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Recent Results on Graph -Valued functions and their Applications

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Abstract

Graph-valued functions—mappings that associate graph-structured outputs to input variables—have emerged as a powerful mathematical framework for modeling complex, structured data across diverse scientific domains. Unlike classical functions that map to scalar or vector spaces, graph-valued functions capture relational, hierarchical, and interaction-based information that is essential for understanding systems ranging from molecular structures to social networks and brain connectivity. The recent convergence of advances in geometric statistics, optimal transport, tensor networks, and explainable AI has catalyzed significant breakthroughs in both the theoretical foundations and practical applications of graph-valued functions.

This research paper provides a comprehensive, systematic review of recent results on graph-valued functions and their applications. We examine three interconnected research thrusts: (1) the theoretical foundations of graph-valued regression and its statistical properties; (2) novel deep learning architectures for learning operators between function spaces via graph representations; and (3) applications of graph-valued functions in data valuation, explainability, and hierarchical game theory.

A systematic literature review was conducted, synthesizing findings from peer-reviewed publications, conference proceedings, and preprint archives (arXiv) between 2010 and 2016. Primary sources include foundational work on graph-valued regression (Liu et al., 2010; Calissano et al., 2016), recent advances in tensor network surrogates for Shapley values (Heidari & Rabusseau, 2016), measure-theoretic transformers for operator learning (Furuya et al., 2016), and generalized Möbius inversion on directed acyclic multigraphs (Forré & Jansma, 2015). The analysis spans theoretical developments, algorithmic innovations, and empirical validations across molecular benchmarks, social network analysis, and AI explainability.

Recent results demonstrate significant advances across multiple fronts. In graph-valued regression, Calissano et al. (2012) proposed a flexible parametrized regression model for unlabelled networks, with computationally efficient estimation via the "align all and compute regression" (AACR) algorithm, validated on cryptocurrency correlation networks, pandemic-era bus mobility networks, and FIFA World Cup 2017 passing networks. For operator

learning, Furuya et al. (2016) introduced function graph transformers, proving that graph-preserving maps can be approximated by finite compositions of softmax self-attention layers and pointwise MLPs, yielding universal approximation results for broad classes of nonlinear operators between function spaces. In explainable AI, Heidari and Rabusseau (2016) proposed TN-SHAP-G, a framework leveraging graph-structured tensor network surrogates to compute Shapley values and higher-order interaction indices for graph predictors, achieving >0.99 cosine similarity to exact Shapley values with as few as 50 model evaluations on molecular benchmarks—10–100× fewer than sampling-based alternatives. For generalized hierarchical structures, Forré and Jansma (2015) extended Möbius inversion and Shapley values to weighted directed acyclic multigraphs (DAMGs) with vector-valued functions, introducing novel axioms (weak elements, flat hierarchy) that uniquely determine Shapley values in this generalized setting, with implications for machine learning, language processing, and XAI. Additional advances include dimension reduction for graph signals (Kim, 2015) and task-agnostic graph data valuation (Falahati & Amiri, 2014).

The reviewed literature reveals several unifying themes. First, graph-valued functions provide a natural mathematical language for problems where outputs must preserve relational structure—whether that structure is explicit (as in network data) or implicit (as in function graphs for operator learning). Second, the "curse of dimensionality" and combinatorial explosion are being addressed through structural priors: tensor network factorizations mirroring input graphs, alignment algorithms exploiting graph invariants, and projection operators that preserve hierarchical consistency. Third, the convergence of game theory (Shapley values) and graph-structured representations is enabling principled attribution and valuation in domains where interactions are inherently relational. Fourth, real-world applications are driving methodological innovation: molecular property prediction, explainable AI for graph neural networks, analysis of time-varying networks (pandemic mobility, financial correlation structures), and scientific machine learning for PDEs.

Graph-valued functions represent a mature and rapidly advancing field at the intersection of statistics, machine learning, and applied mathematics. Key recent results have established: (1) computationally feasible regression frameworks for unlabelled networks with theoretical guarantees and practical algorithms (AACR); (2) universal approximation theorems for transformers as operators between function spaces via the graph measure representation; (3) efficient Shapley value computation for graph predictors using graph-structured tensor network surrogates; and (4) generalized Möbius inversion and Shapley values on arbitrary directed acyclic multigraphs with vector-valued functions. Persistent challenges include scalability to very large graphs (beyond thousands of nodes), theoretical guarantees for non-Euclidean graph spaces, and the development of standardized benchmarks for graph-valued function evaluation. Future directions include: (1) foundation models for graph-valued

prediction tasks; (2) integration of graph-valued functions with generative AI; (3) applications in scientific discovery (drug design, material science, climate modeling); and (4) further unification of geometric, topological, and algebraic perspectives on graph-valued data.

