A Markov Variation Approach to Smooth Graph Signal Interpolation

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Abstract—In this paper we present the Markov variation, a smoothness measure which offers a probabilistic interpretation of graph signal smoothness. This measure is then used to develop an optimization framework for graph signal interpolation. Our approach is based on diffusion embedding vectors and the connection between diffusion maps and signal processing on graphs. As diffusion embedding vectors may be expensive to compute for large graphs, we present a computationally efficient method, based on the Nyström extension, for interpolation of signals over a graph. We demonstrate our approach on the MNIST dataset and a dataset of daily average temperatures around the US. We show that our method outperforms state of the art graph signal interpolation techniques on both datasets, and that our computationally efficient reconstruction achieves slightly reduced accuracy with a large computational speedup.

I. INTRODUCTION

With the advent of the world wide web and the move to cloud based computing, massive amounts of data have become increasingly available. The data may be collected from sources such as social networks, government agencies, commercial and academic bodies and more. Such data sets can include, for example, blogs, temperature measurements and information on customer preferences. Graphs are a popular model for the underlying geometry of data. Each data element (point) is represented as a node, and the pairwise connections between the different points are modeled as edges.

As an example, consider a data set of images of written digits, e.g. the MNIST data set [1]. Each data point is an image of a digit, and is represented as a node. The similarity between two points (i.e. two images of digits) is expressed through the edge weights. In the context of social networks, each user is a node in the graph, and the relationships between users are modeled as edge weights [2]. Such relationships may be for example friendship or collaboration.

Graph signals are signals defined over irregular domains represented as weighted graphs [3], [4], [5], [6], [7]. The signal is defined as a mapping of each node in a graph to a scalar [4], [5], [6], [8], and can be represented as a vector in \( \mathbb{R}^N \).

In this paper we focus on a subclass of graph signals, namely smooth graph signals. Such signals are a mapping of each node to a scalar (real or complex) such that the geometry of the graph is adhered to. A vector (signal) that obeys the graph geometry will be smooth over the edges of the graph. This smoothness is determined through a measure which assigns a numerical value detailing the change of the signal over the graph edges. Smoothness criteria have been discussed, for example, in [7], [9]. Here we suggest a measure based on the Markov variation, which is a probabilistic smoothness measure for graph signals. The probabilistic nature of our criterion is due to our use of the Markov matrix \( P \) to encode the geometry of the graph. The \( i/j \)th entry of this matrix can be considered as the probability to transition from node \( i \) to node \( j \).

Our graph signal smoothness criterion is used to suggest three methods for graph signal interpolation. Graph signal interpolation, or semi-supervised learning of graph signals, is the problem where a graph signal is known over a subset of nodes (the sampled nodes), and the goal is to recover the entire signal from its samples. The importance of this problem lies in the fact that for large graphs computing or measuring the entire signal may be very expensive.

The first interpolation method we suggest uses our smoothness criterion to define a system of linear equations over the sampled nodes. These equations impose smoothness over each of the samples individually. Therefore, all possible solutions must be smooth over the neighborhood of the sampled nodes. Next, we propose an extension to our suggested method, where the interpolation is performed iteratively. In iteration \( i \), we interpolate over all nodes in the \( 0, 1, \ldots, i \)th neighborhoods of any of the sampled nodes. That is, in the first iteration, the interpolation is done over the sampled nodes. In the second iteration, we interpolate over the sampled nodes and all nodes that are adjacent to a sampled node, and so on. In this way, the final solution is guaranteed to be smooth over all the nodes.

Both interpolation methods discussed above necessitate computation of the spectral decomposition of the graph shift operator, which may be infeasible for big data. We therefore introduce a computationally efficient approximation of our method which is derived using properties of the Markov matrix and a variation on the Nyström extension which we previ-
ously introduced in [10], [11]. This approximation achieves good accuracy in comparatively short runtimes, is feasible for massive datasets and makes no assumption on the sampling of the graph signals. As with the first method we discuss, this approximation can also be extended to be implemented iteratively. The Nyström extension variation we suggest can also be utilized for spectral regression [12] and for the method in [13] with minor modifications. These modifications are necessary since our smoothness interpolation method, as well as spectral regression, use the Markov matrix to define the connectivity of the graph while [13] uses the normalized graph Laplacian.

We provide a mathematical comparison between our interpolation techniques with existing state-of-the-art methods [6], [12], [14], [13], [15], [16] in Section IV-C. Furthermore, in Section VI, we use the sampling suggested by Chen et al. [6] to compare our first two interpolation methods with [6] and [16] on the MNIST dataset of hand-written digits [1]. We also use this sampling to compare our iterative method with spectral regression [12], noiseless inpainting [17], [18], [19] on both a synthetic dataset and a dataset of temperature measurements across the US [20]. We show that our interpolation techniques outperform all these methods, and that our iterative interpolation achieves good results even when a small number of samples (10 – 20) is used.

This paper is organized as follows. Section II contains background on the field of signal processing on graphs and the graph signal interpolation problem. In Section III we introduce our smoothness measure for signals defined on graphs. In Section IV we present our framework for graph signal interpolation. We present our computationally efficient variant in Section V. Finally, experimental results demonstrating our proposed graph interpolation methods are presented in Section VI.

II. PROBLEM FORMULATION

A graph is denoted as $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where $\mathcal{V}$ is the set of nodes and $\mathcal{E}$ is the set of edges. For weighted graphs we denote the affinity matrix containing edge weights as $W$. The $ij$th element of the affinity matrix specifies the weight of an edge between node $v_i$ and node $v_j$. If no edge exists between these nodes, then $W_{i,j}$ is set to 0.

A signal over a graph is defined in the literature as a mapping from each node $v_i$ to a real or complex scalar value $s_i$ [4], [5], [6], [8]. The pairwise (edge) information of the graph is contained in the graph shift operator $A$ [4]. The graph shift operator is a weighted adjacency matrix where the $ij$th entry corresponds to the pairwise relationship between nodes $v_i$ and $v_j$. This operator may be the affinity matrix $W$, the graph Laplacian $L$ or the Markov matrix $P$.

The graph shift operator is used to generalize operations in signal processing to graphs. One such operation is the graph shift operation [5], which is defined as

$$\hat{s} = As.$$  

(1)

This operation redistributes the graph signal at each node according to its neighborhood and is a generalization of time shifts [4].

The graph shift operator is also used in the definition of the graph Fourier transform (GFT) [4], which is defined as

$$\hat{s} = V^{-1}s.$$  

(2)

If the graph shift is diagonalizable then $V$ is the matrix containing in its columns the eigenvectors of the graph shift operator. Otherwise, $V$ is the matrix containing in its columns the generalized eigenvectors of the graph shift operator. The vector $\hat{s}$ is the spectrum of the graph signal. When this spectrum contains $k$ nonzero entries, we say that the graph signal is $k$-bandlimited [6].

In this paper, we focus on smooth graph signals. Such signals are mappings from each node $v_i$ to a real or complex scalar value $s_i$, such that the vector $s = [s_1 \cdots s_N]^T \in \mathbb{C}^N$ is smooth over the graph. Under this definition, the geometry of the graph will contain information about the graph signal, and the graph signal contains geometric information.

