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Differential calculus on graphon space ☆

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A B S T R A C T

Recently, the theory of dense graph limits has received attention from multiple disciplines including graph theory, computer science, statistical physics, probability, statistics, and group theory. In this paper we initiate the study of the general structure of differentiable graphon parameters F. We derive consistency conditions among the higher Gâteaux derivatives of F when restricted to the subspace of edge weighted graphs $\mathcal{W}_{\mathbf{p}}$. Surprisingly, these constraints are rigid enough to imply that the multilinear functionals $\Lambda : \mathcal{W}_{\mathbf{p}}^n \to \mathbb{R}$ satisfying the constraints are determined by a finite set of constants indexed by isomorphism classes of multigraphs with n edges and no isolated vertices. Using this structure theory, we explain the central role that homomorphism densities play in the analysis of graphons, by way of a new combinatorial interpretation of their derivatives. In particular, homomorphism densities serve as the monomials in a polynomial algebra that can be used to approximate differential graphon parameters as Taylor polynomials. These ideas are summarized by our main theorem, which asserts that homomorphism densities $t(H, -)$ where H has at most N edges form a basis for the space of smooth graphon parameters whose $(N + 1)$st derivatives vanish. As a consequence of this theory, we also extend and derive new proofs of linear independence of multigraph homomorphism densities, and characterize homomorphism densities. In addition, we develop a theory of series expansions, includ-

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ing Taylor's theorem for graph parameters and a uniqueness principle for series. We use this theory to analyze questions raised by Lovász, including studying infinite quantum algebras and the connection between right- and left-homomorphism densities. Our approach provides a unifying framework for differential calculus on graphon space, thus providing further links between combinatorics and analysis.

1. Introduction

The theory of dense graphs and their limits introduced in [23] has attracted much attention recently (see e.g. [2,4–6,9,10,14]). It has also been observed that limit theories developed in the context of (i) graphons, (ii) exchangeable arrays of random variables [18], and (iii) metric measure spaces ([16, Chapter $3\frac{1}{2}$] and [30]) can often be translated into each other (see [1,12,13]). Several questions have benefited from reformulation in this language – see for instance [17,21,26] and [22, Chapter 16]. The monograph [22] covers many aspects of this development, including topology and analysis on the space of graph limits. Since graphs have become a central abstraction for the modern analysis of complex systems, the theory has also been used to address applied questions in the study of estimable graph parameters [25], machine learning [19], and statistical modelling of networks [3,11,27]. It seems that such a language was needed as much for mathematical theory as for practical application.

The present paper begins the study of functional analysis of dense graph limits. In order to explain our motivation and results, we first briefly review dense graph limit theory and set some notation. By a *graphon* we mean a bounded symmetric measurable function $f : [0,1]^2 \to [0,1]$. Recall that a finite simple labelled graph G with vertices $V = \{1, 2, \dots, n\}$ is identified with the graphon f^G, defined as follows:

$$f^G(x,y) = \mathbf{1}_{(\lceil nx \rceil, \lceil ny \rceil) \in E} = \begin{cases} 1, & \text{if } (\lceil nx \rceil, \lceil ny \rceil) \text{ is an edge in } G, \\ 0, & \text{otherwise.} \end{cases}$$

One description of the topology on isomorphism classes of finite simple graphs in dense graph limit theory is given as follows. The space $\mathcal{W}_{[0,1]}$ of all graphons sits inside $\mathcal{W}$, the vector space of bounded symmetric measurable functions $f : [0,1]^2 \to \mathbb{R}$. The space $\mathcal{W}$ has a seminorm called the *cut norm*

$$\|f\|_{\text{cut}} := \sup_{S,T \subset [0,1]} \left| \int_{S \times T} f(x,y)\, dx\, dy \right|$$

where the supremum is taken over all pairs of Lebesgue measurable subsets S, T of $[0,1]$. The monoid of measure-preserving maps $\overline{S}_{[0,1]}$ acts on $\mathcal{W}_{[0,1]}$ by $f^\sigma(x,y) := f(\sigma(x), \sigma(y))$