Geometric Scattering on Manifolds

Michael Perlmutter
Dept. of CMSE*
Michigan State University
East Lansing, MI 48824
perlmut6@msu.edu

Guy Wolf†
Applied Math Program
Dept. of Mathematics
Yale University
New Haven, CT 06511
guy.wolf@yale.edu

Matthew Hirn‡
Dept. of CMSE*
Dept. of Mathematics
Michigan State University
East Lansing, MI 48824
mhirn@msu.edu

Abstract

We present a mathematical model for geometric deep learning based upon a scattering transform defined over manifolds, which generalizes the wavelet scattering transform of Mallat. This geometric scattering transform is (locally) invariant to isometry group actions, and we conjecture that it is stable to actions of the diffeomorphism group.

1 Introduction

Convolutional neural networks (CNNs) are revolutionizing imaging science for two and three dimensional images over Euclidean domains. However, many images, and more generally data sets, are intrinsically non-Euclidean and are better modeled through other mathematical structures, such as graphs or manifolds. This has led to the development of *geometric deep learning* [1, 2] (and references therein), which refers to a body of research that aims to translate the principles of CNNs to these non-Euclidean structures. In the process, various challenges have arisen, including how to define such networks, how to train them efficiently, and how to analyze their mathematical properties. In this extended abstract we focus primarily on the last question in a relatively general context, akin to several existing methods, which illustrates the fundamental properties of such networks.

We present a geometric version of the scattering transform (Figure 1), which is similar to the one introduced in [3], but here is defined over manifolds instead of Euclidean space. The Euclidean scattering transform can be, on the one hand, thought of as a mathematical model for standard CNNs, but has, on the other hand, obtained state of the art or near state of the art empirical results in computer vision [4, 5, 6], audio signal processing [7, 8, 9], and even quantum chemistry [10, 11]. In Section 3 we define the geometric scattering transform, and provide results showing it encodes localized isometry invariant descriptions of signal data defined on a manifold. These

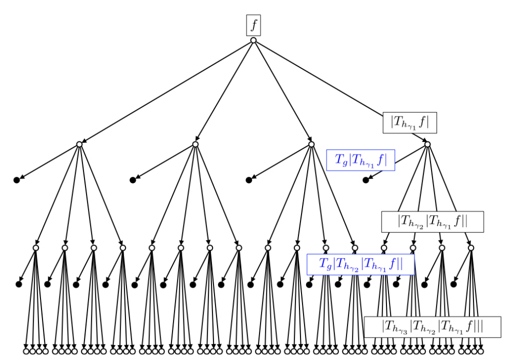

Figure 1: *The geometric scattering transform. Black: Equivariant intermediate layers. Blue: Invariant output coefficients at each layer.*

*Computational Mathematics, Science & Engineering
†http://guywolf.org/
‡https://matthewhirn.com/

NIPS 2018 Integration of Deep Learning Theories Workshop, Montréal, Canada.

results generalize local translation and rotation invariance on Euclidean domains. The underlying spectral integral operators that are the foundation of the geometric scattering transform are presented in Section 2. In Section 4 we discuss the stability of the geometric scattering transform to the action of diffeomorphisms. We provide a framework in which to quantify how much a diffeomorphism differs from being an isometry, provide results proving that individual spectral integral operators are Lipschitz stable to diffeomorphism actions within this framework, and conjecture that these results can be extended to the geometric scattering transform. Finally, we provide a short conclusion in Section 5.

