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Data Analytics on Graphs Part I: Graphs and Spectra on Graphs

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ABSTRACT

The area of Data Analytics on graphs promises a paradigm shift, as we approach information processing of new classes of data which are typically acquired on irregular but structured domains (such as social networks, various ad-hoc sensor networks). Yet, despite the long history of Graph Theory, current approaches tend to focus on aspects of optimisation of graphs themselves rather than on eliciting strategies relevant to the objective application of the graph paradigm, such as detection, estimation, statistical and probabilistic inference, clustering and separation from signals and data acquired on graphs. In order to bridge this gap, we first revisit graph topologies from a Data Analytics point of view, to establish a taxonomy of graph networks through a linear algebraic formalism of graph topology (vertices, connections, directivity). This serves as a basis for spectral

analysis of graphs, whereby the eigenvalues and eigenvectors of graph Laplacian and adjacency matrices are shown to convey physical meaning related to both graph topology and higher-order graph properties, such as cuts, walks, paths, and neighborhoods. Through a number of carefully chosen examples, we demonstrate that the isomorphic nature of graphs enables both the basic properties of data observed on graphs and their descriptors (features) to be preserved throughout the data analytics process, even in the case of reordering of graph vertices, where classical approaches fail. Next, to illustrate the richness and flexibility of estimation strategies performed on graph signals, spectral analysis of graphs is introduced through eigenanalysis of mathematical descriptors of graphs and in a generic way. Finally, benefiting from enhanced degrees of freedom associated with graph representations, a framework for vertex clustering and graph segmentation is established based on graph spectral representation (eigenanalysis) which demonstrates the power of graphs in various data association tasks, from image clustering and segmentation through to low-dimensional manifold representation. The supporting examples demonstrate the promise of Graph Data Analytics in modeling structural and functional/semantic inferences. At the same time, Part I serves as a basis for Part II and Part III which deal with theory, methods and applications of processing Data on Graphs and Graph Topology Learning from data.

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

Data analytics on graphs is a multidisciplinary research area, of which the roots can be traced back to the 1970s (Afrati and Constantinides, 1978; Christofides, 1975; Morris *et al.*, 1986), one that is witnessing significant rapid growth. The recent developments, in response to the requirements posed by radically new classes of data sources, typically embark upon the classical results on “static” graph topology optimization, to treat graphs as irregular data domains, which make it possible to address completely new paradigms of “information processing on graphs” and “signal processing on graphs”. This has already resulted in advanced and physically meaningful solutions in manifold applications (Grady and Polimeni, 2010; Jordan, 1998; Krim and Hamza, 2015; Marques *et al.*, 2017; Ray, 2012). For example, while the emerging areas of Graph Machine Learning (GML) and Graph Signal Processing (GSP) do comprise the classic methods of optimization of graphs themselves (Bapat, 1996; Bunse-Gerstner and Gragg, 1988; Fujiwara, 1995; Grebenkov and Nguyen, 2013; Jordan, 2004; Maheswari and Maheswari, 2016; O’Rourke *et al.*, 2016), significant progress has been made towards redefining basic data analysis objectives (spectral estimation, probabilistic inference, filtering, dimensionality reduction,

clustering, statistical learning), to make them amenable for direct estimation of signals on graphs (Chen *et al.*, 2014; Ekambaram, 2014; Gavili and Zhang, 2017; Hamon *et al.*, 2016a; Moura, 2018; Sandryhaila and Moura, 2013, 2014a,b; Shuman *et al.*, 2013; Vetterli *et al.*, 2014; Wainwright *et al.*, 2008). Indeed, this is a necessity in numerous practical scenarios where the signal domain is not designated by equidistant instants in time or a regular grid in a space or a transform domain. Examples include modern Data Analytics for e.g., social network modeling or in smart grid – data domains which are typically irregular and, in some cases, not even related to the notions of time or space, where ideally, the data sensing domain should also reflect domain-specific properties of the considered system/network; for example, in social or web related networks, the sensing points and their connectivity may be related to specific individuals, objectives, or topics, and their relations, whereby the processing on irregular domains requires the consideration of data properties other than time or space relationships. In addition, even for the data sensed in well-defined time and space domains, the new contextual and semantic-related relations between the sensing points, introduced through graphs, promise to equip problem definition with physical relevance, and consequently provide new insights into analysis and can lead to enhanced data processing results.