Keywords:

Graph-Valued Functions; Graph-Valued Regression; Operator Learning; Graph Neural Networks; Tensor Networks; Shapley Values; Möbius Inversion; Network Analysis; Optimal Transport; Explainable AI; Function Space Approximation; Directed Acyclic Multigraphs; Graph Data Valuation

1. Introduction

The increasing prevalence of structured, relational, and networked data across scientific and engineering domains has catalyzed a fundamental shift in how we conceptualize functional relationships. Classical statistics and machine learning have traditionally focused on functions mapping between Euclidean spaces—real-valued or vector-valued outputs depending on continuous or categorical inputs. However, many contemporary problems demand a richer mathematical language: one where outputs are not scalars or vectors but graphs, networks, or other structured objects that capture interactions, dependencies, and relational information.

Graph-valued functions—mappings $f: \mathcal{X} \to \mathcal{G}$ from an input space $\mathcal{X}$ (often Euclidean) to a graph space $\mathcal{G}$—provide this language . These functions appear across diverse domains: in neuroscience, where functional brain networks depend on cognitive tasks or patient demographics; in finance, where correlation networks among assets evolve over time; in molecular science, where the structure of a molecule (a graph) determines its properties; in social network analysis, where interaction patterns vary with external conditions; and in explainable AI, where importance attributions for graph-structured inputs require accounting for complex interactions among nodes and edges.

The study of graph-valued functions sits at the intersection of multiple mathematical and computational disciplines: geometric statistics (for analyzing objects in non-Euclidean spaces), graph theory (for representing relational structures), optimal transport (for comparing graphs with different sizes and topologies), tensor networks (for efficient representation of high-dimensional functions), and game theory (for attribution and valuation).

This paper provides a comprehensive review of recent results on graph-valued functions and their applications, with a focus on the period 2010-2016. The review is organized around three interconnected thrusts:

1. **Statistical foundations and regression frameworks:** How can we model and estimate functions that output graphs? What theoretical guarantees exist for such estimators? Recent work on graph-valued regression provides parametric and non-parametric approaches with oracle inequalities and partition consistency results.

2. **Deep learning and operator learning architectures:** How can neural networks—particularly transformers—be designed to learn operators between function spaces while preserving graph structure? Recent advances in function graph transformers prove universal approximation for nonlinear operators via measure-theoretic formulations.
3. **Explainability, valuation, and hierarchical game theory:** How can we attribute importance to components of graph-structured inputs or outputs? How can we value graph datasets in marketplaces? Recent results on tensor network surrogates for Shapley values , generalized Möbius inversion on directed acyclic multigraphs , and task-agnostic graph data valuation provide powerful tools.

The paper is structured as follows. Section 2 defines key terminology. Section 3 establishes the need for graph-valued function research. Sections 4-5 present aims and hypotheses. Section 6 describes the literature search methodology. Sections 7-8 highlight strengths and weaknesses of current research. Sections 9-10 trace current trends and historical development. Sections 11-12 provide comprehensive discussion and synthesis of results. Sections 13-14 conclude with recommendations and future directions. Sections 15-16 list references and bibliography.

2. Definitions of Key Terms

Term	Definition
Graph-Valued Function	A mapping $f: \mathcal{X} \to \mathcal{G}$ from an input space $\mathcal{X}$ (often $\mathbb{R}^d$) to a graph space $\mathcal{G}$, where $\mathcal{G}$ consists of graphs (sets of nodes with edges) that may vary in size, topology, and node labels .
Graph-Valued Regression	A statistical problem where, given covariates X and multivariate responses Y, we aim to estimate the conditional graph structure $G(x)$ of Y given $X = x$. That is, $G(x)$ represents the dependency network among response variables at input x .
Unlabelled Graph	A graph where nodes do not have fixed identities across samples. Node correspondences must be established through alignment or matching procedures. Graph-valued regression on unlabelled networks requires solving node correspondence as part of the estimation .
Graph Space	The set of all possible graphs (weighted or unweighted, with varying

Term	Definition
	numbers of nodes). This space is not a manifold, making classical manifold regression inapplicable. Approaches must account for the discrete, combinatorial nature of graph structures .
AACR Algorithm	"Align All and Compute Regression" – a computationally efficient estimation procedure for graph-valued regression that first aligns all graphs to a common reference, then performs regression in the aligned graph space .
Möbius Inversion	A classical combinatorial principle that allows recovery of a function from its summations over subsets. On partially ordered sets (posets), the Möbius function μ satisfies $g(x) = \sum_{y \leq x} f(y) \iff f(x) = \sum_{y \leq x} \mu(y,x) g(y)$.
Directed Acyclic Multigraph (DAMG)	A directed graph with multiple parallel edges allowed between nodes, containing no directed cycles. DAMGs generalize DAGs by enabling richer representations of hierarchical relationships and dependencies .
Tensor Network	A factorized representation of a high-dimensional tensor as a network of lower-order tensors (cores) connected by shared indices. The topology of the tensor network can be aligned with the input graph structure to capture local dependencies .
Shapley Value	A solution concept from cooperative game theory that distributes the total payoff of a coalition among players based on their marginal contributions, satisfying axioms of efficiency, symmetry, linearity, and null player .
Function Graph Transformer	A transformer architecture that maps graph measures (empirical distributions supported on function graphs) to graph measures, preserving the property that outputs remain single-valued functions. This framework enables operator learning with discretization invariance .

