Gradient flows on Graphons

Sewoong Oh[1], Soumik Pal[2], Raghav Somani[1] and Raghav Tripathi[2]

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- Starting from $\{X_{i,0}\}_{i=1}^{n} \overset{\text{i.i.d.}}{\sim} \rho_0$, one can perform a gradient flow:

$$\mathrm{d}X_{i,t} = -\frac{1}{n}\sum_{j=1}^{n}(X_{i,t} - X_{j,t})\,\mathrm{d}t \,, \qquad \forall\, i \in [n],\ t \geq 0 \,.$$

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- Notice that V_n is essentially a function of the empirical measure of its inputs!

$$V_n(x) = \mathrm{Var}(\mathrm{Emp}_n(x)) .$$

Can we approximate this problem by lifting it over the space of measures?

Particle System to Measures

- If a function $V_n : \mathbb{R}^n \to \mathbb{R}$ is invariant under permutations of its input, then it can be extended to a function $V : \mathcal{P}(\mathbb{R}) \to \mathbb{R}$.

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Upshot

Allows approximability to finite dimensional version, under mild assumptions.

Optimization on Large Graphs

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Triangle density

Let G be a finite simple graph with n vertices,

$$h_{\triangle}(G) = \frac{|\text{Number of triangles in } G|}{n^3} .$$

Scalar Entropy

For a graph G with adjacency matrix A, let $h(p) = p \log p + (1-p) \log(1-p)$,

$$E(G) = \frac{1}{n^2} \sum_{i,j=1}^{n} h(A_{i,j}) .$$

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A Problem on Large Graphs

Consider minimizing $h_{\triangle} + E$ over the set of all graphs. (e.g. Chatterjee & Varadhan)

Is there a symmetry?

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- Notice that unlabeled graphs have a symmetry under vertex relabeling.

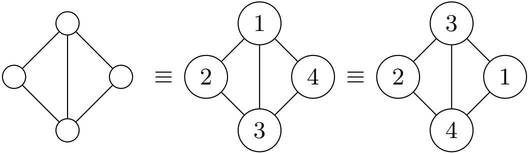

Figure: Symmetry in unlabeled graphs.

- I.e., for an unlabeled graph G with n vertices.
  If A is its adjacency matrix, so is $A_\pi = \left(A_{\pi(i),\pi(j)}\right)_{i,j}$.

$$A = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \equiv \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix} = A_\pi \ .$$

- This makes functions over graphs *invariant* under this symmetry.

Neural Networks: Another Example

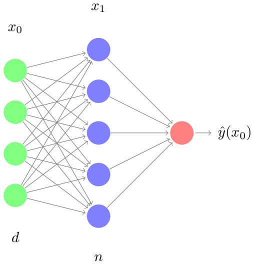

Figure: NN with 1 hidden layer.

$$\hat{y}(x_0) = \frac{1}{n}\sum_{i=1}^{d} \sigma(A_{i,j}x_{0,j}) , \quad A \in \mathbb{R}^{n\times d} ,$$

$$R_n(A) \coloneqq \mathbb{E}_{(X,Y)\sim\mu}[\ell(Y, \hat{y}(X))] .$$

A Mean Field View of the Landscape of Two-Layer Neural Networks - Mei, Montanari & Nguyen, 2018

On the Global Convergence of Gradient Descent for Over-parameterized Models using Optimal Transport - Chizat & Bach, 2018

What we need?

A common set that contains all unlabeled graphs Embedding

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A notion of 'gradient flow' on this space	'Differentiable structure'

Kernels and Graphons

Kernels $\mathcal{W}$

A kernel is a measurable function $W\colon [0,1]^2 \to [-1,1]$ such that $W(x,y) = W(y,x)$.

