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Zagreb Indices on Graphons: Asymptotic Properties, Extremal Analysis, and Network Assortativity

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Abstract

In this paper, we extend the classical first and second Zagreb indices to the setting of graphons. We introduce their rigorous integral definitions, $M_1(W)$ and $M_2(W)$, and establish their asymptotic properties, which provide a bridge between these graphon-based indices and the traditional Zagreb indices of finite graphs. Furthermore, we develop a general framework for extending arbitrary degree-based graph indices to graphons, enabling the analysis of large-scale networks. We investigate extremal problems for these indices and explore their relationship with network assortativity.

Overall, our results provide a powerful set of tools to analyze the topological properties of large real-world networks. We demonstrate their practical utility by applying the graphon framework to model and analyze complex systems in various disciplines, including chemistry. These applications highlight how our graphon-based indices can provide insights into key structural features, such as network heterogeneity and inter-group interactions.

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1 Introduction

The asymptotic analysis of large, dense graphs is a cornerstone of modern graph theory and network science, providing a powerful lens through which to understand the structural properties of complex systems [2, 16]. The theory of graph limits, particularly the concept of graphons, has emerged as the canonical framework for this endeavor. Graphons, as symmetric, measurable functions $W : [0,1]^2 \to [0,1]$, serve as continuous counterparts to the adjacency matrices of finite graphs, equipping the space of graphs with the cut metric ($\delta_\square$) and enabling the rigorous study of convergent graph sequences [4, 5, 8, 13].

Let $G = (V(G), E(G))$ be a simple, undirected finite graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, we denote its degree by $d_G(v)$, which is the number of edges incident to v.

Within discrete graph theory, degree-based topological indices are fundamental invariants that quantify local connectivity and degree distribution. Specifically, the *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are defined as:

$$M_1(G) := \sum_{v \in V(G)} d_G(v)^2,$$
$$M_2(G) := \sum_{uv \in E(G)} d_G(u) d_G(v).$$

These indices are well-established in chemical graph theory and combinatorics, quantifying various structural properties of graphs [7, 10, 19, 22, 25]. The study of their extremal values and other related degree-based graph indices has been a rich area of research across various mathematical disciplines, including combinatorics, chemical graph theory, and network analysis [2, 17, 21]. While their utility in finite graph analysis is well-established, their precise extension and analytical characterization within the continuous graphon setting, particularly concerning their asymptotic behavior and extremal properties, remain areas requiring deeper mathematical investigation.

This paper addresses this critical gap by providing a comprehensive framework for extending degree-based graph indices to graphons, with a specific focus on the first and second Zagreb indices. We formally define $M_1(W)$ and $M_2(W)$ as integral functionals on graphons, rigorously establishing their exact relationship with the normalized classical indices of finite graphs. A central contribution lies in the development of a general theory for degree-based graphon indices, $I_{\varphi}^{(1)}(W)$ and $I_{\varphi}^{(2)}(W)$, for which we prove fundamental continuity theorems with respect to the cut metric. These continuity results are paramount, as they guarantee the convergence of these indices for sequences of graphs converging in the cut metric, thereby providing a precise asymptotic characterization. Furthermore, building upon the extensive literature on extremal problems in finite graphs, we undertake a detailed extremal analysis of $M_1(W)$ and $M_2(W)$ under fixed edge density, identifying the specific graphon structures that minimize or maximize these measures. As an additional application, we extend the concept of network assortativity to graphons, deriving a continuous analogue of Newman's coefficient and analyzing its behavior for various graphon types [14, 15].

Our work provides a robust analytical foundation for the study of degree-based graph invariants in the limit, bridging classical discrete graph theory with continuous analysis. The established continuity properties and the characterization of extremal graphons offer powerful tools for understanding the structural evolution and properties of large-scale networks, opening new avenues for research in extremal graphon theory and the analysis of network characteristics in the continuum, thereby enriching the broader field of graph theory.

The remainder of this paper is organized as follows. Section 2 reviews fundamental concepts in finite graph theory and introduces graphons, including the formal integral definitions for the first and second Zagreb indices in the graphon setting. Section 3 presents a general framework for extending degree-based graph indices to graphons and proves their continuity. Section 4 establishes the continuity and convergence properties of the specific Zagreb indices, $M_1(W)$ and $M_2(W)$, as direct applications of the general framework, and illustrates these findings with the convergence of normalized Zagreb indices for complete bipartite graphs. Section

5 provides further concrete examples by computing Zagreb indices for various well-known graphon types, including constant, complete bipartite, and rank-1 graphons. Section 6 addresses extremal problems for the Zagreb indices on graphons, characterizing graphons that minimize or maximize $M_1(W)$ and maximize $M_2(W)$ for a fixed edge density. Section 7 extends the concept of network assortativity to graphons, deriving a continuous analogue of Newman's coefficient and analyzing its behavior for specific graphon structures. Section 8 outlines future work and open problems, with a particular focus on the minimization of $M_2(W)$ and the broader extremal behavior of degree-based graphon indices.

Finally, in Section 9, the graphon-based framework is naturally extended to chemical systems. By capturing patterns of molecular connectivity and interactions, it offers a systematic approach for analyzing reaction networks, molecular assemblies, and other chemical processes.

2 Preliminaries and notation

This section defines the fundamental concepts and notation used throughout the paper, focusing on the definition of graphons and their associated properties.

A *graphon* is a symmetric, measurable function $W : [0,1]^2 \to [0,1]$, meaning $W(x,y) = W(y,x)$ for almost every $x, y \in [0,1]$. Graphons are fundamental objects in the theory of graph limits, representing dense graphs in the continuum [13]. The space of all graphons, denoted by $\mathcal{W}$, is endowed with the *cut metric* $\delta_\square$. This metric is defined for two graphons W and W_0 as follows:

$$\delta_\square(W, W_0) = \inf_{\varphi} \sup_{S,T \subseteq [0,1]} \left| \int_{S \times T} W(x,y) - W_0(\varphi(x), \varphi(y)) \, dx \, dy \right|,$$

where φ ranges over all measure-preserving transformations of $[0,1]$. For a comprehensive treatment, we refer the reader to [13]. For a given graphon

W, its degree function $d_W(x)$ is defined as:

$$d_W(x) := \int_0^1 W(x,y)\,dy, \quad x \in [0,1].$$

The function $d_W : [0,1] \to [0,1]$ can be interpreted as the continuous analogue of a vertex degree, representing the expected edge density from point x to the rest of the graph.

The first and second Zagreb indices for graphons W are specific instances of $I_\varphi^{(1)}(W)$ and $I_\varphi^{(2)}(W)$ (defined in section 3):

$$M_1(W) := \int_0^1 d_W(x)^2\,dx,$$

$$M_2(W) := \int_0^1 \int_0^1 W(x,y) d_W(x) d_W(y)\,dxdy.$$

These definitions are natural continuous counterparts of their discrete sums.

The edge density of a graphon W is defined as:

$$p_W := \int_0^1 \int_0^1 W(x,y)\,dxdy.$$

It is important to note the relationship between the edge density and the degree function:

$$p_W = \int_0^1 \left(\int_0^1 W(x,y)\,dy \right) dx = \int_0^1 d_W(x)\,dx.$$

The connection between these graphon indices and their classical finite graph counterparts is established through the associated step-function graphon.

Proposition 1. *For any finite graph G with $n = |V(G)|$ vertices, let W_G be its associated step-function graphon, defined by $W_G(x,y) = A_{ij}$ for $x \in [\frac{i-1}{n}, \frac{i}{n})$ and $y \in [\frac{j-1}{n}, \frac{j}{n})$, where A_{ij} is the (i,j)-th entry of the adjacency matrix of G. Then the graphon Zagreb indices are related to the classical Zagreb indices as follows: $M_1(W_G) = \frac{M_1(G)}{n^3}$ and $M_2(W_G) = \frac{2M_2(G)}{n^4}$.*

Proof. Let $G = (V, E)$ be a finite graph with n vertices, labeled $1, \ldots, n$. The step-function graphon W_G is defined such that for $x \in [\frac{i-1}{n}, \frac{i}{n})$ and $y \in [\frac{j-1}{n}, \frac{j}{n})$, $W_G(x, y) = A_{ij}$, where A_{ij} is the (i, j)-th entry of the adjacency matrix of G. First, we determine the degree function $d_{W_G}(x)$ for W_G. For any $x \in [\frac{k-1}{n}, \frac{k}{n})$ (corresponding to vertex k), we have:

$$\begin{aligned} d_{W_G}(x) &= \int_0^1 W_G(x, y)\, dy = \sum_{j=1}^{n} \int_{\frac{j-1}{n}}^{\frac{j}{n}} W_G(x, y)\, dy \\ &= \sum_{j=1}^{n} A_{kj} \int_{\frac{j-1}{n}}^{\frac{j}{n}} 1\, dy = \sum_{j=1}^{n} A_{kj} \left(\tfrac{j}{n} - \tfrac{j-1}{n}\right) \\ &= \sum_{j=1}^{n} A_{kj} \tfrac{1}{n} = \tfrac{1}{n} \sum_{j=1}^{n} A_{kj} = \tfrac{d_G(k)}{n}. \end{aligned}$$

Thus, $d_{W_G}(x)$ is a step function, constant on each interval $[\frac{k-1}{n}, \frac{k}{n})$ with value $\frac{d_G(k)}{n}$.