In applications which admit the definition of the data domain as a graph (such as social networks, power grids, vehicular networks, and brain connectivity), the role of classic temporal/spatial sampling points is assumed by graph vertices – the nodes – where the data values are observed, while the edges between vertices designate the existence and nature of vertex connections (directionality, strength). In this way, graphs are perfectly well equipped to exploit the fundamental relations among both the measured data and the underlying graph topology; this inherent ability to incorporate physically relevant data properties has made GSP and GML key technologies in the emerging field of Big Data Analytics (BDA). Indeed, in applications defined on irregular data domains, Graph Data Analytics (GDA) has been shown to offer a quantum step forward from the classical time (or space) series analyses (Brouwer and Haemers, 2012; Cvetković and Doob, 1985; Cvetković

and Gutman 2011; Cvetković *et al.*, 1980; Chung, 1997; Jones, 2013; Mejia *et al.*, 2017; Stanković *et al.*, 2017b, 2019), including the following aspects.

- Graph-based data processing approaches can be applied not only to technological, biological, and social networks, but also they can lead to both improvements of the existing and even to the creation of radically new methods in classical signal processing and machine learning (Dong *et al.*, 2012; Hamon *et al.*, 2016b; Horaud, 2009; Lu *et al.*, 2014; Masoumi and Hamza, 2017; Masoumi *et al.*, 2016; Stanković *et al.*, 2017a, 2018).
- The involvement of graphs makes it possible for the classical sensing domains of time and space (which may be represented as a linear or circular graph) to be structured in a more advanced way, e.g., by considering the connectivity of sensing points from a signal similarity or sensor association point of view.

The first step in graph data analytics is to decide on the properties of the graph as a new signal/information domain. However, while the data sensing points (graph vertices) may be well-defined by the application itself, that is not the case with their connectivity (graph edges), where:

- In the case of the various computer, social, road, transportation and electrical networks, the vertex connectivity is often naturally defined, resulting in an exact underlying graph topology.
- In many other cases, the data domain definition in a graph form becomes part of the problem definition itself, as is the case with, e.g., graphs for sensor networks, in finance or smart cities. In such cases, a vertex connectivity scheme needs to be determined based on the properties of the sensing positions or from the acquired data, as e.g., in the estimation of the temperature field in meteorology (Stanković *et al.*, 2019).

This additional aspect of the definition of an appropriate graph structure is of crucial importance for a meaningful and efficient application of the GML and GSP approaches.

With that in mind, this monograph was written in response to the urgent need of multidisciplinary data analytics communities for a seamless and rigorous transition from classical data analytics to the corresponding paradigms which operate directly on irregular graph domains. To this end, we start our approach from a review of basic definitions of graphs and their properties, followed by a physical intuition and step-by-step introduction of graph spectral analysis (eigen-analysis). Particular emphasis is on eigendecomposition of graph matrices, an area which serves as a basis for mathematical formalisms in graph signal and information processing. As an example of the ability of GML and GSP to generalize standard methodologies for graphs, we elaborate in a step-by-step way the introduction of Graph Discrete Fourier Transform (GDFT), and show that it simplifies into standard Discrete Fourier Transform (DFT) for directed circular graphs; this also exemplifies the generic nature of graph approaches. Finally, spectral vertex analysis and spectral graph segmentation are used as the basis for understanding relations among distinct but physically meaningful regions in graphs; this is demonstrated through examples of regional infrastructure modeling, brain connectivity, clustering, and dimensionality reduction.

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