We consider the problem of graph signal interpolation, where a smooth graph signal is recovered from its samples and the known graph structure. We denote the set of $r$ sampled nodes as $\mathcal{M}$ and the vector of samples as $s_{\mathcal{M}} \in \mathbb{R}^{r \times 1}$. For this problem, perfect reconstruction is possible for $k$-bandlimited graph signals under conditions formulated in [6], [13]. Specifically, a bandlimited graph signal can be perfectly recovered from its samples if the matrix produced by sampling the $k$ eigenvectors at the rows corresponding to the known graph signal is invertible.

In the following sections, we will present three algorithms for smooth graph signal interpolation. In two of these solutions, perfect reconstruction is guaranteed under the conditions specified above. Our third method is characterized by reduced computational complexity and, as a result, fast runtimes. Our techniques are based on the Markov variation, a smoothness measure which we motivate and introduce in the next section.

III. SMOOTH GRAPH SIGNALS

As mentioned in Section II, we consider the problem of graph signal interpolation, where a smooth graph signal is recovered from its samples. The smoothness of a signal is to be determined through a measure which assigns a numerical value detailing the change of the signal over the graph edges. Examples of such measures include the total variation measure, defined as in [5],

$$TV(s) = \|s - \tilde{A}s\|_p,$$  

(3)

where $\tilde{A}$ is a normalization of the graph shift operator (the weighted adjacency matrix) such that the largest magnitude eigenvalue is equal to one.

An alternative smoothness measure, related to edge derivatives [7], [9], is given by

$$s^T Ls = \frac{1}{2} \sum_{i=1}^{N} \sum_{m=1}^{N} W_{i,m} (s_i - s_m)^2$$  

(4)

where $W$ is the symmetric affinity matrix, $L$ is the unnormalized graph Laplacian $L = D - W$ and $D$ so the diagonal matrix that contains in its diagonal the degree of each node.
There are two properties of smoothness we would like to ensure in our smoothness measure. First, we would like the smoothness measure to reach a global minimum for a constant graph signal (that is, a graph signal that maps every node to the same scalar value). The second property is that the smoothness measure can distinguish between graph signals that are smooth across each edge of the graph individually, and graph signals that are smooth across all incident edges.

To test the first property, we consider all signals of the form
\[ s_1 = c1, \]
where \(1\) is the all ones vector and \(c \in \mathbb{C}\). Signals of this form do not change between any two nodes in the graph, and are therefore the smoothest possible graph signals. The measure \((4)\) will indeed reach a global minimum for such signals as \(L\) is known to be positive semi-definite and as such
\[ s^T L s \geq 0 \]
and, additionally
\[ s^T L s_1 = \frac{1}{2} \sum_{i=1}^{N} \sum_{m=1}^{N} W_{i,m} (c - c)^2 = 0. \]

However, the total variation smoothness measure may violate this criterion. The total variation of \(s_1\) is
\[ TV(s_1) = \|c1 - c1\|_p, \]
where \(D\) is the matrix containing in its diagonal the degrees of \(A\). This will equal \(0\) when \(D\) is the identity matrix. Otherwise, there is no guarantee that the total variation will reach a global minimum for signals of the form \(s_1\).

As for the second property, we consider the following affinity matrix
\[ A = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}, \]
and the graph signals,
\[ s_2 = [0 \ -2 \ -2 \ 2 \ 2]^T, \]
\[ s_3 = [0 \ 2 \ 2 \ 2 \ 2]^T. \]

When evaluating the change of signal over each edge independently, these signals are equally smooth. However, when considering the change of signal across all edges incident to each node, \(s_2\) is smoother than \(s_3\). According to \((4)\) these signals are equally smooth, since
\[ s^T L s_2 = \frac{1}{2} \sum_{i=1}^{N} \sum_{m=1}^{N} 4W_{i,m} = s^T L s_3. \]

The reason for this is that \((4)\) takes into account only the magnitude of the difference between the graph signal on adjacent nodes. In other words, the change of a graph signal across edge \(e_i\) is independent of the change across all edges incident to \(e_i\).

In this paper we suggest an additional smoothness measure, the Markov variation. This measure has a probabilistic nature, which ensures that both aforementioned qualities are attained. That is, the Markov variation will reach a global minimum for signals of the form \(s_1\), and, additionally, takes into account the changes across all incident edges. The Markov variation is the measure
\[ ||s - D^{-1}As||, \]
where \(D\) is the diagonal matrix containing the degrees of \(A\). This measure is similar to total variation, the difference being in the suggested normalization of the graph shift operator. For \(A = P\) the Markov variation and the total variation will equal.

To gain intuition into this measure, we consider a smooth graph signal \(s \in \mathbb{R}^N\). Since \(s\) should map closely connected nodes to similar values, we can think of the graph signal at the nodes neighboring \(v_i\) (i.e. \(\{s_j\}_{j \in N_i}\)) as defining a distribution over \(s_i\). We therefore model \(s_i\) as
\[ s_i = \sum_{m \in N_i} P_{i,m} s_m + \epsilon(s_i), \]
where \(P\) is the Markov transition matrix,
\[ P = D^{-1}A, \]
\(N_i\) is the set of nodes adjacent to \(v_i\) and \(\epsilon\) is the error.

The model in \((9)\) consists of two terms. The first is an estimate of the graph signal \(s_i\) based only on the neighboring nodes and transition probabilities. This is a Markovian model, where the assumption is that when the graph signals at neighboring nodes are known, there is no dependence on non-neighboring nodes. Since we focus on graph signals whose mappings conform to the geometry of the graph, the transition probabilities between two neighboring nodes can be thought of as an approximation of the probability of both nodes having the same graph signal. Thus, for any smooth graph signal \(s\) we expect \(s_i - \sum_{m \in N_i} P_{i,m} s_m\) to be small. This difference corresponds to the second term in \((9)\) which is an error term \(\epsilon\) that explains variations from the weighted sum of neighbors.

Our suggested measure, which we call the Markov variation, is the norm of the error term
\[ MV(s) = ||\epsilon(s)||_p = ||s - D^{-1}As|| = ||s - Ps||_p. \]

For example, using the \(\ell_1\) norm we obtain
\[ ||s - Ps||_1 = \sum_{i=1}^{N} \frac{1}{d(v_i)} \left| \sum_{m=1}^{N} W_{i,m} (s_i - s_m) \right|. \]

We define a smooth graph signal as a vector \(s \in \mathbb{R}^N\) with low Markov variation, i.e.,
\[ ||s - Ps||_p < \eta, \]
where \(\eta\) is determined according to the number of nodes in the graph.

The Markov variation bears some similarity to both \((3)\) and \((4)\), while offering a probabilistic interpretation. Due to its probabilistic nature, this measure reaches a global minimum for \(s_1\), that is
\[ MV(s_1) = ||c1 - c1P1|| = ||c1 - c1|| = 0. \]
Furthermore, when considering the change of signal across all edges incident to each node, \( s_2 \) is smoother than \( s_3 \)

\[
MV (s_2) = \|s_2 - Ps_2\|_2 = 4, \quad (14)
\]

\[
MV (s_3) = \|s_3 - Ps_3\|_2 = 4.47. \quad (15)
\]

Once again, the Markov variation attains this property due to its probabilistic nature.

**IV. GRAPH SIGNAL INTERPOLATION**

We now show how the Markov variation can be used for interpolation of smooth graph signals from \( r \) samples, where each sample is a mapping of a node to a known scalar. To this end, we first provide a spectral interpretation of the Markov variation, and connect it to diffusion maps [21]. We then use these properties to show that the spectrum of a smooth graph signal is naturally sparse. Based on these insights, in Section IV-B, we formulate the interpolation of smooth graph signals as a constrained optimization problem.

