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A GRAPHON PERSPECTIVE FOR FRACTIONAL ISOMORPHISM

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Abstract. Fractional isomorphism of graphs plays an important role in practical applications of graph isomorphism test by means of the color refinement algorithm. We introduce a suitable generalization to the space of graphons in terms of Markov opertors on a Hilbert space, provide characterizations in terms of a push-forward of the graphon to a quotient space and also in terms of measurable partitions of the underlying space. Our proofs use a weak version of the mean ergodic theorem, and correspondences between objects such as Markov projections, sub-σ-algebras, measurable decompositions, etc. That also provides an alternative proof for the characterizations of fractional isomorphism of graphs without the use of Birkhoff–von Neumann Theorem.

1. Introduction

A graphon is a symmetric measurable function $W\colon X \times X \to [0,1]$, where X is a standard probability space. Graphons are the main object of study in the theory of dense graph limits introduced in [**7, 2**]. By using a suitable metric, the so-called cut distance, graphons arise as a limit object of sequences of graphs. The fundamental result in the theory states that the space of graphons is compact with respect to the cut distance, thus providing the compactification on the space of graphs. Given two graphs F and G, we denote by $t(F,G)$ the homomorphism density of F into G. Homomorphism densities in graphs extend to homomorphism densities in graphons, which we denote by $t(F,W)$ the homomorphism density of F into W. Remarkably, the authors of [**7, 2**] prove the equivalence between two types of convergence: a sequence of graphs G_n converges to W in the cut distance if and only if for every finite graph F it holds that $t(F,G_n) \to t(F,W)$.

In the fundaments of the theory of graphons there are distinct notions of isomorphisms. For instance, we say that two graphons U and W are isomorphic if there is a measure preserving measurable bijection $\varphi\colon X \to X$ such that $U(\varphi(x),\varphi(y)) = W(x,y)$ for almost all points x and y, i.e., W can be regarded as a permutation of U. For the discrete counterpart – isomorphism of graphs – permutations play the role of measure preserving bijections, thus providing a suitable generalization in the graphon space. However, a more important notion of

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isomorphism in this theory is a weaker definition of isomorphism: two graphons U and W are said to be weakly isomorphic if and only if $t(F, U) = t(F, W)$ for every finite graph F. At this point it is worthwhile to state two characterizations of weak isomorphism that are essential in the theory. In the first, two graphons U and W are weakly isomorphic if and only if their cut distance is zero. In the second, two graphons U and W are weakly isomorphic if and only if there exist measure preserving maps (not necessarly invertible) $\varphi, \psi \colon X \to X$ such that $U(\varphi(x), \varphi(y)) = W(\psi(x), \psi(y))$, i.e., U and W share the same pull-back. It follows that the limit object of a sequence of graphs is unique up to weak isomorphisms.

In this paper we introduce the notion fractional isomorphism of graphons, which is the suitable counterpart for fractional isomorphism of graphs. To this end, we need to work with special quotients of a given graphon, i.e., a graphon defined on a quotient space of the original graphon. We call this special quotient a fraction of the graphon. The reason for the name will be clear in the next section when we define a fractional condition that must be fulfilled. For now, it is important to understand that the fraction of a graphon can be considered as an inverse notion of the pull-back. For example, when U is a pull-back of W, then it follows from our definition of fraction that W is a fraction of U. However we note that in general two graphons V and W need not be weakly isomorphic to share the same fraction. We will see that many difficulties appear when trying to extend the definitions and proving meaningful characterizations. Before we discuss that in the next section, let us try to convince the reader of the importance of this concept for the isomorphism problem at the same time that we give some basics of fractional isomorphism of graphs.

Recall that a doubly stochastic matrix S is a square matrix with nonnegative entries such that each row and each column sum up to one, i.e., $S \geq 0$ and $S\,\mathbf{1} = S^T\,\mathbf{1} = \mathbf{1}$. For example, permutation matrices are doubly stochastic. Let G and H be graphs and A and B its corresponding adjacency matrices. We say that G and H and fractionally isomorphic if there exists a doubly stochastic matrix S such that $AS = SB$. Notice that G and H are isomorphic if and only if there exists a permutation matrix P such that $AP = PB$. Finding such permutation matrix is a notorious difficult problem in computer science. It is not known if this problem can be solved in polynomial time nor to be NP-complete. Nevertheless, many relaxations of the isomorphism problem have been investigated, one in particular has theoretical and practical interest; the fractional isomorphism decision problem which can be resolved in polynomial time.

