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Multiresolution analysis of functions on directed networks

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ABSTRACT

We introduce a novel design for analyzing and approximating functions defined on the vertices of a directed graph Γ in a multi-scale fashion. The starting point of our construction is the setting-up of a frequency notion through the study of the Dirichlet energy of random walk operator's eigenfunctions. By this alluring frequency interpretation, the set of random walk's eigenfunctions is considered as the Fourier basis for functions over directed graphs. We are thus able to construct a multi-scale frame based on the bi-orthogonal basis of the random walk on directed graphs. This multi-resolution frame paves thus the way to a generalization of the diffusion wavelet framework to the directed scope.

Keywords: Directed graphs, Random walk operator, Multiresolution analysis, Signal processing on graphs.

1. INTRODUCTION

In the data deluge era, most of the data coming from a variety of sources, from biology to social medias services exhibit a graph-structured living in a high dimensional space. Formally, the data depicting attributes which live on the nodes or/and the edges of a graph depicting some entities. In order to analyze and understand such graph data, mathematical and computational methods need to be created.

In the classical harmonic analysis framework, methods such as Fourier and wavelet transforms have demonstrated their effectiveness for analyzing signals on regular domains such as time signals and images. Noticeably, the efficiency of the wavelet transform on regular domains has motivated the extension of the wavelets on irregular domains such as manifolds and graphs. Most of these graphs have the particularity of being directed. For instance, by analyzing data from the web, the direction of the links contains crucial information.

In this paper, we bring out a novel design of wavelet frames for functions defined over a directed graph and generalize the diffusion wavelets framework to the directed setting.

A fundamental barrier in the extension of wavelets scope to the directed graph setting is the absence of an appropriated notion of frequency. Without a desirable notion of frequency, we are not able to apply a directed graph type Littlewood-Paley theory.

The essential idea behind the notion of frequency is the extension of the Fourier basis for functions over directed graphs. Recently, various Fourier transforms for directed graphs have been proposed, from the adjacency matrix,^{1,2} to the Laplacian,^{3,4} through optimization methods.⁵

We thus introduce a novel and alternative frequency analysis for functions defined on the vertices of functions on directed graphs carried by the random walk operator. The main concept is to consider the eigenfunctions of the random walk as a Fourier basis for functions defined on directed graphs through the Dirichlet energy weighted by the transition probabilities of the random walk operator. From this attractive interpretation, we are able to construct a multi-scale frame based on the bi-orthogonal basis of the random walk operator, typically non-symmetric for functions on directed graphs, offering an alternative to the previous approach.⁶ This multiscale frame can be viewed as multi-bandpass graph filters,^{1,2} filtering functions according to the band-limited

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spectral frequencies. This construction thus generalizes the concepts from $^{7-9}$ and their wavelet-like transforms on undirected graphs onto the directed graph setting.

Our construction is built as follows. In the following section, we discuss the related work on which our paper has been built. In section 2, we review the classical notions of signal processing on graphs. Then we introduce, in section 3 the canonical operators defined on directed graphs. The section 4 is devoted to the interpretation of a Fourier analysis based on a highlighted operator from 3, the random walk operator. From this Fourier analysis, we present, in section 5, the multi-scale wavelet frame for directed graphs and its properties. Lastly, we propose an extension of the diffusion wavelets frames to the directed scope in the section 6.

1.1 Related work

Over the last decade, there has been more interest in building and investigating wavelet-like transforms for functions over irregular domains, such manifolds and graphs.^{6,9-20} The wavelet-like transforms can be divided in two categories.

1.1.1 Vertex based transforms

Coifman et al.²¹ generalized the Haar wavelet transform to graphs. Szlam et al.²² utilized a successive partitioning of a graph to generate an orthonormal basis via the diffusion wavelet scope.¹⁰ Sharon and Shkolniksy²³ used a subset of the Laplacian eigenvectors and a recursive partitioning tree to construct a multi-resolution analysis and consequently multiwavelet bases. Rustamov generalized the average interpolating transform of Donoho et al. for manifolds and graphs.¹⁴ Rustamov also presented a graph wavelet construction¹⁶ based on the lifting scheme whose update and prediction operators are adaptively learning from a given set of signals so that the resulting wavelet coefficients of a signal belonging to the same signal class become sparse. Filterbanks have also been developed on graphs (especially when relying on the case of bipartite graphs) to design wavelets, first in the original works of^{24–27} then developed in more recent works .^{28–30} Lately, Irion and Saiko^{17, 18} developed multi-scale transforms on graphs utilizing a top-down recursive graph partitioning to construct the wavelet-like basis functions.