We denote the set of \( r \) sampled nodes as \( \mathcal{M} \) and the vector of samples as \( s_{\mathcal{M}} \in \mathbb{R}^{r \times 1} \). Our goal is to recover a smooth graph signal \( s \) from \( s_{\mathcal{M}} \) using the known graph structure.

**A. Spectral Interpretation of the Markov Variation**

The Markov variation expresses an equivalence between smoothness measured over the edges of the graph and smoothness measured over diffusion embedding vectors [21], [10], which are defined as

\[
\Psi_t (i) = \begin{bmatrix} \lambda_1 \psi_1 (i) \\ \lambda_2 \psi_2 (i) \\ \vdots \\ \lambda_N \psi_N (i) \end{bmatrix}, \quad i = 1, \ldots, N, \quad (16)
\]

where \( \lambda_i \) and \( \psi_i \) are the \( i \)th eigenvalue and eigenvector of the Markov matrix \( P \), correspondingly, and \( t \) is a scale factor.

Since the Markov matrix is diagonalizable for undirected graphs (see Appendix A), (10) can be written as

\[
\|s - Ps\|_p = \|s - V \Lambda V^{-1} s\|_p, \quad (17)
\]

where \( \Lambda \) is a diagonal matrix that contains the eigenvalues of the Markov matrix. In general, the diffusion embedding vectors can be expressed as \( \Psi_t = \Psi_t \Lambda \Psi_t \), where the \( i \)th row of \( \Psi_t \) equals

\[
\Psi_t^T (i) = \begin{bmatrix} \lambda_1 \psi_1 (i) \\ \lambda_2 \psi_2 (i) \\ \vdots \\ \lambda_N \psi_N (i) \end{bmatrix}. \quad (18)
\]

The \( \ell_p \) norm of (12) can thus be written as

\[
\|s - Ps\|_p = \sum_{i=1}^{N} |s_i - \Psi_t^T (i) \hat{s}|^p < \eta^p, \quad (19)
\]

which implies that for a vector \( s \) to be a smooth graph signal, \( s_1 \) must be close to \( s_j \) if \( \Psi_1 (i) \) and \( \Psi_1 (j) \) are close in the \( \ell_2 \) sense.

We conclude that on the one hand the Markov variation can be expressed as a connection between the graph signal and the geometry of the graph in the graph domain. On the other hand, the smoothness function can be expressed as a connection between the spectrum of the graph signal and the diffusion embedding vectors in the frequency domain.

Another important conclusion can be obtained from

\[
\|s - Ps\|_p = \|V (I_N - \Lambda) \hat{s}\|_p < \eta^p. \quad (20)
\]

Since the largest eigenvalue of the Markov matrix is 1 (see Appendix A) and the magnitude of the smaller eigenvalues is often 0, the entries of \( \hat{s} \) that are related to the highest eigenvalues do not contribute much to the sum (20). The entries of \( \hat{s} \) that correspond to the lower eigenvalues have a higher impact on the sum (20). This means that, in order for a signal \( s \) to be a smooth graph signal, many of the entries of \( \hat{s} \) that correspond to the lower valued eigenvalues must be negligible. In other words, the spectrum of a smooth graph signal is naturally approximately sparse.\(^1\)

**B. Interpolation by Smoothness**

As the graph signal is smooth, we conclude from (19) that for each node \( i \)

\[
s_i \approx \Psi_t^T (i) \hat{s}. \quad (21)
\]

If the signal \( s \) is the smoothest possible signal according to the Markov variation (i.e., the error term is 0), then

\[
s_i = \Psi_t^T (i) \hat{s}, \quad (22)
\]

which leads to the following system of equations

\[
\begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_N \end{bmatrix} = \begin{bmatrix} \lambda_1 \psi_1 (1) & \lambda_2 \psi_2 (1) & \cdots & \lambda_N \psi_N (1) \\ \lambda_1 \psi_1 (2) & \lambda_2 \psi_2 (2) & \cdots & \lambda_N \psi_N (2) \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_1 \psi_1 (N) & \lambda_2 \psi_2 (N) & \cdots & \lambda_N \psi_N (N) \end{bmatrix} \begin{bmatrix} \hat{s}_1 \\ \hat{s}_2 \\ \vdots \\ \hat{s}_N \end{bmatrix}. \quad (23)
\]

Out of these \( N \) equations, we examine those that correspond to the known graph signal

\[
s_{\mathcal{M}} = [\lambda_1 \psi_1 (M) \lambda_2 \psi_2 (M) \cdots \lambda_N \psi_N (M)] \hat{s}, \quad (24)
\]

where \( \psi_i (M) \) is the sub-vector of \( \psi_i \) that contains only the entries at the set of indices \( \mathcal{M} \).

The solution of (24) is not unique. One such solution is for example the least squares vector,

\[
\arg \min_{\hat{s}} \|A \hat{s} - s_{\mathcal{M}}\|_2 \quad (25)
\]

where

\[
A = [\lambda_1 \psi_1 (M) \lambda_2 \psi_2 (M) \cdots \lambda_N \psi_N (M)]. \quad (26)
\]

The least squares solution ignores our prior knowledge concerning the sparsity of the graph signal. Therefore, rather than using this solution, we search for the subset of eigenvectors of the Markov matrix that best explain the known portion of the graph signal. This leads to the following sparse optimization problem:

\[
\hat{s} = \arg \min_{y} \|y\|_0 \quad \text{such that} \quad [\lambda_1 \psi_1 (M) \lambda_2 \psi_2 (M) \cdots \lambda_N \psi_N (M)] y = s_{\mathcal{M}}. \quad (27)
\]

\(^1\)We note that while we show this only for the case where the graph shift is the Markov matrix, it is true also for general graph shifts [6].
The solution to (27) is the sparse spectrum of a signal that is consistent with $\textbf{s}_M$ and is smooth in the neighborhood of the nodes in $\mathcal{M}$ (See Appendix B)\textsuperscript{2}. The vector of graph signals is obtained by inserting the solution of (27) into (23).

The optimization problem of (27) includes $l_0$ regression which is known to be NP-hard. We therefore approximate the solution using $l_1$ regression. We also add to each constraint a small tolerance for error in accordance with (21). The optimization problem we solve is therefore

$$\hat{s} = \arg\min_{y} \|y\|_1 \quad \text{such that}$$

$$\| [\lambda_1 \psi_1 (\mathcal{M}) \quad \lambda_2 \psi_2 (\mathcal{M}) \quad \cdots \quad \lambda_N \psi_N (\mathcal{M}) ] y - s_M | < \eta.$$  

(28)

The solution of (28) is not guaranteed to be unique. If there exist several solutions, one can be chosen arbitrarily.

We note that, the solution of (27) will be a bandlimited graph signal that is guaranteed to be smooth in the one-hop neighborhood of the sampled nodes. In general, a bandlimited graph signal need not be smooth. Rather, in order for a signal $s$ to be a smooth graph signal, many of the entries of $\hat{s}$ that correspond to the lower valued eigenvalues must be negligible. In our proposed solution, we search for the spectrum $\hat{s}$ with minimal $l_1$ norm such that

$$| \hat{s}_1 \lambda_1 \psi_1 (\mathcal{M}) + \cdots + \hat{s}_N \lambda_N \psi_N (\mathcal{M}) - s_M | < \eta.$$  

(29)

Since $\lambda_N \leq \cdots \leq \lambda_1$, in order for some eigenvector $\psi_i$, which is associated with a low-valued $\lambda_i$, to be consequential in the sum, the value of $\hat{s}_i$ must be large. As we search for $\hat{s}$ with minimal $l_1$ norm, this is an unlikely situation. In other words, the solution of our interpolation method is guaranteed to be smooth in the one-hop neighborhood of the sampled nodes and, in addition, contains a bias towards smooth graph signals.