The notion of fractional isomorphism have different characterizations that are pertinent for our investigation and we shall state them now before we attempt to come up with a proper definition for graphons. For a graph $G = (V, E)$, let $d(v, S)$ be the degree of a vertex v in a subset of vertices S. Equivalently, $d(v, S) = |N(v) \cap S|$. A partition $\{C_1, C_2, \ldots, C_s\}$ of V is called equitable if and only if for all $u, v \in C_i$, we have $d(u, C_j) = d(v, C_j)$ for all i and j. That is to say that each induced subgraph $G[C_i]$ must be regular and each of the bipartite graphs $G[C_i, C_j]$ must be biregular. That also defines a trivial equivalence relation between vertices, which turns out to be the correct approach when we generalize this kind of partition to the underlying space where the graphon is defined. The relevant characterizations for the purposes of this article are collected bellow.

Theorem 1.1 ([**10**],[**9**]). *Let G and H be graphs. The following statements are equivalent.*

1. *G and H are fractionally isomorphic.*
2. *G and H have some common equitable partition.*
3. *G and H have a common coarsest equitable partition.*

Equivalences (1) and (3) were proved by Tinhofer in [**10**]. Equivalence (2) was proved in [**9**] by Ramana, Scheinerman, and Ullman. Perhaps the most important characterization of fractional isomorphism is due to its practical applications to graph isomorphism test. This application comes from color refinement which is a simple and efficient heuristic to test whether two graphs are isomorphic. The algorithm computes a coloring of the vertices of two graphs based on its iterated degree sequences and compare its colorings. Whenever they are different, we say that color refinement distinguishes the graphs. Whenever they are the same, we do not know whether or not they are isomorphic. Regardless, in [**1**] Babai, Erdős, and Selkow showed that color refinement distinguishes almost all non-isomorphic graphs, and in practice this algorithm performs well. Other advanced graph isomorphism algorithms and almost all practical isomorphism softwares uses color refinement underneath. This heuristic goes beyond isomorphism testing and is also useful in a number of other problems. (See [**6**] for further reading) Noticeable, and most relevant for our investigation, is that color refinement does not distinguish G and H if and only if G and H are fractionally isomorphic, which was proved by Tinhofer [**10, 11**]. That suggests the importance of this notion.

2. Fractional isomorphism of graphons

In this section we define fractional isomorphism of graphons which we show to be characterized in terms of measurable decompositions of the underlying space X. In what follows we define graphons on a standard Borel space. We remark that people usually work with standard probability spaces but since every standard probability space is a completion of some standard Borel space with a probability measure we do not lose anything. This is similar to the fact that in this theory working on any probability space is essentially the same as using a standard probability space, which was showed in [**3**] by Borgs, Chayes and Lovász. They provide a simple procedure to transform a graphon on an arbitrary probability space into a graphon on a standard probability space. The reason we use a standard Borel spaces is to be able to use the Measure Disintegration Theorem which we believe describes better the connection with finite graphs.

An operator $T\colon L^2(X,\mu) \to L^2(Y,\nu)$ is said to be doubly stochastic if $Tf \geq 0$ whenever $f \geq 0$, $T\mathbf{1}_X = \mathbf{1}_Y$, and $T^*\mathbf{1}_Y = \mathbf{1}_X$, where T^* is its adjoint operator $T^*\colon L^2(Y,\nu) \to L^2(X,\mu)$. Doubly stochastic operators are also called in the literature by the name Markov operators. Our reference for the theory of Markov operators is [**5**]. Notice that this is a generalization of doubly stochastic matrices in the context of Hilbert spaces. We consider the graphon operator $T_W: L^2(X,\lambda) \to L^2(X,\lambda)$ defined by $T_W(f)(x) = \int_X f(y) W(x,y)\, \mathrm{d}\lambda$. It is well-known that T_W is a self-adjoint Hilbert-Schmidt operator, which enjoys many nice properties. The graphon operator T_W plays the role of the adjacency matrix as in the discrete case.

Definition 2.1 (Fractional isomorphism of graphons)**.** Let W and U be graphons on spaces X and Y, respectively. We say that U and W are fractionally isomorphic if there exists a doubly stochastic operator $S\colon L^2(X,\mu) \to L^2(Y,\nu)$ such that $S \circ T_W = T_U \circ S$.

