Scaling limits of SGD over large networks

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August 23, 2022







Neural Networks (NN) and a permutation symmetry

- Minimize Risk function over weights of the NN.

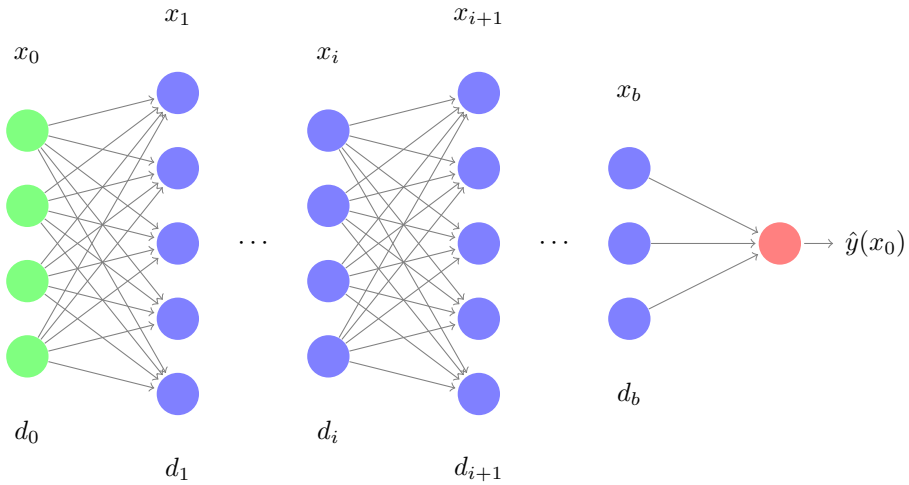

Figure: A feedforward NN as a *computational graph*.

$$x_0 \in \mathbb{R}^{d_0}, \qquad x_i = \sigma(c_i \cdot A_i x_{i-1} + b_i), \quad i \in [b], \qquad \hat{y} = \frac{1}{d_b} \sum_{j=1}^{d_b} x_b(j),$$

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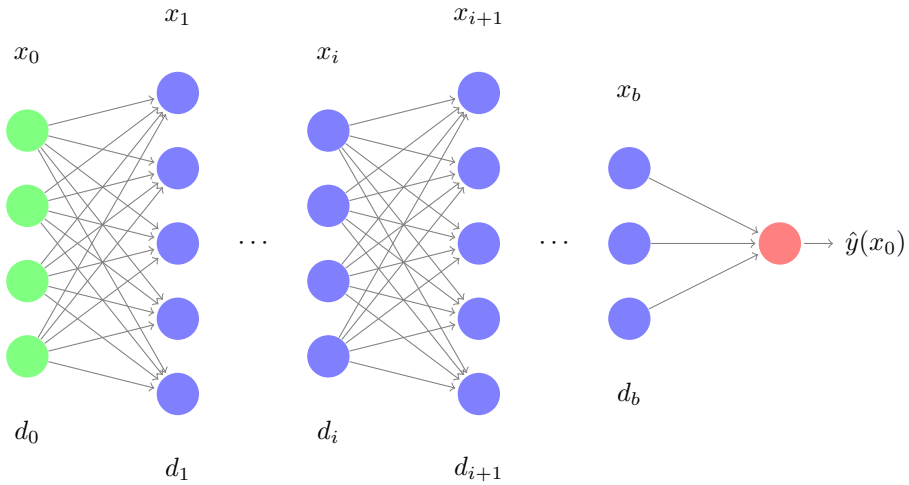

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- There is a **permutation symmetry** within each layer that keeps the output of the NN unchanged.
- This leads us to treat this problem as an **optimization problem over graphs** invariant under a permutation of vertex labels.

Optimization under permutation invariance

As an example consider a simple function $R_n : \mathbb{R}^{n\times n} \to \mathbb{R}$:

$$R_n(A) := \mathrm{Tr}\left[A^3\right]$$

- Matrix A can be thought of as *adjacency matrix* of an edge-weighted graph.
- This is a spectral function (only depends on eigenvalues of A), counts # of $\triangle$s.
- Symmetry: Does not depend on the labeling of vertices.

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Question

How do Euclidean GD and SGD behave when we scale the problem size ($n \to \infty$) under the presence of such a symmetry?

Graphons

- There is already a space of **graphons** that exactly captures this symmetry[1].

