The Graph Scattering Transform(s)

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Why is this talk different than all other talks?

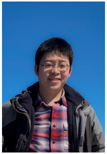
Outline

- Several Formulations of Graph Scattering Transform
- Comparison of constructions and theoretical guarantees
- A new formulation which seeks to unify the differing approaches

Joint Work With

Guy Wolf - University of Montreal

Matthew Hirn - Michigan State University



Feng Gao - Yale University

The (Euclidean) Scattering Transform - S. Mallat (2012)

Overview:

- Model of Convolutional Neural Networks.
- Predefined (wavelet) filters.

Advantages:

- Provable stability and invariance properties.
- Near state of the art numerical results in certain situations.
- Needs less training data.

The Scattering Transform

The Scattering Transform:

- Multilayered nonlinear measurements

$$\mathbf{x} \to W_{j_1}\mathbf{x} \to \sigma(W_{j_1}\mathbf{x}) \to W_{j_2}\sigma(W_{j_1}\mathbf{x}) \to \sigma(W_{j_2}\sigma(W_{j_1}\mathbf{x}))$$

  where $\{W_j\}_{j=0}^{J}$ is a collection of Wavelets.

- $$U[j]\mathbf{x} = \sigma(W_j\mathbf{x}) \quad U[j_1, j_2]\mathbf{x} = \sigma(W_{j_2}\sigma(W_{j_1}\mathbf{x}))$$

- Apply averaging operator or take the ℓ^1 norm

$$S[j_1, j_2]\mathbf{x} = A_J U[j_1, j_2]\mathbf{x} \quad \text{(windowed)}$$
$$\bar{S}[j_1, j_2]\mathbf{x} = \|U[j_1, j_2]\mathbf{x}\|_1 \quad \text{(non-windowed)}$$

The Graph Scattering Transform(s)

- Several Different Versions, developed independently
  - Zou and Lerman: ACHA 2019
  - Gama, Bruna, and Ribiero: NeurIPS 2019, ICLR 2019
  - Gao, Wolf, and Hirn ICML 2019
- Windowed vs Non-windowed (Averaging operator vs $\|\cdot\|_1$)
  - Zou and Lerman: Windowed
  - Others: Non-windowed
- Different Wavelet Constructions
  - Zou and Lerman: Spectral Decomposition of the Unnormalized Laplacian
  - Others: Diffusion Wavelets á la Coifman and Maggioni

Questions

- Can we unify these constructions and their guarantees?
- Windowed Scattering for diffusion wavelets?
- Theoretical Guarantees for asymmetric wavelets, e.g. Gao et al?

Diffusion Wavelets

Lazy Symmetric Diffusion

The wavelets in Gama et al. are polynomials of

$$T := \frac{1}{2}\left(I + D^{-1/2}AD^{1/2}\right)$$

If we let N be the normalized graph Laplacian

$$N := I - D^{-1/2}AD^{-1/2} = V\Omega V^T.$$

We can rewrite T as a Fourier multiplier

$$T = I - \frac{N}{2} = V\left(I - \frac{\Omega}{2}\right)V^T.$$

Isometries and frame bounds

Symmetric Diffusion Wavelets

The wavelets in Gama et al. are given by

$$W_j = p_j(T) = \begin{cases} I - T & \text{if } j = 0 \\ T^{2^{j-1}} - T^{2^j} & \text{otherwise} \end{cases}$$

Frame bounds

$$C\|\mathbf{x}\|_2^2 \leq \sum_j \|W_j\mathbf{x}\|_2^2 \leq \|\mathbf{x}\|_2^2.$$

To get an isometry ($C = 1$) replace $p_j(T)$ with $q_j(T) = p_j(T)^{1/2}$.