Our goal now is to provide the graphon counterpart of Theorem 1.1. However, the notion of equitable partition is not straightforward. A reasonable definition should reflect the properties from the finite case. For example, if $G = (V,E)$ is a finite graph and η is a equivalence relation on V that induces an equitable partition $\{C_1, C_2, \ldots, C_s\}$, then every pair $v,w \in C_i$ must have the same degree, i.e., $d(v,V) = d(w,V)$. The corresponding notion of degree in a graphon is defined for each point $x \in X$ by $d(x) = \int_X W(x,y)\mathrm{d}\lambda$. Consider the example where $X = [0,1]$ with the Lebesgue measure and define the graphon $W(x,y) = xy$. Then $d(x) \neq d(y)$ for all different $x,y \in X$. For this example, the correct generalization of equitable partition must be given by a equivalence relation η with the property that for any $y,x \in [0,1]$ with $x\eta y$ it holds that $x = y$. Therefore, there are uncountably many equivalence classes, all of them with measure zero. That suggests we need to be more careful than in the discrete case to provide a proper definition, which in turn creates some extra difficulties for the proofs.

Let $(X,\mathcal{B},\mu)$ be a standard Borel space with a probability measure. An equivalence relation η on X is said to be a measurable partition if there is a standard Borel space $(Y,\mathcal{C})$ and a measurable map $f_\eta\colon X \to Y$ such that $x\eta y$ if and only if $f_\eta(x) = f_\eta(y)$ and $f(X) \in \mathcal{C}$. Similarly, every surjective measurable function $f\colon X \to Y$ induces a measurable partition η_f. There is a natural equivalence relation on the set of all measurable partitions. Equivalently, this concept can be described by relatively complete (with respect to μ) sub-σ-algebra of $\mathcal{B}$. Namely, for every measurable partition η we assign the sub-σ-algebra $\mathcal{B}_\eta \subset \mathcal{B}$ by $\mathcal{B}_\eta = \{A \in \mathcal{B}:$ for every $x,y \in X$ if $x\eta y$ and $x \in A$ then $y \in A\}$. Assigning back a measurable partition to a relatively complete sub-σ-algebra is possible in our situation because we work with a standard Borel spaces. The reason why we introduce both concepts is that the measurable partition allow us to apply the Measure Disintegration Theorem and generalize the local condition from equitable partition from finite graphs, while the sub-σ-algebra allows us to correlate η with conditional expectation $\mathbb{E}(\cdot|\mathcal{B}_\eta)$ and easily define globally the quotient of a given graphon with respect to a measurable partition. We note that since both concepts are equivalent there is a translation between both approaches which we describe in the next definitions.

It is a standard fact that whenever $(X,\mathcal{B})$ is a standard Borel space, then the space of all probability measures, that we denote as $\mathcal{P}(X)$, carries naturally standard Borel structure. Recall that for every measurable partition η, the Measure

Disintegration Theorem gives a measurable function $\Lambda_\eta \colon X \to \mathcal{P}(X)$ that disintegrates μ with respect to η. We denote an equivalence class of $x \in X$ as x/η.

Definition 2.2 (Fractional partition)**.** Let W be a graphon on X. We say that a measurable partition η is a fractional partition of W if there is a μ-conull Borel set $C \subseteq X$ such that for every $a, b \in C$ where $a\eta b$ we have

$$\int_X W(a,z)\,\mathrm{d}\Lambda_\eta(\mathrm{y})(\mathrm{z}) = \int_{\mathrm{X}} \mathrm{W}(\mathrm{b},\mathrm{z})\,\mathrm{d}\Lambda_\eta(\mathrm{y})(\mathrm{z})$$

for μ-almost every $y \in X$, or equivalently, $\mathbb{E}(W(a,\cdot)|\mathcal{B}_\eta) = \mathbb{E}(W(b,\cdot)|\mathcal{B}_\eta)$, where the equality is μ-almost everywhere.

A fractional partition can be interpreted as a generalization of an equitable partition. In the previous example, where $W(x,y) = xy$, the correct fractional partition η is such that for each point $x \in [0,1]$ it holds $\{x\} = x/\eta$. The disintegration of μ is given by the Dirac measure $\Lambda_\eta(x) = \delta_x$ for each $x \in [0,1]$. Therefore, for all $y, a \in X$ it holds $\int_X W(a,z)\,\mathrm{d}\Lambda_\eta(\mathrm{y})(\mathrm{z}) = \mathrm{W}(\mathrm{a},\mathrm{y})$.

Given a graphon W on X and a measurable partition η it is natural to create a quotient graphon $W_\eta \colon X/\eta \times X/\eta \to [0,1]$ by the push-forward of $\mathbb{E}(W|\mathcal{B}_\eta \times \mathcal{B}_\eta)$ to the quotient space $X/\eta \times X/\eta$ (the space of equivalence classes of η). Note that $(X/\eta, \mathcal{B}_\eta, \mu/\eta)$ is a standard Borel space, due to our definition of measurable partition. The concept of quotient was used before to show for example that every graphon is weakly isomorphic to a twin-free graphon. Recall that two points $x, x' \in X$ are twins if and only if $W(x,y) = W(x',y)$ for almost all $y \in X$. That defines a equivalence relation on X. We remark that this equivalence relation satisfies the notion of fractional partition and the corresponding quotient is the twin-free graphon (see [**8**]). Next, we define the core object of this paper.

