FRACTIONALLY ISOMORPHIC GRAPHS AND GRAPHONS

(EXTENDED ABSTRACT)

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Abstract

Fractional isomorphism is a well-studied relaxation of graph isomorphism with a very rich theory. Grebík and Rocha [Combinatorica 42, pp 365–404 (2022)] developed a concept of fractional isomorphism for graphons and proved that it enjoys an analogous theory. In particular, they proved that if $G_1, G_2, \ldots$ converge to a graphon U, $H_1, H_2, \ldots$ converge to a graphon W and each G_i is fractionally isomorphic to H_i, then U is fractionally isomorphic to W. Answering the main question from *ibid*, we prove the converse of the statement above: If U and W are fractionally isomorphic graphons, then there exist sequences of graphs $G_1, G_2, \ldots$ and $H_1, H_2, \ldots$ which converge to U and W respectively and for which each G_i is fractionally isomorphic to H_i. As an easy but convenient corollary of our methods, we get that every regular graphon can be approximated by regular graphs.

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1   Introduction and the statement of the main result

This work connects the notions of fractional isomorphism for graphs and for graphons. The former was introduced by Tinhofer in 1986 [7], and subsequently several important equivalent characterizations were added by Ramana, Scheinerman, and Ullman [6], by Dvořák [2] and by Dell, Grohe, and Rattan [1]. We recall these characterizations. Of these, (FGI-2) and (FGI-3) play an important role in our contribution to the corresponding theory for graphons. The remaining two are included only to illustrate the mathematical beauty of the theory, which has important applications in designing fast algorithms for fractional isomorphism testing (which is often used as a proxy to isomorphism testing).

Suppose that G and H are two graphs on the same vertex set V.

(FGI-1) *Characterization via bistochastic matrices.* G and H are fractionally isomorphic if and only if there is a bistochastic matrix S such that for the adjacency matrices A_G and A_H of the respective graphs we have $SA_G = A_H S$.

(FGI-2) *Characterization via counting trees.* For two graphs F and J, let $\hom(F, J)$ be the number of homomorphisms of F in J. The graphs G and H are fractionally isomorphic if and only if $\hom(T, G) = \hom(T, H)$ for every tree T.

(FGI-3) *Characterization via equitable partitions.* Let $V(F) = Y_1 \sqcup \ldots \sqcup Y_\ell$ be a partition of the vertex set of a graph F into nonempty sets. We say that $\mathcal{E} = (Y_1, \ldots, Y_\ell)$ is an *equitable partition* if there are numbers $(d_{i,j})_{i,j \in [\ell]}$ such that for every $i, j \in [\ell]$ and every $v \in Y_i$ we have

$$d_{i,j} = \deg_F(v, Y_j) \, . \tag{1}$$

We call the pair $(|Y_i|)_{i \in [\ell]}$ and $(d_{i,j})_{i,j \in [\ell]}$ *the parameters of $\mathcal{E}$.* The graphs G and H are fractionally isomorphic if and only if there are equitable partitions $\mathcal{E}_G$ of G and $\mathcal{E}_H$ of H that have the same parameters.

(FGI-4) *Characterization via iterated degree sequences.* For every vertex $v \in V$ first define $s_{1,G}(v) := \deg_G(v)$ and then inductively define multisets $s_{\ell+1,G}(v) := \{s_{\ell,G}(u) : u \in N_G(v)\}$. The ℓ-*th iteration of the degree sequence of G* is the (multiset) collection $\mathcal{S}_{\ell,G} = \{s_{\ell,G}(v) : v \in V\}$. We can make analogous definitions for H. The graphs G and H are fractionally isomorphic if and only if $\mathcal{S}_{\ell,G} = \mathcal{S}_{\ell,H}$ for every $\ell \in \mathbb{N}$.