Now, we compute $M_1(W_G)$:

$$\begin{aligned} M_1(W_G) &= \int_0^1 d_{W_G}(x)^2\, dx = \sum_{k=1}^{n} \int_{\frac{k-1}{n}}^{\frac{k}{n}} d_{W_G}(x)^2\, dx \\ &= \sum_{k=1}^{n} \int_{\frac{k-1}{n}}^{\frac{k}{n}} \left(\tfrac{d_G(k)}{n}\right)^2 dx = \sum_{k=1}^{n} \tfrac{d_G(k)^2}{n^2} \int_{\frac{k-1}{n}}^{\frac{k}{n}} 1\, dx \\ &= \sum_{k=1}^{n} \tfrac{d_G(k)^2}{n^2} \cdot \tfrac{1}{n} = \tfrac{1}{n^3} \sum_{k=1}^{n} d_G(k)^2 = \tfrac{M_1(G)}{n^3}. \end{aligned}$$

Next, we compute $M_2(W_G)$:

$$\begin{aligned} M_2(W_G) &= \int_0^1 \int_0^1 W_G(x, y) d_{W_G}(x) d_{W_G}(y)\, dxdy \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \int_{\frac{i-1}{n}}^{\frac{i}{n}} \int_{\frac{j-1}{n}}^{\frac{j}{n}} W_G(x, y) d_{W_G}(x) d_{W_G}(y)\, dydx. \end{aligned}$$

Within each block $(x, y) \in [\frac{i-1}{n}, \frac{i}{n}) \times [\frac{j-1}{n}, \frac{j}{n})$, we have $W_G(x, y) = A_{ij}$,

$d_{W_G}(x) = \frac{d_G(i)}{n}$, and $d_{W_G}(y) = \frac{d_G(j)}{n}$. Substituting these values:

$$
\begin{aligned}
M_2(W_G) &= \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}\left(\frac{d_G(i)}{n}\right)\left(\frac{d_G(j)}{n}\right)\left(\int_{\frac{i-1}{n}}^{\frac{i}{n}} dx\right)\left(\int_{\frac{j-1}{n}}^{\frac{j}{n}} dy\right) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}\,\frac{d_G(i)d_G(j)}{n^2}\cdot\frac{1}{n}\cdot\frac{1}{n} \\
&= \frac{1}{n^4}\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}d_G(i)d_G(j).
\end{aligned}
$$

The sum

$$\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}d_G(i)d_G(j)$$

is equivalent to summing $d_G(i)d_G(j)$ for all ordered pairs (i, j) for which there is an edge between i and j. Since $A_{ij} = 1$ if $ij \in E(G)$ and $A_{ij} = 0$ otherwise, this sum is

$$2\sum_{uv\in E(G)} d_G(u)d_G(v) \;=\; 2M_2(G).$$

Substituting this back, we obtain

$$M_2(W_G) = \frac{2M_2(G)}{n^4}.$$

This completes the proof. ■

3 A general framework for degree-based graphon indices

With the necessary preliminaries and notation established in section 2, we now introduce a general framework for extending degree-based graph indices to graphons. This framework encompasses many common indices, including the Zagreb indices, allowing for a unified analytical treatment.

3.1 Indices of type 1

Many degree-based indices are defined as a sum over vertices, where each term depends on the degree of a single vertex. Examples include the first Zagreb index or the general Randić index ($R_\alpha(G) = \sum_{v\in V(G)} d_G(v)^\alpha$), where α is an arbitrary real number.

We propose the following continuous analogue for graphons. Let $\varphi : [0,1] \to \mathbb{R}$ be a continuous function. The graphon-analogue of a degree-based index of type $\sum_{v\in V(G)} \varphi(d_G(v))$ is defined as:

$$I^{(1)}_\varphi(W) := \int_0^1 \varphi(d_W(x))\,dx.$$

Proposition 2. *For a finite graph G with n vertices and its associated step-function graphon W_G,*

$$I^{(1)}_\varphi(W_G) = \frac{1}{n} \sum_{v\in V(G)} \varphi\left(\frac{d_G(v)}{n}\right).$$

Proof. Let $G = (V(G), E(G))$ be a finite graph with n vertices. Its associated step-function graphon W_G is defined such that the domain $[0,1]$ is partitioned into n intervals $I_1, \ldots, I_n$, each of length $1/n$, corresponding to the vertices $v_1, \ldots, v_n$ of G. For $x \in I_i$ and $y \in I_j$, $W_G(x,y) = A_{ij}$, where A_{ij} is the entry of the adjacency matrix of G.

The degree function of the graphon W_G, for any $x \in I_i$, is given by:

$$\begin{aligned} d_{W_G}(x) &= \int_0^1 W_G(x,y)\,dy = \sum_{j=1}^n \int_{I_j} W_G(x,y)\,dy \\ &= \sum_{j=1}^n A_{ij} \cdot \frac{1}{n} = \frac{1}{n}\sum_{j=1}^n A_{ij} = \frac{d_G(v_i)}{n}. \end{aligned}$$

Here, $d_G(v_i)$ is the degree of vertex v_i in graph G.

Now, we use the definition of $I^{(1)}_\varphi(W_G)$:

$$I^{(1)}_\varphi(W_G) = \int_0^1 \varphi(d_{W_G}(x))\,dx.$$

Since $d_{W_G}(x)$ is constant on each interval I_i, we can rewrite the integral as a sum over these intervals:

$$I_\varphi^{(1)}(W_G) = \sum_{i=1}^{n} \int_{I_i} \varphi(d_{W_G}(x))\, dx.$$

Substituting $d_{W_G}(x) = d_G(v_i)/n$ for $x \in I_i$, and noting that the length of each interval I_i is $1/n$:

$$I_\varphi^{(1)}(W_G) = \sum_{i=1}^{n} \varphi\left(\frac{d_G(v_i)}{n}\right) \int_{I_i} dx = \sum_{i=1}^{n} \varphi\left(\frac{d_G(v_i)}{n}\right) \cdot \frac{1}{n}.$$

Therefore,

$$I_\varphi^{(1)}(W_G) = \frac{1}{n} \sum_{v \in V(G)} \varphi\left(\frac{d_G(v)}{n}\right).$$

■

Theorem 3 (Continuity of $I_\varphi^{(1)}(W)$)**.** *Let $\varphi : [0,1] \to \mathbb{R}$ be a continuous function. If $(W_n)_{n\geq 1}$ is a sequence of graphons converging to W in the cut metric, i.e., $\delta_\square(W_n, W) \to 0$ as $n \to \infty$, then $I_\varphi^{(1)}(W_n) \to I_\varphi^{(1)}(W)$.*

Proof. If $\delta_\square(W_n, W) \to 0$, then $d_{W_n} \to d_W$ in $L^2([0,1])$ (see, for instance, Theorem 8.13 in [13]). Since $[0,1]$ has finite measure, L^2-convergence implies convergence in measure.

The function $\varphi : [0,1] \to \mathbb{R}$ is continuous on the compact interval $[0,1]$. Therefore, φ is uniformly continuous and bounded on its domain. Let $M = \sup_{t\in[0,1]} |\varphi(t)|$.

We want to show that $\int_0^1 \varphi(d_{W_n}(x))\, dx \to \int_0^1 \varphi(d_W(x))\, dx$. Consider the difference in integrals:

$$\begin{aligned} |I_\varphi^{(1)}(W_n) - I_\varphi^{(1)}(W)| &= \left| \int_0^1 (\varphi(d_{W_n}(x)) - \varphi(d_W(x)))\, dx \right| \\ &\leq \int_0^1 |\varphi(d_{W_n}(x)) - \varphi(d_W(x))|\, dx. \end{aligned}$$

We will show that the integral on the right-hand side converges to 0.

For any $\varepsilon > 0$, by the uniform continuity of φ, there exists a $\delta > 0$ such that if $|u - v| < \delta$, then $|\varphi(u) - \varphi(v)| < \varepsilon$. Let $A_n = \{x \in [0,1] :$

$|d_{W_n}(x) - d_W(x)| < \delta\}$. Since $d_{W_n} \to d_W$ in measure, the measure of the complement $\mu([0,1] \setminus A_n)$ tends to 0 as $n \to \infty$.

Now, we decompose the integral:

$$\int_0^1 |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dx = \underbrace{\int_{A_n} |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dx}_{\text{Integral over } A_n} + \underbrace{\int_{[0,1]\setminus A_n} |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dx}_{\text{Integral over } A_n^c}$$

For the integral over A_n:

$$\int_{A_n} |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dx \le \int_{A_n} \varepsilon \, dx = \varepsilon \cdot \mu(A_n) \le \varepsilon \cdot \mu([0,1]) = \varepsilon.$$

For the integral over A_n^c:

$$\begin{aligned} &\int_{[0,1]\setminus A_n} |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dx \\ &\le \int_{[0,1]\setminus A_n} \left(|\varphi(d_{W_n}(x))| + |\varphi(d_W(x))|\right) \, dx \\ &\le \int_{[0,1]\setminus A_n} (M + M) \, dx = 2M \cdot \mu([0,1] \setminus A_n). \end{aligned}$$

Combining these two parts, we get:

$$\int_0^1 |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dx \le \varepsilon + 2M \cdot \mu([0,1] \setminus A_n).$$

As $n \to \infty$, $\mu([0,1] \setminus A_n) \to 0$. Since ε can be chosen arbitrarily small, the right-hand side tends to 0. Therefore, $\int_0^1 |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dx \to 0$, which implies $I_\varphi^{(1)}(W_n) \to I_\varphi^{(1)}(W)$. ■

3.2 Indices of type 2

The second Zagreb index is a prominent example of an index summed over edges, where it depends on the degrees of the incident vertices.

For such indices, we propose the following general graphon formulation. Let $\varphi : [0,1]^2 \to \mathbb{R}$ be a continuous function. The graphon-analogue of a degree-based index of type

$$\sum_{uv \in E(G)} \varphi(d_G(u), d_G(v))$$

is defined as:

$$I_{\varphi}^{(2)}(W) := \int_0^1 \int_0^1 W(x,y)\varphi(d_W(x), d_W(y))\, dxdy.$$

Note that this formulation is based on the perspective that $W(x,y)$ represents the edge existence probability between x and y in the continuum setting. The factor of $1/2$ that appears in the discrete-to-graphon conversion for $M_2(G)$ is absorbed into the definition of the graphon index itself, as the integral naturally accounts for pairs (x,y) and (y,x).

