal{K}_\epsilon f - f \mathcal{K}_\epsilon 1\right) \ d \text{ Vol} = \int_{\mathcal{M}} \langle \text{grad } \phi, \text{grad } f \rangle_g \ d \text{ Vol} + \mathcal{O}(\epsilon).$$

In order to prove this Theorem, we first prove the following lemma

Lemma 5.2.2. *For any $z \in \mathbb{N}$,*

$$\int_0^\infty m_1^\partial(b_x) \ db_x = \frac{m_2}{2} + \mathcal{O}(\epsilon^z)$$

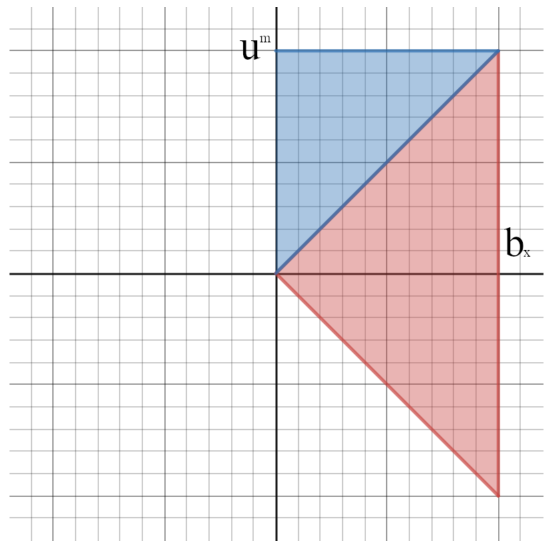

Figure 5.1: The domain of integration for b_x and u^m. The red region indicates the domain which cancels due to symmetry. The remaining blue region is evaluated.

Proof. We have that:

$$\int_0^{\infty} m_1^{\partial}(b_x)\ db_x = \int_0^{\epsilon^\gamma} m_1^{\partial}(b_x) db_x + \mathcal{O}(\epsilon^z)$$

$$= \int_0^{\epsilon^\gamma} \int_{-b_x}^{\epsilon^\gamma} \int_{\mathbb{R}^{m-1}} u^m k(\|u\|^2_{\text{sem}}) du^1 ... du^{m-1} du^m db_x$$

We notice that there is considerable symmetry in the domain of integration between the b_x and u^m variables. Since $u^m k(\|u\|^2_{\text{sem}})$ is an odd function with respect to u^m, we obtain cancellation of the domain in the area indicated in red:

This leads to the simplification to which we then apply Fubini's theorem:

$$\int_0^{\epsilon^\gamma} \int_{-b_x}^{\epsilon^\gamma} \int_{\mathbb{R}^{m-1}} u^m k(\|u\|^2_{\text{sem}}) du^1 ... du^{m-1} du^m db_x = \int_0^{\epsilon^\gamma} \int_{b_x}^{\epsilon^\gamma} \int_{\mathbb{R}^{m-1}} u^m k(\|u\|^2_{\text{sem}}) du^1 ... du^{m-1} du^m db_x$$

$$= \int_0^{\epsilon^\gamma} \int_0^{u^m} \int_{\mathbb{R}^{m-1}} u^m k(\|u\|_{\text{sem}}^2) du^1 ... du^{m-1} db_x du^m$$

$$= \int_0^{\epsilon^\gamma} \int_{\mathbb{R}^{m-1}} \int_0^{u^m} u^m k(\|u\|_{\text{sem}}^2) db_x du^1 ... du^{m-1} du^m$$

$$= \int_0^{\epsilon^\gamma} \int_{\mathbb{R}^{m-1}} (u^m - 0) u^m k(\|u\|_{\text{sem}}^2) du^1 ... du^{m-1} du^m$$

$$= \int_0^{\epsilon^\gamma} \int_{\mathbb{R}}^d (u^m)^2 k(\|u\|_{\text{sem}}^2) du^1 ... du^m$$

$$= \frac{m_2}{2} + \mathcal{O}(\epsilon^z).$$

□

We are now ready to prove the main result of this chapter:

Theorem 5.2.3. *Let $\mathcal{M}$ be a compact Riemannian manifold with boundary isometrically embedded into $\mathbb{R}^d$ via $\iota : \mathcal{M} \hookrightarrow \mathbb{R}^d$. Let $\mathcal{K}_\epsilon$ be the kernel integral operator on $C^\infty(\mathcal{M})$ induced by a kernel k and uniform distribution $q \equiv 1$ on $\mathcal{M}$ satisfying the previous conditions. Then for $f \in C^\infty(M)$ and test function $\phi \in C^\infty(M)$, we have:*

$$\frac{2}{m_2 \epsilon^{d+2}} \int_{\mathcal{M}} \phi \left(\mathcal{K}_\epsilon f - f \mathcal{K}_\epsilon 1 \right) \ d \text{ Vol} = \int_{\mathcal{M}} \langle \text{grad } \phi, \text{grad } f \rangle_g \ d \text{ Vol} + \mathcal{O}(\epsilon).$$

Proof. Using Proposition 2.3.11, we see that for points $x \in M_{\epsilon^\gamma}$:

$$\begin{aligned}\frac{1}{\epsilon^m} \int_{x \in M_{\epsilon^\gamma}} \phi \left(\mathcal{K}_\epsilon f - f \mathcal{K}_\epsilon(1) \right) \ d \text{ Vol} &= \int_{x \in \mathcal{M}_{\epsilon^\gamma}} \phi \left(m_0 f(x) + \frac{\epsilon^2 m_2}{2} \Big(f(x) S(x) - \Delta(f)(x) \Big) + \mathcal{O}(\epsilon^3) \right) \\ &\quad - f(x) \left(m_0 + \frac{\epsilon^2 m_2}{2} S(x) + \mathcal{O}(\epsilon^3) \right) \ d \text{ Vol} \\ &= -\epsilon^2 \frac{m_2}{2} \int_{x \in M_{\epsilon^\gamma}} \phi(x) \Delta f(x) \ \ d \text{ Vol} + \mathcal{O}(\epsilon^3).\end{aligned}$$

Using Proposition 3.4.16, we have that for points in N_{ϵ^γ}:

$$\frac{1}{\epsilon^m}\int_{x\in N_{\epsilon^\gamma}} \phi\left(\mathcal{K}_\epsilon f - f\mathcal{K}_\epsilon(1)\right)\ d\ \mathrm{Vol} = \int_{x\in N_{\epsilon^\gamma}} \phi\Big(m_0^\partial f(x) + \epsilon m_1^\partial(x)\left\langle \mathrm{grad}\ f, \eta\right\rangle_g$$

$$- \frac{m-1}{2}H(x)f(x) + \mathcal{O}(\epsilon^2)\ d\ \mathrm{Vol} + \mathcal{O}(\epsilon^2)$$

$$- f(x)m_0^\partial(x) + \frac{m-1}{2}H(x)f(x) + \mathcal{O}(\epsilon^2)\Big)\ d\ \mathrm{Vol}$$

$$= \epsilon\int_{N_{\epsilon^\gamma}} m_1^\partial(x)\phi\left\langle \mathrm{grad}\ f, \eta\right\rangle_g\ d\ \mathrm{Vol} + \mathcal{O}(\epsilon^2)$$

We then notice that the function $m_1^\partial(x)$ is purely a function of the distance to the boundary b_x and that it decays to zero exponentially as $b_x \to \infty$. Hence, we may apply the result of Theorem 4.3.1. We then have that:

$$\frac{1}{\epsilon^m}\int_{x\in N_{\epsilon^\gamma}} \phi\left(\mathcal{K}_\epsilon f - f\mathcal{K}_\epsilon(1)\right)\ d\ \mathrm{Vol} = \epsilon\int_{N_{\epsilon^\gamma}} m_1^\partial(x)\phi\left\langle \mathrm{grad}\ f, \eta\right\rangle_g\ d\ \mathrm{Vol} + \mathcal{O}(\epsilon^2)$$

$$= \epsilon^2\overline{m_0}\int_{\partial M} \left\langle \phi\ \mathrm{grad}\ f, \eta\right\rangle_g\ d\ \mathrm{Vol}_\partial + \mathcal{O}(\epsilon^3).$$