1.1 Notation

Let $\mathcal{M}$ be a smooth, compact, and connected, d-dimensional Riemannian manifold without boundary contained in $\mathbb{R}^n$. Let $r : \mathcal{M} \times \mathcal{M} \to \mathbb{R}$ denote the geodesic distance between two points, and let Δ be the Laplace-Beltrami operator on $\mathcal{M}$. The eigenfunctions and non-unique eigenvalues of $-\Delta$ are denoted by φ_k and λ_k, respectively. Since $\mathcal{M}$ is compact, the spectrum of $-\Delta$ is countable and we may assume that $\{\varphi_k\}_{k\in\mathbb{N}}$ forms an orthonormal basis for $\mathbf{L}^2(\mathcal{M})$. The set of unique eigenvalues of $-\Delta$ is denoted by Λ, and for $\lambda \in \Lambda$ we let $m(\lambda)$ and E_λ denote the corresponding multiplicities and eigenspaces. For a diffeomorphism $\zeta : \mathcal{M} \to \mathcal{M}$, we let V_ζ be the operator $V_\zeta f(x) = f(\zeta^{-1}(x))$, and let $\|\zeta\|_\infty = \sup_{x\in\mathcal{M}} r(x, \zeta(x))$.

2 Spectral Integral Operators

For a smooth function η, we define a *spectral kernel* K_η by

$$K_\eta(x,y) = \sum_{k\in\mathbb{N}} \eta(\lambda_k)\varphi_k(x)\overline{\varphi}_k(y)$$

and refer to the operator T_η, with kernel K_η, as a *spectral integral operator*. It can be verified that

$$T_\eta f(x) = \sum_{k\in\mathbb{N}} \eta(\lambda_k)\langle f, \varphi_k\rangle \varphi_k(x).$$

Since $\{\varphi_k\}_{k\in\mathbb{N}}$ is an orthonormal basis for $\mathbf{L}^2(\mathcal{M})$, it follows that

$$\|T_\eta f\|_2^2 = \sum_{k\in\mathbb{N}} |\eta(\lambda_k)|^2 |\langle f, \varphi_k\rangle|^2.$$

Therefore, if $\|\eta\|_\infty \leq 1$, then T is a nonexpansive operator on $L^2(\mathcal{M})$. Operators of this form are analogous to convolution operators defined on $\mathbb{R}^d$ since like the latter they are diagonalized in the Fourier basis. To further emphasize this connection, we note the following theorem which shows that spectral integral operators are equivariant with respect to isometries.

Theorem 2.1. *Let T_η be a spectral integral operator. Then, if ζ is an isometry,*

$$T_\eta V_\zeta f = V_\zeta T_\eta f$$

for all $f \in L^2(\mathcal{M})$.

We will consider frame operators that are constructed using a countable family of spectral integral operators. In particular, we assume that we have a low-pass filter g and a family of high-pass filters $\{h_\gamma\}_{\gamma\in\Gamma}$ which satisfy a Littlewood-Paley type condition

$$A \leq m(\lambda)\left[|g(\lambda)|^2 + \sum_{\gamma\in\Gamma} |h_\gamma(\lambda)|^2\right] \leq B, \quad \forall\, \lambda \in \Lambda \tag{1}$$

for some $0 < A \leq B$. A frame analysis operator is then defined by

$$\Phi f = \left\{T_g f,\ T_{h_\gamma} f : \gamma \in \Gamma\right\},$$

where T_g and T_{h_γ} are the spectral integral operators corresponding to $\eta = g$ and $\eta = h_\gamma$, respectively.

Proposition 2.2. *Under the Littlewood-Paley condition (1), Φ is a bounded operator from $\mathbf{L}^2(\mathcal{M})$ to $\ell^2(\mathbf{L}^2(\mathcal{M}))$ and $A\|f\|_2^2 \leq \|\Phi f\|_{2,2}^2 := \|T_g f\|_2^2 + \sum_{\gamma\in\Gamma} \|T_{h_\gamma} f\|_2^2 \leq B\|f\|_2^2$ for all $f \in \mathbf{L}^2(\mathcal{M})$. In particular, if $A = B = 1$, then Φ is an isometry.*

Remark 2.3. In [13], R. Coifman and M. Maggioni used the heat semigroup to construct a class filters such that the high-pass filters $\{h_j\}_{j\in\mathbb{Z}}$ form a wavelet frame and a low-pass filter g_J is chosen so that $\{g_J, h_j : j \geq J\}$ satisfies (1). This construction can be generalized to the manifold setting after making suitable adjustments to account for the multiplicities of the eigenvalues.