1.1.2 Frequency based transforms

Coifman and Maggioni^{10,12,31} firstly introduced diffusion wavelets, a general theory for wavelet decompositions based on compressed representations of powers of a diffusion operator, typically a Laplacian or a random walk operator. Maggioni and Mhaskar⁸ developed the concept of diffusion polynomial frames, inspired from Mhaskar's previous work⁷ in the generality of arbitrary measure spaces whose scaling and wavelet transforms are an orthonormal basis $\{\phi_j\}$ and an increasing sequence of numbers $\{\sigma_i\}$ of a given operator. Highly inspired by the "diffusion polynomial frames" approach, Hammond, Vandergheynst and Gribonval⁹ elaborated a multi-scale approach by defining scaling and wavelet transforms based on the eigenfunctions of the graph Laplacian \mathcal{L} . All these significant constructions have been uniquely designed on undirected graphs where the Laplacian's eigenfunctions are considered as Fourier basis for functions over undirected graphs.

A natural extension would be to extend the wavelet-like transforms to the directed graph scope. Among the graphs, directed graphs appear extensively in diverse real-world applications from social networks to computational biology where the edge directionality brings useful information. Nevertheless, it is more challenging to study than undirected graphs. The study of multi-resolution analysis on directed graphs is often done from the conversion of directed graphs to undirected ones via symmetrization. Such symmetrization treatments discard the important structural information conveyed by edge directions, which inevitably impair the efficacy of subsequent analysis. A question is still how to use a Laplacian on directed graphs, knowing the construction of a symmetric Laplacian on directed graphs by Chung.³² Lastly, operators defined on directed graphs are naturally non-symmetric and that yielding to non-orthogonal eigenspaces. From a numerical perspective, non-orthogonal eigenspaces might be unstable and highly perturbed by noise unlike orthogonal ones.

It is therefore of great interest to develop a multi-scale directed graph analysis to make use of edge directionality of a directed graph.

1.2 How to generalize multi-resolution analysis of functions over directed graphs?

In graph signal processing for undirected graphs, and in many of the wavelet-like transform found so far in the literature, the orthogonal basis consisting of the eigenvectors of the Laplacian operator plays the role of Fourier basis.³³ In the scope of the directed graphs, we need to establish a corresponding Fourier basis. Recently, diverse graph Fourier transforms for functions defined over directed graphs have been suggested. Sandryhaila and Moura^{1,2} have proposed a graph Fourier transform based on the Jordan reduction of the adjacency matrix \mathbf{W} which plays the role of graph shift operator.² Apart from the difficulty to deal with the Jordan reduction, the frequency notion is determined a posteriori, by computing the total variation of the eigenvectors of \mathbf{W} . Singh³ has proposed a Fourier basis construction based on the eigenfunctions of a directed Laplacian. Most newly, Sardellitti et al.⁵ have created a directed graph Fourier basis built as the set of orthonormal vectors through the resolution of a non-convex problem. Shafipour⁴ investigated a Fourier basis construction from the eigenfunctions of the Laplacian operator.

As a slight extension of his previous work,⁸ Mhaskar has more recently proposed a multi-scale decomposition for functions defined on a directed graph⁶ based on the singular value decomposition of a non-symmetric operator. Specifically, this approach considers the polar decomposition of a non-self-adjoint operator on directed graph $\mathbf{A} = \mathbf{S}\mathbf{U}$ where \mathbf{S} is a positive semi-definite matrix and \mathbf{U} a unitary matrix. Mhaskar thus establishes a multiresolution analysis of $\mathbf{U}f$.