Let us now move to graphons. The basic theory of graphons and their role as limits of sequences of dense graphs is by now well-understood. We refer to [5] for the basics and borrow notation from there. Unless stated otherwise, the ground space for graphons is the square of a standard Borel space $(\Omega, \mathcal{B})$ equipped with a Borel probability measure π. Grebík and Rocha [4] developed a theory of fractional isomorphism for graphons. In particular, they showed that all the above characterizations of fractional graph isomorphism have graphon counterparts and are indeed equivalent. To formulate some of these counterparts, one needs to develop nontrivial analytic machinery. Here, we do that only for (FGI-2) and (FGI-3), which we require.
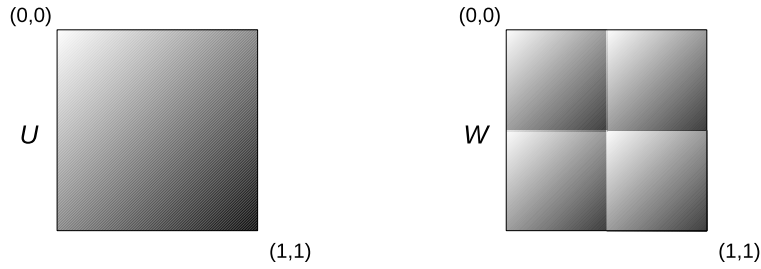
Figure 1: Graphons U and W from (FGI'-3).

(FGI'-2) Two graphons U and W are fractionally isomorphic if and only if $t(T, U) = t(T, W)$ for every tree T. Here, $t(\cdot, \cdot)$ is the usual homomorphism density function.

(FGI'-3) A naive counterpart to (FGI-3) would involve partitions $\Omega = Y_1 \sqcup \ldots \sqcup Y_\ell$ into sets of positive measure. This approach, however, does not work. Consider $\Omega = [0, 1)$ with the Lebesgue measure π and two graphons U and W defined by $U(x, y) = (x + y)/2$ and $W(x, y) = 2((x + y) \mod 0.5)$; see Figure 1. It is easy to check that U and W are fractionally isomorphic in the sense of (FGI'-2). (As a matter of fact, U and W satisfy an even stronger condition called weak isomorphism.) But the requirement from (FGI-3) that all the vertices within one cell have the same degree dictates that the minimum (and only) equitable partition for U be $\{x\}_{x \in [0,1)}$ with uncountably many singleton cells. In W, we can pair up x and $x + \frac{1}{2}$ to get the minimum equitable partition $\left\{x, x + \frac{1}{2}\right\}_{x \in [0, \frac{1}{2})}$. This shows that one has to work with *sigma-algebras* instead of finite partitions into sets of positive measure. Here, we briefly recall the construction, referring to [3, 4] for details. We say that a sigma-algebra[*] $\mathcal{C} \subset \mathcal{B}$ is *U-invariant* if for every $f \in L^2(\Omega, \mathcal{C})$ and for the function $T_U f$ defined by the kernel operator T_U as $(T_U f)(x) = \int_y U(x, y) f(y)$ we have $T_U f \in L^2(\Omega, \mathcal{C})$. With this definition it can be shown that there is a unique minimum U-invariant sigma-algebra, denoted by $\mathcal{C}(U)$. Let us then consider the quotient space $\Omega/\mathcal{C}(U)$, the Borel probability measure $\pi/\mathcal{C}(U)$ on $\Omega/\mathcal{C}(U)$ and a measurable surjection $q_U \colon \Omega \to \Omega/\mathcal{C}(U)$ such that $\pi/\mathcal{C}(U)$ is the pushforward of π via q_U. With these notions, we can naturally transfer the conditional expectation $\mathbb{E}\left(U \mid \mathcal{C}(U) \times \mathcal{C}(U)\right)$ to the domain $(\Omega/\mathcal{C}(U))^2$ by requiring that for the resulting graphon $U/\mathcal{C} : (\Omega/\mathcal{C}(U))^2 \to [0, 1]$ we have $\mathbb{E}\left(U \mid \mathcal{C}(U) \times \mathcal{C}(U)\right)(x, y) = U/\mathcal{C}(q_U(x), q_U(y))$ for all $x, y \in \Omega$. We can repeat the same construction for another graphon W. The graphons U and W are then fractionally isomorphic if there is a measure preserving bijection $b : \Omega/\mathcal{C}(U) \to \Omega/\mathcal{C}(W)$ so that $U/\mathcal{C}(U)(x, y) = (W/\mathcal{C}(W))(b(x), b(y))$ for every $x, y \in \Omega/\mathcal{C}(U)$. To summarize in nontechnical terms, the initial naive approach where the notion of grouping comes from a partition $\Omega = Y_1 \sqcup \ldots \sqcup Y_\ell$ has to be replaced by "grouping" according to sigma-algebra $\mathcal{C}(U)$ and conditional expectation $\mathbb{E}\left(U \mid \mathcal{C}(U) \times \mathcal{C}(U)\right)$ serves as the refined version of the numbers $d_{i,j}$ from (FGI-3).

