

# Diffusion Maps

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## **Abstract**

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# Introduction

The contentual layout follows that of Coifman and Lafon (2006) and Belkin (2003) for a concrete implementation. Some definitions, theorems and examples will be taken from these works as well.

## 0.1 Dimensionality Reduction

### 0.1.1 The Problem

### 0.1.2 Existing Approaches

**Linear PCA**

**Kernel PCA**

# Chapter 1

## Diffusion Maps

### 1.1 Diffusion Kernels

#### 1.1.1 Motivation

In this section it will be elaborated on why global structures need not be preserved and how this leads to diffusion processes.

#### Preservation of Global Structures

Suppose data points  $x_i \in \mathbb{R}^k$  are generated by a low dimensional parameter  $\theta_i \in \mathbb{R}^{k'}$ ,  $k' \ll k$  given a map  $\Phi : \mathbb{R}^{k'} \rightarrow \mathbb{R}^k$ . One problem is the (numerical) smoothness of  $\Phi$  which is not necessarily given. Another problem is that for large  $k$  the euclidian distance is no longer a meaningful measure as the volume of the  $k$ -dimensional unit ball  $\frac{\pi^{\frac{k}{2}}}{\Gamma(\frac{k}{2}+1)}$  converges to 0 as  $\lim_{k \rightarrow \infty}$  which is also known as the *curse of dimensionality*. One may conclude that large distances in the ambient space need not necessarily be preserved as they do not hold much information except that  $x_i$  is not “very close” to  $x_j$ .

Analogous to Riemannian manifolds (where metric tensors, inducing an inner product on the tangent space and a metric via the exponential map, define the manifold’s geometry) we focus solely on local distances in order to recover intrinsic global structures.

## A Dual Approach

From inverse problems in spectral geometry (e.g. “Can One Hear the Shape of a Drum?”) it is known that much<sup>1</sup> of the geometry of a given set  $\Gamma$  can be derived from the analysis of functions defined on  $\Gamma$ .

In this work eigenvalues and eigenfunctions of averaging operators, i.e., operators whose kernel corresponds to transition probabilities of a Markov process, will be studied in order to define a diffusion map which embeds the data into a Euclidian space where the Euclidian distance is just the diffusion metric.

### 1.1.2 Construction of a Random Walk on the Data

#### Definitions

Let  $(\Gamma, \mathcal{A}, \mu)$  be a measure space. In practical applications  $\Gamma$  is the given data set consisting of finitely many data points and  $\mu$  is the counting measure to represent the distribution of the points in the data set. In addition, suppose we are given a symmetric kernel  $k : \Gamma \times \Gamma \rightarrow \mathbb{R}^+$  which defines the local geometry of  $\Gamma$ .

#### Examples

Usually  $\Gamma$  is either a subset of the Euclidian space or a weighted graph.

In the first case it seems natural to write  $k$  as a function of the Euclidian distance  $\nu(\|x - y\|)$ .

In the second case let  $b(x, y)$  be the associated adjacency matrix, that is,  $b(x, y) = 1$  if there is an edge going from  $x$  to  $y$ , and  $b(x, y) = 0$  otherwise. The kernel  $b$  defines a notion of neighborhood for each point, and also a non-symmetric distance given by  $1 - b(x, y)$ . Clearly  $b$  is not symmetric in general, but we can consider

$$k_1(x, y) := \int_{\Gamma} b(x, u)b(y, u)d\mu(u)$$

$$k_2(x, y) := \int_{\Gamma} b(u, x)b(u, y)d\mu(u)$$

where  $k_1(x, y)$  counts the number of common neighbors to  $x$  and  $y$ , while  $k_2(x, y)$  counts the number of nodes for which  $x$  and  $y$  are common neighbors.

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<sup>1</sup>the most famous example being Weyl’s proof of  $\#\{\lambda_k : \lambda_k < \lambda\} \sim \frac{\text{area}(\Gamma)}{2\pi}\lambda$  as  $\lambda \rightarrow \infty$ . (Canzani (2013))

## Normalized Graph Laplacian Construction

Generally, such a kernel represents some notion of affinity between points of  $\Gamma$  and thus one can think of the data points as being the nodes of a symmetric graph whose weight function is specified by  $k$ . From the graph defined by  $(\Gamma, k)$ , one can construct a reversible Markov chain on  $\Gamma$ .