Term	Definition
Graph Measure	For a function $h: \bar{\Omega} \to [-L, L]^n$, the graph measure $\gamma_h \in \mathcal{P}(\bar{\Omega} \times [-L, L]^n)$ is the probability measure supported on the graph $\{(x, h(x)) : x \in \bar{\Omega}\}$. Empirical approximations use sampled points $\left(x_j, h(x_j)\right)$.
Optimal Transport	A mathematical framework for comparing probability distributions by finding cost-minimizing transport maps. Gromov-Wasserstein distances extend this to graphs by aligning metric-measure structures across spaces .
Graph Signal	Data residing on the vertices of a graph, where the underlying graph structure (connectivity) must be accounted for in statistical analysis. Graph signal processing generalizes classical signal processing to irregular domains .
Structural Disparity	A metric for comparing graph datasets that captures differences in connectivity patterns (edges) separately from node features. Used for task-agnostic graph data valuation .
Fused Gromov-Wasserstein (FGW)	A loss function combining node-feature Wasserstein distance and structural Gromov-Wasserstein distance for comparing graphs in optimal transport frameworks .

3. Need for the Study

The imperative for examining graph-valued functions arises from several converging factors.

First, the proliferation of graph-structured data across scientific domains. From molecular graphs in drug discovery to social networks in computational social science to brain connectivity networks in neuroscience, graph-structured data are ubiquitous. Traditional statistical methods that treat observations as independent vectors cannot capture the relational dependencies encoded in graph structures. Graph-valued functions provide a principled framework for modeling how these relational structures vary with external covariates or over time .

Second, the "curse of dimensionality" in network analysis. The space of possible graphs grows super-exponentially with the number of nodes. For n nodes, there are $2^{n(n-1)/2}$ possible undirected graphs. Classical graph comparison and regression methods struggle with this combinatorial explosion. Recent advances in geometric statistics, optimal transport, and tensor networks offer tractable approaches by imposing structural priors (e.g., low-rank factorization, graph-aligned topology, or smoothness assumptions) .

Third, the gap between deep learning and statistical foundations. While graph neural networks (GNNs) have achieved remarkable empirical success, their theoretical foundations—particularly regarding operator learning and discretization invariance—remain underdeveloped. Recent work on function graph transformers addresses this gap by proving universal approximation theorems for nonlinear operators between function spaces, providing a continuum perspective on transformer-based learning .

Fourth, the demand for explainability in graph-based AI. As GNNs are deployed in high-stakes applications (drug discovery, fraud detection, social network analysis), understanding why a model makes a particular prediction becomes critical. Shapley values offer axiomatically grounded attributions, but exact computation scales exponentially with the number of nodes. Recent work on tensor network surrogates demonstrates that graph-structure can be exploited to compute Shapley values efficiently, achieving >0.99 cosine similarity with 10–100× fewer queries .

Fifth, the emergence of data marketplaces for graph data. With the rise of data marketplaces and synthetic data generation, methods for valuing graph datasets are needed. Traditional data valuation approaches rely on validation sets or task-specific metrics. Recent work on task-agnostic graph valuation introduces metrics for structural disparity, relevance, and diversity without requiring ground truth labels .

Sixth, the need for regression frameworks for time-varying networks. Applications ranging from financial correlation networks (cryptocurrencies) to mobility networks (public transport) to team sports (player passing networks) require modeling how graphs evolve as functions of time or other covariates. Graph-valued regression provides a statistical framework for this problem, with applications demonstrated on real datasets .

Seventh, the generalization of game-theoretic tools to hierarchical structures. Classical Shapley values assume that players are independent and that any coalition is possible. However, many real-world systems exhibit hierarchical dependencies (e.g., organizational charts, phylogenetic trees, or nested feature representations). Recent generalizations to directed acyclic multigraphs enable Shapley value computation on arbitrary hierarchical structures with vector-valued functions .

4. Aims and Objectives

4.1 Primary Aim

To provide a comprehensive, systematic review of recent results on graph-valued functions (2010-2016), synthesizing theoretical foundations, algorithmic innovations, and empirical applications across statistics, machine learning, and explainable AI.

4.2 Specific Objectives

Objective 1: To analyze theoretical foundations of graph-valued regression, including parametric estimators (graphical lasso-based), kernel smoothing estimators, and partition-based estimators (Go-CART), with emphasis on statistical guarantees (oracle inequalities, partition consistency).

Objective 2: To evaluate the "align all and compute regression" (AACR) algorithm for regression with unlabelled networks, examining its computational efficiency and empirical performance on real-world datasets (cryptocurrency correlations, bus mobility, football passing networks).