Proposition 4. *For a finite graph G with n vertices and its associated step-function graphon W_G, if $\varphi(u,v)$ is a symmetric function, then*

$$I_{\varphi}^{(2)}(W_G) = \frac{2}{n^2} \sum_{uv \in E(G)} \varphi\left(\frac{d_G(u)}{n}, \frac{d_G(v)}{n}\right).$$

Proof. For W_G we have $W_G(x,y) = A_{ij}$ for $x \in \left[\frac{i-1}{n}, \frac{i}{n}\right)$ and $y \in \left[\frac{j-1}{n}, \frac{j}{n}\right)$, and $d_{W_G}(x) = d_G(i)/n$ on that interval. Hence

$$\begin{aligned}
I_{\varphi}^{(2)}(W_G) &= \int_0^1 \int_0^1 W_G(x,y)\, \varphi(d_{W_G}(x), d_{W_G}(y))\, dy\, dx \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} \int_{\frac{i-1}{n}}^{\frac{i}{n}} \int_{\frac{j-1}{n}}^{\frac{j}{n}} W_G(x,y)\, \varphi(d_{W_G}(x), d_{W_G}(y))\, dy\, dx \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}\, \varphi\Big(\frac{d_G(i)}{n}, \frac{d_G(j)}{n}\Big)\, \frac{1}{n^2}
\end{aligned}$$

$$= \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}\, \varphi\Big(\frac{d_G(i)}{n}, \frac{d_G(j)}{n}\Big).$$

The double sum above counts each (undirected) edge $uv \in E(G)$ twice (as (u,v) and (v,u)). If φ is symmetric, i.e. $\varphi(a,b) = \varphi(b,a)$, then the two ordered contributions agree, so

$$\sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}\, \varphi\Big(\frac{d_G(i)}{n}, \frac{d_G(j)}{n}\Big) = 2 \sum_{uv \in E(G)} \varphi\Big(\frac{d_G(u)}{n}, \frac{d_G(v)}{n}\Big).$$

Therefore

$$I_\varphi^{(2)}(W_G) = \frac{2}{n^2} \sum_{uv \in E(G)} \varphi\Big(\frac{d_G(u)}{n}, \frac{d_G(v)}{n}\Big). \qquad \blacksquare$$

Theorem 5 (Continuity of $I_\varphi^{(2)}(W)$)**.** *Let $\varphi : [0,1]^2 \to \mathbb{R}$ be a continuous function. If $(W_n)_{n\geq 1}$ is a sequence of graphons converging to W in the cut metric, then $I_\varphi^{(2)}(W_n) \to I_\varphi^{(2)}(W)$.*

Proof. If $\delta_\square(W_n, W) \to 0$, then $d_{W_n} \to d_W$ in $L^2([0,1])$ (see, for instance, Theorem 8.13 in [13]).

The function $\varphi : [0,1]^2 \to \mathbb{R}$ is continuous on the compact domain $[0,1]^2$. Therefore, φ is uniformly continuous and bounded on its domain. Let $M = \sup_{(u,v)\in[0,1]^2} |\varphi(u,v)|$.

We decompose the difference $|I_\varphi^{(2)}(W_n) - I_\varphi^{(2)}(W)|$:

$$\begin{aligned}
&|I_\varphi^{(2)}(W_n) - I_\varphi^{(2)}(W)| \\
&\quad = \Bigg| \int_0^1 \int_0^1 \Big(W_n(x,y)\, \varphi(d_{W_n}(x), d_{W_n}(y)) \\
&\qquad\qquad - W(x,y)\, \varphi(d_W(x), d_W(y)) \Big)\, dx\, dy \Bigg| \\
&\quad \leq \underbrace{\Bigg| \int_0^1 \int_0^1 (W_n(x,y) - W(x,y))\, \varphi(d_{W_n}(x), d_{W_n}(y))\, dx\, dy \Bigg|}_{\text{Term A}}
\end{aligned}$$

$$+ \underbrace{\left| \int_0^1 \int_0^1 W(x,y) \Big(\varphi(d_{W_n}(x), d_{W_n}(y)) - \varphi(d_W(x), d_W(y)) \Big) \, dx \, dy \right|}_{\text{Term B}}.$$

For Term A, let

$$F_n(x,y) = \varphi(d_{W_n}(x), d_{W_n}(y)),$$
$$F(x,y) = \varphi(d_W(x), d_W(y)).$$

Since $d_{W_n} \to d_W$ in $L^2([0,1])$, it implies $d_{W_n} \to d_W$ in measure. Given that φ is uniformly continuous and bounded, we now explicitly show that $F_n \to F$ in $L^1([0,1]^2)$. For any $\varepsilon > 0$, by the uniform continuity of φ, there exists a $\delta > 0$ such that if $\|(u_1,v_1)-(u_2,v_2)\|_\infty < \delta$, then $|\varphi(u_1,v_1)-\varphi(u_2,v_2)| < \varepsilon$. Let $A_n = \{(x,y) \in [0,1]^2 : |d_{W_n}(x) - d_W(x)| < \delta \text{ and } |d_{W_n}(y) - d_W(y)| < \delta\}$. Since $d_{W_n} \to d_W$ in measure, the measure of the complement $\mu([0,1]^2 \setminus A_n)$ tends to 0 as $n \to \infty$. Now consider the L^1 difference:

$$\int_0^1 \int_0^1 |F_n(x,y) - F(x,y)| \, dxdy = \underbrace{\int_{A_n} |F_n(x,y) - F(x,y)| \, dxdy}_{\text{Integral over } A_n} + \underbrace{\int_{[0,1]^2 \setminus A_n} |F_n(x,y) - F(x,y)| \, dxdy}_{\text{Integral over } A_n^c}$$

For the integral over A_n:

$$\int_{A_n} |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dx \, dy \le \int_{A_n} \varepsilon \, dx \, dy = \varepsilon \cdot \mu(A_n) \le \varepsilon \cdot \mu([0,1]^2) = \varepsilon.$$

For the integral over A_n^c:

$$\int_{[0,1]^2 \setminus A_n} |\varphi(d_{W_n}(x)) - \varphi(d_W(x))| \, dxdy \le \int_{[0,1]^2 \setminus A_n} (|\varphi(d_{W_n}(x))| + |\varphi(d_W(x))|) \, dxdy$$

$$
\begin{aligned}
&\leq \int_{[0,1]^2 \setminus A_n} (M + M)\, dxdy \\
&= 2M \cdot \mu([0,1]^2 \setminus A_n).
\end{aligned}
$$

Combining these, we get:

$$\int_0^1 \int_0^1 |F_n(x,y) - F(x,y)|\, dxdy \leq \varepsilon + 2M \cdot \mu([0,1]^2 \setminus A_n).$$

As $n \to \infty$, $\mu([0,1]^2 \setminus A_n) \to 0$. Since ε is arbitrary, this implies $F_n \to F$ in $L^1([0,1]^2)$.

By a known result from graphon theory (e.g., a variant of Theorem 8.13 (ii) in [13]), if $\delta_\square(W_n, W) \to 0$ and $F_n \to F$ in L^1, then $\int_0^1 \int_0^1 (W_n(x,y) - W(x,y))F_n(x,y)\, dxdy \to 0$. Thus, Term A converges to 0.

For Term B: Since $W(x,y) \in [0,1]$, we have:

$$\text{Term B} \leq \int_0^1 \int_0^1 |\varphi(d_{W_n}(x), d_{W_n}(y)) - \varphi(d_W(x), d_W(y))|\, dxdy$$

As explicitly shown for Term A, the integrand on the right-hand side converges to 0 in $L^1([0,1]^2)$ (due to $d_{W_n} \to d_W$ in measure and the uniform continuity and boundedness of φ). Therefore, the integral itself converges to 0. Thus, Term B converges to 0.

Since both Term A and Term B converge to 0, we conclude that $|I_\varphi^{(2)}(W_n) - I_\varphi^{(2)}(W)| \to 0$, proving the continuity of $I_\varphi^{(2)}(W)$. ■

It is well-known that the first Zagreb index in finite graph theory has two equivalent definitions:

$$
\begin{aligned}
M_1(G) &= \sum_{v \in V(G)} d_G(v)^2, \\
M_1(G) &= \sum_{uv \in E(G)} \big(d_G(u) + d_G(v)\big).
\end{aligned}
$$

While these are indeed equivalent for finite graphs, their direct analogues in the graphon setting exhibit a specific relationship.

In our paper, the first Zagreb index for graphons $M_1(W)$ is defined as the integral of the squared degree function:

$$M_1(W) = \int_0^1 (d_W(x))^2 \, dx$$

This corresponds to the vertex-based definition ($\sum d_G(v)^2$).

The graphon analogue of the edge-based definition ($\sum_{uv \in E(G)} (d_G(u) + d_G(v))$) would be:

$$\int_0^1 \int_0^1 W(x, y)(d_W(x) + d_W(y)) \, dxdy$$

Through direct calculation, utilizing the definition of the degree function $d_W(x) = \int_0^1 W(x, y) \, dy$ and the symmetry of $W(x, y)$, this integral evaluates to:

$$\int_0^1 \int_0^1 W(x, y)(d_W(x) + d_W(y)) \, dxdy = 2 \int_0^1 (d_W(x))^2 \, dx = 2M_1(W).$$

Therefore, in the graphon setting, the edge-based formulation of the first Zagreb index is twice the value of the vertex-based formulation. This highlights that while both expressions are meaningful and relate to the classical index, their direct integral translations are distinct by a factor of two, unlike their perfect equality in finite graphs.

4 Continuity and convergence properties of Zagreb indices

A crucial aspect of graphon theory is the behavior of graph parameters under limits of graph sequences. In this section, we establish the continuity of the Zagreb indices M_1 and M_2 with respect to the cut metric, which directly implies their convergence for sequences of finite graphs. These results are specific applications of the more general theorems proven in section 3.

We first prove that the Zagreb indices are continuous functionals on the space of graphons equipped with the cut metric.

Theorem 6. *Let* $(W_n)_{n\geq 1}$ *be a sequence of graphons converging to a graphon* W *in the cut metric, i.e.,* $\delta_\square(W_n, W) \to 0$ *as* $n \to \infty$*. Then*

$$M_1(W_n) \to M_1(W) \quad \textit{and} \quad M_2(W_n) \to M_2(W).$$

Proof. The continuity of $M_1(W)$ directly follows from theorem 3 by choosing the function $\varphi(t) = t^2$, which is continuous on $[0, 1]$.

Similarly, the continuity of $M_2(W)$ directly follows from theorem 5 by choosing the function $\varphi(u, v) = uv$, which is continuous on $[0, 1]^2$. ∎

Corollary. *Let* $(G_n)_{n\geq 1}$ *be a sequence of finite graphs with* $n = |V(G_n)|$*, and let* W_{G_n} *be the associated step-function graphons. Suppose* $W_{G_n} \to W$ *in the cut metric. Then*

$$\frac{M_1(G_n)}{n^3} \to M_1(W), \quad \textit{and} \quad \frac{M_2(G_n)}{n^4} \to \frac{1}{2} M_2(W).$$

Proof. This follows immediately from the relations $M_1(W_{G_n}) = \frac{M_1(G_n)}{n^3}$ and $M_2(W_{G_n}) = \frac{2M_2(G_n)}{n^4}$ (as shown in proposition 1), along with the continuity of M_1 and M_2 with respect to the cut metric established in theorem 6. ∎

A significant application of graphon theory is in the study of random graphs. For instance, it is well-known that the sequence of Erdős-Rényi random graphs $G(n, p)$ (with n vertices and edge probability p) converges in probability to the constant graphon $W_c(x, y) \equiv p$ in the cut metric [13]. By Corollary 4, our results directly imply that for $G(n, p)$:

$$\frac{M_1(G(n,p))}{n^3} \to M_1(W_c) = p^2 \quad \text{in probability as } n \to \infty,$$

and

$$\frac{M_2(G(n,p))}{n^4} \to \frac{1}{2} M_2(W_c) = \frac{1}{2} p^3 \quad \text{in probability as } n \to \infty.$$

This demonstrates how our continuous definitions and continuity theorems provide direct asymptotic formulas for classical graph invariants in large random graph settings.