3 The Geometric Scattering Transform

The *geometric scattering transform* is a nonlinear operator constructed through an alternating cascade of spectral integral operators and nonlinearities. Let $M : \mathbf{L}^2(\mathcal{M}) \to \mathbf{L}^2(\mathcal{M})$ be the modulus operator, $Mf(x) = |f(x)|$, and for each $\gamma \in \Gamma$, we let $U_\gamma f(x) = MT_{h_\gamma} f(x) = |T_{h_\gamma} f(x)|$. We define an operator $U : \mathbf{L}^2(\mathcal{M}) \to \ell^2(\mathbf{L}^2(\mathcal{M}))$, called the one-step scattering propagator, by

$$Uf = \{T_g f,\ U_\gamma f : \gamma \in \Gamma\}.$$

The m-step scattering propagator is constructed by iteratively applying the one-step scattering propagator. For $m \geq 1$, let Γ_m be the set of all paths of the form $\vec{\gamma} = (\gamma_1, \ldots, \gamma_m)$. Let Γ_0 denote the empty set, and let $\Gamma_\infty = \cup_{m=1}^{\infty} \Gamma_m$ denote the set of a all finite paths. For $\vec{\gamma} \in \Gamma_m$, let

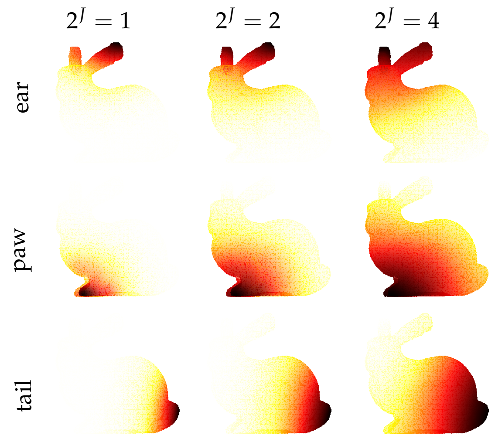

Figure 2: *Illustration of $T_{g_J}\delta_x$ over the Stanford bunny manifold [12] with Gaussian g_J, three J scales, and three Diracs δ_x centered at different regions of the manifold.*

$$U_{\vec{\gamma}} f(x) = U_{\gamma_m} \cdots U_{\gamma_1} f(x), \quad \vec{\gamma} = (\gamma_1, \ldots, \gamma_m),$$

and for $\mathcal{P} \subset \Gamma_\infty$, we define $U[\mathcal{P}]f$ as the collection of all path propagators with paths in $\mathcal{P}$,

$$U[\mathcal{P}]f = \{U_{\vec{\gamma}} f : \vec{\gamma} \in \mathcal{P}\}.$$

The scattering transform $S_{\vec{\gamma}}$ over a path $\vec{\gamma} \in \Gamma_\infty$ is defined as the integration of U_γ against the low-pass integral operator T_g, i.e.

$$S_{\vec{\gamma}} f(x) = T_g U_{\vec{\gamma}} f(x).$$

Analogously to $U[\mathcal{P}]$, we define

$$S[\mathcal{P}]f = \{S_{\vec{\gamma}} f : \vec{\gamma} \in \mathcal{P}\}.$$

The operator $S[\Gamma_\infty] : \mathbf{L}^2(\mathcal{M}) \to \ell^2(\mathbf{L}^2(\mathcal{M}))$ is referred to as the scattering transform. The following proposition shows that $S[\Gamma_\infty]$ is nonexpansive.

Proposition 3.1. *If the Littlewood-Paley condition* (1) *holds, then*

$$\|S[\Gamma_\infty]f_1 - S[\Gamma_\infty]f_2\|_{2,2} \leq \|f_1 - f_2\|, \quad \forall f_1, f_2 \in \mathbf{L}^2(\mathcal{M}).$$

The scattering transform is invariant to the action of the isometry group on the inputted signal f up to a factor that depends upon the decay of the low-pass spectral function g. If the low-pass spectral function g is rapidly decaying and satisfies $|g(\lambda)| \leq Ce^{-t\lambda}$ for some constant C and $t > 0$ (e.g., the heat kernel), then the following theorem establishes isometric invariance up to the scale t^d.

