TOWARDS THEORETICAL UNDERSTANDING OF GEOMETRIC DEEP LEARNING WITH GEOMETRIC WAVELET SCATTERING TRANSFORMS

Speaker: Michael Perlmutter; Co-authors: Feng Gao, Guy Wolf, and Matthew Hirn

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Summary

Recent advances in machine learning have shown impressive performance of increasingly complex deep neural networks on a multitude of tasks. However, some of their most significant achievements are in settings where the analyzed data has an inherent Euclidean structure (e.g., spatial in computer vision or temporal in audio and signal processing applications). This realization gave rise to an emerging field of geometric deep learning that aims to leverage the extensive body of work studying non-Euclidean geometries to process data with intrinsic graph and manifold structures. The mathematics of geometric deep learning is not well understood, though. Inspired by the success of the wavelet scattering model for Euclidean ConvNets, several recent papers have generalized its construction to graphs and manifolds (which numerically are approximated by graphs) with the goal of better understanding the intricacies of geometric deep learning. Referring to such works collectively as geometric wavelet scattering transforms, in this proposed talk we will give an overview of the geometric scattering transform for graphs and manifolds, focusing on its utility as a model for graph ConvNets. We will describe recent theoretical results that quantify the invariance and stability properties of geometric scattering networks on graphs, and which are illustrated via numerical experiments.

Abstract

The processing of signal-based data such as auditory recordings, images, and videos for learning tasks is often carried out with convolutional neural networks (ConvNets) and related architectures. A primary reason for the success of ConvNets is the use of convolution operators, which reduces the number of learned parameters while taking advantage of the underlying Euclidean geometry of the data. However numerous data types of interest, including social networks, molecules in chemistry, two-dimensional surfaces as in certain types of medical diagnostic imaging, and computer graphics, amongst others, do not have an underlying Euclidean structure but do have an underlying geometric structure. In many such cases, this non-Euclidean structure can be modelled as an abstract graph or Riemannian manifold, the latter of which is approximated, numerically, by a mesh graph.

Motivated by the desire to develop learning algorithms for non-Euclidean data and the success of ConvNets for Euclidean data, the nascent field of geometric deep learning [2] seeks to develop ConvNet-type architectures for graph and manifold based data. The resulting developments are revolutionizing several learning tasks on non-Euclidean data, including graph classification, generative graph and manifold models, shape retrieval, and shape alignment, among others. Despite these early successes, many open questions remain, including how to structure such networks to best capture relevant information in graphs and manifolds, how to compute and train them efficiently, and how to identify the mathematical properties of the resulting learning algorithms.

In this proposed talk we focus on the latter topic, namely the theoretical understanding of geometric deep learning. As geometric deep learning algorithms have evolved, they have become more specialized on either graph based data or manifold based data (particularly two-dimensional surfaces in the latter case, motivated in large part by computer graphics). However, spectral analysis of geometric ConvNets relies on studying the eigenvalues and eigenvectors of the graph Laplacian in the case of graphs, and the eigenvalues and eigenfunctions of the Laplace-Beltrami operator for manifolds. In both settings, one defines a generalized notion of Fourier series on the graph or manifold, which is a core component of graph signal processing [14]. Furthermore, nonlinear dimension reducing algorithms, and in particular so-called manifold learning algorithms, e.g., [13, 1, 3], have long relied on the close relationship between spectral graph theory (i.e., the study of the spectral properties of the graph Laplacian) and spectral geometry (i.e., the study of the spectral properties of the Laplace-Beltrami operator).

In this talk we will deliver a unified treatment of mathematical properties of graph and manifold based ConvNets through the lens of recently developed geometric versions of the wavelet scattering transform. The Euclidean wavelet scattering transform, first introduced by S. Mallat in [9], has proven to be a powerful mathematical model for Euclidean ConvNets [10]. Similar to the convolutional layers of a standard ConvNet, the wavelet scattering transform consists of a cascade of convolutional operators and nonlinearities. However, it replaces the learned filters of ConvNets with complex-valued wavelet filters, and utilizes the nonlinear modulus operator as its activation function. The power of the Euclidean wavelet scattering model is that it provably has several desirable properties, such as guaranteed local translation/rotation invariance and Lipschitz stability to the action of small diffeomorphisms (see the results in [9]), while simultaneously has been shown to be a powerful data representation for processing 1D, 2D, and 3D signal based data [10].

In the past two years, several research articles have generalized the Euclidean wavelet scattering transform to graphs [16, 15, 6, 4, 5, 7] and manifolds [12, 11], using geometric notions of wavelets [8]. We collectively refer to these types of wavelet scattering transforms as *geometric wavelet scattering transforms*. Many of these articles focus on the theoretical properties of the geometric wavelet scattering transform, although [7, 15] illustrate its utility and competitive performance in supervised and unsupervised learning tasks associated to graphs. Both the graph and manifold versions of the geometric wavelet scattering transform are designed to have provable invariance properties to graph permutations and manifold isometries, which generalize the translation and rotation invariance of Euclidean wavelet scattering transforms. They are also provably stable to graph perturbations and manifold diffeomorphisms under certain conditions, but the existing theorems provide only partial results and warrant additional study. This talk will present an overview of the geometric wavelet scattering transform with a focus on the current state of the art. It provides a unified geometric signal processing framework for analyzing both graph and manifold based ConvNets with theory and empirical performance that show the promise of the model, and yet many questions and unexplored research directions remain open that would be of interest to the network science community.

Submission

Please consider this submission for a 20 minute talk. Also, if this abstract is accepted, in order to avoid scheduling conflicts, please note I am organizing a mini-symposium for the SIAM annual meeting titled "Multiscale data science inspired by physical and biological systems."

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