



An Algebraic Approach to Inference in Complex Networked Structures

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14. ABSTRACT Analysis and processing of very large data sets, or big data, poses a significant challenge. Massive data sets are collected and studied in numerous domains, from engineering sciences to social networks, biomolecular research, commerce, and security. Extracting valuable information from big data requires innovative approaches that efficiently process large amounts of data and utilize their structure. This research project developed a paradigm for large-scale data analysis based on the discrete signal processing (DSP) on graphs (DSPG). DSPG extends signal processing concepts and methodologies from the classical signal processing theory to data indexed by general graphs. We introduced fundamental concepts of DSPG, including graph signals and graph filters, graph Fourier transform, graph frequency, and spectrum ordering that extended their counterparts from classical signal processing theory. Big data analysis presents several challenges to DSPG, in particular, in filtering and frequency analysis of very large data sets. We showed how to analyze these large data sets by considering product graphs as a graph model that helps extend the application of DSPG methods to large data sets through efficient implementations based on parallelization and vectorization. We illustrated the applicability of DSPG with numerous studies that are relevant in applications			
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THERE is an explosion of interest in processing and analyzing large datasets collected in very different settings, including social and economic networks, information networks, internet and the world wide web, immunization and epidemiology networks, molecular and gene regulatory networks, citation and coauthorship studies, friendship networks, as well as physical infrastructure networks like sensor networks, power grids, transportation networks, and other networked critical infrastructures. We briefly contrast our approach in this project with existing work.

A. Brief review of the literature

Many authors focus on the underlying *relational structure* of the data by: 1) inferring the structure from community relations and friendships, or from perceived alliances between agents as abstracted through game theoretic models [1], [2]; 2) quantifying the connectedness of the world; and 3) determining the relevance of particular agents, or studying the strength of their interactions. Other authors are interested in the *network function* by quantifying the impact of the network structure on the diffusion of disease, spread of news and information, voting trends, imitation and social influence, crowd behavior, failure propagation, global behaviors developing from seemingly random local interactions [2], [3], [4]. Much of these works either develop or assume network models that capture the interdependencies among the data and then analyze the structural properties of these networks. Models often considered may be deterministic like complete or regular graphs, or random like the Erdős-Rényi and Poisson graphs, the configuration and expected degree models, small world or scale free networks [2], [4], to mention a few. These models are used to quantify network characteristics, such as connectedness, existence and size of the giant component, distribution of component sizes, degree and clique distributions, and node or edge specific parameters including clustering coefficients, path length, diameter, betweenness and closeness centralities.

Another body of literature is concerned with inference and learning from such large datasets. Much work falls under the generic label of graphical models [5], [6], [7], [8], [9], [10]. In graphical models, data is viewed as a family of random variables indexed by the nodes of a graph, where the graph captures

probabilistic dependencies among data elements. The random variables are described by a family of joint probability distributions. For example, directed (acyclic) graphs [11], [12] represent Bayesian networks where each random variable is independent of others given the variables defined on its parent nodes. Undirected graphical models, also referred to as Markov random fields [13], [14], describe data where the variables defined on two sets of nodes separated by a boundary set of nodes are statistically independent given the variables on the boundary set. A key tool in graphical models is the Hammersley-Clifford theorem [13], [15], [16], and the Markov-Gibbs equivalence that, under appropriate positivity conditions, factors the joint distribution of the graphical model as a product of potentials defined on the cliques of the graph. Graphical models exploit this factorization and the structure of the indexing graph to develop efficient algorithms for inference by controlling their computational cost. Inference in graphical models is generally defined as finding from the joint distributions lower order marginal distributions, likelihoods, modes, and other moments of individual variables or their subsets. Common inference algorithms include belief propagation and its generalizations, as well as other message passing algorithms. A recent block-graph algorithm for fast approximate inference, in which the nodes are non-overlapping clusters of nodes from the original graph, is in [17]. Graphical models are employed in many areas; for sample applications, see [18] and references therein.

Extensive work is dedicated to discovering efficient data representations for large high-dimensional data [19], [20], [21], [22]. Many of these works use spectral graph theory and the graph Laplacian [23] to derive low-dimensional representations by projecting the data on a low-dimensional subspace generated by a small subset of the Laplacian eigenbasis. The graph Laplacian approximates the Laplace-Beltrami operator on a compact manifold [21], [24], in the sense that if the dataset is large and samples uniformly randomly a low-dimensional manifold then the (empirical) graph Laplacian acting on a smooth function on this manifold is a good discrete approximation that converges pointwise and uniformly to the elliptic Laplace-Beltrami operator applied to this function as the number of points goes to infinity [25], [26], [27]. One can go beyond the choice of the graph Laplacian by choosing discrete approximations to other continuous operators and obtaining possibly more desirable spectral bases for the characterization of the geometry of the manifold underlying the data. For example, if the data represents a non-uniform sampling of a continuous manifold, a conjugate to an elliptic Schrödinger-type operator can be used [28], [29], [30].