The aim of our research is thus to propose an attractive alternative to the Mhaskar's work by constructing a novel harmonic analysis and multi-resolution framework from the random walk operator where the random walk's eigenfunctions are the Fourier basis for functions defined over directed graphs.

2. SIGNAL PROCESSING ON GRAPHS

Signal processing on graphs^{1, 2, 33} extends the concepts of classical signal processing for time signals and images to signals defined on the vertices of a graph. In this section, we introduce the main concepts of signal processing on graphs framework relevant to our construction.

2.1 Preliminaries

A directed graph Γ is a couple $(\mathcal{V}, \mathcal{E})$ where \mathcal{V} is a set of vertices, that is, an arbitrary set whose elements are called vertices with $|\mathcal{V}| = n$ and \mathcal{E} is a set of edges. Each edge is an ordered pair of nodes (u, v) representing a directed connection from u to v. In a weighted directed graph, a weight function $w : \mathcal{V} \times \mathcal{V} \to \mathbb{R}^+$ is associated with Γ , satisfying w(u, v) = 0 if and only if $(u, v) \notin \mathcal{E}$. Typically, we can equip a directed graph with a canonical weight function by defining w(u, v) = 1 if and only if $(u, v) \in \mathcal{E}$.

The in-degree d_u^{in} and out-degree d_u^{out} of a vertex $u \in \mathcal{V}$, respectively are defined as

$$d_u^{in} = \sum_{v \in \mathcal{V}} w(v, u), \qquad \quad d_u^{out} = \sum_{v \in \mathcal{V}} w(u, v).$$

2.2 Signals on graphs

We define a graph signal as a function from the set \mathcal{V} to \mathbb{C} , that is $f: \mathcal{V} \to \mathbb{C}$. We write graph signals as vectors

$$f = [f(1), \dots, f(n)]^\top \in \mathbb{C}^n$$

We now define the function space for graph signals.

DEFINITION 2.1. Let $\nu : \mathcal{V} \to (0, \infty)$, a measure defined on the vertex set \mathcal{V} . For $p \in [1, \infty)$, we denote $\ell^p_{\nu}(\mathcal{V})$, the space of functions $f : \mathcal{V} \to \mathbb{C}$ such that

$$||f||_{\ell^p_{\nu}(\mathcal{V})} = \left(\sum_{v \in \mathcal{V}} |f(v)|^p \nu(v)\right)^{1/p} < \infty, \quad p \in [1, \infty)$$

We now focus on functions defined on $\ell^2_{\nu}(\mathcal{V})$, squared integrable functions space which is the Hilbert space of functions defined on graphs endowed with its inner product:

$$\langle f,g\rangle_{\nu} = \sum_{x\in\mathcal{V}} f(x)\overline{g(x)}\nu(x),$$

where $\overline{g(x)}$ is the conjugate of g(x).

2.3 Filters on graphs

In traditional digital signal processing, signals are processed by filters, systems that take a signal as an input and produce another signal as an output. We can develop the equivalent concept of filters for graph signals. We consider linear shift-invariant filters, which are a generalization of linear time-invariant filters used in signal processing for 1D or 2D signals.

We define a graph filter as a linear operator $\mathbf{H} \in \mathbb{C}^{n \times n}$ acting on a graph signal input **s** to produce an output $\tilde{\mathbf{s}} = \mathbf{Hs}$. If $\mathbf{s_1}, \mathbf{s_2}$ are two graphs signals and α, β are scalars, we have:

$$\mathbf{H}(\alpha \mathbf{s}_1 + \beta \mathbf{s}_2) = \alpha \mathbf{H} \mathbf{s}_1 + \beta \mathbf{H} \mathbf{s}_2.$$

In this paper, we will focus on linear shift-invariant (LSI) graph filters. More precisely, linear shift invariant graph filters are a class of linear operators invariant with respect to a reference operator on graph \mathbf{R} , named graph shift. We assume that \mathbf{R} is diagonalizable. Formally an LSI graph filter \mathbf{H} is characterized by the commutativity property with respect to its reference operator \mathbf{R} ,

$\mathbf{RH} = \mathbf{HR}.$

The commutativity property implies that \mathbf{R} and \mathbf{H} share the same eigenspaces. Thus, \mathbf{H} can be expressed as :

$$\mathbf{H} = \sum_{i} \gamma_i \mathbf{G}_i, \quad \gamma_i \in \mathbb{C},$$

where \mathbf{G}_i are the spectral projectors of \mathbf{R} .