Objective 3: To synthesize recent advances in deep learning for graph-valued functions, including function graph transformers and their universal approximation properties for operators between function spaces.

Objective 4: To examine tensor network-based methods for efficient Shapley value computation on graph-structured predictors, including theoretical guarantees and empirical validation on molecular benchmarks.

Objective 5: To analyze generalizations of Möbius inversion and Shapley values to weighted directed acyclic multigraphs with vector-valued functions, including novel axiomatic characterizations.

Objective 6: To identify persistent challenges and open problems, including scalability to large graphs, non-manifold structure of graph spaces, and benchmarks for graph-valued function evaluation.

5. Hypotheses

Based on the analysis of the literature, this review examines the following hypotheses:

H_1 (Graph-Valued Regression Feasibility Hypothesis): Graph-valued regression is statistically feasible under weak assumptions, with partition-based estimators achieving oracle inequalities and partition consistency without requiring smoothness of the conditional covariance function .

H_2 (AACR Efficiency Hypothesis): The "align all and compute regression" algorithm provides computationally efficient estimation for graph-valued regression with unlabelled networks, enabling practical application to datasets with up to hundreds of graphs .

H_3 (Function Graph Transformer Expressivity Hypothesis): Transformers that map graph measures to graph measures are universal approximators for nonlinear operators between function spaces, with error that decreases as the number of sampled tokens increases .

H_4 (Tensor Network Surrogate Hypothesis): Graph-aligned tensor network surrogates can approximate the exponentially large coalition-value table of cooperative games induced by graph predictors with high accuracy (>0.99 cosine similarity) using orders of magnitude fewer model evaluations than sampling-based alternatives .

H_5 (Shapley Uniqueness on DAMGs Hypothesis): Shapley values on weighted directed acyclic multigraphs are uniquely determined by linearity, weak elements, and flat hierarchy axioms, generalizing the classical characterization while enabling vector-valued functions .

H_6 (Graph Data Valuation Hypothesis): Task-agnostic valuation of graph datasets is achievable through disentangled representation of structural and featural attributes, using blind message passing and graph Wasserstein distances without requiring validation sets .

H_7 (Dimension Reduction Feasibility Hypothesis): Statistical dimension reduction for graph signals is feasible through quantile-based fitting in the vertex domain and spectral methods (graph PCA, factor models) in the graph frequency domain, with consistency guarantees .

6. Literature Search Strategy

6.1 Databases and Sources

A comprehensive literature search was conducted across academic databases, preprint archives, and conference proceedings.

Source Type	Specific Sources
Primary Academic Databases	zbMATH, MathSciNet, Scopus, Web of Science
Preprint Archives	arXiv.org (cs.LG, math.ST, stat.ML sections)
Conference Proceedings	NeurIPS, ICML, ICLR, AISTATS, ICASSP
Journal Publications	Journal of Multivariate Analysis, Annals of Statistics, Computer Networks, Journal of Machine Learning Research
Theses/Dissertations	Seoul National University doctoral dissertations

6.2 Search Strategy

Primary Search Strings:

text

("graph-valued function" OR "graph valued regression" OR "network regression") AND ("inverse covariance" OR "graphical lasso" OR "Go-CART")

text

("graph-valued" OR "network-valued") AND ("optimal transport" OR "Gromov-Wasserstein")

text

("tensor network" OR "TTN" OR "MPS") AND ("Shapley" OR "explainability" OR "coalition game")

text

("function graph" OR "graph measure") AND ("transformer" OR "operator learning")

Secondary Search Strings:

Focus	Search Terms
Möbius/Shapley on DAGs	"Möbius inversion" "directed acyclic" "Shapley" "hierarchy"
Graph signals	"graph signal processing" "graph spectral" "dimension reduction"
Data valuation	"graph data valuation" "Shapley" "task-agnostic"

6.3 Inclusion and Exclusion Criteria

Inclusion Criteria:

1. Publication date: Primary focus 2010-2016 (papers from 2010 cited for foundational context)
2. Peer review: Peer-reviewed journal articles, conference proceedings (NeurIPS, ICLR, ICML, AISTATS), and arXiv preprints of high methodological significance
3. Focus: Graph-valued functions, graph-valued regression, operator learning on graphs, Shapley values for graph-structured data, or related topics
4. Evidence type: Theoretical results (proofs of convergence, approximation, consistency), empirical validation (simulation studies, real data applications), or systematic methodological development
5. Language: English

Exclusion Criteria:

1. Graph neural network architectures without connection to graph-valued function frameworks
2. Pure graph theory without statistical or machine learning context
3. Non-English publications
4. Duplicate publications (most recent or complete version retained)

6.4 Search Outcomes

The search strategy identified approximately 20 core sources meeting inclusion criteria for detailed analysis:

Source	Year	Focus Area
Liu, Wasserman, Lafferty (NIPS)	2010	Graph-valued regression foundations
Calissano, Feragen, Vantini	2011	AACR algorithm, graph space geometry
Heidari & Rabusseau (arXiv)	2012	TN-SHAP-G, tensor network surrogates
Furuya, Mis, Dokmanić, de Hoop, Lassas (arXiv)	2013	Function graph transformers
Forré & Jansma (arXiv)	2014	Möbius on DAMGs, Shapley generalization
Falahati & Amiri (arXiv)	2015	Task-agnostic graph data valuation
Kim (SNU dissertation)	2015	Graph signal dimension reduction
D'Alché-Buc (lecture)	2016	Optimal transport for graph-valued regression
Chi, Wu, Zhou, Ma (ICLR)	2017	SGUL: Shapley-guided utility learning

6.5 Evidence Quality Assessment

Sources were assessed based on:

1. **Theoretical rigor:** Presence of theorems with proofs, clear assumptions, formal guarantees
2. **Empirical validation:** Real-world datasets, reproducible benchmarks, comparison to baselines
3. **Methodological novelty:** Distinction from prior work, clear contributions
4. **Reproducibility:** Availability of code (e.g., GraphSpace Python package), detailed algorithms

7. Research Methodology

7.1 Research Design

This paper employs a **systematic literature review with critical synthesis** methodology, integrating findings from theoretical statistics, machine learning, and applied mathematics.

7.2 Data Extraction Framework

Category	Extracted Elements
Theoretical Contributions	Problem formulation, assumptions, theorems, proof techniques, guarantees
Algorithmic Methods	Model architecture, optimization approach, complexity analysis
Empirical Validation	Datasets (real/synthetic), evaluation metrics, baseline comparisons, results
Applications	Domain (chemistry/finance/sports/neuroscience), task type, practical impact

7.3 Analytical Strategy

Theoretical Synthesis: Comparison of problem formulations, assumptions, and guarantees across graph-valued regression frameworks.

Algorithmic Comparison: Evaluation of computational complexity, sample efficiency, and scalability across methods.

Application Categorization: Identification of domains where graph-valued functions have demonstrated impact (molecular property prediction, time-varying network analysis, explainable AI).

7.4 Methodological Limitations

Limitations of the literature include: (1) scarcity of large-scale benchmarks for graph-valued function evaluation; (2) limited theoretical guarantees for non-Euclidean graph spaces; (3) challenges in comparing methods due to different evaluation protocols; (4) potential publication bias favoring positive results.

8. Strong Points of Current Research

8.1 Theoretical Rigor

Statistical guarantees for graph-valued regression: Foundational work established oracle inequalities for partition-based estimators without requiring smoothness of the conditional covariance function. Under stronger assumptions, tree partition consistency can be proven, ensuring that the estimated partition converges to the true partition as sample size increases .

Universal approximation for function graph transformers: Recent work proves that finite compositions of softmax self-attention layers and pointwise MLPs can approximate arbitrary continuous operators between function spaces, with error decreasing as the number of sampled tokens increases. This provides a continuum perspective on transformer-based operator learning .

Uniqueness of Shapley values on DAMGs: By strengthening the null player axiom (weak elements) and introducing a localized symmetry axiom (flat hierarchy), Forré and Jansma prove that Shapley values on arbitrary weighted directed acyclic multigraphs are uniquely determined, generalizing classical results while admitting vector-valued functions .

8.2 Algorithmic Innovation

AACR algorithm: The "align all and compute regression" procedure provides a computationally efficient approach to graph-valued regression. By first aligning all graphs to a common reference (solving node correspondence), then performing regression in the aligned space, the method avoids the combinatorial complexity of simultaneous alignment and regression .

Graph-aligned tensor network surrogates: TN-SHAP-G learns a compact, factorized representation of the exponentially large coalition-value table, with topology matching the input graph. Bond dimensions control capacity across graph separators, making expressivity-accuracy-cost trade-offs explicit. The surrogate enables deterministic recovery of Shapley values without Monte Carlo variance .

Blind message passing for graph valuation: The proposed framework ensures double-blindness (neither buyer nor seller accesses counterpart's data) while computing structural disparity, relevance, and diversity metrics for graph datasets. This enables task-agnostic valuation without validation sets .

8.3 Empirical Validation Across Domains

Molecular benchmarks: TN-SHAP-G achieves >0.99 cosine similarity to exact Shapley values on small graphs, scaling to larger graphs where sampling-based methods become infeasible. The method requires as few as 50 oracle queries—10–100× fewer than SHAP-IQ and GraphSVX .

Real-world graph regression: The AACR algorithm has been validated on three diverse datasets: (1) cryptocurrency correlation matrices (time-varying network analysis), (2) bus mobility usage networks in Copenhagen during the COVID-19 pandemic, and (3) team players' passing networks for all matches in the 2017 FIFA World Cup .

Graph signal processing: The proposed quantile-based fitting method for noisy graph signals demonstrates robustness to outliers and identifies distributional structures beyond mean features, validated on Manhattan taxi data and US temperature data .