[1] Limits of dense graph sequences - Lovász & Szegedy, 2006

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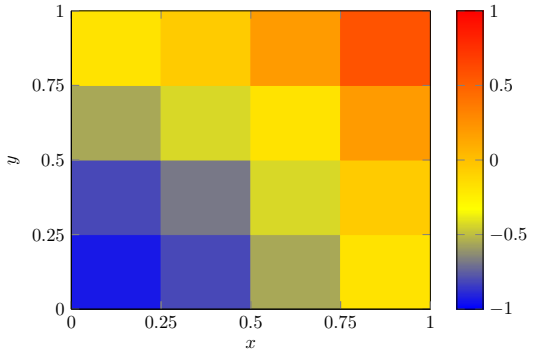
- A matrix can be converted to a *kernel*.

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

Symmetric matrix A



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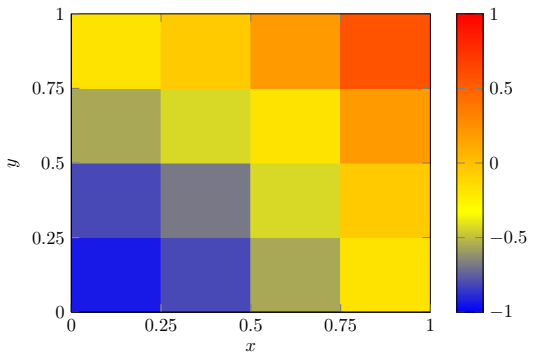

Kernel representation of A

- This allows us to take $n \to \infty$!

Kernels $\mathcal{W}$

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

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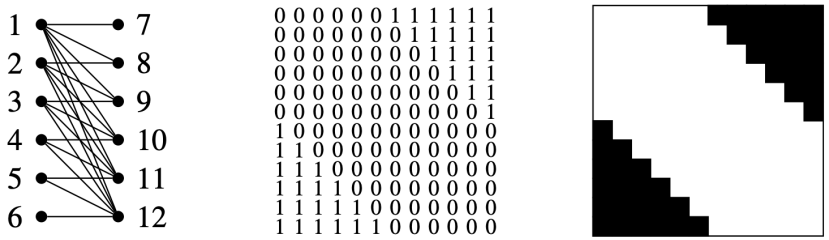
Graphons

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



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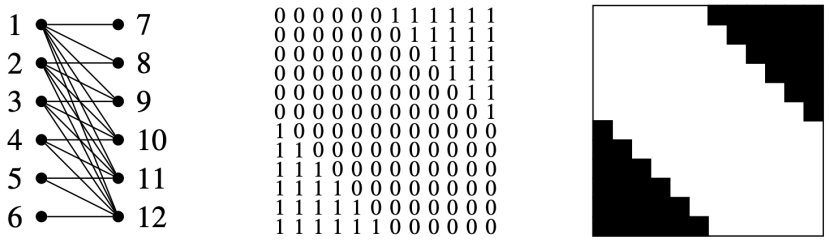

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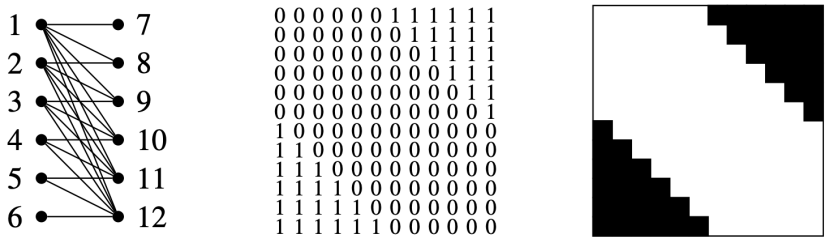

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Graphons $\widehat{\mathcal{W}}$ (Lovász & Szegedy, 2006)

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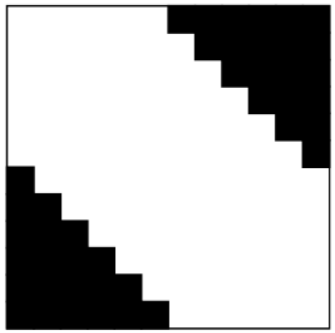
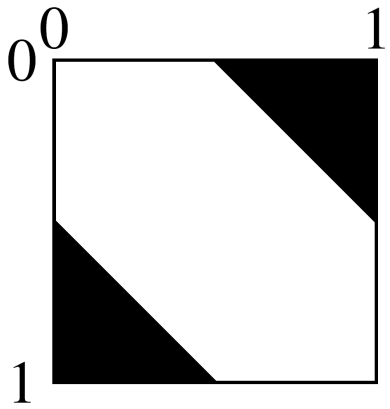
Convergence of Graph(ons) ($n \to \infty$)



