Gradient flows on Graphons

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Objective

Study large scale optimization problems that have permutation symmetries.

- Exploiting symmetries allow taking limits of the size of optimization problems.

For $n \in \mathbb{N}$, consider minimizing the following interaction energy $V_n \colon \mathbb{R}^n \to \mathbb{R}_+$

$$V_n(x) \coloneqq \frac{1}{n^2} \sum_{i,j=1}^{n} \frac{1}{2} (x_i - x_j)^2 \, .$$

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

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

- 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 probability measures?

Particle System to Measures

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

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- For the interaction energy V_n, we know that $V(\rho) = \mathrm{Var}(\rho)$ for $\rho \in \mathcal{P}(\mathbb{R})$.
- Notice that for all $n \in \mathbb{N}$,

$$\min_{\mathbb{R}^n} V_n = \min_{\mathcal{P}(\mathbb{R})} \mathrm{Var} .$$

- One can solve the latter using *Wasserstein gradient flows*!
- One may also add a noise term.

$$\mathrm{d}X_{i,t} = -\frac{1}{n}\sum_{j=1}^{n}(X_{i,t} - X_{j,t}) + \sqrt{2\beta}\,\mathrm{d}B_{i,t}, \quad \forall\, i \in [n],\ t \geq 0,$$

  where B_t is the standard Brownian motion on $\mathbb{R}^n$, and $\beta \geq 0$.
- This SDE captures the Wasserstein gradient flow of $\mathrm{Var} + \beta\mathrm{Ent} \colon \mathcal{P}(\mathbb{R}) \to \mathbb{R}$, the entropy-regularized optimization.

Benefits

Approximations and universal limits.

Optimization on Large Graphs

Q. What about optimization over dense unlabeled (weighted) graphs?

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Triangle density

Let G be a finite simple graph with n vertices,

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

For a graph with adjacency matrix A one can define

$$\text{Number of triangles in } G = \sum_{\phi\colon [3]\to V(G)} \prod_{\{i,j\}\in E(G)} A_{\phi(i),\phi(j)} .$$

The above formula works even when A is a symmetric matrix of real edge weights.

Optimization on Large Graphs

Scalar Entropy

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

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

- Scalar Entropy is 0 for all unweighted graphs.

Optimization on Large Graphs

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A Problem on Statistics of Exponential Random Graphs

Consider minimizing $h_{\triangle} + E$ over the set of all graphs.

See Diaconis and Janson 2008, Chatterjee & Varadhan 2011, Lovász 2012, Lubetzky and Zhao 2015 etc.

Is there a symmetry?

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

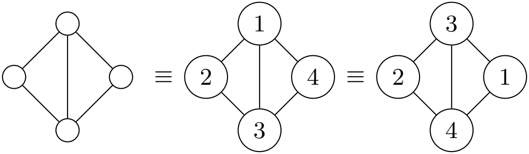


Figure: Symmetry in unlabeled graphs.

- 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 these graphs *exchangeable* under this symmetry. See Aldous '81, '82, and Austin '08, '12.

Neural Networks: Another Example

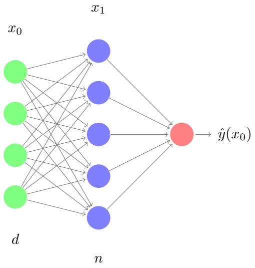


Figure: NN problem is optimization over unlabeled networks.

$$\hat{y}(x_0) = \frac{1}{n}\sum_{i=1}^{d} \sigma(A_{i,j} x_{0,j}) , \quad A \in \mathbb{R}^{n\times d} , \quad R_n(A) := \mathbb{E}_{(X,Y)\sim\mu}[\ell(Y, \hat{y}(X))] .$$

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 embedding that contains all unlabeled graphs
- A suitable topology of ‘graph convergence’
- Completion under a metric
- A notion of ‘differentiable structure’ to define ‘gradient flow’ on this space.

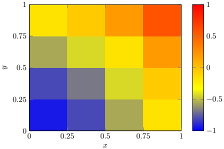
Kernels and Graphons

Kernels $\mathcal{W}$

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

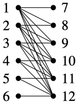
- Symmetric matrices can be converted into a kernel.

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



Symmetric matrix A Kernel representation of A

- (Weighted) Graphs $\Leftrightarrow$ adjacency matrix $\Leftrightarrow$ kernel.