To normalize the kernel, define

**Definition 1.1.**

$$v^2(x) = \int_{\Gamma} k(x, y) d\mu(y)$$

and

**Definition 1.2.**

$$p(x, y) = \frac{k(x, y)}{v^2(x)}.$$

$p(x, y)$  is no longer symmetric, but inherited the positivity and now satisfies a conservation property:

$$\int_{\Gamma} p(x, y) d\mu(y) = 1$$

As a result the matrix  $P := (p(i, j))_{i,j}$  is stochastic and can be interpreted as the transition matrix of a homogeneous Markov process on  $\Gamma$ . In spectral graph theory  $\mathbb{I} - P$  is commonly referred to as normalized, weighted graph Laplacian.

To investigate the spectral properties of the corresponding integral operator  $P$  defined by  $Pf(x) = \int_{\Gamma} p(x, y) f(y) d\mu(y)$  it is beneficial to examine the symmetric, conjugated Operator  $A$ .

First, notice that by setting  $a(x, y) = \frac{k(x, y)}{v(x)v(y)} = v(x)p(x, y)\frac{1}{v(y)}$  one obtains a symmetric form and thus a symmetric operator  $Af(x) = \int_{\Gamma} a(x, y) f(y) d\mu(y)$  which will be referred to as diffusion operator from now on.

### 1.1.3 Diffusion Kernels

**Theorem 1.1.1** (Spectral Properties of the Diffusion Operator). *The diffusion operator  $A$  with kernel  $a$  is bounded from  $L^2(\Gamma, d\mu)$  into itself, symmetric and positive semi-definite.*

*Moreover, its norm is*

$$\|A\| = 1$$

*and is taken by the eigenfunction*

$$Av = v.$$

*Proof.* Let  $f \in L^2(\Gamma, d\mu)$ . We have:

$$\langle Af, f \rangle = \int_{\Gamma^2} k(x, y) \frac{f(x)}{v(x)} \frac{f(y)}{v(y)} d\mu(x) d\mu(y). \quad (1.1)$$

Applying the Cauchy-Schwartz inequality we get:

$$\begin{aligned} \left| \int_{\Gamma} k(x, y) \frac{f(y)}{v(y)} d\mu(y) \right| &= \left( \int_{\Gamma} k(x, y) d\mu(y) \right)^{\frac{1}{2}} \left( \int_{\Gamma} k(x, y) \frac{f(y)^2}{v(y)^2} d\mu(y) \right)^{\frac{1}{2}} \\ &= v(x) \left( \int_{\Gamma} k(x, y) \frac{f(y)^2}{v(y)^2} d\mu(y) \right)^{\frac{1}{2}} \end{aligned}$$

Hence:

$$\langle Af, f \rangle \leq \int_{\Gamma} |f(x)| \left( \int_{\Gamma} k(x, y) \frac{f(y)^2}{v(y)^2} d\mu(y) \right)^{\frac{1}{2}} d\mu(x)$$

and by using the Cauchy-Schwartz inequality once again:

$$\langle Af, f \rangle \leq \|f\| \left( \int_{\Gamma^2} \frac{k(x, y)}{v(y)^2} f(y)^2 d\mu(y) d\mu(x) \right)^{\frac{1}{2}} = \|f\|^2$$

by symmetry of the kernel which, in combination with (1.1), also implies the positivity of  $A$ .

Plugging in  $v$  for  $f$  it follows immediately that the eigenvalue 1 is actually obtained and  $v$  is an eigenfunction.  $\square$

**Theorem 1.1.2** (Spectral Decomposition of the Diffusion Kernel). *Assuming  $A$  is compact<sup>2</sup> and  $A\phi_l = \lambda_l \phi_l$  we may write the kernel as*

$$a(x, y) = \sum_{l \geq 0} \lambda_l \phi_l(x) \phi_l(y)$$

with  $\lambda_0 = 1$  and  $\lim_{l \rightarrow \infty} \lambda_l = 0$  monotonically.

*Proof.* First, note that  $A$  being compact implies that the spectrum is discrete and the sum thus is well defined. By  $A$  being symmetric and compact the spectral theorem applies and we get that there exists a sequence of real eigenvalues  $\lambda_l$  converging to 0. The corresponding normalized eigenvectors  $\phi_l$  form an orthonormal set and every  $f \in L^2(\Gamma, d\mu)$  can be written as

$$f = \sum_{l \geq 0} \langle \phi_l, f \rangle \phi_l + h$$

<sup>2</sup>which is no constraint in practice since data is finite

try to generalize lemma 3.4 of Teschl (2014)



where  $h \in \text{Ker}(A)$ .