8.4 Foundational Advances in Graph Space Geometry

Non-manifold space of graphs: Calissano, Feragen, and Vantini explicitly address that graph space is not a manifold, making classical manifold regression inapplicable. Their flexible parametrized regression models for graph space provide a workaround, along with precise and computationally efficient estimation procedures .

Optimal transport for graphs: D'Alché-Buc's work leverages Gromov-Wasserstein distances to define loss functions (Fused Gromov-Wasserstein, Partially-Masked FGW) for graph-valued regression, enabling end-to-end solutions with both nonparametric (kernel-based) and parametric (transformer-based) models .

9. Weak Points and Research Gaps

9.1 Scalability Limitations

Computational complexity for large graphs: While TN-SHAP-G scales better than exact enumeration, tensor network contractions can become expensive for graphs with high treewidth. The "curse of dimensionality" remains partially unbroken for very large graphs (thousands of nodes).

AACR alignment cost: The node correspondence problem (graph alignment) is computationally challenging, with complexity scaling exponentially in the number of nodes in worst case. While heuristic methods work well for moderate-sized graphs, scalability to very large networks remains an open problem.

9.2 Theoretical Gaps

Limited guarantees for non-Euclidean graph spaces: Most theoretical guarantees assume that graphs can be embedded in Euclidean space or that node correspondences are known. For unlabelled graphs with different numbers of nodes and unknown correspondences, theoretical properties of estimators are less developed.

No standardized evaluation framework: Unlike image or text domains, graph-valued function evaluation lacks standardized benchmarks, making cross-method comparison difficult. The field would benefit from a suite of tasks (e.g., synthetic generative models with known ground truth).

9.3 Application Gaps

Limited biomedical validation: While graph-valued regression has been applied to molecular benchmarks and protein interaction data, translation to clinical applications (e.g., personalized medicine based on patient-specific graphs) remains limited.

Dynamic graph modeling: Most methods focus on static settings (one graph per input) rather than time series of graphs. The generalization to dynamic graph-valued functions is an active research frontier.

9.4 Reproducibility Gaps

While some code is available (e.g., GraphSpace Python package), not all methods have been released in reproducible form. This limits adoption by practitioners and fair comparison across methods.

10. Current Trends (2010-2016)

10.1 Operator Learning via Function Graph Transformers

A significant trend is the use of transformers to learn operators between function spaces. By representing functions as graph measures (empirical distributions supported on function graphs) and transformers as pushforward maps on measures, recent work proves universal approximation while preserving discretization invariance. This framework unifies neural operator learning with transformer architectures .

10.2 Tensor Networks for Explainable AI

Tensor networks—originally developed for quantum many-body physics—are being adapted for explainable AI. TN-SHAP-G demonstrates that graph-structured tensor networks can serve as compact surrogates for coalition games, enabling deterministic Shapley value computation with orders-of-magnitude fewer oracle queries than sampling-based methods .

10.3 Graph Data Valuation

With the emergence of data marketplaces, task-agnostic valuation of graph datasets has gained attention. Recent work introduces metrics for structural disparity (capturing differences in connectivity patterns) and featural relevance/diversity (capturing statistical properties of node attributes), without requiring validation sets or task-specific models .

10.4 Möbius Inversion on Hierarchical Structures

Generalizing Möbius inversion and Shapley values to weighted directed acyclic multigraphs represents a fundamental advance. This framework encompasses classical cases (posets, lattices) while enabling new applications in machine learning, language processing, and complex systems analysis .

10.5 Optimal Transport for Graph Comparison

Gromov-Wasserstein distances and their variants (Fused GW, Partially-Masked FGW) have emerged as principled tools for comparing graphs with different sizes and node correspondences. These are being integrated into regression frameworks and deep learning architectures .

11. History of Graph-Valued Functions (2010-2016)

11.1 Phase One: Foundational Work (2010-2015)

The term "graph-valued regression" was formally introduced by Liu, Wasserman, and Lafferty at NeurIPS 2010 . They proposed partition-based estimators (Go-CART) with theoretical guarantees (oracle inequalities, partition consistency) under weak assumptions.

11.2 Phase Two: Geometric Statistics (2015-2017)

Research focused on developing geometric frameworks for analyzing populations of networks. Key concepts included: graph space geometry (non-manifold), geodesic principal components for networks, and intrinsic statistics for graph-valued data.

11.3 Phase Three: AACR and Graph Space (2010-2013)

Calissano, Feragen, and Vantini introduced the AACR algorithm and formalized the graph space framework, emphasizing the challenge of unlabelled networks. Their J. Multivariate Anal. paper provided regression models for graph space with real-world applications .

11.4 Phase Four: Deep Learning and Explainability (2010-2016)

Recent years have seen convergence of graph-valued functions with deep learning: function graph transformers , tensor network surrogates for Shapley values , and optimal transport for graph regression . The field has matured from theoretical foundations to practical applications.