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

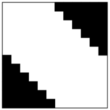


Figure: Example 4.1.6, Graph Theory and Additive Combinatorics, Zhao

Graphons

- 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)

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

- For finite labeled graphs, the corresponding graphons are the equivalent classes for identification modulo graph isomorphisms.
- Compare with a measure given by two different pushforwards $T_1, T_2\colon [0,1] \to \mathbb{R}$.

Invariant functions on Kernels = functions on graphons

- Recall the triangle density function

$$h_{\triangle}(G) = \frac{\text{Number of triangles in G}}{n^3} = \frac{1}{n^3} \sum_{\phi:\ [3]\to V(G)} \prod_{\{i,j\}\in E(G)} A_{\phi(i),\phi(j)}.$$

- For a kernel W, the triangle density can be defined as

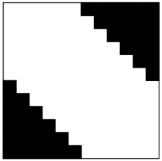
$$h_{\triangle}(W) = \int_{[0,1]^3} W(x_1, x_2)W(x_2, x_3)W(x_3, x_1)\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3\ .$$

- $h_{\triangle}$ is a function on the corresponding graphon. That is,

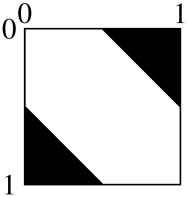
$$h_{\triangle}(V) = h_{\triangle}(W),$$

if V can be obtained from W by vertex permutations.

Convergence of Graph(ons)



(a) Half Graph (Kernel)



(b) Limit of Half Graph

Graph Theory and Additive Combinatorics, Yufei Zhao

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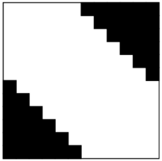

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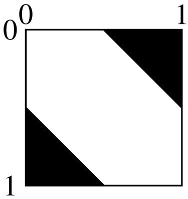
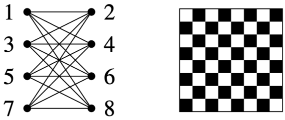


(b) Limit of Half Graph

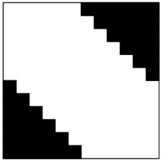


(a) Checkerboard

Q. Where does this sequence of graphons converge?

Graph Theory and Additive Combinatorics, Yufei Zhao

Convergence of Graph(ons)



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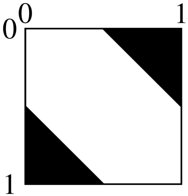
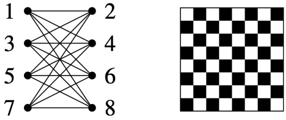


(b) Limit of Half Graph



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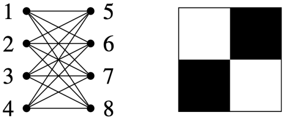
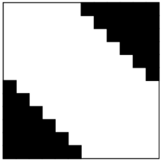


(b) Checkerboard after vertex relabeling

Graph Theory and Additive Combinatorics, Yufei Zhao

Convergence of Graph(ons)



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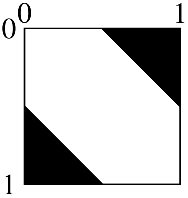

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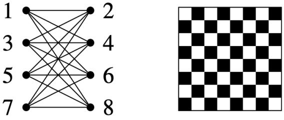

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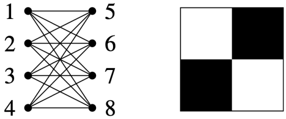

(b) Checkerboard after vertex relabeling

A. Both (a) and (b) are the *same* graphon, but two different kernel representations.

Graph Theory and Additive Combinatorics, Yufei Zhao

Metrics on Graphons

- Recall: $W_1 \cong W_2$ if there is a measure preserving transform $\varphi\colon [0,1] \to [0,1]$ such that
$$W_1^{\varphi}(x,y) \coloneqq W_1(\varphi(x), \varphi(y)) = W_2(x,y)\ .$$
- How to define metrics for graphon convergence?