Where

$$\overline{m_0} = \int_0^\infty m_1^\partial(b_x)\ db_x.$$

We now treat the interior term:

$$\overline{m_0} = \int_{\mathbb{R}^{m-1}}\int_{-b_x}^{\epsilon^\gamma}\int_0^{\epsilon^\gamma} u^m k(\|u\|_{\mathrm{sem}})du^1...du^{m-1}...db_x du^m$$

Apply integration by parts:

$$\frac{1}{\epsilon^m}\int_{x\in M_{\epsilon^\gamma}} \phi\left(\mathcal{K}_\epsilon f - f\mathcal{K}_\epsilon(1)\right)\ d\ \mathrm{Vol} = -\epsilon^2\frac{m_2}{2}\int_{x\in M_{\epsilon^\gamma}} \phi(x)\Delta f(x)\ \ d\ \mathrm{Vol} + \mathcal{O}(\epsilon^3)$$

$$= -\frac{\epsilon^2 m_2}{2}\Big(\int_{\mathcal{M}_{\epsilon^\gamma}} \left\langle \mathrm{grad}\ \phi, \mathrm{grad}\ f\right\rangle_g\ d\ \mathrm{Vol}$$

$$- \int_{\partial \mathcal{M}_{\epsilon^\gamma}} \langle \phi \text{grad } f, \eta \rangle_g \ d \text{ Vol}_\partial \Big) + \mathcal{O}(\epsilon^3)$$

We now treat the boundary term:

$$\frac{1}{\epsilon^m} \int_{x \in N_{\epsilon^\gamma}} \phi \left(\mathcal{K}_\epsilon f - f \mathcal{K}_\epsilon(1) \right) \ d \text{ Vol} = \epsilon^2 \overline{m_0} \int_{\partial M} \langle \phi \text{ grad } f, \eta \rangle_g \ d \text{ Vol}_\partial + \mathcal{O}(\epsilon^3)$$

$$= \epsilon^2 \frac{m_2}{2} \int_{\partial M} \langle \phi \text{ grad } f, \eta \rangle_g \ d \text{ Vol}_\partial + \mathcal{O}(\epsilon^3)$$

Gathering the boundary terms from both the interior and boundary computations, we then apply the Divergence theorem on the closure of the boundary region $\overline{N}_\epsilon^\gamma$.

$$\epsilon^2 \frac{m_2}{2} \int_{\partial \overline{N}_{\epsilon^\gamma}} \langle \phi \text{grad } f, \eta \rangle_g \ d \text{ Vol}_\partial = \epsilon^2 \frac{m_2}{2} \int_{\overline{N}_{\epsilon^\gamma}} \text{div}(\phi \text{grad } f) \ d \text{ Vol}_\partial$$

$$= \epsilon^2 \frac{m_2}{2} \int_{\overline{N}_{\epsilon^\gamma}} \phi \text{ div}(\text{grad } f) + \langle \text{grad } \phi, \text{grad } f \rangle_g \ d \text{ Vol}_\partial$$

$$= \epsilon^2 \frac{m_2}{2} \int_{\overline{N}_{\epsilon^\gamma}} \phi \Delta f + \langle \text{grad } \phi, \text{grad } f \rangle_g \ d \text{ Vol}$$

By Theorem 4.3.1, we have that

$$\epsilon^2 \frac{m_2}{2} \int_{\overline{N}_{\epsilon^\gamma}} \phi \Delta f \ d \text{ Vol} = \epsilon^3 \overline{m}_0 \int_{\partial M} \phi \Delta f \ d \text{ Vol}_\partial + \mathcal{O}(\epsilon^4)$$