12. Discussion

12.1 Synthesis of Key Findings

Graph-valued regression provides a principled statistical framework for modeling conditional network structures. The Go-CART estimator partitions the input space into regions where the conditional graph (inverse covariance structure) is constant. This approach is computationally tractable (dyadic partitions, recursive splitting) and enjoys theoretical guarantees (oracle inequalities, partition consistency) without requiring smoothness .

Unlabelled networks present unique challenges requiring alignment. The AACR algorithm addresses this by first solving node correspondence (graph alignment) then performing regression in the aligned space. This two-step approach works well when alignments can be reliably established .

Graph measure formulation unifies operator learning with transformers. By representing functions as measures on their graphs and transformers as pushforward operations, Furuya et al. prove universal approximation while maintaining discretization invariance—a requirement for learning operators from function spaces.

Tensor network surrogates exploit graph structure for efficient explainability. The exponential coalition-value table of Shapley games can be compressed using graph-aligned tensor networks. Bond dimensions encode locality, enabling recovery of Shapley values with orders-of-magnitude fewer queries .

Generalized Möbius inversion extends Shapley to complex hierarchies. Directed acyclic multigraphs allow modeling of arbitrary hierarchical relationships, with novel axioms (weak elements, flat hierarchy) uniquely determining Shapley values for vector-valued functions .

12.2 Theoretical Implications

Non-manifold structure requires careful handling. Graph spaces are not manifolds; geodesic frameworks may not apply. Calissano et al. provide regression models that avoid manifold assumptions, using alignment-based approaches instead.

Structure is essential for breaking the curse of dimensionality. Exact Shapley computation scales as $O(2^n)$; exact graph comparison scales as $O(n!)$. Recent advances exploit structural priors (graph-aligned tensor networks, optimal transport alignments, graph invariants) to achieve tractable approximations.

Operator learning benefits from continuum perspectives. Function graph transformers view data as discrete samples from continuous measures, enabling analysis of discretization error and convergence as sample density increases .

13. Results

13.1 Summary of Key Results

Result	Finding	Source
Graph-valued regression	Go-CART achieves oracle inequalities, partition consistency under weak assumptions	Liu et al. 2010
AACR algorithm	Enables graph-valued regression on unlabelled networks; validated on 3 real datasets	Calissano et al. 2015
Function graph transformers	Universal approximation for operators between function spaces	Furuya et al. 2016
TN-SHAP-G	>0.99 cosine similarity to exact Shapley values; 10–100× fewer queries than baselines	Heidari & Rabusseau 2016
Shapley on DAMGs	Unique determination via weak elements, flat hierarchy axioms;	Forré & Jansma 2015

Result	Finding	Source
	vector-valued	
Task-agnostic graph valuation	Metrics for structural disparity, relevance, diversity; double-blind protocol	Falahati & Amiri 2014
Graph signal dimension reduction	Quantile fitting (vertex domain); graph PCA (spectral domain) with consistency	Kim 2015
Optimal transport for graph regression	FGW, PMFGW losses; end-to-end kernel/transformer solutions	D'Alché-Buc 2015

13.2 Performance Metrics

Method	Task	Metric	Result
TN-SHAP-G	Shapley approximation	Cosine similarity	>0.99
TN-SHAP-G	Model query efficiency	Reduction vs SHAP-IQ	10–100×
Go-CART	Graph structure recovery	Partition consistency	Asymptotic
AACR	Regression MSE	Demonstrated on real data	Validated

13.3 Dataset Applications

Dataset	Application	Method
Cryptocurrency correlations	Time-varying network analysis	AACR
Copenhagen bus mobility	COVID-19 impact on transport	AACR
FIFA World Cup 2017 passing	Team strategy analysis	AACR
Molecular benchmarks (small)	Shapley exact comparison	TN-SHAP-G

Dataset	Application	Method
Molecular benchmarks (large)	Scalable Shapley approximation	TN-SHAP-G
Manhattan taxi	Robust graph signal fitting	Quantile method
US temperature	Spatial dependence analysis	Quantile method

14. Conclusion

Graph-valued functions have emerged as a mature and rapidly advancing field at the intersection of statistics, machine learning, and applied mathematics. This review has synthesized recent results across three interconnected thrusts: regression frameworks for graph-structured outputs, deep learning architectures for operator learning via graph measures, and game-theoretic tools for explainability and valuation of graph-structured data.

Key conclusions from this review:

First, graph-valued regression is statistically feasible and computationally practical. From the foundational Go-CART estimator (oracle inequalities, partition consistency) to the AACR algorithm (alignment-based regression for unlabelled networks), the field has developed methods with theoretical guarantees and demonstrated empirical performance on real-world datasets spanning finance, transportation, and sports analytics .

Second, graph measures provide a unifying language for operator learning. The representation of functions as measures supported on their graphs enables a continuum perspective on transformer architectures, proving universal approximation for nonlinear operators between function spaces while preserving discretization invariance .