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[*]an additional technical condition is needed in the actual definition

We can start connecting the notions of fractional isomorphism for graphs and for graphons. The direction "finite graphs⇒graphons" was already observed in [4].

Proposition 1. *Suppose that $G_1, G_2, \ldots$ and $H_1, H_2, \ldots$ are sequences of graphs which converge in cut distance to graphons U and W respectively and for which G_i and H_i are fractionally isomorphic for each $i \in \mathbb{N}$. Then U and W are fractionally isomorphic.*

Since the proof in [4] is not very explicit ('follows from the fact that fractional isomorphism of graphons is an equivalence relation closed in the cut distance'), we give further details here.

Proof. Let T be an arbitrary tree on, say, k vertices. By (FGI-2) we have $\hom(T, G_i) = \hom(T, H_i)$ for each $i \in \mathbb{N}$. Since G_i and H_i are of the same order, we have equality of homomorphism densities, that is, $\frac{\hom(T,G_i)}{v(G_i)^k} = \frac{\hom(T,H_i)}{v(H_i)^k}$. Convergence in the cut distance implies convergence of all homomorphism densities, so in particular we have

$$t(T, U) = \lim_{i \to \infty} \frac{\hom(T, G_i)}{v(G_i)^k} = \lim_{i \to \infty} \frac{\hom(T, H_i)}{v(H_i)^k} = t(T, W) \ .$$

The fact that U and W are fractionally isomorphic now follows from (FGI'-2). □

Let us look at the reverse direction "graphons⇒finite graphs". It is not true in general that if U and W are fractionally isomorphic graphons and $G_1, G_2, \ldots$ and $H_1, H_2, \ldots$ are sequences of graphs converging in cut distance to U and W respectively, then G_i and H_i are fractionally isomorphic for each $i \in \mathbb{N}$. Indeed, G_i and H_i might have different orders, which would automatically make them not fractionally isomorphic. Even if G_i and H_i had the same order, a single-edge edit of one of them would preserve convergence in cut distance but make them not fractionally isomorphic. Hence, a sensible question in this direction needs to have an existential quantification for the sequences instead of a universal one. Indeed, this was the main open question of [4].

Question 2 (Question 3.2 in [4])**.** *Suppose that U and W are fractionally isomorphic graphons. Do there exist sequences $\{G_i\}_{i \in \mathbb{N}}$ and $\{H_i\}_{n \in \mathbb{N}}$ of graphs which converge in cut distance to U and W respectively and for which G_i and H_i are fractionally isomorphic for each $i \in \mathbb{N}$?*

The main result of our work is a positive answer to Question 2. In fact, we prove a slightly stronger statement in which we simultaneously approximate an arbitrary (even infinite) family of mutually fractionally isomorphic graphons.

Theorem 3. *Suppose that $\mathcal{U}$ is a family of mutually fractionally isomorphic graphons. Then for each $\varepsilon > 0$ there exists $n_0 \in \mathbb{N}$ such that for each $n \geq n_0$ there exists a family $\{H_U\}_{U \in \mathcal{U}}$ of mutually fractionally isomorphic graphs on vertex set $[n]$ with the property that for each $U \in \mathcal{U}$ the cut distance between U and H_U is at most ε.*

It is easy to check that for each $d \in [0, 1]$ the family $\mathcal{U}_d$ of all d-regular graphons[†] is a family of mutually fractionally isomorphic graphons. Our proof of Theorem 3 gives the following corollary for d-regular graphons.

Theorem 4. *Suppose that $d \in [0, 1]$ and $\mathcal{U}_d$ is the family of all d-regular graphons. Then for every $\varepsilon > 0$ there exists $n_0 \in \mathbb{N}$ such that for each $n \geq n_0$ there exists $D \in \mathbb{N}$ and a family $\{H_U\}_{U \in \mathcal{U}_d}$ of D-regular graphs on vertex set $[n]$ such that for each $U \in \mathcal{U}_d$ the cut distance between U and H_U is at most ε.*

2 Sketch of proof of Theorem 3

While we explained in (FGI'-3) that an infinitesimal approach using sigma-algebras is needed, we begin the following proof overview under the assumption that for a graphon $U \in \mathcal{U}$ the sigma-algebra $\mathcal{C}(U)$ is generated by a finite partition $\mathcal{Q} = \{Q_i\}_{i \in [M]}$ of Ω sets of positive measure; we shall return to the general case at the end of this exposition.