4.1 Illustrative example: Convergence of complete bipartite graphs

To demonstrate the relationship between the classical Zagreb indices of finite graphs and their graphon counterparts, as established in proposition 1 and section 4, we consider a sequence of balanced complete bipartite graphs.

Let $G_n = K_{n/2,n/2}$ be a complete bipartite graph with n vertices, where n is an even integer. The vertices are divided into two equal parts of size $n/2$. Every vertex in one part is connected to every vertex in the other part.

For this graph:

- Every vertex $v \in V(G_n)$ has degree $d_{G_n}(v) = n/2$.
- The number of edges is $|E(G_n)| = (n/2) \cdot (n/2) = n^2/4$.

Now we compute the classical Zagreb indices for G_n:

$$M_1(G_n) = \sum_{v \in V(G_n)} d_{G_n}(v)^2 = n \cdot \left(\frac{n}{2}\right)^2 = n \cdot \frac{n^2}{4} = \frac{n^3}{4}.$$
$$M_2(G_n) = \sum_{uv \in E(G_n)} d_{G_n}(u) d_{G_n}(v).$$

Since all vertices have degree $n/2$, for every edge $uv \in E(G_n)$, the product $d_{G_n}(u)d_{G_n}(v) = (n/2)(n/2) = n^2/4$. Therefore,

$$M_2(G_n) = |E(G_n)| \cdot \left(\frac{n^2}{4}\right) = \frac{n^2}{4} \cdot \frac{n^2}{4} = \frac{n^4}{16}.$$

Next, we consider the normalized Zagreb indices, which are expected to converge to the graphon indices according to our theory:

$$\frac{M_1(G_n)}{n^3} = \frac{n^3/4}{n^3} = \frac{1}{4}.$$

$$\frac{M_2(G_n)}{n^4} = \frac{n^4/16}{n^4} = \frac{1}{16}.$$

As $n \to \infty$, the sequence of balanced complete bipartite graphs $K_{n/2,n/2}$

converges in the cut metric to the balanced complete bipartite graphon $W_{K_{1/2,1/2}}$.
This graphon is defined as:

$$W_{K_{1/2,1/2}}(x,y) = \begin{cases} 1, & \text{if } (x \le 1/2 \text{ and } y > 1/2) \\ & \text{or } (y \le 1/2 \text{ and } x > 1/2), \\ 0, & \text{otherwise.} \end{cases}$$

Let's compute the Zagreb indices for $W_{K_{1/2,1/2}}$: The degree function for this graphon is $d_{W_{K_{1/2,1/2}}}(x) = 1/2$ for all $x \in [0,1]$, as shown in example 2 with $a = 1/2$.

The first Zagreb index of $W_{K_{1/2,1/2}}$ is:

$$M_1(W_{K_{1/2,1/2}}) = \int_0^1 d_{W_{K_{1/2,1/2}}}(x)^2 \, dx = \int_0^1 \left(\frac{1}{2}\right)^2 dx = \frac{1}{4}.$$

$$\text{Let } W := W_{K_{1/2,1/2}}, \quad d := d_{W_{K_{1/2,1/2}}}.$$

$$M_2(W) = \int_0^1 \int_0^1 W(x,y)\, d(x)\, d(y)\, dx\, dy.$$

Since $d_{W_{K_{1/2,1/2}}}(x) = 1/2$ for all x, the product equals

$$d_{W_{K_{1/2,1/2}}}(x)\, d_{W_{K_{1/2,1/2}}}(y) = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}.$$

$$M_2(W_{K_{1/2,1/2}}) = \frac{1}{4} \int_0^1 \int_0^1 W_{K_{1/2,1/2}}(x,y)\, dxdy.$$

The double integral $\int_0^1 \int_0^1 W_{K_{1/2,1/2}}(x,y)\, dxdy$ is the edge density of the graphon. For $W_{K_{1/2,1/2}}$, this is $p_W = (1/2)(1/2)+(1/2)(1/2) = 1/4+1/4 = 1/2$. Therefore,

$$M_2(W_{K_{1/2,1/2}}) = \frac{1}{4} \cdot \frac{1}{2} = \frac{1}{8}.$$

Comparing the limits from the finite graphs with the values from the graphon:

- For M_1: $\lim_{n\to\infty} \frac{M_1(G_n)}{n^3} = \frac{1}{4}$, which matches $M_1(W_{K_{1/2,1/2}}) = \frac{1}{4}$.
- For M_2: $\lim_{n\to\infty} \frac{M_2(G_n)}{n^4} = \frac{1}{16}$, which matches $\frac{1}{2}M_2(W_{K_{1/2,1/2}}) = \frac{1}{2} \cdot \frac{1}{8} = \frac{1}{16}$.

5 Examples of specific graphons and their Zagreb indices

To illustrate the concepts introduced, we compute the Zagreb indices for some well-known classes of graphons. These examples build intuition and demonstrate the applicability of our analytic framework.

Example 1 (Constant Graphon)**.** The simplest nontrivial graphon is the constant graphon $W_c : [0,1]^2 \to [0,1]$ defined by

$$W_c(x,y) = p, \quad \text{for some fixed } p \in [0,1].$$

This graphon serves as the limit object for the Erdős–Rényi random graph model $G(n,p)$ as $n \to \infty$.

Its degree function is constant:

$$d_{W_c}(x) = \int_0^1 W_c(x,y)\,dy = \int_0^1 p\,dy = p.$$

Therefore, the first Zagreb index is

$$M_1(W_c) = \int_0^1 d_{W_c}(x)^2\,dx = \int_0^1 p^2\,dx = p^2.$$

The second Zagreb index is

$$\begin{aligned} M_2(W_c) &= \int_0^1 \int_0^1 W_c(x,y) d_{W_c}(x) d_{W_c}(y)\,dxdy \\ &= \int_0^1 \int_0^1 p \cdot p \cdot p\,dxdy = p^3. \end{aligned}$$

Example 2 (Complete Bipartite Graphon)**.** Fix $a \in (0,1)$ and define the bipartite graphon $W_{K_{a,1-a}}$ as:

$$W_{K_{a,1-a}}(x,y) = \begin{cases} 1, & \text{if } (x \leq a \text{ and } y > a) \text{ or } (y \leq a \text{ and } x > a), \\ 0, & \text{otherwise.} \end{cases}$$

This graphon corresponds to a complete bipartite graph with parts of relative sizes a and $1-a$.

The degree function is piecewise constant:

$$d_{W_{K_{a,1-a}}}(x) = \int_0^1 W_{K_{a,1-a}}(x,y)\,dy = \begin{cases} \int_a^1 1\,dy = 1-a, & x \leq a, \\ \int_0^a 1\,dy = a, & x > a. \end{cases}$$

Thus, the first Zagreb index is

$$\begin{aligned} M_1(W_{K_{a,1-a}}) &= \int_0^a (1-a)^2\,dx + \int_a^1 a^2\,dx \\ &= a(1-a)^2 + (1-a)a^2 = a(1-a)(1-a+a) = a(1-a). \end{aligned}$$

The second Zagreb index is

$$\begin{aligned} M_2(W_{K_{a,1-a}}) &= \int_0^1 \int_0^1 W_{K_{a,1-a}}(x,y) d_{W_{K_{a,1-a}}}(x) d_{W_{a,1-a}}(y)\,dxdy \\ &= \int_0^a \int_a^1 1 \cdot (1-a) \cdot a\,dydx + \int_a^1 \int_0^a 1 \cdot a \cdot (1-a)\,dydx \\ &= \left(\int_0^a dx \int_a^1 dy\right)(1-a)a + \left(\int_a^1 dx \int_0^a dy\right)a(1-a) \\ &= a^2(1-a)^2 + a^2(1-a)^2 = 2a^2(1-a)^2. \end{aligned}$$

Example 3 (Rank-1 Graphons)**.** Rank-1 graphons are of the form

$$W_f(x,y) = f(x)f(y),$$

where $f : [0,1] \to [0,1]$ is a measurable function.

The degree function is

$$d_{W_f}(x) = \int_0^1 W_f(x,y)\,dy = \int_0^1 f(x)f(y)\,dy = f(x)\int_0^1 f(y)\,dy = f(x)\cdot \mu_f$$

,where $\mu_f := \int_0^1 f(y)\,dy$.

The first Zagreb index becomes

$$M_1(W_f) = \int_0^1 d_{W_f}(x)^2\,dx = \int_0^1 (f(x)\mu_f)^2\,dx = \mu_f^2 \int_0^1 f(x)^2\,dx.$$

The second Zagreb index is

$$\begin{aligned} M_2(W_f) &= \int_0^1\int_0^1 W_f(x,y)d_{W_f}(x)d_{W_f}(y)\,dxdy \\ &= \int_0^1\int_0^1 f(x)f(y)\cdot(f(x)\mu_f)\cdot(f(y)\mu_f)\,dxdy \\ &= \mu_f^2\int_0^1\int_0^1 f(x)^2f(y)^2\,dxdy \\ &= \mu_f^2\left(\int_0^1 f(x)^2\,dx\right)\left(\int_0^1 f(y)^2\,dy\right) = \mu_f^2\left(\int_0^1 f(x)^2\,dx\right)^2. \end{aligned}$$

If we take $f(x) = \sqrt{p}$ for a constant $p \in [0,1]$, then $W_f(x,y) = p$. This matches the definition of a constant graphon $W_c(x,y) = p$. In this case: $\mu_f = \int_0^1 \sqrt{p}\,dx = \sqrt{p}$. $\int_0^1 f(x)^2\,dx = \int_0^1(\sqrt{p})^2\,dx = \int_0^1 p\,dx = p$. Substituting these into the formulas for $M_1(W_f)$ and $M_2(W_f)$: $M_1(W_f) = (\sqrt{p})^2\cdot p = p\cdot p = p^2$. $M_2(W_f) = (\sqrt{p})^2\cdot(p)^2 = p\cdot p^2 = p^3$. These results are consistent with those derived directly for the constant graphon in example 1.