(a) Half Graph (Kernel)



(b) Limit of Half Graph ($n \to \infty$)

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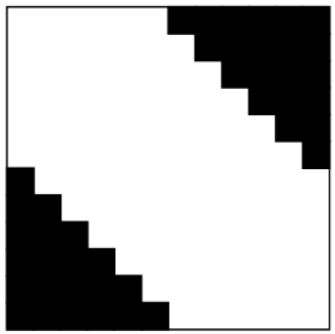

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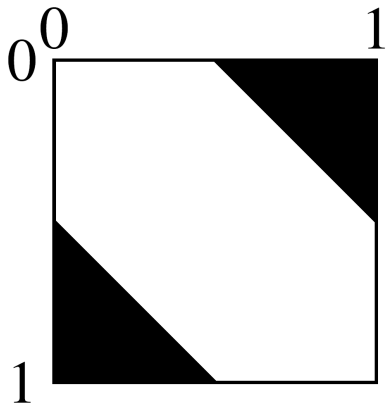

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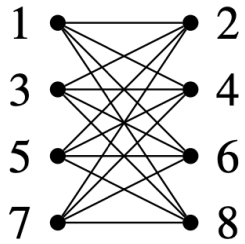

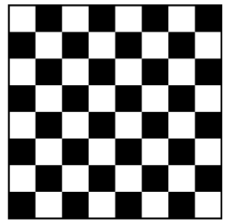

(a) Checkerboard

Q. Where do these graphons converge?

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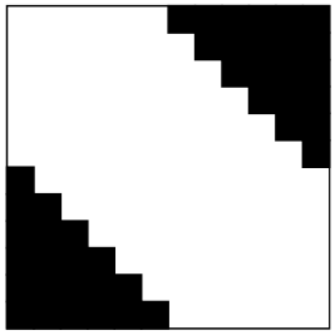

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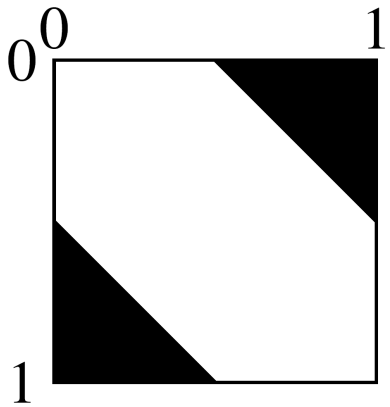

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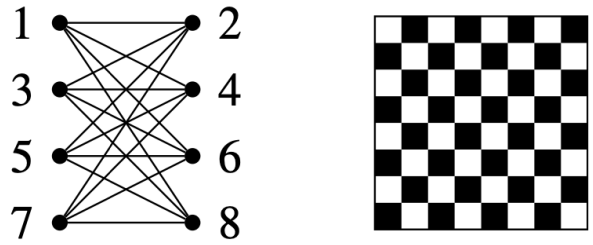

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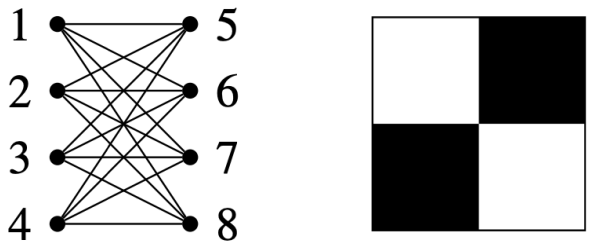

(b) Checkerboard after vertex relabeling

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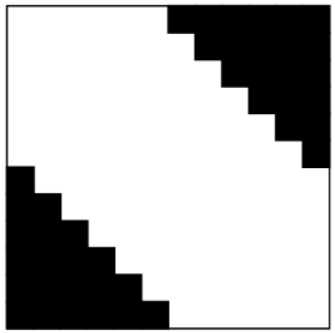