Spectral Square Roots

$$q_j(T) = \left(p_j(V\Lambda V^T)\right)^{1/2} = \left(Vp_j(\Lambda)V^T\right)^{1/2} = Vq_j(\Lambda)V^T$$

Asymmetric Diffusion Wavelets

Asymmetric Diffusion Wavelets

The wavelets in Gao et al. polynomials of

$$P = D^{1/2} T D^{-1/2} = \frac{1}{2}\left(I - AD^{-1}\right),$$

where $D = \mathrm{diag}(\mathbf{d})$.
Not symmetric, so the theorems of Gama et al. don't apply.

Unified Construction

$$W_j = p_j(K), \text{ (or } q_j(K) = p_j(K)^{1/2}) \quad K = MTM^{-1}$$

$$K = \begin{cases} T & \text{if } M = I \\ P & \text{if } M = D^{-1/2} \\ P^T & \text{if } M = D^{1/2} \end{cases}.$$

Frame Bounds for the K Wavelets

Lemma: (Weighted L^2 space)

$K = MTM^{-1}$ is self-adjoint on the weighted ℓ^2 space

$$\langle \mathbf{x}, \mathbf{y} \rangle_M = \langle M^{-1}\mathbf{x}, M^{-1}\mathbf{y} \rangle_2.$$

Example: If $M = diag(\mathbf{d}^{1/2})$, $K = P^T$

$$\langle \mathbf{x}, \mathbf{y} \rangle_M = \sum_i x_i y_i d_i$$

Proposition (Nonexpansive Frames)

$$C\|\mathbf{x}\|_M^2 \leq \sum_j \|p_j(K)\mathbf{x}\|_M^2 \leq \|\mathbf{x}\|_M^2,$$

$$\sum_j \|q_j(K)\mathbf{x}\|_M^2 = \|\mathbf{x}\|_M^2, \text{ where } q_j(t) = p_j(t)^{1/2}.$$

Invariance

Non-windowed Scattering

For all of the graph scattering transforms it is true that $U[j_1, j_2]$ commutes with permutations meaning that for a permutation π,

$$U_{\pi(G)}[j_1, j_2]\pi(\mathbf{x}) = \pi\left(U_G[j_1, j_2]\mathbf{x}\right).$$

From this is follow that

$$\bar{S}_{\pi(G)}[j_1, j_2]\pi(\mathbf{x}) = \|U_{\pi(G)}[j_1, j_2]\pi(\mathbf{x})\|_1 = \bar{S}_G[j_1, j_2]\mathbf{x}.$$

Windowed-Scattering

Zou et al. showed that with their wavelet's

$$\|S_{\pi(G)}[j_1, j_2]\pi(\mathbf{x}) - S_G[j_1, j_2]\mathbf{x}\| = O\left(2^{-J}\right)$$

Invariance Continued

Windowed-Scattering

Zou and Lerman showed that with their wavelets

$$\|S_{\pi(G)}[j_1, j_2]\pi(\mathbf{x}) - S_G[j_1, j_2]\mathbf{x}\| = O\left(2^{-J}\right)$$

Is the same true for the Diffusion wavelets, equipped with a low-pass averaging operator?

Yes ... if $K = P^T$

- For large J, $A_J \approx$Projection onto the bottom eigenvector.
- For the unnormalized Laplacian, the bottom eigenvector is constant.
- For $A_J = K^{2^J}$, $\mathbf{u}_0 = M^{-1}\mathbf{d}^{1/2}$ =constant, if $M = \text{diag}(\mathbf{d}^{1/2})$.

Continuity and Conservation of Energy

Continuity

For the windowed-scattering transform: As long as the wavelet transform is non-expansive,

$$\|S\mathbf{x} - S\mathbf{y}\|_{\ell^2(L^2(G,M))} \leq \|\mathbf{x} - \mathbf{y}\|_M.$$

For the non-windowed scattering transform:

$$\|\bar{S}\mathbf{x} - \bar{S}\mathbf{y}\|_{\ell^2} \leq C\|\mathbf{x} - \mathbf{y}\|_M$$

Conservation of Energy

If the wavelet transform is an isometry,

$$\|S\mathbf{x}\|_{\ell^2(L^2(G,M)} = \|\mathbf{x}\|_M.$$

Note, this relies on a energy-decay result which is much easier on graphs than on $\mathbb{R}^n$ as first observed by Zou and Lerman.