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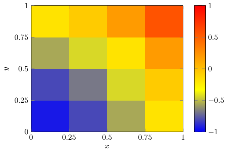
- Symmetric matrices can be converted into a kernel.

$$\frac{1}{16}\begin{bmatrix} -16 & -15 & -12 & -14 \\ -15 & -14 & -11 & 1 \\ -12 & -11 & -6 & 4 \\ -7 & 1 & 4 & 9 \end{bmatrix}$$

Symmetric matrix A



Kernel representation of A

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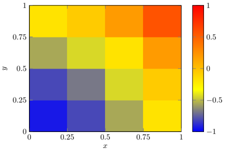
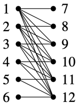


Kernel representation of A

- Therefore graphs can be made into kernel.



$$\begin{matrix} 0&0&0&0&0&0&1&1&1&1&1&1 \\ 0&0&0&0&0&0&0&1&1&1&1&1 \\ 0&0&0&0&0&0&0&0&1&1&1&1 \\ 0&0&0&0&0&0&0&0&0&1&1&1 \\ 0&0&0&0&0&0&0&0&0&0&1&1 \\ 0&0&0&0&0&0&0&0&0&0&0&1 \\ 1&0&0&0&0&0&0&0&0&0&0&0 \\ 1&1&0&0&0&0&0&0&0&0&0&0 \\ 1&1&1&0&0&0&0&0&0&0&0&0 \\ 1&1&1&1&0&0&0&0&0&0&0&0 \\ 1&1&1&1&1&0&0&0&0&0&0&0 \\ 1&1&1&1&1&1&0&0&0&0&0&0 \end{matrix}$$

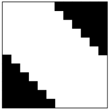
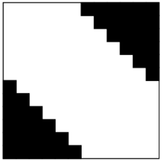
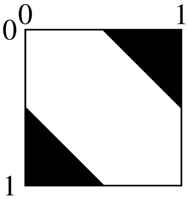


Figure: Example 4.1.6, Graph Theory and Additive Combinatorics, Yufei Zhao

Convergence of Graph(ons)



(a) Half Graph (Kernel)



(b) Limit of Half Graph

Graph Theory and Additive Combinatorics, Yufei Zhao

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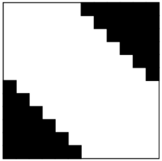

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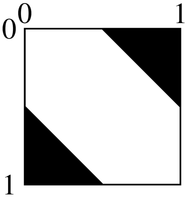

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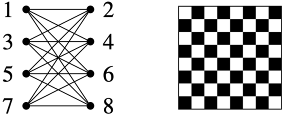

(a) Checkerboard

Q. Where does this sequence of kernels converge?

Graph Theory and Additive Combinatorics, Yufei Zhao

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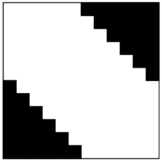

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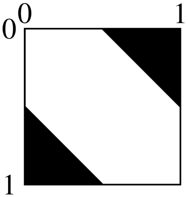

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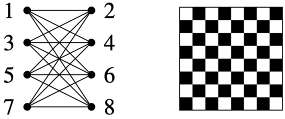

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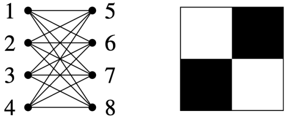

(b) Checkerboard after vertex relabeling

Graph Theory and Additive Combinatorics, Yufei Zhao

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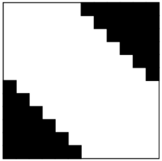

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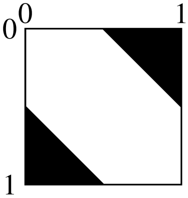

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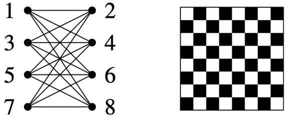

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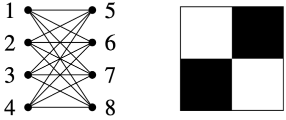

(b) Checkerboard after vertex relabeling

A. The limit of a bipartite graph is **not** the 1/2.

Graph Theory and Additive Combinatorics, Yufei Zhao

Graphons

- We should identify two kernels if one can be obtained by 'permuting' the other.
- $W_1 \cong W_2$ if there is a measure preserving transform $\varphi\colon [0,1] \to [0,1]$ such that

$$W_1^{\varphi}(x,y) := W_1(\varphi(x), \varphi(y)) = W_2(x,y) \ .$$

Space of Graphons $\widehat{\mathcal{W}}$ (Lovász & Szegedy, 2006)

$$\widehat{\mathcal{W}} := \mathcal{W}/\cong \ .$$

A general recipe

Start with a norm $\|\cdot\|$ on $\mathcal{W}$. Define δ as

$$\delta(W_1, W_2) = \inf_{\varphi_1, \varphi_2} \|W_1^{\varphi_1} - W_2^{\varphi_2}\| \ ,$$

where $W^{\varphi}(x,y) = W(\varphi(x), \varphi(y))$.