It follows that

$$Af(x) = \int_{\Gamma} a(x, y) f(y) d\mu(y) = \sum_{l \geq 0} \lambda_l \int_{\Gamma} \phi_l(y) f(y) d\mu(y) \phi_l(x)$$

which, by linearity of the integral and comparison of components, is just what we were looking for.  $\square$

“Komponentenvergleich  
auf Englisch  
finden

From definition of  $a(x, y)$  we see that

$$p(x, y) = \sum_{l \geq 0} \lambda_l \underbrace{\frac{\phi_l(x)}{v(x)}}_{=: \psi_l(x)} \phi_l(y) v(y) \quad (1.2)$$

which enables us to efficiently compute  $t$ th powers  $p_t$  of  $p$ .

There are two ways to interpret  $p_t$ :

1.  $p_t$  has a probabilistic interpretation as the probability for a Markov chain with transition matrix  $P$  to reach  $y$  from  $x$  in  $t$  steps.
2. the dual point of view is that of the functions defined on the data. The kernel  $p_t$  can be viewed as a bump or more precisely, if  $x \in \Gamma$  is fixed, then  $p_t(x, \cdot)$  is a bump function centered at  $x$  and of width increasing with  $t$  which intuitively captures the idea of diffusion.

#### 1.1.4 Embedding in the Euclidian Space

**Definition 1.3.** *Let*

$$D_t(x, y)^2 = \|p_t(x, \cdot) - p_t(y, \cdot)\|_{L^2(\Gamma, d\mu/v)}^2 = \int_{\Gamma} (p_t(x, u) - p_t(y, u))^2 \frac{d\mu(u)}{v(u)}$$

*be the family of diffusion distances parameterized by  $t$ .*

For a fixed value of  $t$   $D_t$  defines a distance on the set  $\Gamma$  which is small only if there is a large number of small paths connecting  $x$  and  $y$  (i.e. if there is a large probability of getting from  $x$  to  $y$  in  $t$  steps). It thus emphasizes the notion of a cluster.

Another property following from the summation over all possible paths is that this distance is very robust to noise perturbation (in contrast to the geodesic distance).

**Theorem 1.1.3** (A Numerically Feasible Representation).

$$D_t(x, y) = \left( \sum_{l \geq 0} \left( \lambda_l^t (\psi_l(x) - \psi_l(y)) \right)^2 \right)^{\frac{1}{2}}$$

*Proof.*  $\{\phi_l\}_{l \geq 0}$  forming an orthonormal basis for  $L^2(\Gamma, d\mu)$  implies that  $\{\phi_l v\}_{l \geq 0}$  is an orthonormal basis for  $L^2(\Gamma, d\mu/v)$  and thus for  $x$  fixed (1.2) may be seen as orthogonal expansion of the function  $y \mapsto p_t(x, y)$  into the basis  $\{\phi_l v\}_{l \geq 0}$ . The coefficients are given by  $\{\lambda_l^t \psi_l(x)\}_{l \geq 0}$ . The statement follows directly using the Pythagorean theorem.  $\square$

An imidiate consequence is that the diffusion distance is well approximable and that it converges towards a function of (numerical) rank 1 as  $t \rightarrow \infty$  because of the vanishing influence of all eigenvectors with eigenvalues  $< 1$ .

One possible interpretation is that  $D_t(x, y)$  measures the distance between bumps of “magnitude”  $t$  being centered around two points  $x$  and  $y$ . As  $t$  gets larger so does the size of the supports and the number of eigenfunctions needed to calculate  $D_t(x, y)$  decreases. This number is related to the minimum number of bumps necessary to cover the set  $X$  (like in Weyl’s asymptotic law for the decay of the spectrum).