Putting this all together, we see that:

$$\frac{1}{\epsilon^m} \int_{x \in M_{\epsilon^\gamma}} \phi \left(\mathcal{K}_\epsilon f - f \mathcal{K}_\epsilon(1) \right) \ d \text{ Vol} = -\epsilon^2 \frac{m_2}{2} \int_M \langle \text{grad } \phi, \text{grad } f \rangle_g \ d \text{ Vol} + \mathcal{O}(\epsilon^3)$$

□

5.3 Normalized Laplacian

We now show using Theorem 1.4.4 that the same consistency result holds for the bias of the normalized graph Laplacian estimator. The proof is a straightforward computation.

Corollary 5.3.1. *With the same conditions as Theorem 1.4.4,*

$$\frac{2}{m_2\epsilon^{d+2}}\int_{\mathcal{M}}\phi\left(\frac{\mathcal{K}_\epsilon f - f\mathcal{K}_\epsilon 1}{\mathcal{K}_\epsilon 1}\right)\ d\ \mathrm{Vol} = \int_{\mathcal{M}}\langle \mathrm{grad}\ \phi, \mathrm{grad}\ f\rangle_g\ d\ \mathrm{Vol} + \mathcal{O}(\epsilon).$$

Proof. We begin by applying Theorem 1.4.4 to the test function $\tilde{\phi} = \frac{\phi}{\mathcal{K}_\epsilon 1}$. We then obtain, by product rule:

$$\begin{aligned}\frac{2m_0}{m_2\epsilon^{d+2}}\int_{\mathcal{M}}\phi\left(\frac{\mathcal{K}_\epsilon f - f\mathcal{K}_\epsilon 1}{\mathcal{K}_\epsilon 1}\right)\ d\ \mathrm{Vol} &= \int_{\mathcal{M}}\left\langle \mathrm{grad}\ \left(\phi\mathcal{K}_\epsilon^{-1}1\right), \mathrm{grad}\ f\right\rangle_g\ d\ \mathrm{Vol} + \mathcal{O}(\epsilon)\\ &= \int_{\mathcal{M}}\left\langle \mathrm{grad}\ \mathcal{K}_\epsilon^{-1}1, \mathrm{grad}\ f\right\rangle_g\ d\ \mathrm{Vol}\\ &+ \int_{\mathcal{M}}\langle \mathrm{grad}\ \phi, \mathrm{grad}\ f\rangle_g\ d\ \mathrm{Vol}\\ &+ \mathcal{O}(\epsilon)\end{aligned}$$

We now see that since $\mathcal{K}_\epsilon^{-1}1 = m_0 + \mathcal{O}(\epsilon)$, on M_ϵ^γ and $\mathcal{K}_\epsilon^{-1}1 = m_0^\partial(x) + \mathcal{O}(\epsilon)$ on N_{ϵ^γ}, that

$$\begin{aligned}\frac{2m_0}{m_2\epsilon^{d+2}}\int_{\mathcal{M}}\phi\left(\frac{\mathcal{K}_\epsilon f - f\mathcal{K}_\epsilon 1}{\mathcal{K}_\epsilon 1}\right)\ d\ \mathrm{Vol} &= \int_{N_{\epsilon^\gamma}}\left\langle \mathrm{grad}\ m_0^\partial(x), \mathrm{grad}\ f\right\rangle_g\ d\ \mathrm{Vol}\\ &+ \int_{\mathcal{M}}\langle \mathrm{grad}\ \phi, \mathrm{grad}\ f\rangle_g\ d\ \mathrm{Vol}\\ &+ \mathcal{O}(\epsilon)\end{aligned}$$

We then apply Theorem 4.3.1 to obtain:

$$\int_{N_{\epsilon\gamma}} \left\langle \text{grad } m_0^{\partial}(x), \text{grad } f \right\rangle_g \, d \text{ Vol} = \epsilon \int_{\partial M} \left\langle \text{grad } m_0^{\partial}(x), \text{grad } f \right\rangle_g \, d \text{ Vol}$$

which shows that the remaining term is of order ϵ.