2.1 Desired graph profile from the graphon profile

The U-invariance of $\mathcal{C}(U)$ implies that for all $i, j \in [M]$ and $x \in Q_i$ we have a counterpart to (1), namely

$$\int_{z \in Q_j} U(x, z) = d_{i,j} \pi(Q_j) \tag{2}$$

where $d_{i,j} := \frac{1}{\pi(Q_i)\pi(Q_j)} \cdot \int_{y \in Q_i} \int_{z \in Q_j} U(z, y)$. The fact that each graphon $U' \in \mathcal{U}$ is fractionally isomorphic to U then means that there is a partition $\mathcal{Q}' = \{Q'_i\}_{i \in [M]}$ of Ω with $\pi(Q'_i) = \pi(Q_i)$ such that quantities $d'_{i,j}$ defined in analogy with $d_{i,j}$ satisfy $d'_{i,j} = d_{i,j}$. So, to prove the theorem in this simplified setting, it is enough to approximate (for a given $\varepsilon > 0$ and sufficiently large n) U in cut distance by an n-vertex graph H_U with an equitable partition (in the sense of (FGI-3)) whose parameters depend solely on the vector $\mathbf{r} = (\pi(Q_i))_{i \in [M]}$ and the matrix $\mathcal{D} = (d_{i,j})_{i,j \in [M]}$. Indeed, repeating the construction detailed below for any other $U' \in \mathcal{U}$ yields a graph $H_{U'}$ that has an equitable partition with the same parameters. Hence, it follows by (FGI-3) that $H_{U'}$ and H_U are fractionally isomorphic.

Our construction of H_U has two main steps, as detailed in the following two subsections.

2.2 Approximating by $\mathbb{G}(n, U)$

First, we use the inhomogeneous random graph model $\mathbb{G}(n, U)$ (see [5, Section 10.1]) to generate H_U^*. Let the points $x_1, \dots, x_n \in \Omega$ sampled in the procedure represent the respective vertices $1, \dots, n$ of $V(H_U^*)$. For $i \in [M]$ define $X_i^* := \{\ell \in V(H_U^*) : x_\ell \in Q_i\}$. By the 'Second sampling lemma' (see [5, Lemma 10.15]) H_U^* is close to U in cut distance

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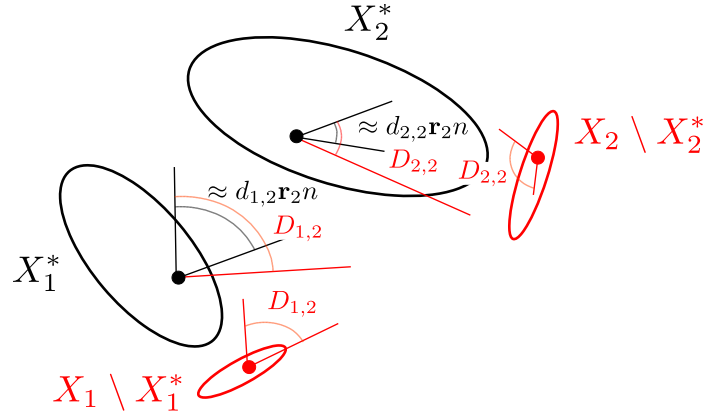[†]A graphon W is d-regular, if for each $x \in \Omega$ we have $\int_y W(x, y) = d$.

Figure 2: An example of the fine-tuning of the degree sequence. The figure focuses on the degrees within X_2 and from X_1 to X_2. The original graph H_U^* is shown in black. The parts added on the way to constructing H_U are shown in red. Theorems of Erdős–Gallai and of Gale–Ryser are used for the red parts.