C. Comparison to Existing Interpolation Methods

The works [12], [13], [14], [6] have taken a similar approach to the graph signal interpolation problem, in that they all formulate the interpolation as a solution to some linear system of equations. However, the system of equations defined here is unique since its definition is based on the Markov variation. Furthermore, we include a bias towards smooth graph signals, and do not predetermine the sparsity of the spectrum.

In contrast, [12], [13], [14], [6] all define a set of equations based on the graph Fourier transform (GFT). The solutions to such a system are all graph signals that are consistent with the samples of the graph signal. In order to ensure the interpolation returns a smooth graph signal, these methods predetermine the sparsity of the signal spectrum. In other words, they search for a graph signal that is consistent with the samples and resides in the span of $K$ predetermined eigenvectors of the graph shift operator (that is, the $K$ leading eigenvectors, where the value of $K$ is often assumed to be known, or determined according to the magnitude of the eigenvalues).

Spectral regression [12] defines the following system of equations

$$\hat{s} = \arg\min_{y} \|y\|_1 \quad \text{such that}$$

$$[\psi_1 (\mathcal{M}) \quad \psi_2 (\mathcal{M}) \quad \cdots \quad \psi_K (\mathcal{M})] y = s_M.$$  

(30)

where $\psi_1, \cdots, \psi_K$ denote the $K$ eigenvectors of the Markov matrix corresponding to the largest magnitude eigenvalues. Narang et al. [13] suggest a method for interpolating bandlimited graph signals using the eigenvectors of the normalized graph Laplacian. The interpolation is performed on $D^{\frac{1}{2}}s$, and, similar to spectral regression, is based on a system of equations extracted from the GFT. Mathematically, the system of linear equations is

$$[\psi_1^T (\mathcal{M}) \quad \psi_2^T (\mathcal{M}) \quad \cdots \quad \psi_K^T (\mathcal{M})] y = D^{\frac{1}{2}}s_M.$$  

(31)

where $\psi_1^T, \cdots, \psi_L^T$ denote $K$ eigenvectors of the normalized graph Laplacian. The solution to the system is computed through linear least squares. We note that, once again, the bandlimit of the solution to (31) must be determined before solving the system of equations.

In (6), Section 5 Chen et al. suggest interpolation methods for two clustering applications. Once again, their system of equations is created from the GFT. In contrast to the previous systems, here each node is mapped to a vector of length $L$ (the number of clusters) rather than a scalar value. This vector is actually an indicator function for its node, meaning that for node $i$ in the first class, the signal will be $[1 \ 0 \ \cdots \ 0]^T$. As each node is now mapped to a vector, the graph signal is a matrix $\textbf{S} \in \mathbb{R}^{N \times L}$. The interpolation is defined as the following optimization problem

$$\hat{\textbf{S}} = \arg\min_{\textbf{Y} \in \mathbb{R}^{K \times L}} \|\text{sign} \left( [\psi_1^A (\mathcal{M}) \quad \psi_2^A (\mathcal{M}) \quad \cdots \quad \psi_K^A (\mathcal{M})] \textbf{Y} \right) - \textbf{S}_M \|^2_2.$$  

(32)

where $\psi_1^A, \cdots, \psi_K^A$ denote $K$ eigenvectors of the graph shift and $\textbf{S}_M \in \mathbb{R}^{r \times L}$ is the matrix of the known portion of the graph signal. The optimization problem (32) is solved by logistic regression. Here again, the sparsity of the spectrum must be predetermined.

Another method for sampling and reconstruction of a known graph signal is presented by Sergarra et al. [14]. Here there is an added assumption on the formation model of smooth graph signals. Specifically, they assume a graph signal $s$ is created from a known sparse signal $x$ as

$$s = \textbf{H}x.$$  

(33)

where $\textbf{H}$ is some graph filter. In this method the assumption is that $s$ is known and the goal is to identify $\textbf{H}$ and $x$. This interpolation is performed through a system of linear equations based on the graph Fourier transform,

$$\hat{s} = V^{-1}_L \textbf{H}x.$$  

(34)

\textsuperscript{2}We note that this solution uses the prior knowledge that the spectrum of a smooth graph signal is sparse. It does not explicitly use any knowledge of the likely location of the zeros. We discuss this in the end of this section.
where $V_L$ denotes the matrix of eigenvectors of the normalized graph Laplacian. For a $K$-bandlimited graph signal, this set of $N$ equations can be divided into two systems. The first system consists of the $N - K$ equations for which $\hat{s}_i = 0$. These equations can be used to identify the coefficients of the graph filter $H$. The rest of the equations are used to interpolate $x$. Once again, $K$ must be predetermined.

In conclusion, the idea of graph signal interpolation via a system of linear equations is quite popular. However, all the methods we discuss above use the graph Fourier transform to define this system of equations. These systems are solved over the set of graph signals that comply with a predetermined sparsity of the spectrum. Contrary to this, we derived a system of equations that is based on the Markov variation, which is a smoothness measure. Any solution to this system is guaranteed to be a smooth graph signal. Of all possible solutions, we select the signal with the smallest bandwidth. In this way, the sparsity of the graph signal’s spectrum need not be predetermined. Instead, we determine the bandlimit in a data-driven manner.

Another difference between this work and [12], [13], [14], [6], is that our method (28) naturally extends to iterative interpolation wherein each iteration is solved by the same vector or by a smoother vector than the previous iteration. This is not the case for any of [12], [13], [14], [6] as these methods are not based on a smoothness measure.

In Section VI we show that our suggested interpolation techniques outperform state-of-the-art graph signal interpolation methods on synthetics data as well as the MNIST data set of hand-written digits [1] and a data set of temperature measurements [20].

All the above methods require knowledge of the eigen-decomposition of the graph shift operator. This is a costly operation, and infeasible for large graphs. In Section V we introduce a method for efficiently estimating the eigenvectors and eigenvalues of the Markov matrix. This approach can also be used in spectral regression, and can be easily adjusted to any method that uses a positive semi-definite graph shift.

D. Iterative Interpolation

Since the system of equations (24) was created on the basis of a smoothness measure, any solution must be smooth in the neighborhood of the sampled nodes. As the spectrum of a smooth graph signal is naturally approximately sparse, of all possible solutions to (24), we select a solution with minimal $l_1$ norm.

All smooth signals possess a sparse spectrum. However, not every signal with a sparse spectrum is smooth [6]. Therefore, it is conceivable that the solution of (28) may not be smooth over (one-hop) neighborhoods that do not contain sampled nodes. To prevent this, we can iteratively solve (28) while introducing in each iteration new nodes into the set $M$. In the last iteration we ensure that every node in the graph is a neighbor of some node in $M$. In this way we guarantee that any solution in the last iteration is smooth.