More in line with the research we developed in this project, several works have proposed multiple transforms for data indexed by graphs. Examples include regression algorithms [31], wavelet decompositions [30], [32], [33], [34], [35], filter banks on graphs [36], [37], de-noising [38], and compression [39]. Some of these transforms focus on distributed processing of data from sensor fields while addressing sampling irregularities due to random sensor placement. Others consider localized processing of signals on graphs in multiresolution fashion by representing data using wavelet-like bases with varying “smoothness” or defining transforms based on node neighborhoods. In the latter case, the graph Laplacian and its eigenbasis are sometimes used to define a spectrum and a Fourier transform of a

signal on a graph. This definition of a Fourier transform was also proposed for use in uncertainty analysis on graphs [40], [41]. This graph Fourier transform is derived from the graph Laplacian and restricted to undirected graphs with real, non-negative edge weights, not extending to data indexed by directed graphs or graphs with negative or complex weights.

The algebraic signal processing (ASP) theory [42], [43], [44], [45] is a formal, algebraic approach to analyze data indexed by special types of line graphs and lattices. The theory uses an algebraic representation of signals and filters as polynomials to derive fundamental signal processing concepts. This framework has been used for discovery of fast computational algorithms for discrete signal transforms [42], [46], [47]. It was extended to multidimensional signals and nearest neighbor graphs [48], [49] and applied in signal compression [50], [51]. The framework proposed that we developed in this project generalizes and extends the ASP to signals on arbitrary graphs.

B. Overview of our contributions

Our goal was to develop a linear discrete signal processing (DSP) framework and corresponding tools for datasets arising from social, biological, and physical networks. DSP has been very successful in processing time signals (such as speech, communications, radar, or econometric time series), space-dependent signals (images and other multidimensional signals like seismic and hyperspectral data), and time-space signals (video). We refer to data *indexed* by nodes of a graph as a *graph signal* or simply signal and to our approach as *DSP on graphs* DSP_G . We developed the basics of linear DSP_G , including the notion of a shift on a graph, graph filter structure, graph filtering and graph convolution, graph signal and graph filter spaces and their algebraic structure, the graph Fourier transform, graph frequency, graph spectrum, graph spectral decomposition, and graph impulse and graph frequency responses. With respect to other works, ours is a deterministic framework to signal processing on graphs rather than a statistical approach like graphical models. Our work is an extension and generalization of the traditional DSP, and generalizes the Algebraic Signal Processing theory [42], [43], [44], [45] and its extensions and applications [49], [50], [51]. We emphasize here the contrast between the DSP_G and the approach to the graph Fourier transform that takes the graph Laplacian as a point of departure [32], [35], [36], [38], [39], [41]. In the latter case, the Fourier transform on graphs is given by the eigenbasis of the graph Laplacian. However, this definition is not applicable to directed graphs, which often arise in real-world problems, and graphs with negative weights. In general, the graph Laplacian is a second-order operator for signals on a graph, whereas an adjacency matrix is a first-order operator. Deriving a graph Fourier transform from the graph Laplacian is analogous in traditional DSP to restricting signals to be even (like correlation sequences) and Fourier transforms to represent power spectral densities of signals. Instead, we demonstrated that the graph Fourier transform is properly defined through the Jordan normal form and generalized eigenbasis of the adjacency matrix. Finally, we illustrate the DSP_G with applications like classification, compression, and linear prediction for datasets that include blogs, customers of a mobile operator, or collected by a network of irregularly placed weather stations, under many other applications.

Summary of results

DSP_G extended the algebraic signal processing (ASP) theory introduced in [42],[43],[44], [45],[46] where the shift is the elementary non-trivial filter that generates, under an appropriate notion of shift invariance, all linear shift-invariant filters for a given class of signals. Our key insight in DSP_G to build the theory of signal processing on graphs is to identify the shift operator. We adopted the weighted adjacency matrix of the graph as the shift operator and then developed appropriate concepts of z-transform, impulse and frequency response, filtering, convolution, and Fourier transform. In particular, the graph Fourier transform in this framework expands a graph signal into a basis of eigenvectors of the adjacency matrix, and the corresponding spectrum is given by the eigenvalues of the adjacency matrix.