Cut Metric: $\delta_\square$

$$\|W\|_\square := \sup_{S,T} \left| \int_{S\times T} W(x,y)\,\mathrm{d}x\,\mathrm{d}y \right|.$$

[1] Lovász & Szegedy, 2006, using Szemerédi's regularity lemma
Frieze & Kannan, 1999

Cut Metric: $\delta_\square$

$$\|W\|_\square := \sup_{S,T} \left| \int_{S\times T} W(x,y)\,\mathrm{d}x\,\mathrm{d}y \right|.$$

- Captures graph convergence.
  - $(G_n)_n$ converges in $\delta_\square$ if
    $$\lim_{n\to\infty} h_F(G_n)$$
    exists for all simple graphs $F \in \{-, \wedge, \triangle, \leftthreetimes, \sqcup, \square, \boxtimes, \ltimes, \bowtie, \ldots\}$.
- $(\widehat{\mathcal{W}}, \delta_\square)$ is compact.[1]

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Invariant L^2 metric δ_2

For $\|\cdot\| = \|\cdot\|_{L^2([0,1]^2)}$, we get the Invariant L^2 metric δ_2.

Borgs, Chayes, Lovász, Sós & Vesztergombi, 2008

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For $\|\cdot\| = \|\cdot\|_{L^2([0,1]^2)}$, we get the Invariant L^2 metric δ_2.

- Stronger than the cut metric (i.e., $\delta_\square \leq \delta_2$).
- Gromov-Wasserstein distance between the metric measure spaces $([0,1], \mathrm{Leb}, W_1)$ and $([0,1], \mathrm{Leb}, W_2)$.
- Provides geodesic metric structure on $\widehat{\mathcal{W}}$. Allows notion of (geodesic) convexity.

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What is a ‘gradient flow’?

On $\mathbb{R}^d$

The ‘gradient flow’ u of a function $F\colon \mathbb{R}^d \to \mathbb{R}$ is given by solutions of

$$u'(t) = -\nabla F(u(t)) \ ,$$

Gradient Flows in Metric Spaces and in the Space of Probability Measures - Ambrosio, Gigli & Savare, 2005

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On $(\widehat{\mathcal{W}}, \delta_2)$

Consider a curve ω and a function F on $\widehat{\mathcal{W}}$.

- Speed of ω: Metric derivative $|\omega'|$

Metric Derivative of ω

$$|\omega'|(t) = \lim_{s \to t} \frac{\delta_2(\omega_t, \omega_s)}{|t-s|} \ .$$

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$$\frac{\mathrm{d}}{\mathrm{d}t} F(u(t)) = \langle u'(t), \nabla F(u(t)) \rangle$$

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On $(\widehat{\mathcal{W}}, \delta_2)$

Consider a curve ω and a function F on $\widehat{\mathcal{W}}$.

- Speed of ω: Metric derivative $|\omega'|$

Metric Derivative of ω

$$|\omega'|(t) = \lim_{s \to t} \frac{\delta_2(\omega_t, \omega_s)}{|t-s|} \ .$$

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Fréchet-like derivative of F: DF

Provides a local linear approximation of F.

Gradient Flows in Metric Spaces and in the Space of Probability Measures - Ambrosio, Gigli & Savare, 2005

What is a 'gradient flow'?