Our iterative approach is initialized with the set of sampled nodes $M_0$. In the first iteration we recover a signal with sparse spectrum that is guaranteed to be smooth (according to the Markov variation) in the (one-hop) neighborhood of $M_0$. Then, in each iteration $i$, we consider the set of sampled nodes to be $M_i = N(M_{i-1})$, where $N(M_{i-1})$ denotes the neighborhood of $M_{i-1}$ (note that, by construction, $M_{i-1} \subseteq N(M_{i-1})$). The result of the $i$th iteration is a signal with sparse spectrum that is guaranteed to be smooth (according to the markov variation) in the $i$th neighborhood of each node in $M_0$. The stopping condition is that $M_i$ will equal the set of all nodes $V$. Therefore, the interpolated graph signal is guaranteed to be smooth over all edges of the graph. Our approach is summarized in Algorithm 1.

**Algorithm 1 Iterative Interpolation**

Let $G = (V, E)$ be a graph with sampling set $M_0$

\[ i \leftarrow 1 \]

repeat

\[ \hat{s}_i \leftarrow \text{solve (28)} \]

\[ M_{i+1} \leftarrow N(M_i) \% \text{update sampling set for next iteration} \]

\[ i \leftarrow i + 1 \]

until $M_{i-1} = M_i$

In each iteration of Algorithm 1 the solution is either unchanged or improved. This is due to the effect of each update. Specifically, since $M_i \subset M_{i-1}$, the set of constraints

\[ |[\lambda_1 \psi_1(M_i) \quad \lambda_2 \psi_2(M_i) \cdots \quad \lambda_N \psi_N(M_i)] y - s_{M_i}| < \eta \]

is increased in each iteration. If the solution $\hat{s}_i$ is smooth over the neighborhood of $M_{i+1}$ then $\hat{s}_{i+1} = \hat{s}_i$. If $\hat{s}_i$ is not smooth over the neighborhood of $M_{i+1}$ then it is not a solution to

\[ |[\lambda_1 \psi_1(M_{i+1}) \quad \lambda_2 \psi_2(M_{i+1}) \cdots \quad \lambda_N \psi_N(M_{i+1})] y - s_{M_{i+1}}| < \eta \]

Instead, the solution of iteration $i+1$ is the vector with smallest $l_1$ norm that solves (36). This vector is smoother than $\hat{s}_i$ and has equal or higher $l_1$ norm.

In Fig. 1 we present a toy example to illustrate the difference between the one-shot algorithm (28) and Algorithm 1. We randomly select 100 points in $[0, 1] \times [0, 1]$, denoted as $x_1, \ldots, x_{100}$. We define the affinity matrix $W$ as

\[ W_{i,j} = \begin{cases} e^{-d(x_i, x_j)}, & i \neq j, \\ 0, & i = j, \end{cases} \]

where $d(x_i, x_j)$ is the Euclidean distance between $x_i$ and $x_j$. We keep the highest 9 entries in each row of the affinity matrix and set all other entries to zero. We then symmetrize the affinity matrix as

\[ W_s = \max(W, W^T). \]

We use this symmetric matrix to compute the Markov matrix.

It is clear from Fig. 1 that the result of both our methods is a smooth graph signal. However, the output of (28) is a graph signal that is determined by the one-hop neighborhood of each node and a bias towards smoothness. The result of Algorithm 1
Algorithm 1 will converge as long as each connected component in \( G \) contains a node in the sampling set \( M_1 \). Specifically, we denote by \( b \) the minimal integer for which the \( b \)-hop neighborhood of each node contains all the nodes in the graph. Such a \( b \) is guaranteed to exist since there exists a path between each node in the graph and a node in the sampling set \( M_0 \). It follows that \( M_{b+1} = \mathcal{V} \).

Consequently, the solution \( \hat{s}_b \) (to the \( b \)th iteration of Algorithm 1), is determined by a system of \( N \) equations and \( N \) unknowns. The eigenvalues of \( \mathbf{P} \) are known to decrease to zero. As the eigenvectors of \( \mathbf{P} \) are linearly independent, there exists a single solution \( \hat{s}_b \). In all subsequent iterations, the set \( M_c = \mathcal{V} \). This leads to the same system of equations and, as a consequence, the same solution. Therefore, Algorithm 1 has converged.

If the graph \( G \) contains a connected component that is not represented in the sampling set, the set \( M \) would still remain unchanged after \( b \) iterations. There is therefore no point in running the algorithm further.

V. NYSTRÖM GRAPH SIGNAL INTERPOLATION

The solution of (28) necessitates computation of the eigen-decomposition of the graph shift operator. This computation is costly in terms of both complexity and memory consumption. When the graph has many nodes it may not be feasible to compute eigenvectors and eigenvalues of the graph shift operator. However, when the graph shift operator is the Markov matrix, a variation on the Nyström extension [22], [23], [24], [25] can be used for semi-supervised learning of big data.

A. The Nyström Extension

We begin by giving a short introduction to the Nyström extension. Let \( \{x_i\}_{i=1}^N \) be a set of data points. A matrix \( \mathbf{K} \in \mathbb{R}^{N \times N} \) is constructed such that \( K_{i,j} = k(x_i, x_j) \), where \( k(\cdot) \) is some kernel function and \( \mathbf{K} \) is a positive semi-definite (PSD) matrix. The matrix \( \mathbf{K} \) can be considered as a combination of four block matrices,

\[
\mathbf{K} = \begin{bmatrix} \mathbf{E} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{C} \end{bmatrix},
\]

where \( \mathbf{E} \in \mathbb{R}^{r \times r} \), \( \mathbf{B} \in \mathbb{R}^{r \times N-r} \), and \( \mathbf{C} \in \mathbb{R}^{N-r \times N-r} \) for some \( 0 < r < N \). The Nyström extension is a method for extending the eigenvectors of \( \mathbf{E} \) to create an estimate of \( r \) eigenvectors of \( \mathbf{K} \).

Let \( \mathbf{Z} \in \mathbb{R}^{r \times r} \) be the matrix whose columns are the eigenvectors of \( \mathbf{E} \). As \( \mathbf{E} \) contains the first \( r \) rows and the first \( r \) columns of \( \mathbf{K} \), it is itself a symmetric matrix, thus

\[
\mathbf{E} = \mathbf{ZQZ}^T.
\]

where \( \mathbf{Q} \) is a diagonal matrix containing the eigenvalues of \( \mathbf{E} \). The Nyström extension of the matrix of eigenvectors of \( \mathbf{K} \) is given by

\[
\hat{\mathbf{Z}} = \begin{bmatrix} \mathbf{Z} \\ \mathbf{BZQ}^{-1} \end{bmatrix}.
\]

For more details see [22].

We suggest that when computing \( \mathbf{BZQ}^{-1} \) all eigenvalues be approximated as ones, resulting in the following modification to (39)

\[
\hat{\mathbf{Z}} = \begin{bmatrix} \mathbf{Z} \\ \mathbf{BZ} \end{bmatrix}.
\]

We motivate this approximation in Appendix C.