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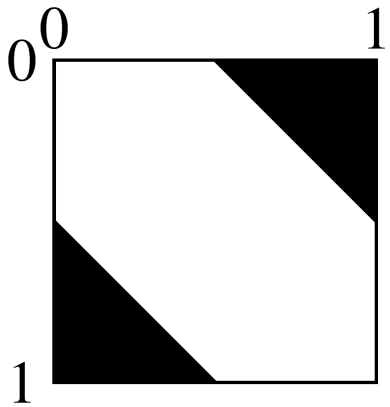

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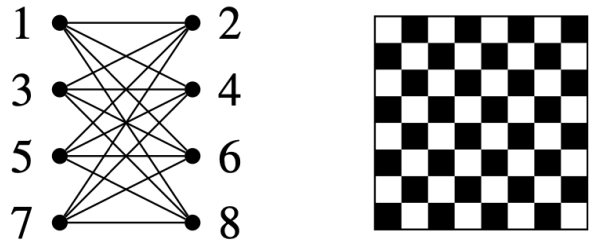

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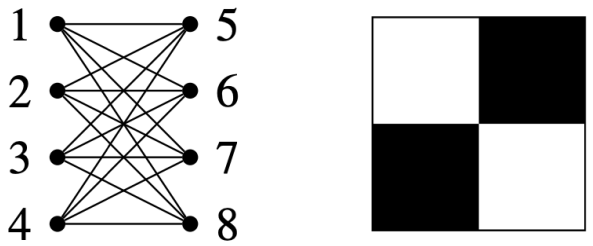

(b) Checkerboard after vertex relabeling

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

Topology and Metric over Graphons

The set of Graphons comes with nice topological and geometrical properties.

- Topology induced by **Cut metric**:[2]
  - Provides a natural topology over graphons that **captures graph convergence**.
  - Provides **compactness** when edge-weights are bounded, say in $[-1, 1]$.

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  - We show that it is a **geodesic** metric.[4]
  - Allows defining geodesic convexity on $(\widehat{\mathcal{W}}, \delta_2)$.
  - Allows a notion of 'gradient' on $(\widehat{\mathcal{W}}, \delta_2)$.
  - Allows construction of 'gradient flows' on $(\widehat{\mathcal{W}}, \delta_2)$.

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Our Results

Algorithms over Euclidean spaces allow us to access this geometry suitably.
Under suitable assumptions, we show that as the step size goes to zero and $n \to \infty$:

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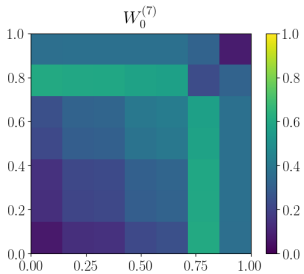
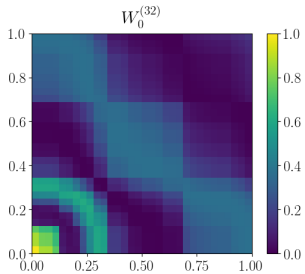
Scaling limits of SGD with added non-trivial noise

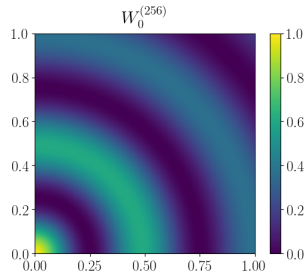
Euclidean SGD with non-trivial added noise converge to curves that are not gradient flows, but can be characterized as fixed points of an iteration scheme.

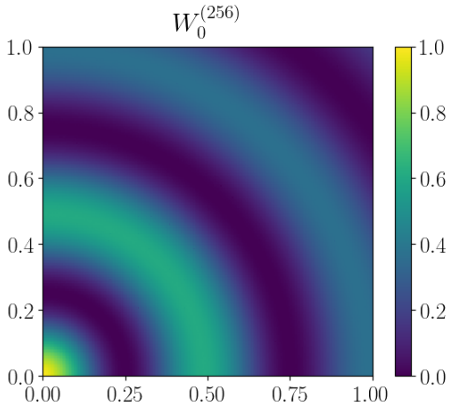
Simulations

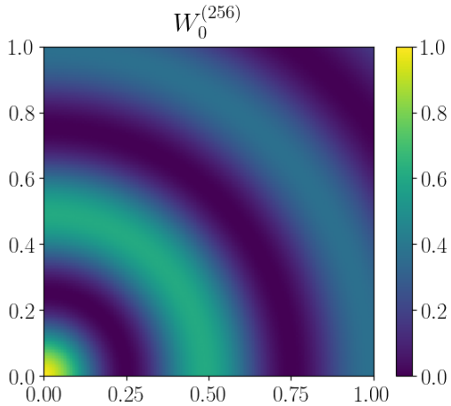
- Turán's theorem: The n-vertex triangle-free graph with the maximum number of edges is a complete bipartite graph.