A general recipe

Start with any norm $\|\cdot\|$ on functions $[0,1]^2 \to [-1,1]$. Define δ as
$$\delta(W_1, W_2) = \inf_{\varphi} \|W_1^{\varphi} - W_2\|.$$

Cut Metric: $\delta_\square$

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

- Cut metric (Frieze & Kannan, 1999) metrizes *graph convergence* (Lovász & Szegedy, 2006).
  - $(G_n)_n$ converges in $\delta_\square$ if
    $$\lim_{n\to\infty} h_F(G_n)$$
    exists for all simple graphs $F \in \{-, \wedge, \triangle, \curlywedge, \sqcup, \square, \boxtimes, \ltimes, \bowtie, \ldots\}$.
- $(\widehat{\mathcal{W}}, \delta_\square)$ is compact.[1]
- Analogous to the weak topology over probabilities.
- Example: Almost surely, random graph $G(n, 1/2)$ converges to constant graphon

$$W(x,y) = 1/2 \ , \ \forall\,(x,y) \in [0,1]^2 \ .$$

[1] uses Szemerédi's regularity lemma

Invariant L^2 metric δ_2

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.
- Analogous to the Wasserstein-2 metric over measures.

Borgs, Chayes, Lovász, Sós & Vesztergombi, 2008

What is a 'gradient flow' on a metric space?

On $\mathbb{R}^d$

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

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

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

$$\geq -\frac{1}{2}|u'|^2(t) - \frac{1}{2}|\nabla F(u(t))|^2 \ .$$

A curve u is a gradient flow of F if

$\frac{\mathrm{d}}{\mathrm{d}t} F(u(t)) \leq -\frac{1}{2}|u'|^2(t) - \frac{1}{2}|\nabla F(u(t))|^2.$

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

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

- Gradient of F: Fréchet-like derivative

Fréchet-like derivative of F: DF

Provides a local linear approximation of F.

A curve u is a gradient flow of F if

$$\frac{\mathrm{d}}{\mathrm{d}t} F(\omega(t)) \leq -\tfrac{1}{2} \left| \omega' \right|^2 (t) - \tfrac{1}{2} \left| DF(\omega(t)) \right|^2 .$$

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Fréchet-like derivative and existence of gradient flow

Theorem [OPST '21]

If F

- has a Fréchet-like derivative,
- is geodesically semiconvex in δ_2,

then starting from any $W_0 \in \widehat{\mathcal{W}}$, there exists a unique gradient flow curve $(W_t)_{t \in \mathbb{R}_+}$ for F.
The curve satisfies ODE

$$W_t := W_0 - \int_0^t DF(W_s)\,\mathrm{d}s\ ,$$

inside $\widehat{\mathcal{W}}$. At the boundary of $\widehat{\mathcal{W}}$, add constraints to contain it.

Gradient flows on graphons

- For the triangle density function $h_\triangle$,

$$h_\triangle(W) = \int_{[0,1]^3} W(x_1, x_2)W(x_2, x_3)W(x_3, x_1)\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3,$$

  its Fréchet-like derivative is

$$(Dh_\triangle)(W)(x, y) = 3\int_0^1 W(x, z)W(z, y)\,\mathrm{d}z\ .$$

- Example of "potential energy". Similarly, one has interaction energy and internal energy.

Example

- For the scalar entropy function

$$E(W) = \int_{[0,1]^2} h(W(x,y))\,\mathrm{d}x\,\mathrm{d}y\ ,\ \ h(p) = p\log(p) + (1-p)\log(1-p),$$

  if $0 < W < 1$, its Fréchet-like derivative is

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

- Gradient flow

$$W_t'(x,y) = -(DE)(W_t)(x,y)\ ,$$

  converges to the constant $W \equiv 1/2$.

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 $x, y \in [0,1]$,

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

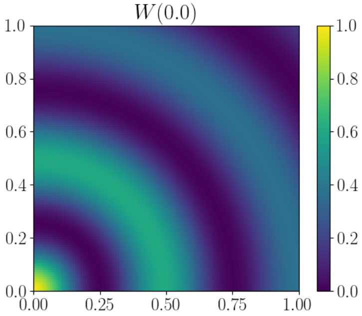


Figure: Gradient flow of $h_\triangle + 10^{-1}E$

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

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

$$W(t) = W_0 - \int_0^t DF(W(s))\,\mathrm{d}s\ .$$

- Note that the function F can be regarded as a function on symmetric matrices $F_n\colon \mathcal{M}_n \to R$. Suppose that F_n has a gradient flow. It is then given by

$$V^{(n)}(t) = V_0^{(n)} - \int_0^t \nabla_n F_n\Big(V^{(n)}(s)\Big)\,\mathrm{d}s\ .$$

Question?