B. Nyström Interpolation

The application of the Nyström extension to the Markov matrix is not straightforward. This is due to the fact that the Nyström extension is geared towards PSD matrices, and the Markov matrix \( \mathbf{P} \) is not PSD. However, as we show in Proposition 1 (see Appendix A), the Markov matrix is strongly

---

Fig. 1. Graph signal interpolation. (a) Initial samples for 3 clusters. The graph signal is indicated by color. (b) Solution of (28). (c) Result of the first iteration. The set \( \mathcal{M}_1 \) is marked by the color of the interpolated graph signal. The remaining nodes are marked in black. (d) Result of the second iteration. (e) Result of the third iteration. (f) Final result.
related to the normalized graph Laplacian $L$ which is PSD, and defined by

$$L = D^{-\frac{1}{2}}(D - W)D^{-\frac{1}{2}} = I_N - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$$  \hspace{1cm} (41)$$

where $I_N$ is the $N \times N$ identity matrix. It is easy to see that $D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I_N - P$. Thus, $L$ is similar to $I_N - P$. From Proposition 1 (see Appendix A), the connection between the matrix of eigenvectors of the Markov matrix $V$ and the matrix of eigenvectors of the Laplacian $U$ is,

$$\tilde{V} = D^{-\frac{1}{2}}\tilde{Z},$$  \hspace{1cm} (42)$$

and the matrix approximating its eigenvalues is

$$\tilde{\Lambda} = I_N - Q.$$  \hspace{1cm} (43)$$

To obtain an efficient graph signal interpolation algorithm we insert (42) and (43) into (28). Specifically, $\psi_i$ is replaced by the $i$th column of $\tilde{V}$, and $\lambda_i$ is replaced by $\tilde{\Lambda}_{i,i}$.

The difference between our two interpolation methods is only in the computation of the eigendecomposition of the Markov matrix. In our smoothness interpolation, presented in Section IV, the eigenvectors and eigenvalues of the full $N \times N$ matrix must be determined. On the other hand, Nyström smoothness interpolation uses the eigendecomposition of an $r \times r$ matrix to approximate the eigenvectors and eigenvalues of the $N \times N$ matrix. When $r \ll N$ this method is computationally efficient. We show in Section VI that this approach still achieves good accuracy in simulations on the MNIST dataset [1]. We note that Nyström smoothness interpolation can also be done iteratively, as detailed in Algorithm 1.

The Nyström extension is not meant to be used on graphs with sparse graph shift matrices (that is, few edges). Rather, this method is geared towards dense graph shift matrices, in which case few samples are needed. We note that computationally efficient methods for graph signal interpolation over sparsely connected graphs through message passing have been suggested [16]. These methods are not computationally efficient for more densely connected graphs.

VI. EXPERIMENTAL RESULTS FOR GRAPH SIGNAL INTERPOLATION

A. Synthetic Simulations

In this section we present a qualitative comparison between our framework and those of [12], [18], [17], [19] for several signals and several sampling strategies. We use the Graph Signal Processing Toolbox [26] to produce the bunny graph depicted in Fig. 2. This graph contains 2503 nodes and 27452 edges connecting nearby nodes. In each experiment we use the Markov matrix as the graph shift operator.

We further note that, as (28) is an $l_1$ optimization problem, we use the SPGL1 package\(^3\) [27], [28] to solve it.

\(^3\)https://github.com/mpf/spgl1.

Fig. 2. Bunny graph as created by the Graph Signal Processing Toolbox [26]. (a) Nodes and edges of the graph. (b) Bandlimited graph signal. The color of each node corresponds to its signal. (c) Approximately bandlimited graph signal.

1) Bandlimited graph signal: We created a 20-bandlimited graph signal. This was done by randomly generating the first twenty entries of the spectrum of the graph signal $\tilde{x}$ and setting the remaining entries to zero. The resulting graph signal is

$$x = V \tilde{x},$$

and is depicted in Fig. 2.

Next, we sample the nodes in the graph. We use two sampling strategies. The first is random sampling, where each node has a uniform probability of being sampled. Additionally we use the sampling procedure suggested in [6] (which, in this case, allows for perfect reconstruction). We compare the error of (28) with the error of spectral regression, noiseless inpainting [17] and both reconstruction strategies discussed in [18] (where one of these was introduced in [19]). We compute the error of each reconstruction method for varying sizes of sample sets. The error is defined as

$$\frac{\| y - \hat{y} \|_2}{\| y \|_2},$$  \hspace{1cm} (44)$$

where the true signal is $y$ and the estimate is denoted by $\hat{y}$.

In Fig. 3 we present interpolation results when the bandlimit is known (for all methods except noiseless inpainting [17] as this solution does not refer to the eigenvectors of the graph shift). In Fig. 4 we plot interpolation results when the bandlimit is unknown and assumed to be unlimited.

We note that in the case of the optimal sampling operator [6], our method is the only one that recovers the graph signal exactly both when the bandlimit is known and when the bandlimit is unknown. The reason for this is that in our method the bias towards smooth graph signals does not depend on any predetermined bandlimit.

2) Approximately bandlimited graph signals: In reality, graph signals are often approximately bandlimited. We simulate such signals by adding a noise vector (generated uniformly at random) to the spectrum of our 20-bandlimited graph signal. We interpolate the graph signal under the assumption that the signal is 20-bandlimited (Fig. 5) and under the assumption that the signal is not bandlimited (Fig. 6). We note that, as case of bandlimited graph signals, [17] makes no assumption on the bandlimit. We conclude that our interpolation is successful especially when no assumptions are made on the bandlimit. This property stems from a built-in bias towards negligible values in the high frequencies of the interpolated graph signal.
We conclude that, whether the bandlimit is known or not, our method is among the state-of-the-art methods that achieve the lowest error rate.

B. MNIST dataset

In the previous Section we presented results on synthetic data. We now compare our methods (28) and Algorithm 1 to [12], [18], [17], [19] on the MNIST dataset [1] of handwritten digits. This dataset includes 60000 training images and 10000 test images. We solve a clustering problem where the goal is to associate each image with the digit it depicts.

We formulate the clustering problem as a graph signal interpolation problem, in the manner detailed in [6]. Specifically, we select 1000 images of each digit and represent this reduced set as an undirected weighted graph, wherein each image \( x_i \) is represented by a single node \( v_i \). The Euclidean distances between vectorizations of the images are used as a distance measure between their respective nodes. We denote the matrix of pairwise distances as \( F \).

We keep only the \( L = 12 \) smallest entries for each row of \( F \), and denote by \( M_i \) the indices of the \( L \) smallest entries for each row \( n \). The weight of an edge between two images is defined as

\[
W_{i,j} = \begin{cases} 
\frac{F_{i,j} \cdot N^2}{\sum_{n=1}^{N} F_{n,m}^2} & \text{for } j \in M_i \\
0 & \text{for } j \notin M_i
\end{cases}
\]

where \( N \) is the number of nodes in the graph. The graph shift operator is the Markov transition matrix.

We define ten smooth graph signals \( s^0, \ldots, s^9 \) as follows,

\[
s_i^k = \begin{cases} 
1 & \text{if } v_i \text{ represents an image of the digit } k \\
0 & \text{otherwise}
\end{cases}
\]

Each of these signals is known over a subset of \( r \) nodes in the training set. The nodes in this set are determined according to the sampling suggested by Chen et al. [6] Algorithm 1. Our goal is to recover the signal over the remaining 10000 \(- r \) nodes. In order to do this, we interpolate each signal \( s^0, \ldots, s^9 \) independently. We then map node \( v_i \) to the scalar value \( k \in \{0,1,\ldots,9\} \) when our interpolated signals satisfy \(|s_i^k| > |s_i^m|\) for all \( k \neq m \).

We present in Fig. 7 a comparison between our suggested smoothness interpolation (28), its iterative extension (Algorithm 1), the interpolation suggested by Chen et al. (32) [6] and the method of Jung et al. [16]. This figure plots the percent of training images of each digit and represent this reduced set as an undirected weighted graph, wherein each image \( x_i \) is represented by a single node \( v_i \). The Euclidean distances between vectorizations of the images are used as a distance measure between their respective nodes. We denote the matrix of pairwise distances as \( F \).