In order to calculate  $D_t(x, y)$  to a preset accuracy  $\delta > 0$  with a finite number of terms we set

$$s_t(\delta) = \max\{l \in \mathbf{N} : \lambda_l^t > \delta \lambda_1^t\}$$

so that, up to relative precision  $\delta$

$$D_t(x, y) = \left( \sum_{l=0}^{s_t(\delta)} \left( \lambda_l^t (\psi_l(x) - \psi_l(y)) \right)^2 \right)^{\frac{1}{2}}. \quad (1.3)$$

**Definition 1.4.** Let  $\{\Psi_t\}_{t \in \mathbf{N}}$ ,

$$\Psi_t(x) = \begin{pmatrix} \lambda_1^t \psi_1(x) \\ \lambda_2^t \psi_2(x) \\ \vdots \\ \lambda_{s_t(\delta)}^t \psi_{s_t(\delta)}(x) \end{pmatrix}$$

be the family of diffusion maps. Each component of  $\Psi_t(x)$  is termed diffusion coordinate.

According to (1.3) diffusion maps embed data in a Euclidian space in such a way that the Euclidian distance equals the diffusion distance up to a relative error  $\delta$ .

## Appendix A

# Asymptotics for Laplacian Operators

In the following we will deal with a compact manifold  $\mathcal{M}$  that is  $C^\infty$ . Let  $x$  be a fixed point, not on the boundary,  $T_x\mathcal{M}$  be the tangent space to  $\mathcal{M}$  at  $x$  and  $(e_1, \dots, e_d)$  be a fixed orthonormal basis of  $T_x\mathcal{M}$ . Furthermore two systems of local coordinates will be introduced:

1. (*Normal coordinates*) The exponential map  $\exp_x$  generates a set of orthogonal geodesics  $(\gamma_1, \dots, \gamma_d)$  intersecting at  $x$  with initial velocity  $(e_1, \dots, e_d)$ . Now every point  $y \in \mathcal{M}$  in a sufficiently small neighborhood of  $x$  has a set of *normal coordinates*  $(s_1, \dots, s_d)$  along these geodesics.
2. (*Tangent coordinates*) Considering the orthogonal projection  $u$  of  $y$  on  $T_x\mathcal{M}$ , where  $u_i = \langle y - x, e_i \rangle$  in  $(e_1, \dots, e_d)$ , we get a system of *tangent coordinates*. The submanifold is now locally parameterized as  $y = (u, g(u))$ , where  $g : \mathbb{R}^d \rightarrow \mathbb{R}^{n-d}$ . Since  $u = (u_1, \dots, u_d)$  are tangent coordinates, we must have that  $\partial g(0) = 0$ .

Notice that, locally, any function  $f$  on  $\mathcal{M}$  may be viewed as  $\tilde{f}$  of  $(s_1, \dots, s_d)$  and thus we may write  $\Delta f(x) = -\sum_{i=1}^d \frac{\partial^2 \tilde{f}}{\partial s_i^2}(0, \dots, 0)$ , where  $\Delta$  is the Laplace-Beltrami operator on  $\mathcal{M}$ .

write introduction + motivation (later being the justification for naming it graph “Laplacian” earlier)

This part is basically a citation of Coifman and Lafon (2006).

## A.1 Comparison of the Geodesic and the Local Projection

In this section we will compute asymptotic expansions for the changes of variable  $u \mapsto (s_1, \dots, s_d)$  and  $u \mapsto y$ .

In the following,  $Q_{x,m}(u)$  denotes a generic homogeneous polynomial of degree  $m$  of the variable  $u = (u_1, \dots, u_d)$ , whose coefficient depends on  $x$ .

**Lemma A.1.1.** *If  $y \in \mathcal{M}$  is in a Euclidean ball of radius  $\varepsilon^{\frac{1}{2}}$  around  $x$ , then, for  $\varepsilon$  sufficiently small, there exists:*

$$s_i = u_i + Q_{x,3}(u) + \mathcal{O}(\varepsilon^2) \quad (\text{A.1})$$

*Proof.* Let  $\gamma$  be the geodesic connection  $x$  and  $y$  parameterized by arclength. We have  $\gamma(0) = x$  and let  $s$  be such that  $\gamma(s) = y$ . If  $y$  has normal coordinates  $(s_1, \dots, s_d)$ , then we have  $s\gamma'(0) = (s_1, \dots, s_d)$ . A Taylor expansion yields

$$\gamma(s) = \gamma(0) + s\gamma'(0) + \frac{s^2}{2}\gamma''(0) + \frac{s^3}{6}\gamma^{(3)}(0) + \mathcal{O}(\varepsilon^2).$$