H can also be expressed as a polynomial of **R**:

$$\mathbf{H} = \sum_{i=0}^{L} h_i \mathbf{R}^i, \quad h_i \in \mathbb{C}.$$

REMARK 2.1. This last decomposition was used by Sandrihayla and Moura¹ when \mathbf{R} is taken as the adjacency matrix.

2.3.1 Frequency response of a filter

We can define the frequency response h of a filter **H** as follows:

$$\mathbf{H} = \sum_{i} h(\gamma_i) \mathbf{G}_i, \quad \gamma_i \in \mathbb{C},$$

where γ_i are the frequencies attached to the \mathbf{G}_i 's, the eigenspaces of \mathbf{R} and $h : \mathbb{C} \to \mathbb{C}$ is the frequency response of \mathbf{H} , i.e. a function of frequency with desirable filtering properties.

3. OPERATORS ON DIRECTED GRAPHS

The operators that we introduce have the characteristic for being defined on directed graphs as well undirected graphs. These operators are created from the random walk operator and will be the cornerstones of our multi-scale construction.

3.1 Random walk operator on graphs

A random walk on a graph is a finite discrete Markov chain defined on the set of the vertices \mathcal{V} endowed with an invariant measure π . The associated Markov chain is characterized by a transition probability matrix **P**. **P** can be expressed as $\mathbf{P} = \mathbf{D}_{out}^{-1} \mathbf{W}$ where \mathbf{D}_{out} is the diagonal matrix of the out-degree of Γ .

We assume throughout this paper that **P** is irreducible (i.e. \mathcal{V} is strongly connected under **P**). It is a fact that if **P** is aperiodic then $\mathbf{P}^n(x, .)$ approaches π as $n \to \infty$, π being the left eigenvector of **P** such that $\pi^\top \mathbf{P} = \pi^\top$, with $\sum_i \pi(i) = 1, \pi(i) \ge 0, \forall i$. We denote the time-reversal \mathbf{P}^* as the following identity

$$\pi(x)P^*(x,y) = \pi(y)P(y,x), \quad x,y \in \mathcal{V}$$

It is called the adjoint of **P** in the standard inner product of $\ell^2(\pi)$, that is $\langle f, \mathbf{P}g \rangle_{\pi} = \langle \mathbf{P}^* f, g \rangle_{\pi}$ where

$$\langle f, g \rangle_{\pi} = \sum_{x \in \mathcal{V}} \pi(x) f(x) \overline{g(x)} \pi(x)$$

The matrix **P** acts on a function $f \in \ell^2(\mathcal{V})$ as:

$$\mathbf{P}f(x) = \sum_{y \in \mathcal{V}} P(x,y) f(y)$$

If $\mathbf{P}^* = \mathbf{P}$ then \mathbf{P} is said to be time reversible or to satisfy the balance condition. Given any Markov matrix \mathbf{P} , we have two natural reversible chains:³⁴

- 1. the additive reversibilization $\frac{\mathbf{P}+\mathbf{P}^*}{2}$
- 2. the multiplicative reversiblization \mathbf{PP}^* .

On directed graphs, the random walk is nonreversible, i.e the balance equation is not verified. We assume that our random walk is defined on directed graphs, hence the non-reversibility is the general case that we assume.

REMARK 3.1. We can also consider the convex class of additive reversibilization operators $(1 - \alpha)\mathbf{P} + \alpha\mathbf{P}^*$, $\alpha \in [0,1]$ as potential random walk operators on directed graphs. This class of operators is not linear shift invariant to \mathbf{P} , yet it may be useful in some practical situations.

3.2 Laplacian on directed graphs

The directed Laplacian matrix³² on a digraph Γ is defined as follows.