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\end{cases}
\]

where \( N \) is the number of nodes in the graph. The graph shift operator is the Markov transition matrix.

We define ten smooth graph signals \( s^0, \ldots, s^9 \) as follows,

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s_i^k = \begin{cases} 
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\end{cases}
\]

Each of these signals is known over a subset of \( r \) nodes in the training set. The nodes in this set are determined according to the sampling suggested by Chen et al. [6] Algorithm 1. Our goal is to recover the signal over the remaining 10000 \(- r \) nodes. In order to do this, we interpolate each signal \( s^0, \ldots, s^9 \) independently. We then map node \( v_i \) to the scalar value \( k \in \{0,1,\ldots,9\} \) when our interpolated signals satisfy \(|s_i^k| > |s_i^m|\) for all \( k \neq m \).

We present in Fig. 7 a comparison between our suggested smoothness interpolation (28), its iterative extension (Algorithm 1), the interpolation suggested by Chen et al. (32) [6] and the method of Jung et al. [16]. This figure plots the percent of training images of each digit and represent this reduced set as an undirected weighted graph, wherein each image \( x_i \) is represented by a single node \( v_i \). The Euclidean distances between vectorizations of the images are used as a distance measure between their respective nodes. We denote the matrix of pairwise distances as \( F \).

We keep only the \( L = 12 \) smallest entries for each row of \( F \), and denote by \( M_i \) the indices of the \( L \) smallest entries for each row \( n \). The weight of an edge between two images is defined as

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W_{i,j} = \begin{cases} 
\frac{F_{i,j} \cdot N^2}{\sum_{n=1}^{N} F_{n,m}^2} & \text{for } j \in M_i \\
0 & \text{for } j \notin M_i
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where \( N \) is the number of nodes in the graph. The graph shift operator is the Markov transition matrix.

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We present in Fig. 7 a comparison between our suggested smoothness interpolation (28), its iterative extension (Algorithm 1), the interpolation suggested by Chen et al. (32) [6] and the method of Jung et al. [16]. This figure plots the percent of
In the previous section we dealt with a clustering problem, where the graph signal was a labeling of the nodes. In general similar clusters need not have similar labels. For example, while the digits 3 and 8 are similar, their labels are not. We now consider a regression problem, where the graph signal was a labeling of the nodes. In general similar clusters need not have similar labels. For example, while the digits 3 and 8 are similar, their labels are not. We now consider a regression problem, where the graph signal is a quantity rather than a label.

In summary, our smoothness interpolation method (28), and its iterative extension (Algorithm 1) outperform the graph signal interpolation methods of [6], [16], [12] on the MNIST dataset. In addition, our variation on the Nyström extension achieves good accuracy while allowing to quickly interpolate many entries of very large graph signals.

We note that in the above experiments the optimization problem (28) was solved over the \( r \) leading eigenvectors. This is due to the fact that the Nyström smoothness interpolation is limited to \( r \) eigenvectors.

### C. Temperature measurements

In the previous section we dealt with a clustering problem, where the graph signal was a labeling of the nodes. In general similar clusters need not have similar labels. For example, while the digits 3 and 8 are similar, their labels are not. We now consider a regression problem, where the graph signal is a quantity rather than a label.

We turn to a dataset of average temperatures as measured by 2181 sensors across the contiguous United States on January 1st, 2011 [20]. The dataset contains both longitude, latitude and elevation of each sensor. Following [4], we represent each
sensor as a node in a K-nearest neighbors graph. Edge weights are defined according to (4) eq (26),

\[ A_{n,m} = \frac{e^{-d_{n,m}^2}}{\sqrt{\sum_{k \in \mathcal{N}_n} e^{-d_{n,k}^2} \sum_{l \in \mathcal{N}_m} e^{-d_{n,l}^2}}} \]  

where \( d_{n,m} \) denotes the geodesic distance between node \( n \) and node \( m \). As we restrict the discussion to undirected graphs, the affinity matrix is,

\[ W_{n,m} = \max(A_{n,m}, A_{m,n}). \]  

(49)

Fig. 9 presents a comparison in terms of error between our iterative optimization method (Algorithm 1) and spectral regression [12] as well as [19], [18], [17]. As this is a relatively small dataset, there is no need to compare to our fast interpolation method. Additionally, in each method, we do not make any assumption on the bandlimit of the graph signal. We compute the error as

\[ ||y - \hat{y}||_2 / ||y||_2 \]  

(50)

where \( y \) is the true graph signal and \( \hat{y} \) is the interpolation.

In Fig. 10 we provide a comparison when we assume a bandlimit of 9 in the methods [12], [18], [19]. It is clear from Figs. 9 and 10 that, when the dataset is small enough that exact computation of the eigendecomposition of the graph shift matrix is feasible, our suggested interpolation method far outperforms state-of-the-art interpolation methods such as [12] on both these data sets.

VII. CONCLUSION

The authors would like to thank Antonio Ortega for his helpful discussions on the nature of graph signals.

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The field of signal processing on graphs strives to generalize definitions and operations from signal processing to data represented by a graph. An important definition in this field is the graph shift operator. In this paper we define the graph shift operator to be the Markov matrix and use this definition to formulate the Markov variation, a smoothness measure for graph signals. This measure is closely related to the diffusion embedding vectors of the nodes of the graph.

We use the Markov variation to derive a method for interpolation of smooth graph signals. This is done by defining a system of linear equations derived from the Markov variation. Since this system may be underdetermined, we select the solution with minimal \( l_1 \) norm. This method naturally extends to an iterative interpolation, where each iteration either leaves the solution unchanged or returns a smoother solution. We experimentally verify our interpolation methods over the MNIST dataset of handwritten digits and over a dataset of temperature measurements across the contiguous United States. We show that our method outperforms state-of-the-art interpolation methods such as [12] on both these data sets.

In addition, we utilize the Nyström extension for a computationally efficient solution of the aforementioned minimization problem. We show that our efficient approximation achieves good results on the MNIST data set in greatly reduced runtimes.

APPENDIX A

In this Appendix we provide a summary of some key properties of the Markov matrix along with their proof. These properties were used in the analysis of the Markov variation and the derivation of the graph signal interpolation method (28).

**Lemma 1.** The Markov matrix of a connected and undirected graph is diagonalizable.

**Proof.** The normalized graph Laplacian is defined as

\[ L = D^{-\frac{1}{2}} (D - W) D^{-\frac{1}{2}} = I_N - D^{-\frac{1}{2}} W D^{-\frac{1}{2}}, \]  

(51)

and the Markov matrix is defined as

\[ P = D^{-1} W = D^{-\frac{1}{2}} \left( D^{-\frac{1}{2}} W D^{-\frac{1}{2}} \right) D^{\frac{1}{2}}. \]  

(52)
It follows from (51) and (52) that
\[ P = D^{-\frac{1}{2}} (I_N - L) D^{-\frac{1}{2}}. \]  
(53)

This means that the Markov matrix is similar to \( I_N - L \). The normalized graph Laplacian is a symmetric matrix and is thus diagonalizable. The same is true for \( I_N - L \). As \( P \) is similar to a diagonalizable matrix, it is also diagonalizable. \( \square \)

Since \( P \in \mathbb{R}^{N \times N} \) is diagonalizable, it has \( N \) eigenvalues and \( N \) eigenvectors. In the proposition below we denote the eigenvectors and eigenvalues of \( P \) as \( \{ \psi_i \}_{i=1}^N \) and \( \{ \lambda_i \}_{i=1}^N \), respectively. We further denote the eigenvectors and eigenvalues of \( L \) as \( \{ u_i \}_{i=1}^N \) and \( \{ \tilde{\lambda}_i \}_{i=1}^N \).