The association of the graph shift with the adjacency matrix in DSP_G is natural and has multiple intuitive interpretations. The graph shift is an elementary filter, and its output is a graph signal with the value at vertex n of the graph given approximately by a weighted linear combination of the input signal values at graph neighbors of n . With appropriate edge weights, the graph shift can be interpreted as a (minimum mean square) first-order linear predictor. Another interpretation in DSP_G of the graph shift comes from Markov chain theory [52], where the adjacency matrix represents the one-step transition probability matrix of the chain governing its dynamics. Finally, the graph shift can also be seen as a stencil approximation of the first-order derivative on the graph.

Because the eigenvalues of the graph shift are in general complex valued, there is an issue that arises in DSP_G with defining low and high frequencies, and low-pass, band-pass, and high-pass graph signals or graph filters. In DSP_G , we defined low and high frequencies and low-, high-, and band-pass graph signals and filters on generic graphs in a novel way. In traditional discrete signal processing (DSP), these concepts have an intuitive interpretation, since the frequency contents of time series and digital images are described by complex or real sinusoids that oscillate at different rates [33]. The oscillation rates provide a physical notion of “low” and “high” frequencies: low-frequency components oscillate less and high-frequency ones oscillate more. However, these concepts do not have a similar interpretation on graphs, and it was not obvious how to order graph frequencies to describe the low- and high-frequency contents of a graph signal.

In DSP_G , we developed an ordering of the graph frequencies that is based on how “oscillatory” the graph spectral components are with respect to the indexing graph, i.e., how much they change from a node to neighboring nodes. To quantify this amount, we introduced the graph total variation function that measures how much signal samples (values of a graph signal at a node) vary in comparison to neighboring samples. This approach is analogous to the approach taken in classical DSP theory, where the oscillations in time and image signals are also quantified by appropriately defined total variations [33]. Once we have an ordering of the frequencies based on the graph total variation function, we define the notions of low and high frequencies, as well as low-, high-, and band-pass graph signals and graph filters.

We applied DSP_G in a number of important applications, demonstrating not only its wide applicability as well as the gains of performance it affords when analyzing signals indexed by nodes of a graph. Applications we considered included: signal recovery on graphs, classification, compression, semi-supervised learning, detection of anomalies, and sensor network analysis. For example, signal recovery on graphs recovers one or multiple smooth graph signals from noisy, corrupted, or incomplete measurements. We formulated graph signal recovery as an optimization problem, for which we provided a general solution through the alternating direction methods of multipliers. We showed how signal inpainting, matrix completion, robust principal component analysis, and anomaly detection all relate to graph signal recovery and provided corresponding specific solutions and theoretical analysis. We validated the proposed methods on real-world recovery problems, including online blog classification, bridge condition identification, temperature estimation, recommender system for jokes, and expert opinion combination of online blog classification. On another set of studies, we showed that naturally occurring graph signals, such as measurements of physical quantities collected by sensor networks or labels of objects in a dataset, tend to be low-frequency graph signals, while anomalies in sensor measurements or missing data labels can amplify high-frequency parts of the signals. We demonstrated how these anomalies can be detected using appropriately designed high-pass graph filters, and how unknown parts of graph signals can be recovered with appropriately designed regularization techniques. In particular, our experiments showed that classifiers designed using the graph shift matrix lead to higher classification accuracy than classifiers based on the graph Laplacian matrices, combinatorial or normalized.

The specific framework, theoretical results, analysis methods, and application studies carried out were detailed in papers [1] through [12], see Section C.

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Abstract

Analysis and processing of very large data sets, or big data, poses a significant challenge. Massive data sets are collected and studied in numerous domains, from engineering sciences to social networks, biomolecular research, commerce, and security. Extracting valuable information from big data requires innovative approaches that efficiently process large amounts of data and utilize their structure. This research project developed a paradigm for large-scale data analysis based on the discrete signal processing (DSP) on graphs (DSPG). DSPG extends signal processing concepts and methodologies from the classical signal processing theory to data indexed by general graphs. We introduced fundamental concepts of DSPG, including graph signals and graph filters, graph Fourier transform, graph frequency, and spectrum ordering that extended their counterparts from classical signal processing theory. Big data analysis presents several challenges to DSPG, in particular, in filtering and frequency analysis of very large data sets. We showed how to analyze these large data sets by considering product graphs as a graph model that helps extend the application of DSPG methods to large data sets through efficient implementations based on parallelization and vectorization. We illustrated the applicability of DSPG with numerous studies that are relevant in applications.

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Changes in research objectives (if any):

None

Change in AFOSR Program Manager, if any:

Initially, our PM was Dr. Robert Bonneau. After Dr. Bonneau left AFOSR, our PM is Fr. Benjamin Knott.

Extensions granted or milestones slipped, if any:

None.

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, \$K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

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