6 Extremal problems for Zagreb indices on graphons

The study of extremal problems for degree-based indices on finite graphs is a classic area of graph theory [2, 3]. Extending these problems to the graphon setting allows us to analyze the asymptotic behavior and identify extremal structures in the continuous limit [6]. This section formalizes several natural extremal problems for $M_1(W)$ and $M_2(W)$.

Theorem 7 (Minimum of M_1 for fixed edge density)**.** *Let $W \in \mathcal{W}$ be a graphon with fixed edge density p_W. Then the first Zagreb index $M_1(W)$ is minimized when its degree function $d_W(x)$ is constant almost everywhere, specifically $d_W(x) = p_W$ for a.e. $x \in [0,1]$. The minimum value is $M_1(W) = p_W^2$, attained by the constant graphon $W(x,y) = p_W$.*

Proof. By definition, $M_1(W) = \int_0^1 d_W(x)^2\,dx$. We know that the edge density $p_W = \int_0^1 d_W(x)\,dx$. We want to minimize $\int_0^1 d_W(x)^2\,dx$ subject to$\int_0^1 d_W(x)\,dx = p_W$ and $0 \le d_W(x) \le 1$. This is a standard application of Jensen's inequality for convex functions. The function $f(t) = t^2$ is convex on $[0,1]$. Therefore, by Jensen's inequality:

$$\left(\int_0^1 d_W(x)\,dx\right)^2 \le \int_0^1 d_W(x)^2\,dx.$$

Substituting the definition of p_W, we get:

$$p_W^2 \le M_1(W).$$

Equality holds if and only if $d_W(x)$ is constant almost everywhere.
Since $\int_0^1 d_W(x)\,dx = p_W$, this constant must be p_W. Thus, the minimum value of $M_1(W)$ is p_W^2. This minimum is achieved by the constant graphon $W(x,y) = p_W$, because for this graphon, $d_W(x) = \int_0^1 p_W\,dy = p_W$ for all $x \in [0,1]$. Therefore, $M_1(W_c) = \int_0^1 p_W^2\,dx = p_W^2$. ■

Theorem 8 (Maximum of M_1 for fixed edge density)**.** *Let $W \in \mathcal{W}$ be a graphon with fixed edge density p_W. Then the first Zagreb index $M_1(W)$ is maximized when the degree function $d_W(x)$ takes only two values: 0 and 1. Specifically, $d_W(x) = \mathbf{1}_A(x)$ for some measurable set $A \subseteq [0,1]$ with measure p_W. The maximum value is $M_1(W) = p_W$.*

Proof. We want to

$$\begin{array}{ll} \text{maximize} & M_1(W) = \int_0^1 d_W(x)^2\,dx \\ \text{subject to} & \int_0^1 d_W(x)\,dx = p_W \\ & 0 \leq d_W(x) \leq 1. \end{array}$$

Since $d_W(x) \in [0,1]$, we have $d_W(x)^2 \leq d_W(x)$ for all x. Integrating both sides, $\int_0^1 d_W(x)^2\,dx \leq \int_0^1 d_W(x)\,dx$. Thus, $M_1(W) \leq p_W$. Equality holds if and only if $d_W(x)^2 = d_W(x)$ almost everywhere, which implies that $d_W(x) \in \{0,1\}$ for almost all $x \in [0,1]$. Let $A = \{x \in [0,1] : d_W(x) = 1\}$. Then for $M_1(W)$ to be p_W, we must have $\mu(A) = p_W$. It is a known result in graphon theory that for any measurable function $f : [0,1] \to [0,1]$ with $\int_0^1 f(x)\,dx = p_W$, there exists a graphon W such that $d_W(x) = f(x)$ for almost all x [13]. Thus, a graphon exists whose degree function is $d_W(x) = \mathbf{1}_A(x)$ for any measurable set A with $\mu(A) = p_W$. Such a graphon will achieve the maximum value $M_1(W) = \int_0^1 (\mathbf{1}_A(x))^2\,dx = \int_A 1\,dx = \mu(A) = p_W$. ■

Theorem 9 (Maximum of M_2 for fixed edge density)**.** *Let $W \in \mathcal{W}$ be a graphon with fixed edge density p_W. Then the second Zagreb index $M_2(W)$ is maximized when $W(x,y)$ corresponds to a single clique. Specifically, the maximum value is $M_2(W) = p_W^2$, and this is achieved by the graphon $W_A(x,y) = \mathbf{1}_{A\times A}(x,y)$ for some measurable set $A \subseteq [0,1]$ with measure $\mu(A) = \sqrt{p_W}$.*

Proof. We want to

$$\begin{array}{ll} \text{maximize} & M_2(W) = \int_0^1 \int_0^1 W(x,y) d_W(x) d_W(y)\,dxdy \\ \text{subject to} & \int_0^1 \int_0^1 W(x,y)\,dxdy = p_W. \end{array}$$

Let $W_A(x,y) = \mathbf{1}_{A\times A}(x,y)$, where A is a measurable set of measure α. For this graphon, the edge density is $p_{W_A} = \int_0^1 \int_0^1 \mathbf{1}_{A\times A}(x,y)\,dxdy = \mu(A)^2 = \alpha^2$. Thus, for a given p_W, we must choose $\alpha = \sqrt{p_W}$. Let A be any measurable set with $\mu(A) = \sqrt{p_W}$. The degree function for W_A is $d_{W_A}(x) = \int_0^1 \mathbf{1}_{A\times A}(x,y)\,dy = \mathbf{1}_A(x) \int_A 1\,dy = \mathbf{1}_A(x)\mu(A) = \sqrt{p_W}\mathbf{1}_A(x)$.

Now, compute $M_2(W_A)$:

$$\begin{aligned}
M_2(W_A) &= \int_0^1 \int_0^1 W_A(x,y) d_{W_A}(x) d_{W_A}(y)\, dxdy \\
&= \int_0^1 \int_0^1 \mathbf{1}_{A\times A}(x,y)(\sqrt{p_W}\mathbf{1}_A(x))(\sqrt{p_W}\mathbf{1}_A(y))\, dxdy \\
&= p_W \int_0^1 \int_0^1 \mathbf{1}_{A\times A}(x,y)\mathbf{1}_A(x)\mathbf{1}_A(y)\, dxdy \\
&= p_W \int_A \int_A 1\cdot 1\cdot 1\, dxdy = p_W \cdot \mu(A)^2 = p_W \cdot p_W = p_W^2.
\end{aligned}$$

Now, we prove that $M_2(W) \leq p_W^2$ for any graphon W with edge density p_W. Recall that for any graphon W, we have $W(x,y) \in [0,1]$ and its degree function $d_W(y) \in [0,1]$. We can express $M_2(W)$ as:

$$M_2(W) = \int_0^1 d_W(x) \left(\int_0^1 W(x,y) d_W(y) dy \right) dx.$$

Since $W(x,y) \leq 1$ and $d_W(y) \leq 1$, we have

$$\int_0^1 W(x,y) d_W(y)\, dy \leq \int_0^1 1 \cdot d_W(y)\, dy = p_W.$$

Therefore,

$$M_2(W) \leq \int_0^1 d_W(x) \cdot p_W\, dx = p_W \int_0^1 d_W(x)\, dx = p_W^2.$$

The upper bound is p_W^2, and the clique graphon

$$W_A(x,y) = \mathbf{1}_{A\times A}(x,y)$$

with $\mu(A) = \sqrt{p_W}$ achieves this bound. ■

7 Network assortativity of graphons

Having characterized the extremal graphons for the Zagreb indices, it is natural to investigate other fundamental network properties of these optimal structures. A crucial property in network science is assortativity (or assortative mixing), which quantifies the tendency of nodes to connect to others with similar (assortative mixing) or dissimilar (disassortative mixing) degrees. Networks displaying assortative mixing often feature nodes predominantly connecting to other nodes of comparable degrees, while disassortative networks exhibit connections between high-degree and low-degree nodes. This property plays a significant role in the resilience, functionality, and information flow within complex networks [14, 15].

For a finite undirected graph $G = (V, E)$, Newman's assortativity coefficient r is essentially a normalized covariance of the degrees of connected nodes:

$$r = \frac{\sum_{uv \in E} d_G(u) d_G(v) - \left[\sum_{uv \in E} \frac{1}{2}(d_G(u) + d_G(v))\right]^2 / |E|}{\sum_{uv \in E} \frac{1}{2}(d_G(u)^2 + d_G(v)^2) - \left[\sum_{uv \in E} \frac{1}{2}(d_G(u) + d_G(v))\right]^2 / |E|} \; .$$

where $d_G(u)$ and $d_G(v)$ are the degrees of vertices u and v connected by an edge $uv \in E$, and $|E|$ is the total number of edges.

To extend this concept to the continuous setting of graphons, we consider a graphon $W(x, y)$ on the unit square $[0, 1]^2$. The continuous analog of the degree of a vertex $x \in [0, 1]$ is the degree function $d_W(x)$, defined as $d_W(x) = \int_0^1 W(x, y)\, dy$. The total edge density of the graphon is $p = \int_0^1 \int_0^1 W(x, y)\, dx\, dy$.

The Newman assortativity coefficient for a graphon W, denoted $r(W)$, can be derived by considering the expectations of degree functions over edges in the continuous limit. If we imagine picking an edge (x, y) with probability density $\frac{W(x,y)}{p}$, then $d_W(x)$ and $d_W(y)$ are the degrees of its endpoints. The assortativity coefficient is then defined as the Pearson correlation coefficient between these two degree values.