Theorem 3.2. *Let ζ be an isometry. If the Littlewood-Paley condition* (1) *holds and $|g(\lambda)| \leq Ce^{-t\lambda}$ for some constant C and $t > 0$, then there exists a constant $C(\mathcal{M}) < \infty$, such that*

$$\|S[\Gamma_\infty]f - S[\Gamma_\infty]V_\zeta f\|_{2,2} \leq C(\mathcal{M})t^{-d}\|\zeta\|_\infty \|U[\Gamma_\infty]f\|_{2,2} \qquad \forall f \in L^2(\mathcal{M}).$$

4 Stability to Diffeomorphisms

As stated in Theorem 2.1, spectral integral operators are equivariant to the action of isometries. This fact is crucial to proving Theorem 3.2 because it allows us to estimate

$$\|S[\Gamma_\infty]f - V_\zeta S[\Gamma_\infty]f\|_{2,2} \tag{2}$$

instead of

$$\|S[\Gamma_\infty]f - S[\Gamma_\infty]V_\zeta f\|_{2,2}. \tag{3}$$

In [3], it is shown that the Euclidean scattering transform S_{Euc} is stable to the action of certain diffeomorphisms which are close to being translations. A key step in the proof is a bound on the commutator norm $\|[S_{Euc}[\Gamma_\infty], V_\zeta]\|$, which then allows the author to bound a quantity analogous to (2) instead of bounding (3) directly. This motivates us to study the commutator of spectral integral operators with V_ζ for diffeomorphisms which are close to being isometries.

For technical reasons, we will assume that $\mathcal{M}$ is two-point homogeneous, that is, for any two pairs of points, $(x_1, x_2), (y_1, y_2)$ such that $r(x_1, x_2) = r(y_1, y_2)$, there exists an isometry $\zeta : \mathcal{M} \to \mathcal{M}$ such that $\zeta(x_1) = y_1$ and $\zeta(x_2) = y_2$. In order to quantify how far a diffeomorphism ζ differs from being an isometry we will consider two quantities:

$$A_1(\zeta) = \sup_{\substack{x,y\in\mathcal{M}\\ x\neq y}} \left| \frac{r\left(\zeta(x), \zeta(y)\right) - r(x,y)}{r(x,y)} \right|,$$

and

$$A_2(\zeta) = \sup_{x\in\mathcal{M}} \left| |\det[D\zeta(x)]| - 1 \right|.$$

We let $A(\zeta) = \max\{A_1(\zeta), A_2(\zeta)\}$ and note that if ζ is an isometry, then $A(\zeta) = 0$.

Theorem 4.1. *Assume that $\mathcal{M}$ is two-point homogeneous, and let T_η be a spectral integral operator. Then there exists a constant $C(\mathcal{M}) > 0$ such that for any diffeomorphism $\zeta : \mathcal{M} \to \mathcal{M}$,*

$$\|[T, V_\zeta]\| \leq C(\mathcal{M}) A(\zeta) B(\eta) \tag{4}$$

where

$$B(\eta) = \max\left\{ \sum_{k\in\mathbb{N}} \eta(\lambda_k)\lambda_k^{(d-1)/4}, \left(\sum_{k\in\mathbb{N}} \eta(\lambda_k)^2 \right)^{\frac{1}{2}} \right\}.$$

Remark 4.2. We conjecture that when Φ is constructed to be a wavelet frame as in Remark 2.3, we can use (4) to prove a bound on $\|[S[\Gamma_\infty], V_\zeta]\|$ in terms of $A(\zeta)$. If true, this result would allow us to show that the scattering transform is stable to diffeomorphisms using methods analogous to the ones in [3].