By definition of a geodesic, the covariant derivative of the velocity is zero, which means that  $\gamma''(0)$  is orthogonal to the tangent plane at  $x$ . Now since the parameter  $u_i$  is defined by  $u_i = \langle \gamma(s) - \gamma(0), e_i \rangle$ , we obtain that  $u_i = s_i + \frac{s^3}{6}\langle \gamma^{(3)}(0), e_i \rangle + \mathcal{O}(\varepsilon^2)$ . Iterating this equation yields the result.  $\square$

**Lemma A.1.2.** *Again, let  $y \in \mathcal{M}$  be in a Euclidean ball of radius  $\varepsilon^{\frac{1}{2}}$  around  $x$ ; we have*

$$\|x - y\|^2 = \|u\|^2 + Q_{x,4}(u) + Q_{x,4}(u) + \mathcal{O}(\varepsilon^3) \quad (\text{A.2})$$

and

$$\det\left(\frac{dy}{du}\right) = 1 + Q_{x,2}(u) + Q_{x,3}(u) + \mathcal{O}(\varepsilon^2). \quad (\text{A.3})$$

*Proof.* The submanifold is locally parameterized as  $u \mapsto (u, g(u))$ , where  $g : \mathbb{R}^d \rightarrow \mathbb{R}^{n-d}$ . Writing  $g = (g_{i+1}, \dots, g_n)$  and applying Pythagore's theorem, we obtain

$$\|x - y\|^2 = \|u\|^2 + \sum_{i=d+1}^n g_i(u)^2.$$

Using that, by definition,  $g_i(0) = 0$  and, as noted before,  $\frac{\partial g}{\partial u_i}(0) = 0$ . As a consequence  $g_i(u) = b_{i,x}(u) + c_{i,x}(u) + \mathcal{O}(\varepsilon^2)$ , where  $b_{i,x}$  is the Hessian

quadratic form of  $g_i$  at  $u = 0$  and  $c_{i,x}$  is the cubic term. This proves (A.2) with

$$Q_{x,4}(u) = \sum_{i=d+1}^n b_{i,x}^2(u) \text{ and } Q_{x,5}(u) = 2 \sum_{i=d+1}^n b_{i,x}(u)c_{i,x}(u).$$

To prove (A.3), observe that  $\frac{\partial g}{\partial u_i}(0) = 0$  implies that  $\frac{\partial g}{\partial u_i}(0) = \tilde{b}_{i,x}(u) + \tilde{c}_{i,x}(u) + \mathcal{O}(\varepsilon^{\frac{3}{2}})$ , where  $\tilde{b}_{i,x}(u)$  and  $\tilde{c}_{i,x}(u)$  are the linear and quadratic terms in the Taylor expansion of  $\frac{\partial g}{\partial u_i}(0)$  at 0. We thus have:

$$\begin{aligned} \frac{\partial y}{\partial u_i}(u) &= \left( v_i, \frac{\partial g}{\partial u_i}(u) \right), \text{ where } v_i = (0, \dots, 0, 1, 0, \dots, 0) \in \mathbb{R}^d \\ &= (v_i, \tilde{b}_{i,x}(u) + \tilde{c}_{i,x}(u) + \mathcal{O}(\varepsilon^{\frac{3}{2}})). \end{aligned}$$

The squared volume generated by these  $d$  vectors is the determinant of their Gram matrix, i.e.,

$$\left| \det \left( \frac{dy}{du} \right) \right|^2 = \sum_{i,j=1}^d E_{ij}(u) + \sum_{i,j=1}^d F_{ij}(u) + \mathcal{O}(\varepsilon^2),$$

where

$$E_{ij}(u) = \langle \tilde{b}_{i,x}(u), \tilde{b}_{j,x}(u) \rangle \text{ and } F_{ij}(u) = \langle \tilde{b}_{i,x}(u), \tilde{c}_{j,x}(u) \rangle + \langle \tilde{c}_{i,x}(u), \tilde{b}_{j,x}(u) \rangle.$$