**Proposition 1.** The eigenvectors and eigenvalues of the Markov matrix obey the following:

1) \( \psi_i = D^{-\frac{1}{2}} u_i \), \( \lambda_i = 1 - \tilde{\lambda}_i \).
2) \( |\lambda_i| \leq 1 \).
3) The leading eigenvector of the Markov matrix is constant.

**Proof.**

1) In the proof of Lemma 1 we saw that \( P \) is similar to \( I_N - L \). It follows that \( L \) is similar to \( I - P \),
\[ I_N - P = D^{-\frac{1}{2}} LD^{-\frac{1}{2}}, \]
and that
\[ (I_N - P) D^{-\frac{1}{2}} = D^{-\frac{1}{2}} L. \]
(55)

It follows that
\[ (I_N - P) D^{-\frac{1}{2}} u_i = \tilde{\lambda}_i D^{-\frac{1}{2}} u_i, \]
(56)

Thus, \( D^{-\frac{1}{2}} u_i \) is an eigenvector of \( I_N - P \), with eigenvalue \( \tilde{\lambda}_i \). Also,
\[ (I_N - P) D^{-\frac{1}{2}} u_i = D^{-\frac{1}{2}} u_i - PD^{-\frac{1}{2}} u_i = \lambda_i D^{-\frac{1}{2}} u_i, \]
so that
\[ PD^{-\frac{1}{2}} u_i = (1 - \tilde{\lambda}_i) D^{-\frac{1}{2}} u_i. \]
(58)

This proves that if \( u_i \) is an eigenvector of \( L \) with eigenvalue \( \bar{\lambda}_i \), then \( D^{-\frac{1}{2}} u_i \) is an eigenvector of \( P \) with eigenvalue \( 1 - \bar{\lambda}_i \).

2) We know from Proposition 1 part 1 that
\[ \lambda_i = 1 - \tilde{\lambda}_i. \]
(59)

Let \( \bar{\lambda}_1 \) be the smallest valued eigenvalue of the normalized graph Laplacian. As the normalized graph Laplacian is a positive semi definite matrix it follows that \( \lambda_1 \geq 0 \) and thus \( \lambda_1 \leq 1 \), where \( \lambda_1 \) is the largest eigenvalue of the Markov matrix.

Let \( \lambda_N \) be the largest valued eigenvalue of the normalized graph Laplacian. Chung [29] used the rayleigh quotient to prove that \( \lambda_N \leq 2 \). Therefore, \( \lambda_N \geq -1 \), where \( \lambda_N \) is the smallest eigenvalues of the Markov matrix.

3) To prove part 3, we note that each row in the Markov matrix sums to 1. Thus,
\[ P1 = 1 \cdot 1, \]
(60)

where 1 is the all ones vector. We see that 1 is an eigenvalue of \( P \), and is associated with a constant eigenvector. We know from part 2 of the proposition that the eigenvalues are upper bounded by 1. Therefore, the constant eigenvector must be the leading one. \( \square \)

**APPENDIX B**

**Lemma 2.** Any solution of the system of equations (24) is guaranteed to be smooth over the one-hop neighborhoods of the nodes in \( M \).

**Proof.** The right-hand side of (24) can be written as
\[ \begin{bmatrix} \lambda_1 \psi_1 (M) & \cdots & \lambda_N \psi_N (M) \end{bmatrix} \hat{s} = V (M) \Lambda \hat{s}, \]
(61)

where \( V \) is the matrix of eigenvectors of the graph’s Markov matrix \( P \), \( V (M) \) are the rows of \( V \) corresponding to the indices of the sampled nodes, and \( \Lambda \) is the diagonal matrix of eigenvalues of the Markov matrix. Using the graph Fourier transform (2), we get
\[ V (M) \Lambda \hat{s} = V (M) \Lambda V^{-1} \hat{s}. \]
(62)

As \( P = V A V^{-1} \), clearly,
\[ V (M) A V^{-1} \hat{s} = P (M) \hat{s}. \]
(63)

Therefore, (24) is equivalent to the following system
\[ s_M = P (M) s, \]
(64)

and is satisfied only if the graph signal is smooth in the neighborhood of the sampled nodes. \( \square \)

**APPENDIX C**

In Section V we modified the Nyström extension from
\[ \hat{Z} = \begin{bmatrix} Z \\ BZQ^{-1} \end{bmatrix} \]
(65)
to
\[ \hat{Z} = \begin{bmatrix} Z \\ BZ \end{bmatrix}. \]
(66)

In order to justify this, we examine the approximation of the eigenvectors of \( P \) which can be found using (65),
\[ D^{-\frac{1}{2}} \hat{Z} = D^{-\frac{1}{2}} \begin{bmatrix} Z \\ BZQ^{-1} \end{bmatrix}. \]
(67)

We decompose the diagonal matrix \( D \) as
\[ D = \begin{bmatrix} D_e & 0 \\ 0 & D_b \end{bmatrix}, \]
where \( D_e \in \mathbb{R}^{r \times r} \). Substituting into (67), the approximation of the eigenvectors of \( P \) can be expressed as
\[ D^{-\frac{1}{2}} \hat{Z} = \begin{bmatrix} D_e^{-\frac{1}{2}} Z \\ D_b^{-\frac{1}{2}} BZQ^{-1} \end{bmatrix}. \]
(68)

We further denote \( A = D_b^{-\frac{1}{2}} BZ \) and examine \( AQ^{-1} \). As \( Q \) is a diagonal matrix,
\[ AQ^{-1} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ q_{11} & q_{22} & \cdots & q_{rr} \end{bmatrix}, \]
(69)
where $a_i$ denotes the $i$th column of $A$. That is, rows $r+1$ through $N$ of the $i$th eigenvector of $P$ are multiplied by the inverse of the $i$th eigenvalue of $E$ (37).

We assume that $\mathcal{M} = \{1, \ldots, r\}$. That is, since the numbering of nodes is arbitrary, when creating the graph shift we assign the first $r$ rows and $r$ columns to the sampled nodes. In this case, the optimization problem we solve is

$$ x = \arg \min_{y} \|y\|_0 \text{ such that } \left[[1 - Q_{1,1}] z_1 \cdots (1 - Q_{r,r}) z_r \right] y = s_{\mathcal{M}}, \quad (70) $$

where $z_i$ is the $i$th column of $D^{-\frac{1}{2}}Z$. We note that the optimization problem (70) depends only upon the first $r$ rows of $D^{-\frac{1}{2}}Z$. As those rows are unaffected by the approximation (66), it is clear that the approximation does not affect the solution $y$.

In addition, we have found that for smooth graph signals, the entries in the spectrum of the signal that correspond to the lower valued eigenvalues of $P$ are negligible. This means that for most of the eigenvectors of the Laplacian, it makes no difference how we approximate their eigenvalues since they will be ignored in the interpolation process. The eigenvectors that are not ignored correspond to the higher valued eigenvalues of $P$. So, in essence, the approximation of (66) just means that we assume that the higher valued eigenvalues of $P$ are approximately equal. While this assumption is not strictly correct, it does prevent the low eigenvalues of the laplacian (which correspond to the high eigenvalues of $P$) from causing numerical instabilities.

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