Graphons for Machine Learning: Theory, Estimation, and Applications

Sevvandi Kandanaarachchi*
CSIRO
Research Way, Clayton
VIC, 3168

Cheng Soon Ong
CSIRO
Clunies Ross Street, Acton
ACT 2601

The Concept

Graphons are graph limits. Traditionally a graphon is defined on a unit square as $W : [0, 1]^2 \to [0, 1]$ with the output denoting the edge probability. They capture the asymptotic structure of a graph in a size-independent form, enabling graphs of different sizes to be studied and compared within a unified framework.

Graphons are increasingly used in machine learning: for GNN transferability across graphs of different sizes, and for neural network pruning, among other applications. Estimating a graphon from observed graph data is itself an active research problem, with newer approaches, such as IGNR and JGS, offering more flexible, learnable alternatives to classical estimators. At the same time, while a rich body of theory has been developed for sparse graphons and related extensions, these models have seen relatively limited adoption within machine learning, despite the prevalence of sparse graphs in real-world applications.

Together, this combination of graphons' growing role in core ML tasks, a rapidly evolving landscape of estimation methods, and the largely untapped potential of sparse graphon models motivates their inclusion in the Education Track. Such a tutorial would cover both state-of-the-art applications and emerging opportunities for leveraging graphons in machine learning.

Leveling and prerequisite knowledge

Basic graph theory, linear algebra and calculus knowledge assumed.

Learning objectives and outcomes

On completion of this mini-course, participants would be able to

1. understand the mathematical foundations of graphons, including homomorphism densities, cut distance/cut norm, convergence and exchangeability,
2. apply graphons as a base generative model to generate graphs and combine graphons to construct richer and more complex network structures,
3. understand the limitations of classical graphons for modelling sparse graphs and gain hands-on experience with sparse graph extensions covering Kallenberg exchangeable graphs, graphon mixtures, and graphettes,
4. evaluate and understand graphon estimation methods including traditional methods such as SAS, and more recent methods such as Implicit Graphon Neural Representation (IGNR) and Joint Graph Sorting estimator,

*Use footnote for providing further information about author (webpage, alternative address)—*not* for acknowledging funding agencies.

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5. understand and describe how graphons are used in machine learning, for example in GNN transferability and neural network pruning.

Linked Papers: Recent papers using graphons in Machine Learning

[1] Huimin Cheng, Yongkai Chen, Ping Ma, and Wenxuan Zhong. Graphon Cross-Validation: Assessing Models on Network Data. In *The Fourteenth International Conference on Learning Representations*, 2026.

[2] Xinyuan Fan, Feiyan Ma, Chenlei Leng, and Weichi Wu. Low-Rank Graphon Learning for Networks. In *The Thirty-ninth Annual Conference on Neural Information Processing Systems*, 2025.

[3] Hoang Pham, The-Anh Ta, Tom Jacobs, Rebekka Burkholz, and Long Tran-Thanh. The Graphon Limit Hypothesis: Understanding Neural Network Pruning via Infinite Width Analysis. In *The Thirty-ninth Annual Conference on Neural Information Processing Systems*, 2025.

[4] Yuyao Wang, Yu-Hung Cheng, Debarghya Mukherjee, and Huimin Cheng. Transfer Learning on Edge Connecting Probability Estimation Under Graphon Model. In *The Thirty-ninth Annual Conference on Neural Information Processing Systems*, 2025.

Teaching materials summary

Teaching materials consist of videos, slides and Jupyter worksheets detailed as follows:

Videos

1. **Introduction to graphons:** This video introduces graphons as a generative model and samples graphs from different graphons. It combines graphons in 3 different ways: convex addition, disjoint union and joining disjoint graphons.
2. **Mathematical properties of graphons:** This video introduces graphons as graph limits and explores convergence from the lens of homomorphism density and the cut metric. Furthermore, it briefly discusses the assumption of exchangeability.
3. **Sparse graph modelling with graphons:** This video explores different sparse extensions of traditional graphons.
4. **Graphon estimation:** This video introduces graphon estimation when a single graph or multiple graphs are observed.
5. **Graphons in machine learning:** This video discusses 2 applications of graphons – GNN transferability and neural network pruning.

Jupyter Worksheets

1 **Introduction to graphons:** This worksheet introduces graphon sampling and combines graphons in 3 different ways: convex addition, disjoint union and joining disjoint graphons.

2-4 **Sparse graph implementations:** These 3 worksheets explore different graphon-related sparse graph generation mechanisms including Kallenberg exchangeable graphs detailed in [5].

5-6. **Graphon estimation:** These 2 worksheets explores graphon estimation using IGNR [7] and JGS [6].

References

[5] F. Caron and E. B. Fox. Sparse graphs using exchangeable random measures. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 79(5):1295–1366, 2017.

[6] R. B. Sogan and T. Rebafka. Low-Complexity and Consistent Graphon Estimation from Multiple Networks. In *International Conference on Artificial Intelligence and Statistics*, 2026.

[7] X. Xia, G. Mishne, and Y. Wang. Implicit Graphon Neural Representation. In *International Conference on Artificial Intelligence and Statistics*, pages 10619–10634. PMLR, 2023.