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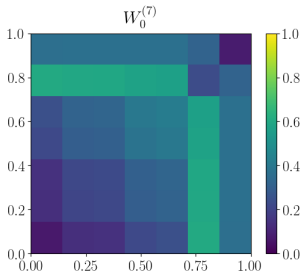

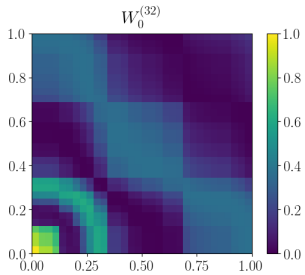

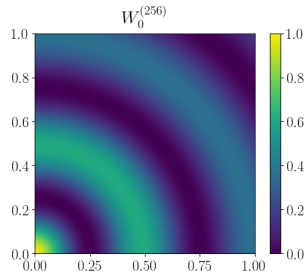

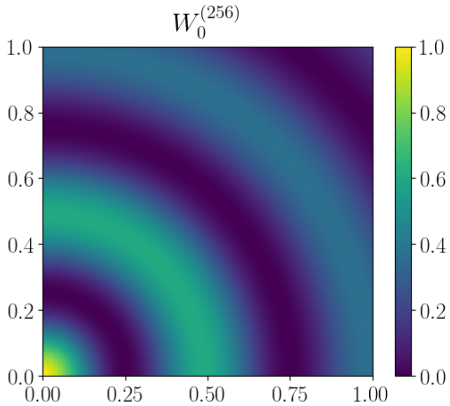

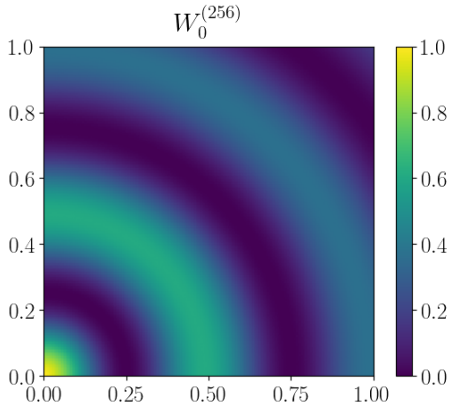

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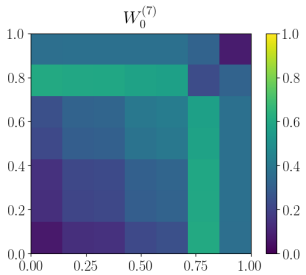
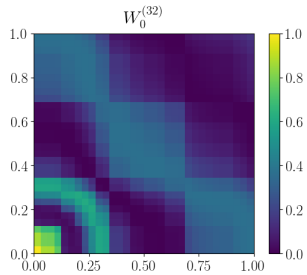
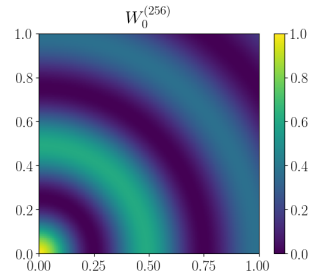


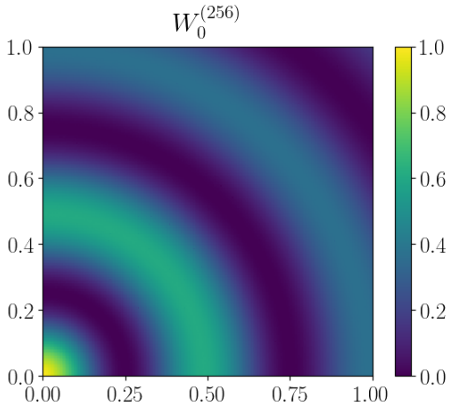
(a) GD ($n = 7$)