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

Euclidean Gradient and Fréchet-like derivative

Fréchet-like derivative [OPST '21]

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 $F_n \colon \mathcal{M}_n \to \mathbb{R}$.

$\lim_{n\to\infty} n^2 \nabla_n F_n(W) = DF(W)$ as graphons.

Scalings of derivatives

Scaling derivatives for mean

$$F_n\left(\frac{1}{n}\sum_{i=1}^{n}\delta_{x_i}\right) = \frac{1}{n}\sum_{i=1}^{n} x_i$$
$$\nabla F_n = \frac{1}{n}\mathbf{1}$$
$$F(\mu) = \int x \,\mathrm{d}\mu$$
$$\nabla_W F(\mu) \equiv 1$$
$$\lim_{n\to\infty} n\nabla F_n = \nabla_W F(\mu)$$

Scaling derivatives for edge density

$$F_n(A_n) = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} A_n(i,j)$$
$$\nabla F_n = \frac{1}{n^2}\mathbf{1}$$
$$F(W) = \int_{[0,1]^2} W(x,y)\,\mathrm{d}x\,\mathrm{d}y$$
$$DF(W) \equiv 1$$
$$\lim_{n\to\infty} n^2\nabla F_n = DF$$

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 $\mathcal{M}_n$

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

- 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 by 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 $W(t)$, $t \geq 0$.
- Consider the Euclidean gradient flow of $F_n\colon \mathcal{M}_n \to \mathbb{R}$ starting at $V_0^{(n)}$, i.e.,

$$V^{(n)}(t) \coloneqq V_0^{(n)} - \int_0^t \nabla_n F_n\Big(V^{(n)}(s)\Big)\,\mathrm{d}s,$$

  with adjustments at the boundary.
- Set $W^{(n)}(t) = V^{(n)}(n^2 t)$.

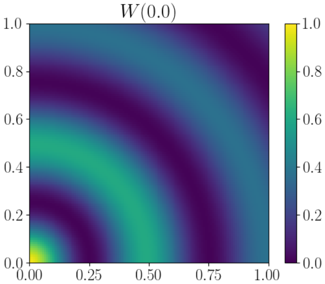
If $W_0^{(n)} \xrightarrow{\delta_\square} W_0$, then

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

uniformly over compact time intervals in $[0, \infty)$.

Simulations

- By Turán's theorem: The n-vertex triangle-free graph with the maximum number of edges is a complete bipartite graph.



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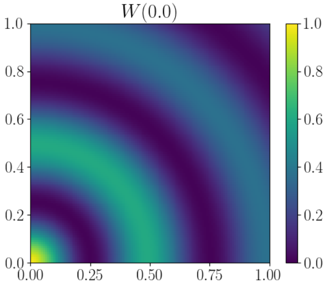

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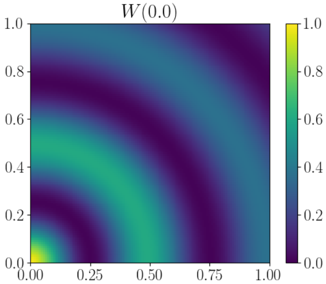

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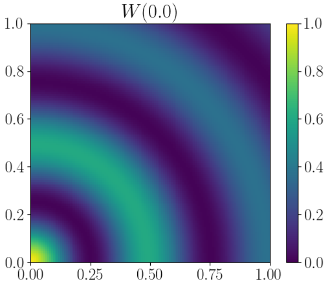

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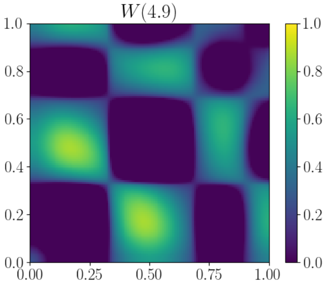

(b) Approximate complete bipartite graphon

Ongoing and Future directions

- Study convergence of stochastic gradient descent with and without added noise.
- Specialize the theory on optimization over multiple layer NNs.
- Limiting curves for other “mean-field interactions” on graphs.

- Optimization on graphs is hard due to discreteness.
- However, gradient flows exist on graphons, their infinite limiting space.
- Analysis is similar to calculus in Wasserstein-2 spaces.
- Approximated by finite dimensional gradient flows on matrices.

Thank you!

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