with high probability. Further, basic concentration results tell us that with high probability, for each $i, j \in [M]$ and each $\ell \in X_i^*$ we have

$$|X_i^*| \approx \mathbf{r}_i n \text{ and} \tag{3}$$

$$\deg_{H_U^*}(\ell, X_j^*) \approx d_{i,j} \mathbf{r}_j n. \tag{4}$$

2.3 Fine-tuning the degree sequence

We shall modify H_U^* in several steps by adding $o(n)$ vertices to each set X_i and $o(n^2)$ edges inside each set X_i and inside each bipartite pair (X_i, X_j), with the aim to achieve after these modifications that

$$|X_i| = N_i \approx \mathbf{r}_i n \text{ and} \tag{5}$$

$$\deg_{H_U}(\ell, X_j) = D_{i,j} \approx d_{i,j} \mathbf{r}_j n \tag{6}$$

for some numbers $(N_i)_{i \in [M]}$ and $(D_{i,j})_{i,j \in [M]}$ which depend only on $\mathbf{r}$, $\mathcal{D}$ and n. Hence, we fulfil the task described in Section 2.1. We apply the classical theorem of Erdős and Gallai on graphic sequences and its bipartite counterpart due to Gale and Ryser. These theorems allow us to construct graphs within the sets $X_i \setminus X_i^*$ and in the pairs $(X_i \setminus X_i^*, X_j)$ (including the case $i = j$) with precisely controlled degree sequences to achieve a state in which each graph $H_U[X_i]$ is regular and each graph $H_U[X_i, X_j]$ is biregular as required by (6). An illustration is given in Figure 2.

2.4 From finite partitions to sigma-algebras

As explained in (FGI'-3), $U/\mathcal{C}(U)$ is defined in terms of a suitable sigma-algebra and does not usually correspond to a finite partition. Here, Szemerédi's regularity lemma comes to

the rescue. Indeed, it is well-known that if $\{\tilde{Q}_i\}_{i \in [M]}$ is a δ-regular Szemerédi partition for a graphon Γ, then in particular we have an approximate version of (2) for most vertices $x \in \tilde{Q}_i$.[‡] We shall take $\delta \ll \varepsilon$.

So, given a graphon U, generate $H_U^* \sim \mathbb{G}(n, U)$ as in Section 2.2. Since we apply Szemerédi's regularity lemma merely to handle degrees, and since we want its application to work in the same way for all graphons in the class $\mathcal{U}$, we shall apply it to the graphon $\Gamma := U/\mathcal{C}(U)$. Let $\Omega/\mathcal{C}(U) = \tilde{Q}_1 \sqcup \ldots \sqcup \tilde{Q}_M$ be a δ-regular Szemerédi partition for Γ. Define $Q_1, \ldots, Q_M$ by $Q_i := q_U^{-1}(\tilde{Q}_i)$. Now, $\Omega = Q_1 \sqcup \ldots \sqcup Q_M$ is in general not a regular Szemerédi partition.[§] However, it can still be proved that an approximate version of (2) holds for most vertices $x \in Q_i$ with respect to the graphon U. This allows us to define again $X_i^* := \{\ell \in V(H_U^*) : x_\ell \in Q_i\}$ and then fine-tune the sequence in a spirit similar to that described in Section 2.3.

2.5 Proving Theorem 4

If U is d-regular then $\Omega/\mathcal{C}(U) = \{a\}$ consists of a single atom and $U/\mathcal{C}(U)(a, a) = d$. So, $M = 1$ and $Q_1 = \Omega$. In particular, the construction above guarantees that the graph $H_U = H_U[X_1]$ is regular, as needed.

[‡]In this overview, we neglect the issue that a Szemerédi partition may involve some irregular pairs. Also, we neglect that the usual regularity lemma does not control behaviour inside clusters whereas we shall need a counterpart to (2) even for $i = j$.

[§]This is perhaps best illustrated with an example. Let $\Omega = A_1 \sqcup A_2$, α_1, α_2 be two distinct numbers and U be such that for $i = 1, 2$ and for every $x \in A_i$ we have

$$\int_{y \in A_i} U(x, y) = \alpha_i \quad \text{and} \quad \int_{y \in A_{3-i}} U(x, y) = 0 . \tag{7}$$

Indeed, in this example $\Omega/\mathcal{C}(U) = \{a_1, a_2\}$ consists of two atoms and we have $U/\mathcal{C}(U)(a_i, a_i) = \alpha_i$ and $U/\mathcal{C}(U)(a_i, a_{3-i}) = 0$. Obviously, the only possible Szemerédi regularization for $U/\mathcal{C}(U)$ has $M = 2$, $\tilde{Q}_1 = \{a_1\}$ and $\tilde{Q}_2 = \{a_2\}$. But the pullbacks $\{Q_i := q_U^{-1}(\tilde{Q}_i) = A_i\}_{i \in [2]}$ clearly need not form a Szemerédi regularization for U, since the restriction (7) leaves a lot of space for wildly structured graphons.

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