Therefore:

$$\frac{2m_0}{m_2 \epsilon^{d+2}} \int_{\mathcal{M}} \phi \left(\frac{\mathcal{K}_\epsilon f - f \mathcal{K}_\epsilon 1}{\mathcal{K}_\epsilon 1} \right) \, d \text{ Vol} = = \int_{\mathcal{M}} \langle \text{grad } \phi, \text{grad } f \rangle_g \, d \text{ Vol} + \mathcal{O}(\epsilon).$$

□

Thus, we have shown that the weak convergence of the associated kernel integral operator to both the unnormalized and the random walks graph Laplacian estimators.

Chapter 6: Outlook

There are several interesting consequences of this work to both the theoretical and applied aspects of manifold learning. On the theoretical side, the weak-sense approach to convergence of diffusion maps is a promising extension which may allow us to better understand the empirical behavior of graph Laplacians on data which does not reside on a Riemannian manifold. On the applied side, our main results can be used to show consistency of a mesh-free method for solving numerical PDEs on Riemannian manifolds.

6.1 Regularity of Manifold Learning

Although the setting of compact Riemannian manifolds is necessary for our pointwise estimates of the Laplacian, such a setting is often too restrictive for real world data sets. Despite this fact, graph Laplacian based methods are often used to great effect in situations which one cannot expect the presence of an underlying smooth manifold. We speculate that the work of this thesis can be extended in order to generalize the hypotheses of manifold learning to a more realistic setting.

6.1.1 Manifolds of Bounded Geometry

The first approach would be to extend the pointwise expansions present in this work to a larger class of manifolds called *manifolds of bounded geometry* [28]. A manifold has C^k bounded geometry if it has nonzero injectivity radius if each of the covariant derivatives of its Riemann curvature tensors is bounded. Manifolds of bounded geometry can also be generalized to boundary manifolds by requiring the existence of a normal collar and bounds on the inward-facing sectional curvature of the boundary. Manifolds of bounded geometry are in essence the largest class of manifolds on which Sobolev spaces behave similarly to the classical theory in the Euclidean case. Thus, they are in some sense the largest class of noncompact manifolds on which the functional-analytic properties are suitable for analysis of the Laplace-Beltrami operator. These manifolds were first studied in the context of graph Laplacian based methods in [21], where pointwise consistency of graph Laplacian based estimators was established. Although the results of [21] hold for manifolds of bounded geometry, they do not hold uniformly and make no use of semigeodesic coordinates.

In the present work, the proofs in Chapters 2 and 3 of this thesis have been written in such a way to be suggestive of generalization to manifolds of bounded geometry. More specifically, most of the proofs depend explicitly on a global upper bound for component functions g_{ij} of the metric in normal or semigeodeisc coordinates. A fundamental result proven in [28] shows that such a global bound holds for all manifolds of bounded geometry. We remark that the pointwise results proved in this work hold exactly on manifolds of bounded geometry if we assume the following three conditions:

(a) The embedding function $\iota : \mathcal{M} \to \mathbb{R}^d$ is uniformly continuous with uniformly continuous inverse.

(b) There exists a $R > 0$ such that for any $\epsilon < R$, each point of $\mathcal{M}_{\epsilon^\gamma}$ is contained in a geodesic ball of radius ϵ^γ.

(c) There exists a $C > 0$ such that for small enough ϵ, every semigeodesic cylinder of radius ϵ near the boundary contains a metric ball of radius $C\epsilon$.