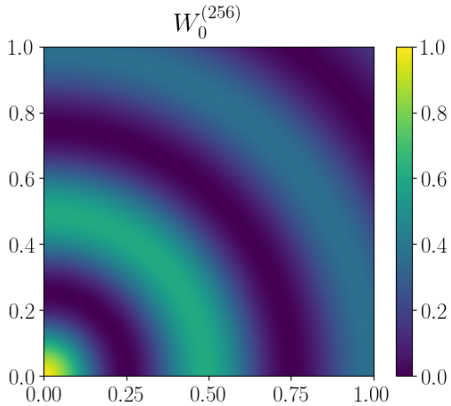


(b) GD ($n = 32$)



(c) GD ($n = 256$)

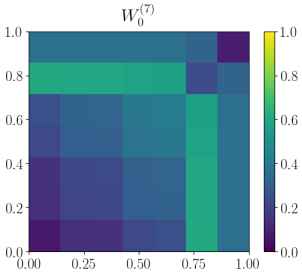




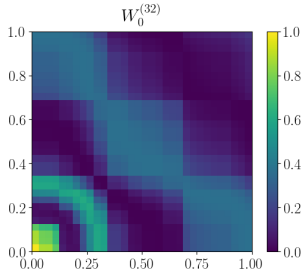
Simulations

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

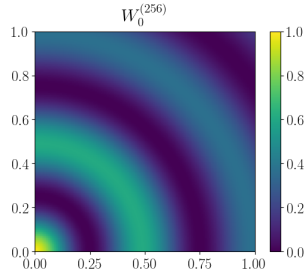
Q. Can we recover this theorem through an optimization problem on graphons?



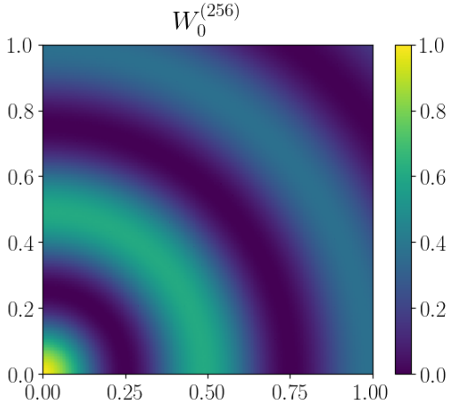
(a) GD ($n = 7$)



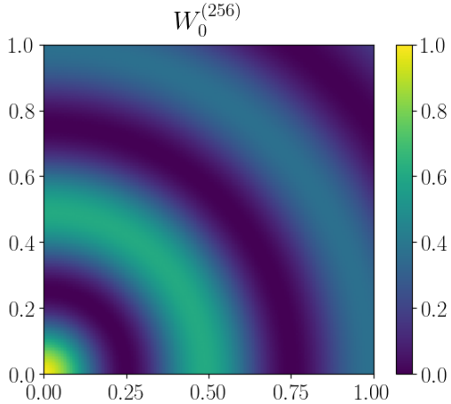
(b) GD ($n = 32$)



(c) GD ($n = 256$)



(a) SGD ($n = 256$)



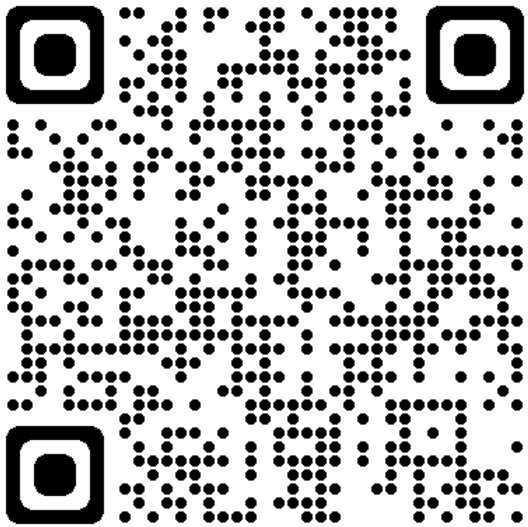
(b) SGD + Brownian noise ($n = 256$)

Future directions

- Extend the geometry to consider symmetry groups in **Deep NNs**.
- What about processes on non-weighted graphs? Sparse graphs? Open.

Thank you!

- ArXiv version[5]: https://arxiv.org/abs/2111.09459



[5] Gradient flows on graphons: existence, convergence, continuity equations - Oh, Pal, Somani, Tripathi, 2021