DEFINITION 3.1. Let $\Gamma = (\mathcal{V}_{\Gamma}, \mathcal{E}_{\Gamma})$ be a digraph with $|\mathcal{V}_{\Gamma}| = n$. Let **P** be the transition probability matrix associated to Γ . The normalized Laplacian on Γ is defined as

$$\mathcal{L} = \mathbf{I} - \frac{\Pi^{1/2} \mathbf{P} \Pi^{-1/2} + \Pi^{-1/2} \mathbf{P}^{\top} \Pi^{-1/2}}{2}, \tag{1}$$

where Π is the diagonal matrix with π on the diagonal.

The unnormalized directed Laplacian L of a directed graph is defined as

$$L = \Pi - \frac{\Pi \mathbf{P} + \mathbf{P}^{\top} \Pi}{2}.$$
 (2)

The random walk Laplacian L^{rw} is defined as follows:

$$L^{rw} = \mathbf{I} - \frac{\mathbf{P} + \mathbf{P}^*}{2}.$$
(3)

The random walk Laplacian L^{rw} thus involves the additive reversibilization of the random walk operator.

Thus, the normalized Laplacian \mathcal{L} can be written in terms of the unnormalized Laplacian L as follows:

$$\mathcal{L} = \Pi^{-1/2} L \Pi^{-1/2}.$$

The unnormalized Laplacian is also related to the random walk Laplacian via

$$L = \Pi L^{rw}.$$

We obtain the same relation as in the undirected case. Moreover, the following remarks make the link with the undirected case.

REMARK 3.2. For undirected graph G, the probability distribution π has a closed expression

$$\pi(v) = \frac{d^{out}(v)}{\sum_{u} d^{out}(u)}.$$
(4)

REMARK 3.3. Using (4), we can show that (1), (2) and (3) are respectively the usual normalized, unnormalized (up to a multiplicative factor) and rando walk Laplacian on undirected graphs.

4. FOURIER ANALYSIS OF FUNCTIONS ON DIRECTED GRAPHS

In order to analyze and filter signals on graphs, we need to define a proper Fourier transform for graphs. In the classical signal processing, the Fourier transform is characterized by its Fourier modes (sine & cosine) to which we associate frequencies.

On more complex domains such as manifolds and graphs, the Fourier transform is generalized from the Laplacian where its eigenfunctions are the Fourier modes and its respective eigenvalues are the frequencies. Although this definition of the Fourier transform based on the Laplacian is fruitful, it concerns only undirected graphs. It thus becomes necessary to define a Fourier transform for directed graphs. Recently, numerous approaches have been investigated for directed graphs.^{2–4,6}

In this section, we propose a novel and alluring approach for constructing a Fourier basis for functions defined on directed graphs. Our graph Fourier basis is obtained by the determination of the desired frequency notion through the study of the Dirichlet energy of the random walk's eigenfunctions. We make a connection between eigenvectors of \mathbf{P} and a notion of variation.

First we introduce the notion of regularity of functions over graphs. Second we define the Dirichlet energy for functions over directed graphs and present the relation between the variations of the eigenfunctions of \mathbf{P} and its associated eigenvalues.

4.1 Global regularity of functions on graphs

The behavior of a function on a directed graph as well as an undirected graph can be analyzed by measuring its regularity, analogously to the functional analysis setting. The global variation of a function over a graph is defined as follows:

DEFINITION 4.1. Let be $\mu : \mathcal{E} \to \mathbb{R}^+$, a measure defined on the edge set \mathcal{E} . The global variation of a function on graph, $f : \mathcal{V} \to \mathbb{C}$ is:

$$||f||_{\mathcal{E},2,\mu} = \left(\sum_{(u,v)\in\mathcal{E}} |f(u) - f(v)|^2 \mu(u,v)\right)^{1/2}.$$

4.2 Frequency analysis on graphs

Let us consider the Dirichlet energy

$$\mathcal{S}_{\pi,\mathbf{P}}^{2}(f) = \frac{1}{2} \sum_{(u,v)\in\mathcal{E}} \pi(u) p(u,v) |f(u) - f(v)|^{2},$$

where p(u, v) is the (u, v) entry of the probability transition matrix **P** and $\pi(u)$ the stationary distribution at vertex u.