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Fréchet-like derivative and existence of gradient flow

Theorem [OPST '21]

If F

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then starting from any $W_0 \in \widehat{\mathcal{W}}$, the curve $(W_t)_{t\in\mathbb{R}_+}$ defined as

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- For the scalar entropy function E, if $0 < W < 1$, then

$$(DE)(W)(x,y) = \log\left(\frac{W(x,y)}{1-W(x,y)}\right).$$

Example

- Given Dh_F and DE, we can now perform a gradient flow to minimize $h_\triangle + E$ on the space of Graphons!
- Given initial conditions, one needs to solve for all $x, y \in [0,1]$,

$$W_t'(x,y) = -\left[3\int_0^1 W(x,z)W(z,y)\,\mathrm{d}z + \log\left(\frac{W(x,y)}{1-W(x,y)}\right)\right].$$

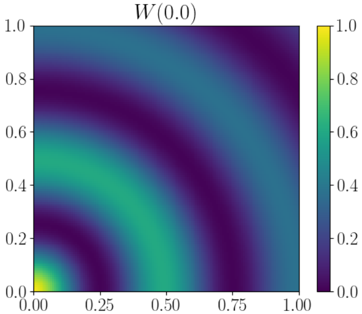

Figure: Gradient flow of $h_\triangle + 10^{-1}E$

Euclidean Gradient flow and Gradient flow on $\widehat{\mathcal{W}}$

Consider a function $F : \widehat{\mathcal{W}} \to \mathbb{R}$ that has following gradient flow

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Question?

Are the curves $V^{(n)}$ and W close (if n is large)?

Euclidean Gradient and Fréchet-like derivative

Fréchet-like derivative

A symmetric measurable function $\phi \in L^\infty([0,1]^2)$ is said to be Fréchet-like derivative $DF(W)$ of F at $W \in \widehat{\mathcal{W}}$ if

$$\lim_{\substack{U \in \mathcal{W}, \\ \|U-W\|_2 \to 0}} \frac{F(U) - F(W) - \langle \phi, U - W \rangle_{L^2([0,1]^2)}}{\|U - W\|_2} = 0 \, .$$

- Recall that $F \colon \widehat{\mathcal{W}} \to \mathbb{R}$ can be regarded as a function $F_n \colon \mathcal{M}_n \to \mathbb{R}$.
- Let $\nabla_n F_n$ be Euclidean derivative of $F_n \colon \mathcal{M}_n \to \mathbb{R}$.

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The graphon corresponding to $n^2 \nabla_n F_n(W)$ equals $DF(W)$.

Euclidean gradient flow and gradient flow on Graphons

Gradient flow on $\widehat{\mathcal{W}}$

$$\frac{\mathrm{d}}{\mathrm{d}t}W(t) = -DF(W(t)) = -n^2\nabla_n F(W(t))$$

Gradient flow on $\mathcal{M}_n$

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t) = -\nabla_n F(V(t))$$

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$$\frac{\mathrm{d}}{\mathrm{d}t} V(t) = -\nabla_n F(V(t))$$

- The curve $\tilde{W}(t) := V(n^2 t)$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t} \tilde{W}(t) = -n^2 \nabla_n F(\tilde{W}(t)) = -DF(\tilde{W}(t)) \,.$$

- That is, it is reasonable to expect that the gradient flow on Graphons can be obtained a scaling limit of Euclidean gradient flows.

Convergence of Euclidean Gradient Flow

Theorem [OPST '21]

- Let $F\colon \widehat{\mathcal{W}} \to \mathbb{R}$ be a function with gradient flow

$$W(t) := W_0 - \int_0^t D_{\widehat{\mathcal{W}}} F(W)\,\mathrm{d}s\ .$$

- Consider the Euclidean gradient flow of $F_n\colon \mathcal{M}_n \to \mathbb{R}$ starting at $V_0^{(n)}$, i.e.,

$$V^{(n)}(t) := V^{(n)}(0) - \int_0^t \nabla_n F_n\Big(V^{(n)}(s)\Big)\,\mathrm{d}s\ .$$

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If $W_0^{(n)} \xrightarrow{\delta_\square} W_0$, then

$$W^{(n)} \overset{\delta_\square}{\rightrightarrows} W \qquad \text{as } n \to \infty\ ,$$

over compact time intervals.

Ongoing and Future directions

- Study convergence of stochastic gradient descent with and without added noise.
- Specialize the theory on optimization over multiple layer NNs.

Thank you!

- ArXiv version: https://arxiv.org/abs/2111.09459