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Contents

Data Analytics on Graphs Part III: Machine Learning on Graphs, from Graph Topology to Applications

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ABSTRACT

Modern data analytics applications on graphs often operate on domains where graph topology is not known a priori, and hence its determination becomes part of the problem definition, rather than serving as prior knowledge which aids the problem solution. Part III of this monograph starts by a comprehensive account of ways to learn the pertinent graph topology, ranging from the simplest case where the physics of the problem already suggest a possible graph structure, through to general cases where the graph structure is to be learned from the data observed on a graph. A particular emphasis is placed on the use of standard "relationship measures" in this context, including the correlation and precision matrices, together with the ways to combine these

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with the available prior knowledge and structural conditions, such as the smoothness of the graph signals or sparsity of graph connections. Next, for learning sparse graphs (that is, graphs with a small number of edges), the utility of the least absolute shrinkage and selection operator, known as (LASSO) is addressed, along with its graph specific variant, the graphical LASSO. For completeness, both variants of LASSO are derived in an intuitive way, starting from basic principles. An in-depth elaboration of the graph topology learning paradigm is provided through examples on physically well defined graphs, such as electric circuits, linear heat transfer, social and computer networks, and spring-mass systems. We also review main trends in graph neural networks (GNN) and graph convolutional networks (GCN) from the perspective of graph signal filtering. Particular insight is given to the role of diffusion processes over graphs, to show that GCNs can be understood from the graph diffusion perspective. Given the largely heuristic nature of the existing GCNs, their treatment through graph diffusion processes may also serve as a basis for new designs of GCNs. Tensor representation of lattice-structured graphs is next considered, and it is shown that tensors (multidimensional data arrays) can be treated as a special class of graph signals, whereby the graph vertices reside on a high-dimensional regular lattice structure. Finally, the concept of graph tensor networks is shown to provide a unifying framework for learning of big data on irregular domains. This part of monograph concludes with an in-dept account of emerging applications in financial data processing and underground transportation network modeling. More specifically, by means of portfolio cuts of an asset graph, we show how domain knowledge can be meaningfully incorporated into investment analysis, while the underground transportation example addresses vulnerability of stations in the London underground network to traffic disruption.

Keywords: graph theory; random data on graphs; big data on graphs; signal processing on graphs; machine learning on graphs; graph topology learning; systems on graphs; vertex-frequency estimation; graph neural networks; graphs and tensors.

1

Introduction

Graph data analytics have already shown enormous potential, as their flexibility in the choice of graph topologies (irregular data domains) and connections between the entities (vertices) allows for both a rigorous account of irregularly spaced information such as locations and social connections, and also for the incorporation of semantic and contextual cues, even for otherwise regular structures such as images.

In Part I and Part II of this monograph, it was assumed that the graph itself is already defined prior to analyzing data on graphs. The focus of Part I has been on defining graph properties through the mathematical formalism of linear algebra, while Part II introduces graph counterparts of several important standard data analytics algorithms, again for a given graph. However, in many modern applications, graph topology is not known a priori (Cioacă *et al.*, 2019; Das *et al.*, 2017; Dong *et al.*, 2015, 2016; Epskamp and Fried, 2018; Friedman *et al.*, 2008; Hamon *et al.*, 2019, Meinshausen *et al.*, 2006; Pavez and Ortega, 2016; Pourahmadi, 2011; Rabiei *et al.*, 2019; Stanković *et al.*, 2018, 2020), and the focus of this part is therefore on simultaneous estimation of data on a graph and the underlying graph topology. Without loss of generality, it is convenient to assume that the vertices are given, while the edges and their associated weights are part of the solution to the problem considered and need to be estimated from the vertex geometry and/or the observed data (Bohannon *et al.*, 2019; Caetano *et al.*, 2009; Camponogara and Nazari, 2015; Dal Col *et al.*, 2019; Gu and Wang, 2019; Mao and Gu, 2019; Pasdeloup *et al.*, 2019; Slawski and Hein, 2015; Segarra *et al.*, 2016; Stanković and Sejdić, 2019; Stanković *et al.*, 2017; Tanaka and Sakiyama, 2019; Thanou *et al.*, 2014; Ubaru *et al.*, 2017; Yankelevsky and Elad, 2016; Zhao *et al.*, 2012; Zheng *et al.*, 2011).

Three scenarios for the estimation of graph edges from vertex geometry or data are considered in this part of the monograph.

- Based on the *geometry of vertex positions.* In various sensor network setups (such as temperature, pressure, and transportation), the locations of the sensing positions (vertices) are known beforehand, while the vertex distances convey physical meaning about data dependence and thus may be employed for edge/weight determination.

- Based on *data association and data similarity.* Various statistical measures are available to serve as data association metrics, with the covariance and precision matrices most commonly used. A strong correlation between data on two vertices would indicate a large weight associated with the corresponding edge. A small degree of correlation would indicate nonexistence of an edge (after weight thresholding).

- *Based on physically well defined relations among the sensing positions.* Examples include electric circuits, power networks, linear heat transfer, social and computer networks, spring-mass systems, to mention but a few. In these cases, edge weighting can usually be well defined based on the underlying context of the considered problem.

After a detailed elaboration of graph definition and graph topology learning techniques, a summary of graph topology learning from data using probabilistic generative models is given. This followed by an account of graph neural networks (GNN), with a special emphasis on graph convolutional networks (GCN). The analysis is considered from the perspective of graph signal filtering presented in Part II. Graph data analysis is further generalized to the tensor representation of lattice-structured graphs, whereby the graph vertices reside on a high-dimensional tensor structure. Finally, two applications of graph-based data analysis are given: (i) an example where domain knowledge is incorporated into financial data analysis (the investment analysis), by means of portfolio cuts; (ii) London underground transportation system. The latter example demonstrates how graph theory can be used to identify the stations in the London underground network which have the greatest influence on the functionality of the traffic, and also to assess the impact of a station closure on service levels across the city.

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