Stability for T wavelets

Polynomial Wavelets

Gama et al. show

$$\sum_j \|p_j(T)\mathbf{x} - p_j(T')\mathbf{x}\|_2^2 \leq C(\|T - T'\|_{2\to2}^2 + \|T - T'\|_{2\to2})\|\mathbf{x}\|_2^2$$

Square Root Wavelets

It can also be shown,

$$\sum_j \|q_j(T)\mathbf{x} - q_j(T')\mathbf{x}\|_2^2 \leq C_J \left(\sup|\lambda_i - \lambda_i'| + \sup\|v_i - v_i'\|_2\right)\|\mathbf{x}\|_2^2$$

Stability for K wavelets

Differences in the weighting matrix

$$\kappa = \max\left\{\|M'M^{-1} - I\|, \|M'^{-1}M - I\Big\|\right\}$$

In prototypical example $M = \text{diag}(\mathbf{d}^{\pm 1/2})$ so

$$\kappa^2 \approx \max\left\{\left|\frac{d_i'}{d_i} - 1\right|, \left|\frac{d_i}{d_i'} - 1\right|\right\}$$

Transferred Stability Bounds

Let $\mathcal{W}^{(T)}$ be wavelets constructed from (square roots of) polynomials of T and $W^{(K)}$ be the wavelets built from the same (square roots of) polynomials of K Then

$$\|W^{(K)} - W^{(K')}\|_{\ell^2(\mathbf{L}^2(G,M))} = \mathcal{O}(\|W^{(T)} - W^{(T')}\|_{\ell^2(\mathbf{L}^2(G))} + \kappa)$$

Asymmetric Diffusion Distances

Transferred Stability Bounds

Combining the previous results gives

$$\sum_j \|p_j(K)\mathbf{x}-p_j(K')\mathbf{x}\|_2^2 \leq C(\|T-T'\|_{2\to 2}^2+\|T-T'\|_{2\to 2}+\kappa^2)\|\mathbf{x}\|_2^2.$$

Bound in terms of $\|K-K'\|_{M\to M}$

$$\|T-T'\|_{2\to 2} \leq \kappa(1+R^3)+R\|K-K'\|_{M\to M}$$

where

$$\kappa = \max\{\|M'M^{-1}-I\|_2, \|M'^{-1}M-I\|_2\}$$
$$R = \|M'M^{-1}\|_2, \|M'^{-1}M\|_2$$

If graphs are well-aligned $\kappa \approx 0, R \approx 1$.

Stability of the scattering transform

ℓ-th layer coefficients

The ℓ-th layer scattering coefficients sastisfy

$$\|S^\ell \mathbf{x} - (S^\ell)'\mathbf{x}\|_{\ell^2(\mathbf{L}^2(G,M))} \leq C_\ell \|W - W'\|_{\mathbf{L}^2(G,M)} \|\mathbf{x}\|_M$$

where

$$C_\ell = \sum_{j=1}^{\ell} \|\mathcal{W}'\|^j_{\ell^2(\mathbf{L}^2(G,M))} \approx \ell \text{ if the graph are well-aligned}$$

Wavelets on the "wrong space"

$$\|\mathcal{W}'\|_{\ell^2(\mathbf{L}^2(G,M))} \leq R^2, \quad \text{where}$$

$$R = \max\{\|M'M^{-1}\|_2, \|M'^{-1}M\|_2\}$$

Conclusion and Future Work

- New formulation of Graph Scattering using asymmetric diffusions $K = MTM^{-1}$.
- Windowed Scattering is only invariant if $K = P^T$
- Theoretical Guarantees of Previous Papers can be extended to these asymmetric diffusion scattering transforms
- Can we learn the best M?

THANK YOU!