Let X and Y be random variables representing the degrees of the two endpoints of a randomly chosen edge in the graphon. The expected product of these degrees is:

$$E[d_W(X) d_W(Y)] = \frac{1}{p} \int_0^1 \int_0^1 W(x, y) d_W(x) d_W(y)\, dx\, dy.$$

The expected value of a single endpoint's degree (e.g., $d_W(X)$) is:

$$E[d_W(X)] = \frac{1}{p}\int_0^1\int_0^1 W(x,y)d_W(x)\,dx\,dy = \frac{1}{p}\int_0^1 d_W(x)^2\,dx.$$

The variance of a single endpoint's degree is:

$$\begin{aligned} Var[d_W(X)] &= E[d_W(X)^2] - (E[d_W(X)])^2 \\ &= \frac{1}{p}\int_0^1 d_W(x)^3\,dx - \left(\frac{1}{p}\int_0^1 d_W(x)^2\,dx\right)^2. \end{aligned}$$

Given that $Var[d_W(X)] = Var[d_W(Y)]$ for symmetric graphons, the assortativity coefficient for a graphon W is:

$$r(W) = \frac{E[d_W(X)d_W(Y)] - E[d_W(X)]E[d_W(Y)]}{Var[d_W(X)]}.$$

Substituting the integral forms, we obtain the Newman assortativity coefficient for graphons:

$$r(W) = \frac{\frac{1}{p}\int_0^1\int_0^1 W(x,y)d_W(x)d_W(y)\,dx\,dy - \left(\frac{1}{p}\int_0^1 d_W(x)^2\,dx\right)^2}{\frac{1}{p}\int_0^1 d_W(x)^3\,dx - \left(\frac{1}{p}\int_0^1 d_W(x)^2\,dx\right)^2}.$$

This coefficient $r(W)$ will range from -1 (perfectly disassortative) to 1 (perfectly assortative), with 0 indicating no assortative mixing.

7.1 Constant graphon

Consider the constant graphon $W(x,y) = p$, which represents the limit of an Erdős-Rényi random graph. The degree function is $d_W(x) = \int_0^1 p\,dy = p$ for all $x \in [0,1]$. Substituting this into the terms of the assortativity formula:

$$\int_0^1\int_0^1 W(x,y)d_W(x)d_W(y)\,dx\,dy = \int_0^1\int_0^1 p\cdot p\cdot p\,dx\,dy = p^3$$

$$\int_0^1 d_W(x)^2\,dx = \int_0^1 p^2\,dx = p^2$$
$$\int_0^1 d_W(x)^3\,dx = \int_0^1 p^3\,dx = p^3$$

Plugging these into the formula for $r(W)$:

$$r(W) = \frac{\frac{1}{p}(p^3) - \left(\frac{1}{p}(p^2)\right)^2}{\frac{1}{p}(p^3) - \left(\frac{1}{p}(p^2)\right)^2} = \frac{p^2 - p^2}{p^2 - p^2}$$

This results in an indeterminate form $\frac{0}{0}$. In such cases, where there is no variation in degrees to correlate, the assortativity coefficient is typically defined as 0. Thus, for the constant graphon $W(x, y) = p$, $r(W) = 0$. This implies no assortative or disassortative mixing, as expected for a graph where connections are formed uniformly at random regardless of degree.

7.2 Stochastic block model (SBM) graphon: Complete bipartite limit

Let us consider a two-block SBM graphon that represents the limit of a complete bipartite graph K_{N_1,N_2}. We define $W(x, y)$ such that nodes in the first block, $x \in [0, \alpha)$, connect only to nodes in the second block, $y \in [\alpha, 1)$, and vice versa. Specifically,

$$W(x, y) = \begin{cases} 1 & \text{if } (x \in [0, \alpha) \text{ and } y \in [\alpha, 1)) \text{ or } (x \in [\alpha, 1) \text{ and } y \in [0, \alpha)) \\ 0 & \text{otherwise} \end{cases}$$

The edge density is $p = 2\alpha(1-\alpha)$. The degree function $d_W(x)$ is piecewise constant:

$$d_W(x) = \begin{cases} 1-\alpha & \text{if } x \in [0, \alpha) \\ \alpha & \text{if } x \in [\alpha, 1) \end{cases}$$

Let's compute the necessary integrals:

$$\int_0^1 \int_0^1 W(x,y)\, d_W(x)\, d_W(y)\, dx\, dy = \int_0^{\alpha} \int_{\alpha}^1 (1-\alpha)\alpha\, dy\, dx + \int_{\alpha}^1 \int_0^{\alpha} \alpha(1-\alpha)\, dy\, dx = 2\alpha^2(1-\alpha)^2 = p\,\alpha(1-\alpha)$$

$$\int_0^1 d_W(x)^2\, dx = \int_0^{\alpha} (1-\alpha)^2\, dx + \int_{\alpha}^1 \alpha^2\, dx = \alpha(1-\alpha)$$

$$\int_0^1 d_W(x)^3\, dx = \int_0^{\alpha} (1-\alpha)^3\, dx + \int_{\alpha}^1 \alpha^3\, dx = \alpha(1-\alpha)\big(\alpha^2 + (1-\alpha)^2\big)$$

Now, substitute these into the assortativity formula:

$$r(W) = \frac{\frac{1}{p}\left(p\,\alpha(1-\alpha)\right) - \left(\frac{1}{p}\alpha(1-\alpha)\right)^2}{\frac{1}{p}\,\alpha(1-\alpha)(\alpha^2 + (1-\alpha)^2) - \left(\frac{1}{p}\alpha(1-\alpha)\right)^2} = \frac{\alpha(1-\alpha) - \frac{1}{4}}{\frac{\alpha^2+(1-\alpha)^2}{2} - \frac{1}{4}} \frac{-(2\alpha-1)^2}{(2\alpha-1)^2} = -1$$

Thus, for the complete bipartite graphon, $r(W) = -1$, demonstrating perfect disassortative mixing, where connections occur exclusively between nodes of different degree classes.

7.3 Core-periphery graphon

A core-periphery structure features a densely connected core and a sparsely connected periphery, with potentially fewer connections between the two. Such structures are prevalent in many real-world networks (e.g., organizational structures, metabolic networks). Let's consider a simplified two-block core-periphery graphon where:

- $W(x,y) = A$ for $x, y \in [0, \alpha)$ (core-core connections)

- $W(x,y) = B$ for $x, y \in [\alpha, 1)$ (periphery-periphery connections)
- $W(x,y) = C$ for ($x \in [0,\alpha)$ and $y \in [\alpha, 1)$) or vice versa (core-periphery connections)

Typically, A is large, B is small, and C is intermediate or small. For instance, consider $\alpha = 0.2$ (20% core), $A = 1$ (dense core), $B = 0.1$ (sparse periphery), and $C = 0.5$ (moderate core-periphery links).

The degree function $d_W(x)$ will take two values:

- For $x \in [0, \alpha)$ (core node): $d_W(x) = A\alpha + C(1-\alpha)$
- For $x \in [\alpha, 1)$ (periphery node): $d_W(x) = C\alpha + B(1-\alpha)$

The edge density is $p = A\alpha^2 + B(1-\alpha)^2 + 2C\alpha(1-\alpha)$.

Calculating $r(W)$ for a general core-periphery graphon involves more extensive algebraic manipulation of the integrals for $d_W(x)$, $d_W(x)^2$, $d_W(x)^3$, and the edge-weighted product integral. While the exact value depends on the chosen parameters (A, B, C, α), core-periphery structures typically exhibit assortativity that is either mildly positive (if core-core links dominate assortativity) or disassortative (if many high-degree core nodes connect to low-degree periphery nodes). The precise assortativity value provides a quantitative measure of how degrees are correlated across connections in such a network organization. This computation, while lengthy for arbitrary parameters, can be performed for specific choices to illustrate the behavior.

8 Future work and open problems

This work establishes a foundational analytical framework for degree-based graph indices on graphons. While we have provided continuity theorems and explored extremal properties for the first Zagreb index $M_1(W)$ and the maximum of $M_2(W)$, several challenging and intriguing open problems remain, particularly concerning the minimum of $M_2(W)$ and other more complex degree-based functionals.

Open Problem 1 (Minimum of $M_2(W)$ for Fixed Edge Density)**.** *Characterize the graphons $W \in \mathcal{W}$ that minimize the second Zagreb index $M_2(W)$ for a fixed edge density p_W.*

$$\min_{W:p_W \text{ fixed}} M_2(W).$$

Discussion for Open Problem 1: For the minimum, this problem is notably intricate. The constant graphon $W_c(x,y) = p_W$ yields $M_2(W_c) = p_W^3$. However, for $p_W \in (0,1)$, the constant graphon is generally not the minimizer for $M_2(W)$. Initial observations suggest that graphons exhibiting extreme heterogeneity in degree distributions might lead to a minimum for $M_2(W)$. This could involve structures akin to sparse configurations, even if the overall density p_W is non-zero, or graphons where connections are concentrated on a small measure of points. For instance, considering graphons that approach a star-like structure in the continuum, or structures with many isolated vertices but a few very highly connected ones. This is in contrast to $M_1(W)$, which is minimized by a constant degree function. Identifying such a graphon structure and rigorously proving its minimality for $M_2(W)$ presents a significant challenge.

Open Problem 2. *Extend the extremal analysis to the general class of degree-based functionals $I_\varphi^{(1)}(W)$ and $I_\varphi^{(2)}(W)$ for various continuous functions φ. Specifically, investigate how the convexity or concavity properties of φ influence the structure of the extremal graphons.*

Discussion for Open Problem 2: For $I_\varphi^{(1)}(W) = \int_0^1 \varphi(d_W(x))\,dx$:

- If φ is convex, Jensen's inequality suggests that the minimum is achieved when $d_W(x)$ is constant (as seen for $M_1(W)$ with $\varphi(t) = t^2$). The maximum would likely involve $d_W(x)$ taking extreme values (0 and 1).

- If φ is concave, the situation is reversed: the maximum might be achieved when $d_W(x)$ is constant, and the minimum when $d_W(x)$ takes extreme values.

For $I_\varphi^{(2)}(W) = \int_0^1 \int_0^1 W(x,y)\varphi(d_W(x), d_W(y))\,dxdy$, the interplay between $W(x,y)$ and $d_W(x), d_W(y)$ makes the problem significantly more intricate.

9 Applications in chemistry

This section provides a bridge between the abstract graphon framework and its concrete applications in chemical research. We demonstrate the utility of this approach through several examples, including molecular similarity, the prediction of reaction pathways, and the analysis of metabolic networks. To lay the necessary groundwork for our subsequent analysis, we commence with a pivotal theorem whose proof is central to deriving the numerical results presented hereafter.