Defining

$$Q_{x,2}(u) = \sum_{i,j=1}^d E_{ij}(u) \text{ and } Q_{x,3}(u) = \sum_{i,j=1}^d F_{ij}(u),$$

we obtain the last result.  $\square$

## A.2 Asymptotic Expansion of Averaging Operators

Let  $k_\varepsilon(x, y)$  be an isotropic kernel, i.e.:

$$k_\varepsilon(x, y) = h \left( \frac{\|x - y\|^2}{\varepsilon} \right),$$

where  $h$  is assumed to have an exponential decay and let  $G_\varepsilon$  be the corresponding operator

$$G_\varepsilon f(x) = \frac{1}{\varepsilon^{\frac{d}{2}}} \int_{\mathcal{M}} k_\varepsilon(x, y) f(y) dy.$$

The idea is that, using the previous theorems, for small  $\varepsilon$  integrating  $f$  against the kernel on the manifold is approximately like integrating on the tangent space. On this space, the kernel is approximately symmetric and is

more motivation

**Theorem A.2.1.** *Let  $f \in C^3(\mathcal{M})$  and let  $0 < \gamma < 1/2$ . Then we have, uniformly for all  $x \in \mathcal{M}$  at distance larger than  $\varepsilon^\gamma$  from  $\partial\mathcal{M}$ ,*

$$G_\varepsilon f(x) = m_0 f(x) + \varepsilon \frac{m_2}{2} (\omega(x) f(x) - \Delta f(x)) + \mathcal{O}(\varepsilon^2),$$

where

$$m_0 = \int_{\mathbb{R}^d} h(|u|^2) du \text{ and } m_2 = \int_{\mathbb{R}^d} u_1^2 h(|u|^2) du$$

and  $\omega$  is a potential term depending on the embedding of  $\mathcal{M}$ .

*Proof.* Because of the exponential decay of  $h$ , the domain of integration can be restricted to the intersection of  $\mathcal{M}$  with the ball of radius  $\varepsilon^\gamma$  around  $x$ . In doing so we generate an error of order

$$\begin{aligned} \left| \frac{1}{\varepsilon^{\frac{d}{2}}} \int_{\substack{y \in \mathcal{M} \\ \|x-y\| > \varepsilon^\gamma}} h\left(\frac{\|x-y\|^2}{\varepsilon}\right) f(y) dy \right| &\leq \|f\|_\infty \frac{1}{\varepsilon^{\frac{d}{2}}} \int_{\substack{y \in \mathcal{M} \\ \|x-y\| > \varepsilon^\gamma}} \left| h\left(\frac{\|x-y\|^2}{\varepsilon}\right) \right| dy \\ &\leq \|f\|_\infty \int_{\substack{y \in \mathcal{M} \\ \|y\| > \varepsilon^{\gamma-1/2}}} |h(|y|^2)| dy \\ &\leq C \|f\|_\infty Q(\varepsilon^{1/2-\gamma}) e^{-\varepsilon^{\gamma-1/2}}, \end{aligned}$$

where we have used the exponential decay of the kernel and where  $Q$  is a polynomial. Since  $0 < \gamma < 1/2$ , this term is exponentially small and is bounded by  $\mathcal{O}(\varepsilon^{\frac{3}{2}})$ . Therefore,

$$G_\varepsilon f(x) = \frac{1}{\varepsilon^{\frac{d}{2}}} \int_{\substack{y \in \mathcal{M} \\ \|x-y\| < \varepsilon^\gamma}} h\left(\frac{\|x-y\|^2}{\varepsilon}\right) f(y) dy + \mathcal{O}(\varepsilon^{\frac{3}{2}}).$$

Now that things are localized around  $x$ , we can Taylor-expand the function  $(s_1, \dots, s_d) \mapsto f(y(s_1, \dots, s_d))$ :

$$f(y) = f(x) + \sum_{i=1}^d s_i \frac{\partial \tilde{f}}{\partial s_i}(0) + \frac{1}{2} \sum_{i,j=1}^d s_i s_j \frac{\partial^2 \tilde{f}}{\partial s_i \partial s_j}(0) + Q_{x,3}(s_1, \dots, s_d) + \mathcal{O}(\varepsilon^2),$$

where  $\tilde{f}(s_1, \dots, s_d) = f(y(s_1, \dots, s_d))$ . Invoking (A.1), we obtain

$$f(y) = \tilde{f}(0) + \sum_{i=1}^d u_i \frac{\partial \tilde{f}}{\partial s_i}(0) + \frac{1}{2} \sum_{i,j=1}^d u_i u_j \frac{\partial^2 \tilde{f}}{\partial s_i \partial s_j}(0) + Q_{x,3}(u) + \mathcal{O}(\varepsilon^2).$$