Definition 2.3 (Fraction of a graphon)**.** Let η be a fractional partition of W. Then a fraction of W is the graphon $W_\eta \colon X/\eta \times X/\eta \to [0,1]$ defined by the push-forward of $\mathbb{E}(W|\mathcal{B}_\eta \times \mathcal{B}_\eta)$ to the quotient space X/η, or equivalently,

$$W_\eta(x/\eta, y/\eta) = \int_{X\times X} W(r,s)\,\mathrm{d}\Lambda_\eta(\mathrm{x})(\mathrm{r}) \times \Lambda_\eta(\mathrm{y})(\mathrm{s}).$$

Note that if $\eta = \{X\}$ the corresponding graphon W_η is the constant graphon on one-point probability space with the value $\int_{X\times X} W(x,y)\,\mathrm{d}\mu \times \mu$. This is a fraction of W exactly when almost all points have the same degree. This clearly shows that there are graphons that are not weakly isomorphic but share the same fraction. Another example that we mentioned in the introduction is when U is a pull-back of W. Then one can easily verify that W is a fraction of U.

Rather surprisingly, for every graphon W on X there is a maximal fractional partition $\eta_{\max}$ in the sense that $\eta_{\max}$ is a partition of any fractional partition η of W. That we show in the following result, which is one of the fundaments in our investigation.

Theorem 2.4. *Let W be a graphon on X. Then there is a fractional partition $\eta_{\max}$ of W with the property that for every fractional partition η of W there is a fractional partition θ of W_η such that $(W_\eta)_\theta = W_{\eta_{\max}}$.*

Comparing to the discrete case, this result is analogue to the fact that any equitable partition has a coarsest equitable partition. To further understand this concept, we provide the following result that characterizes fractional partitions. Notice that whenever η is a measurable partition of X, then $L^2(X/\eta, \mu/\eta)$ can be naturally viewed as a subspace of $L^2(X, \mu)$.

Theorem 2.5. *Let W be a graphon on X. The following are equivalent.*

1. *η is a fractional partition of W.*
2. *T_W is invariant on $L^2(X/\eta, \mu/\eta)$.*
3. *There is an orthonormal basis of $L^2(X/\eta, \mu/\eta)$ that consists of eigenfunctions of $T_W \restriction L^2(X/\eta, \mu/\eta)$.*

We are ready to state our main result that generalizes the conditions from Theorem 1.1.

Theorem 2.6. *Let W and U be graphons on spaces X and Y, respectively. Then the following are equivalent*

1. *W and U are fractionally isomorphic.*
2. *there area fractional partitions η of W and θ of U such that W_η and U_θ are isomorphic.*
3. *the maximal fractional partitions $\eta_{\max}$ of W and $\theta_{\max}$ of U are such that $W_{\eta_{\max}}$ and $U_{\theta_{\max}}$ are isomorphic.*

Let us briefly mention that the proof of this theorem has a very different approach than in the discrete case. First, the proof for graphs given in [**9**] relies on the Birkhoff–von Neumann theorem, which states that any doubly stochastic matrix can be written as a convex combination of permutation matrices. This type of decomposition is not possible for a general doubly stochastic operator in a Hilbert space. To overcome this issue, we provide a proof that uses a weak version of the mean ergodic theorem and correspondences between objects such as Markov projections, sub-σ-algebras, measurable decompositions, etc. Thus, our result also provides an alternative proof for Theorem 1.1 without the use Birkhoff–von Neumann theorem which seems to be unknown.

3. Further directions

There are two further relevant conditions that characterizes fractional isomorphism of graphs. The first is the iterated degree sequence of graphs, providing the relation with the color refinement algorithm, and the second is a condition involving density of trees. The latter condition appeared in [**4**], where the authors showed that two graphs G and H are fractionally isomorphic if and only if for every T it holds $t(T, G) = t(T, H)$. It is expected that a similar condition holds for graphons. However, the graphon case is not fully understood and we expect to report on this matter soon. As a final remark on the current investigation, to provide this type of tree density condition for graphons we first need to understand a similar condition involving the iterated degree sequence in the context of graphon. To this end, we define a distributions on iterated degree distributions which allow us to produce a fraction of a graphon, and further show the equivalence to the existence of isomorphic fractions.

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