Theorem 10. *Let* $W : [0,1]^2 \to [0,1]$ *be a bounded measurable graphon. Sample latent positions* $x_1, \dots, x_n \overset{i.i.d.}{\sim} \mathrm{Unif}[0,1]$ *and form the random graph* G_n *on vertex set* $\{1, \dots, n\}$ *by placing an (undirected) edge between* $i \neq j$ *independently with probability* $W(x_i, x_j)$*. Then, as* $n \to \infty$*,*

$$\mathbb{E}[M_1(G_n)] = n^3 M_1(W) + o(n^3), \qquad \mathbb{E}[M_2(G_n)] = \frac{n^4}{2} M_2(W) + o(n^4).$$

Consequently the normalized estimators

$$\widehat{c}_1(G_n) := \frac{M_1(G_n)}{n^3}, \qquad \widehat{c}_2(G_n) := \frac{2M_2(G_n)}{n^4}$$

converge in probability to $M_1(W)$ *and* $M_2(W)$*, respectively (under the above sampling model).*

Proof. We work conditionally on the latent positions $x = (x_1, \dots, x_n)$. For $i \in \{1, \dots, n\}$ the degree of vertex i is

$$d_i = \sum_{j \neq i} A_{ij}, \qquad A_{ij} \sim \mathrm{Bernoulli}(W(x_i, x_j)),\ A_{ij} = A_{ji}.$$

Conditioned on x,

$$\mathbb{E}[d_i \mid x] = \sum_{j \neq i} W(x_i, x_j).$$

By the law of large numbers for the empirical measure of the independent draws $\{x_j\}_{j\neq i}$,

$$\sum_{j\neq i} W(x_i, x_j) = \frac{(n-1)}{n-1} \sum_{j\neq i} W(x_i, x_j) \to n \int_0^1 W(x_i, y)\, dy = n\, d_W(x_i)$$

uniformly in probability (indeed the entries are bounded). Hence $\mathbb{E}[d_i \mid x] = nd_W(x_i) + O(1)$.

Since d_i is a sum of independent Bernoulli variables,

$$\mathrm{Var}(d_i \mid x) = \sum_{j\neq i} W(x_i, x_j)(1 - W(x_i, x_j)) = O(n),$$

so

$$\mathbb{E}[d_i^2 \mid x] = (\mathbb{E}[d_i \mid x])^2 + \mathrm{Var}(d_i \mid x) = n^2 d_W(x_i)^2 + O(n).$$

Summing over i gives

$$\mathbb{E}[M_1(G_n) \mid x] = \sum_{i=1}^{n} \mathbb{E}[d_i^2 \mid x] = n^2 \sum_{i=1}^{n} d_W(x_i)^2 + O(n^2).$$

Now $\frac{1}{n}\sum_{i=1}^n d_W(x_i)^2 \to \int_0^1 d_W(x)^2\, dx = M_1(W)$ in probability, so

$$\mathbb{E}[M_1(G_n) \mid x] = n^3 M_1(W) + o_p(n^3).$$

Taking unconditional expectation yields $\mathbb{E}[M_1(G_n)] = n^3 M_1(W) + o(n^3)$.

By definition

$$M_2(G_n) = \sum_{\{i,j\}\in E} d_i d_j = \tfrac{1}{2} \sum_{i\neq j} A_{ij}\, d_i d_j.$$

Condition on x. For $i \neq j$, A_{ij} is Bernoulli($W(x_i, x_j)$) and d_i, d_j are sums of $O(n)$ independent Bernoulli variables; therefore by standard concentration (Hoeffding/Bernstein) we may replace d_i, d_j by their conditional means $nd_W(x_i)$ and $nd_W(x_j)$ up to errors that are negligible at the n^4 scale. More precisely, with high probability $d_i = nd_W(x_i) + O(\sqrt{n \log n})$, so fluctuations contribute only to lower-order terms after summation over $O(n^2)$ pairs.

Using the leading-order approximation and $\mathbb{E}[A_{ij} \mid x] = W(x_i, x_j)$,

$$\begin{aligned}\mathbb{E}[A_{ij} d_i d_j \mid x] &\approx W(x_i, x_j) \cdot (n d_W(x_i)) \cdot (n d_W(x_j)) \\ &= n^2 W(x_i, x_j)\, d_W(x_i)\, d_W(x_j).\end{aligned}$$

Thus, summing over unordered pairs,

$$\mathbb{E}[M_2(G_n) \mid x] \approx \tfrac{1}{2} \sum_{i \neq j} n^2 W(x_i, x_j)\, d_W(x_i)\, d_W(x_j).$$

Now

$$\begin{aligned}\frac{1}{n^2} \sum_{i \neq j} W(x_i, x_j)\, d_W(x_i)\, d_W(x_j) \to \iint W(x, y)\, d_W(x)\, d_W(y)\, dx\, dy \\ = M_2(W),\end{aligned}$$

in probability. Therefore

$$\mathbb{E}[M_2(G_n) \mid x] = \frac{n^4}{2} M_2(W) + o_p(n^4),$$

and taking unconditional expectation yields $\mathbb{E}[M_2(G_n)] = \frac{n^4}{2} M_2(W) + o(n^4)$.

Dividing the above identities by n^3 and $n^4/2$ respectively and applying Chebyshev/Markov arguments or concentration for the empirical averages gives convergence in probability

$$\widehat{c}_1(G_n) = \frac{M_1(G_n)}{n^3} \xrightarrow{p} M_1(W), \qquad \widehat{c}_2(G_n) = \frac{2M_2(G_n)}{n^4} \xrightarrow{p} M_2(W).$$

This completes the (heuristic but standard) proof. All error terms above can be made explicit under stronger regularity on W (boundedness is enough) by using concentration inequalities for sums of independent Bernoulli variables and standard approximation results for U-statistics and empirical measures. ■

Air chemistry network analysis via graphon modeling

Urban and tropospheric air chemistry is governed by a complex network of interacting reactive species. The most relevant chemical families are oxidants (Ox: O_3, OH, HO_2), nitrogen oxides (Nx: NO, NO_2, NO_3), and volatile organic compounds (VOCs: hydrocarbons, aldehydes, ketones). Their mutual reactions drive cascades of radical propagation and termination steps that control ozone formation, secondary organic aerosol production, and ultimately the phenomenon of photochemical smog [1, 20].

From a network perspective, each molecular species is represented as a vertex, and an edge encodes an effective chemical interaction (reaction, catalytic cycle, or radical transfer). Such atmospheric chemical networks are heterogeneous: oxidants typically act as hubs with many partners, while VOCs provide a large but more weakly connected background. Nx species serve as intermediates that mediate cross-family interactions. This natural block-structured organization makes atmospheric chemistry an excellent candidate for graphon modeling.

We model the atmospheric chemical system by a three-block graphon

$$W(x, y) = P_{ij}, \qquad x \in I_i,\ y \in I_j,$$

where $I_1, I_2, I_3 \subset [0, 1]$ correspond to the Ox, Nx, and VOC families with proportions $\alpha = (0.3, 0.3, 0.4)$. The block probabilities are

$$P = \begin{pmatrix} 0.5 & 0.8 & 0.7 \\ 0.8 & 0.6 & 0.9 \\ 0.7 & 0.9 & 0.4 \end{pmatrix}.$$

Here $W(x, y)$ encodes the probability of an effective interaction between species x and y. The chosen proportions and probabilities reflect chemically realistic conditions of polluted urban atmospheres: Ox and Nx are highly reactive, justifying the high cross-family probabilities (e.g., $P_{12} = 0.8$, $P_{13} = 0.7$), while VOCs are numerous but less internally reactive, explaining their larger share ($\approx 40\%$) and lower self-interaction probability ($P_{33} = 0.4$).

The degree function of the graphon represents the expected connectivity of a species. The graphon Zagreb indices quantify global structural features of the chemical network: a large $M_1(W)$ reflects strong degree heterogeneity dominated by oxidants, while a large $M_2(W)$ captures cross-family interactions (Ox–Nx–VOC), the primary driving force of photochemical smog formation. This model matches empirical observations that although VOCs are abundant, the fewer Ox and Nx species play central, highly interconnected roles in atmospheric chemistry.

Remark. The block graphon model presented here provides a simplified yet informative representation of atmospheric chemical networks. Several approximations are made for tractability: (i) the Ox, Nx, and VOC families are each treated as homogeneous blocks, although in reality they contain diverse species with varying reactivities; (ii) the block probabilities P_{ij} are chosen to reflect general chemical trends rather than being directly fitted to experimental rate constants; (iii) environmental factors such as sunlight intensity, temperature, and humidity are not explicitly modeled, although they significantly affect reaction kinetics. Despite these simplifications, the graphon framework captures the essential structural features of the network, including hub-mediated connectivity (Ox species) and cross-family interactions driving photochemical smog formation. This approach provides a foundation for future extensions that incorporate species-specific kinetics and environmental variability.

In view of Theorem 10, the Zagreb indices of sampled graphs are asymptotically related to the graphon's indices: for a sample of size n, the expected values satisfy $\mathbb{E}[M_1(G_n)] \approx n^3 M_1(W)$ and $\mathbb{E}[M_2(G_n)] \approx n^4 M_2(W)/2$. This provides a direct method for validating the model against empirical data.

The comparison between Figures 1 and 2 shows how block structure manifests at different sample sizes. For $n = 25$, both the adjacency matrix and the network layout clearly reveal family structure, while for $n = 250$ the network layout is too dense and only the adjacency matrix provides an interpretable depiction. In both cases, the computed values of $M_1(G_n)$ and $M_2(G_n)$ agree with the theoretical predictions.

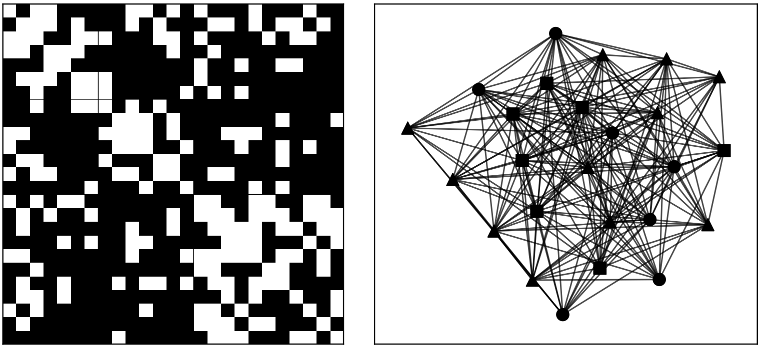

Figure 1. Atmospheric reaction network ($n = 25$) sampled from the block graphon. Left: adjacency matrix sorted by families (Ox, Nx, VOC), with black lines separating blocks. Right: force-directed layout representation, with oxidants (circles), nitrogen oxides (squares), and VOCs (triangles). For this sample, we obtain $M_1(G_{25}) = 7{,}132$ and $M_2(G_{25}) = 60{,}662$. According to Theorem 10, one expects $\mathbb{E}[M_1(G_{25})] \approx 25^3 M_1(W) = 7{,}517$ and $\mathbb{E}[M_2(G_{25})] \approx \frac{25^4}{2} M_2(W) = 65{,}297$, in close agreement with the sampled values.