5 Conclusion

We have presented a path towards understanding the mathematical properties of geometric deep networks through the notion of the geometric scattering transform. Recently, related analyses for graphs have been presented in [14, 15, 16]. We remark that the analysis proposed here applies to compact Riemannian manifolds of arbitrary dimension, thus providing a road map that goes beyond 2D surface or 3D shape matching. Looking ahead, such an approach naturally lends itself to research avenues that synthesize geometric deep learning and geometric data analysis (e.g., manifold learning [17, 18, 19]), which in turn has the potential to bridge the graph and manifold theories for geometric deep networks.

Acknowledgments

M.H. is partially supported by Alfred P. Sloan Fellowship #FG-2016-6607, DARPA YFA #D16AP00117, and NSF grant #1620216.

References

[1] Federico Monti. `http://geometricdeeplearning.com/`, Last accessed in 2018.

[2] Michael M. Bronstein, Joan Bruna, Yann LeCun, Arthur Szlam, and Pierre Vandergheynst. Geometric deep learning: Going beyond euclidean data. *IEEE Signal Processing Magazine*, 34(4):18–42, 2017.

[3] Stéphane Mallat. Group invariant scattering. *Communications on Pure and Applied Mathematics*, 65(10):1331–1398, October 2012.

[4] Laurent Sifre and Stéphane Mallat. Rotation, scaling and deformation invariant scattering for texture discrimination. In *The IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, June 2013.

[5] Joan Bruna and Stéphane Mallat. Invariant scattering convolution networks. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 35(8):1872–1886, August 2013.

[6] Edouard Oyallon and Stéphane Mallat. Deep roto-translation scattering for object classification. In *2015 IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pages 2865–2873, 2015.

[7] Joan Bruna and Stéphane Mallat. Audio texture synthesis with scattering moments. arXiv:1311.0407, 2013.

[8] Joakim Andén and Stéphane Mallat. Deep scattering spectrum. *IEEE Transactions on Signal Processing*, 62(16):4114–4128, August 2014.

[9] Vincent Lostanlen and Stéphane Mallat. Wavelet scattering on the pitch spiral. In *Proceedings of the 18th International Conference on Digital Audio Effects*, pages 429–432, 2015.

[10] Michael Eickenberg, Georgios Exarchakis, Matthew Hirn, and Stéphane Mallat. Solid harmonic wavelet scattering: Predicting quantum molecular energy from invariant descriptors of 3D electronic densities. In *Advances in Neural Information Processing Systems 30 (NIPS 2017)*, pages 6540–6549, 2017.

[11] Michael Eickenberg, Georgios Exarchakis, Matthew Hirn, Stéphane Mallat, and Louis Thiry. Solid harmonic wavelet scattering for predictions of molecule properties. *Journal of Chemical Physics*, 148:241732, 2018.

[12] Greg Turk and Marc Levoy. The stanford bunny, 2005.

[13] Ronald R. Coifman and Mauro Maggioni. Diffusion wavelets. *Applied and Computational Harmonic Analysis*, 21(1):53–94, 2006.

[14] Dongmian Zou and Gilad Lerman. Graph convolutional neural networks via scattering. arXiv:1804:00099, 2018.

[15] Fernando Gama, Alejandro Ribeiro, and Joan Bruna. Diffusion scattering transforms on graphs. arXiv:1806.08829, 2018.

[16] Feng Gao, Guy Wolf, and Matthew Hirn. Graph classification with geometric scattering. arXiv:1810.03068, 2018.

[17] Sam T. Roweis and Lawrence K. Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290(5500):2323–2326, 2000.

[18] Mikhail Belkin and Partha Niyogi. Laplacian eigenmaps for dimensionality reduction and data representation. *Neural Computation*, 15(6):1373–1396, 2003.

[19] Ronald R. Coifman and Stéphane Lafon. Diffusion maps. *Applied and Computational Harmonic Analysis*, 21:5–30, 2006.