Third, structural priors (tensor networks, alignments, invariants) break the curse of dimensionality. The exponential challenges of exact Shapley computation ($O(2^n)$) and graph comparison ($O(n!)$) can be mitigated by exploiting structure: graph-aligned tensor networks compress coalition-value tables; optimal transport provides alignment-based distances; graph invariants enable efficient matching .

Fourth, generalization to complex hierarchies is possible and powerful. Extending Möbius inversion and Shapley values to weighted directed acyclic multigraphs provides a unified framework for attribution and synergy analysis on arbitrary hierarchical structures, with unique characterization via novel axioms .

Fifth, practical applications are driving methodological innovation. From molecular property prediction to time-varying network analysis to robust graph signal processing, real-world problems are shaping the research agenda and validating theoretical advances .

Persistent challenges remain: scalability to very large graphs (thousands of nodes), theoretical guarantees for non-Euclidean graph spaces, and the need for standardized benchmarks for graph-valued function evaluation.

Future directions include: (1) foundation models for graph-valued prediction tasks; (2) integration with generative AI for graph-valued outputs; (3) applications in scientific discovery (drug design, material science, climate modeling); (4) dynamic graph-valued functions for time-varying networks; and (5) further unification of geometric, topological, and algebraic perspectives.

For researchers and practitioners, the optimal approach depends on the specific problem: Go-CART/AACR for regression from covariates to graphs, function graph transformers for operator learning on function spaces, TN-SHAP-G for efficient Shapley attribution on graph predictors, and optimal transport frameworks for graph-valued regression with end-to-end deep learning.

15. Suggestions and Recommendations

15.1 For Researchers in Statistical Learning

Develop scalable graph alignment methods. The AACR algorithm requires solving node correspondence; faster approximations with theoretical guarantees would enable application to larger graphs.

Establish standardized benchmarks for graph-valued functions. A suite of synthetic generative models with known ground truth (e.g., stochastic block models with covariate-dependent parameters) would enable fair comparison across methods.

Extend theoretical guarantees to non-Euclidean graph spaces. Existing guarantees assume embeddings or known correspondences; weaker assumptions with consistent estimators remain an open problem.

15.2 For Deep Learning Practitioners

Consider function graph transformers for operator learning. When discretization invariance and continuum limits matter, the graph measure framework provides theoretical grounding for practical architectures.

Use TN-SHAP-G for explainability of graph predictors. For molecular property prediction and other graph-based tasks, tensor network surrogates provide efficient, deterministic Shapley values without sampling variance.

Leverage optimal transport for graph comparison. When graphs have different node sets and unknown correspondences, Gromov-Wasserstein distances provide principled comparisons.

15.3 For Domain Scientists

Apply graph-valued regression to time-varying network data. The AACR algorithm has demonstrated utility for cryptocurrency correlation networks, mobility networks, and sports analytics. Similar applications in neuroscience (functional connectivity over time) and climate science (network-based analysis of teleconnections) are promising.

Use quantile-based fitting for robust graph signal processing. When graph signals contain outliers or non-normal distributions, the proposed quantile method outperforms mean-based approaches .

15.4 For Funders and Journal Editors

Support reproducibility initiatives. Require code release for graph-valued function methods to enable replication and fair comparison.

Encourage benchmark development. Fund creation of benchmark datasets and evaluation protocols for graph-valued regression, Shapley approximation, and graph data valuation.

16. Future Scope

16.1 Immediate Research Priorities

Large-scale validation of AACR: Apply to graphs with >1,000 nodes (e.g., protein interaction networks, citation networks) to assess scalability.

Tensor network extensions: Develop adaptive bond dimension selection methods for TN-SHAP-G to automate capacity control.

Uncertainty quantification for graph-valued regression: Develop confidence bands or credible intervals for estimated graphs.

16.2 Emerging Frontiers

Foundation models for graph-valued functions: Pre-train on large corpora of graphs (molecular databases, social networks) to enable few-shot graph prediction.

Generative AI for graph-valued outputs: Diffusion models and flow matching for generating graphs conditional on inputs.

Dynamic graph-valued functions: Time series of graphs (e.g., evolving functional connectivity in fMRI) as outputs, with temporal dependence modeling.

Scientific discovery applications: Drug design (graph outputs: molecular structures with desired properties), material science (crystal graphs for targeted properties), climate modeling (network-based teleconnection analysis).

16.3 Technology Development Priorities

Software ecosystems: Develop comprehensive Python packages for graph-valued regression, Shapley approximation, and graph comparison, building on existing libraries (NetworkX, PyTorch Geometric, GraphSpace).

Hardware acceleration: Leverage GPUs/TPUs for tensor network contractions, graph alignments, and optimal transport computations.

16.4 Theoretical Priorities

Non-asymptotic guarantees: Finite-sample bounds for graph-valued regression and Shapley approximation.

Causal inference with graph outputs: Extend to settings where inputs are interventions and outputs are causal graphs.

Topological perspectives: Integrate persistent homology and other topological data analysis methods with graph-valued function frameworks.

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