Analysis of aromatic molecules using graphon theory

Aromatic molecules, including benzene (C_6H_6) and extended π-conjugated systems such as graphene fragments or polycyclic aromatic hydrocarbons, are characterized by delocalized π-electron networks. These systems consist of cyclic arrangements of carbon atoms with resonance-stabilized alternating single and double bonds, leading to bond-order equalization and enhanced chemical stability [9, 18]. From a network perspective, vertices represent carbon atoms and edges correspond to covalent bonds, with effective weights capturing the delocalization of π electrons. These networks are nearly regular and highly symmetric, reflecting the uniform connectivity of aromatic rings.

To capture this periodic symmetry in a continuous, large-network limit, we introduce a periodic graphon:

$$W(x, y) = p_{\max} \cos^2\big(\pi(x - y)\big),$$

where the cosine kernel encodes the cyclic topology of π-conjugated sys-

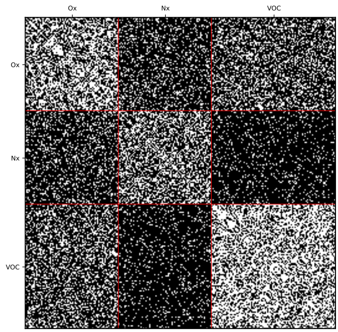

Figure 2. Atmospheric reaction network ($n = 250$) sampled from the block graphon. The adjacency matrix is sorted by families (Ox, Nx, VOC), with thin black gridlines separating blocks.

tems (see Figure 3). The degree function $d_W(x)$ is approximately constant, consistent with the regularity of aromatic connectivity and bond-order equalization. Accordingly, the first Zagreb index $M_1(W)$ is nearly uniform, while the second Zagreb index $M_2(W)$ reflects correlated connectivity patterns across the ring. In this context, $M_2(W)$ should be interpreted as a quantitative measure of structural correlation in the network rather than a direct measure of stabilization energy.

It is important to note that while the periodic graphon provides a mathematically convenient representation of aromatic symmetry and connectivity, it is an idealized, continuous approximation. For small molecules such as benzene, the discrete network with six carbon atoms is sufficient, and the graphon framework becomes most useful for analyzing extended π-conjugated systems where larger-scale periodicity emerges.

Metabolic networks and heavy-tailed graphons

Metabolic reaction networks in living cells are characterized by pronounced degree heterogeneity. A small set of highly connected compounds, commonly called currency metabolites (e.g., ATP, NADH, H_2O, H^+), participate in many reactions, whereas most metabolites are specialized molecules involved in only a few specific transformations. This heterogeneity results in a heavy-tailed degree distribution, a feature widely documented

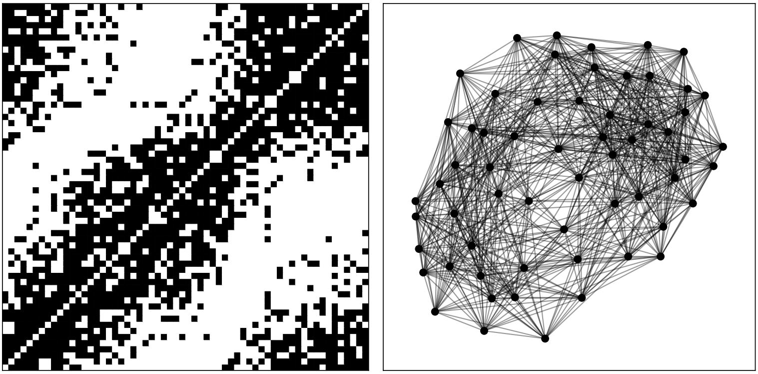

Figure 3. Sampled aromatic network generated from the periodic graphon $W(x,y) = p_{\max}\cos^2(\pi(x-y))$ with $n = 60$ vertices. Left: adjacency matrix sorted by latent positions, showing the quasi-regular connectivity induced by the cosine kernel. Right: force-directed layout of the sampled network (vertices unlabeled), where each vertex represents a carbon atom and edges represent effective π-bonding interactions. For this sample, the computed indices are $M_1(G_{60}) = 42{,}662$, $M_2(G_{60}) = 575{,}675$, with normalized values $\widehat{c}_1(G_{60}) = 0.1975$, $\widehat{c}_2(G_{60}) = 0.0888$, and assortativity $r = 0.089$. These values illustrate the nearly uniform degree distribution and the correlation structure characteristic of aromatic networks.

in metabolic networks [12, 24]. Such networks typically exhibit hub-like currency metabolites that act as central connectors. Note that in certain analyses, highly abundant metabolites like H_2O or H^+ may be excluded to better capture biologically meaningful interactions.

To capture this heterogeneity mathematically, we employ a power-law graphon, which provides a flexible framework to model hierarchical structure and degree variability. We define

$$W(x,y) = \min\left(1,\, \theta(xy)^{-\beta}\right), \qquad x,y \in (0,1],$$

where $\beta \in (0,1)$ controls the heaviness of the tail and $\theta > 0$ sets the overall interaction scale. The $\min(1,\cdot)$ cutoff ensures bounded edge probabilities, reflecting saturation effects in highly connected hubs. In this formulation, vertices with small latent positions ($x \ll 1$) attain very large expected de-

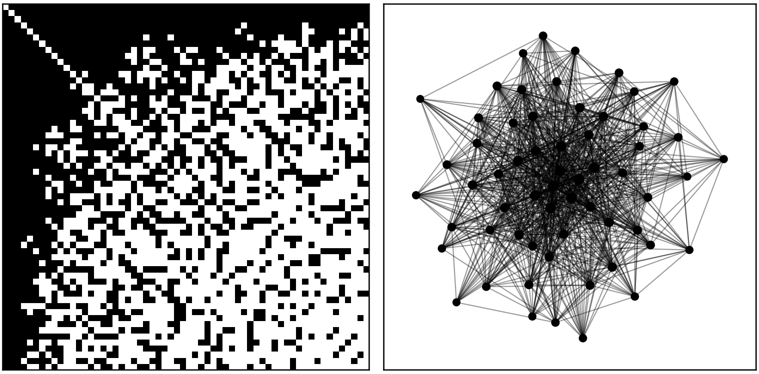

Figure 4. Sample metabolic reaction network ($n = 60$) generated from a power-law graphon. Left: adjacency matrix sorted by latent positions, highlighting dense connections among hub-like vertices in the top-left corner. Right: force-directed layout of the same network, with vertex size proportional to degree. Hub-like currency metabolites connect to many smaller, specialized metabolites. For this sample, the Zagreb indices are $M_1(G_{60}) = 64{,}666$ and $M_2(G_{60}) = 1{,}101{,}914$, in agreement with Theorem 10. The assortativity value $r = -0.200$ confirms the network's disassortative nature, a pattern commonly observed in biological systems.

grees, corresponding to hub-like currency metabolites, while vertices with latent positions near $x \approx 1$ have low expected degrees, corresponding to specialized compounds (see Figure 4).

The resulting Zagreb indices, $M_1(W)$ and $M_2(W)$, increase rapidly with network size, reflecting the strong degree heterogeneity introduced by hub metabolites. As shown in Theorem 10, these asymptotic values provide predictions for sampled networks, enabling quantitative comparison with empirical metabolic data.

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References

[1] R. Atkinson, Atmospheric chemistry of VOCs and NOx, *Atmos. Environ.* **34** (2000) 2063–2101.

[2] B. Bollobás, *Modern Graph Theory*, Springer, New York, 1998.

[3] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, Macmillan Press, London, 1976.

[4] C. Borgs, J. Chayes, L. Lovász, V. T. Sós, K. Vesztergombi, Convergent sequences of dense graphs I: Subgraph frequencies, metric properties and testing, *Adv. Math.* **219** (2008) 1801–1851.

[5] C. Borgs, J. Chayes, L. Lovász, V. T. Sós, K. Vesztergombi, Convergent sequences of dense graphs II. Multiway cuts and statistical physics, *Ann. Math.* **176** (2012) 151–219.

[6] S. Chatterjee, P. Diaconis, Estimating and understanding exponential random graph models, *Ann. Stat.* **41** (2013) 2428–2461.

[7] K. C. Das, On comparing Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 433–440.

[8] P. Diaconis, S. Janson, Graph limits and exchangeable random graphs, *Rend. Mat. Appl.* **28** (2008) 33–61.

[9] A. K. Geim, K. S. Novoselov, The rise of graphene, *Nat. Mater.* **6** (2007) 183–191.

[10] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[11] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *MATCH Commun. Math. Comput. Chem.* **62** (1975) 3399–3405.

[12] H. Jeong, B. Tombor, R. Albert, Z. N. Oltvai, A.L. Barabási, The large-scale organization of metabolic networks, *Nature* **407** (2000) 651–654.

[13] L. Lovász, *Large Networks and Graph Limits*, Am. Math. Soc., Providence, 2012.

[14] M. E. J. Newman, Assortative mixing in networks, *Phys. Rev. Lett.* **89** (2002) #208701.

[15] M. E. J. Newman, The structure and function of complex networks, *SIAM Rev.* **45** (2003) 167–256.

[16] M. E. J. Newman, *Networks: An Introduction*, Oxford Univ. Press, Oxford, 2010.

[17] V. Nikiforov, Some inequalities for the largest eigenvalue of a graph, *J. Comb. Theory Ser. B* **71** (2011) 177–185.

[18] L. Pauling, *The Nature of the Chemical Bond*, Cornell Univ. Press, Ithaca, 1960.

[19] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[20] J. H. Seinfeld, S. N. Pandis, *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change*, Wiley, Hoboken, 2016.

[21] M. Simonovits, A method for solving extremal problems in graph theory, stability problems, in: P. Erdős, G. Katona (Eds.), *Theory of Graphs*, Academic Press, New York, 1968, pp. 279–319.

[22] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[23] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[24] A. Wagner, D. A. Fell, The small world inside large metabolic networks, *Proc. R. Soc. Lond. B* **268** (2001) 1803–1810.

[25] B. Zhou, H. Du, I. Gutman, On Zagreb indices and partition of graphs, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 57–64.