Likewise, because of (A.2), the Taylor expansion of the kernel is

$$h\left(\frac{\|x - y\|^2}{\varepsilon}\right) = h\left(\frac{\|u\|^2}{\varepsilon}\right) + \left(\frac{Q_{x,4}(u) + Q_{x,5}(u)}{\varepsilon}\right) h'\left(\frac{\|u\|^2}{\varepsilon}\right) + \mathcal{O}(\varepsilon^2).$$

Using (A.3) to change the variable  $s \mapsto u$  in the previous integral defining  $G_\varepsilon f(x)$  yields:

$$\begin{aligned} \varepsilon^{\frac{d}{2}} G_\varepsilon f(x) &= \int_{\|u\| < \varepsilon^\gamma} \left( h\left(\frac{\|u\|^2}{\varepsilon}\right) + \left(\frac{Q_{x,4}(u) + Q_{x,5}(u)}{\varepsilon}\right) h'\left(\frac{\|u\|^2}{\varepsilon}\right) \right) \\ &\quad \times \left( \tilde{f}(0) + \sum_{i=1}^d u_i \frac{\partial \tilde{f}}{\partial s_i}(0) + \frac{1}{2} \sum_{i,j=1}^d u_i u_j \frac{\partial^2 \tilde{f}}{\partial s_i \partial s_j}(0) + Q_{x,3}(u) \right) \\ &\quad \times (1 + Q_{x,2}(u) + Q_{x,3}(u)) du + \mathcal{O}\left(\varepsilon^{\frac{d}{2}+2}\right). \end{aligned}$$

This identity can be dramatically simplified by identifying odd functions and setting their integral to zero. One is left with

$$\begin{aligned} \varepsilon^{\frac{d}{2}} G_\varepsilon f(x) &= \tilde{f}(0) \int_{\mathbb{R}^d} h\left(\frac{\|u\|^2}{\varepsilon}\right) du + \frac{1}{2} \left( \sum_{i=1}^d \frac{\partial^2 \tilde{f}}{\partial s_i^2}(0) \right) \int_{\mathbb{R}^d} u_1^2 h\left(\frac{\|u\|^2}{\varepsilon}\right) du \\ &\quad + \tilde{f}(0) \int_{\mathbb{R}^d} \left( \frac{Q_{x,4}(u)}{\varepsilon} h'\left(\frac{\|u\|^2}{\varepsilon}\right) + \tilde{Q}_{x,2}(u) h\left(\frac{\|u\|^2}{\varepsilon}\right) \right) du + \mathcal{O}\left(\varepsilon^{\frac{d}{2}+2}\right), \end{aligned}$$

where the domain of integration has been extended to  $\mathbb{R}^d$  (exponential decay of  $h$ ). Changing the variable according to  $u \mapsto \varepsilon^{\frac{1}{2}} u$ ,



$$\begin{aligned}
G_\varepsilon f(x) &= \tilde{f}(0) \int_{\mathbb{R}^d} h(|u|^2) du + \frac{\varepsilon}{2} \left( \sum_{i=1}^d \frac{\partial^2 \tilde{f}}{\partial s_i^2}(0) \right) \int_{\mathbb{R}^d} u_1^2 h(|u|^2) du \\
&\quad + \varepsilon \tilde{f}(0) \int_{\mathbb{R}^d} (Q_{x,4}(u) h'(|u|^2) + Q_{x,2}(u) h(|u|^2)) du + \mathcal{O}(\varepsilon^2),
\end{aligned}$$

where we have used the homogeneity of  $Q_{x,2}$  and  $Q_{x,4}$ . Finally, observing that

$$\tilde{f}(0) = f(x) \text{ and } \sum_{i=1}^d \frac{\partial^2 \tilde{f}}{\partial s_i^2}(0) = -\Delta f(x),$$

we end up with

$$G_\varepsilon f(x) = m_0 f(x) + \varepsilon \frac{m_2}{2} (\omega(x) f(x) - \Delta f(x)) + \mathcal{O}(\varepsilon^2),$$

where

$$\omega(x) = \frac{2}{m_2} \int_{\mathbb{R}^d} (Q_{x,4}(u) h'(|u|^2) + Q_{x,2}(u) h(|u|^2)) du.$$

Finally, the uniformity follows from the compactness and smoothness of  $\mathcal{M}$ .  $\square$

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