Condition 1 is necessary in order to uniformly relate intrinsic and extrinsic distance in $\mathcal{M}$. Condition 2 is necessary to ensure that the injectivity radius of $\mathcal{M}_{\epsilon^\gamma}$ does not shrink faster than ϵ^γ as $\epsilon \to 0$. A sufficient condition for condition 2 to be satisfied is that the double $D(\mathcal{M})$ has nonzero injectivity radius. Condition 3 is necessary to ensure that one can uniformly localize to both geodesic balls in $\mathcal{M}_{\epsilon^\gamma}$ and semigeodesic cylinders in N_{ϵ^γ} at the same time. The main reason for this condition is that it relates the norm in semigeodesic coordinates to intrinsic distance in $\mathcal{M}$. This allows for the uniform continuity assumption in 1 to be applied to semigeodesic coordinates as well.

We conjecture that condition 3 holds for all manifolds of bounded geometry. Such a result could be proven using Warner's generalizaton of the Rauch comparison theorem. However, this is not quite sufficient due to the fact that metric balls near the boundary are not suitably parameterized by the exponential map. This suggests that by weakening the setting to the study of metric geometry may be a potential solution. In [1], it is shown that manifolds with boundary of bounded curvature are instance of *Alexandrov* metric spaces, upon which many of the triangle comparison theorems in Riemannian geometry still hold.

6.1.2 Manifold Learning on Metric Measure Spaces

Although the pointwise estimates of the Laplace-Beltrami operator done in this work rely heavily on the structure of a Riemannian manifold, such a structure is not a natural assumption in the context of data. Since data is often assumed to be sampled from a probability measure, a more natural class of spaces to study would be the class of *metric measure spaces.* Although metric measure spaces do not have the necessary smoothness to perform the arguments of this work, there is reason to believe that the arguments of this thesis may be adapted to metric measure spaces. First of all, it has been shown in several works including [2] and [18] that nonsmooth versions of the heat kernel and Laplace-Beltrami operator hold on metric measure spaces. In addition, when one assumes an additional *doubling property*, one may also assume the existence of a smooth structure on the metric measure space which is smooth almost everywhere [24]. By using the weak (integrated) sense approach present in this thesis, we believe that it may be possible to adapt the pointwise notions present in this work to the more general case of metric measure spaces.

Another approach could be to consider Gromov-Hausdorff limits of manifolds with curvature bounds. It is well-known [8] that the limit of Riemannian manifolds with sectional curvature bounds are Alexandrov spaces. It then could be possible to study the behavior of metric measure spaces by considering the pointwise results proven in this work on a sequence of manifolds converging in Gromov-Hausdorff distance. It is our hope that by performing this analysis, we may be able to explain the robustness of manifold learning techniques on data that does not reside on manifolds.

6.2 Mesh-Free Methods in Numerical PDE

Much of the results of this thesis are also motivated by applications in numerically solving elliptic PDEs. The Laplace-Beltrami operator is central in the study of elliptic PDEs on manifolds, and thus graph Laplacians might be a natural choice for numerically solving PDEs on data. There has been recently renewed interest[19, 23] in using graph Laplacians for numerically solving PDEs which are difficult or impossible to mesh.

One of the critical issues when considering boundary value problems using graph Laplacians, as noted in [21], is that the boundary of a manifold is of measure zero and thus one can never expect to sample boundary points on which to impose a given boundary condition. The estimation of boundary integrals proved in Theorem 4.3.1 of Chapter 4 allows us to get around this issue through a weak-sense approach. In addition, it has empirically been observed [13] that the Diffusion Maps graph Laplacian returns Neumann functions. This empirical phenomenon is finally explained in our main result in which we show that the diffusion averaging operator converges weakly to the Neumann Laplacian.

In a forthcoming paper [38], we demonstrate the effectiveness of graph Laplacians for solving Neumann, Dirichlet, and Robin boundary value problems on manifolds. In addition to demonstrating their effectiveness, the role of mean curvature in the asymptotic estimates of this work is experimentally verified on simple examples such as the ellipse. It is our hope that the analysis done in this thesis can be used in other areas of elliptic PDE.

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Curriculum Vitae

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