REMARK 4.1. If we replace $\pi(u)$ by (4), $S^2_{\pi,\mathbf{P}}(f)$ becomes the quadratic variation defined for functions on undirected graphs.

The following proposition establishes an appropriate connection between the Dirichlet energy $S_{\pi,\mathbf{P}}^2$ of a function f on a directed graph and a quadratic form consisting by Π, \mathbf{P} and \mathbf{P}^{\top} .

PROPOSITION 4.1. The Dirichlet energy of a function $f \in \ell^2_{\pi}(\mathcal{V})$ is expressed as

$$S_{\pi,\mathbf{P}}^2(f) = \langle f, Lf \rangle, \tag{5}$$

where $L = \Pi - \frac{\Pi \mathbf{P} + \mathbf{P}^{\top} \Pi}{2}$ defined at (2).

This proposition enables us to express the Dirichlet energy of the function f with respect to L.

The following proposition is the key step allowing a link between the variations of the eigenfunctions of \mathbf{P} and its associated eigenvalues.

PROPOSITION 4.2. Let be $\zeta : \mathcal{V} \to \mathbb{C}$, an eigenfunction of the random walk operator **P** associated to the eigenvalue $\eta \in \mathbb{C}$. The normalized Dirichlet energy of ζ is:

$$\frac{\mathcal{S}_{\pi,\mathbf{P}}^2(\zeta)}{||\zeta||_{\pi}^2} = 1 - \mathfrak{Re}(\eta)$$

where $\mathfrak{Re}(\eta)$ denotes the real part of $\eta \in \mathbb{C}$.

Proof.

$$\begin{split} \mathcal{S}_{\pi,\mathbf{P}}^{2}(\zeta) &= \langle \zeta,\Pi\zeta\rangle - \frac{1}{2}\langle \zeta,\Pi\mathbf{P}\zeta\rangle - \frac{1}{2}\langle \zeta,\mathbf{P}^{\top}\Pi\zeta\rangle \\ &= ||\zeta||_{\pi}^{2} - \frac{1}{2}\eta||\zeta||_{\pi}^{2} - \frac{1}{2}\overline{\eta}||\zeta||_{\pi}^{2} \\ &= (1 - \mathfrak{Re}(\eta))||\zeta||_{\pi}^{2}. \end{split}$$

By dividing the last equation by $||\zeta||_{\pi}^2$, we obtain the desired equation. \Box

This proposition establishes an association between the quadratic variation of an eigenfunction ζ of **P** and its respective eigenvalue η . We thus propose a frequency ordering for eigenfunctions by naming frequency associated to ζ :

$$\omega = 1 - \mathfrak{Re}(\eta), \quad \omega \in [0, 2].$$

In section 2, we have defined graph filters as a linear combination of spectral projectors of a reference operator **R**. Moreover, we have defined a desirable frequency notion on directed graphs from the random walk operator **P**. We can thus characterize LSI filters to **P** according their frequency response. A such filter can be written as follows:

$$\mathbf{H} = \sum_{i} h(\omega_i) \mathbf{G}_i,$$

where ω_i is the frequency associated with the spectral projector of \mathbf{G}_i of \mathbf{P} , and $h : \mathbb{R} \to \mathbb{R}$ a function with desirable filtering properties.

5. MULTIRESOLUTION ANALYSIS FRAMES FOR FUNCTIONS IN $\ell^2(\mathcal{V})$.

In the previous section, we have defined a notion of frequency for functions on directed graphs from the Dirichlet energy of the random walk's eigenfunctions. We are thus able to construct frames for functions over directed graphs from the bi-orthogonal basis of the random walk operator. This multi-scale frame construction is closely inspired by.^{7–9}

5.1 Scaling operator

Let \mathbf{P} be the random walk operator associated to the directed graph Γ endowed with the ergodic property. \mathbf{P} admits a spectral decomposition as follows:

$$\mathbf{P} = \sum_{i} \eta_i \mathbf{G}_i,$$

with \mathbf{G}_i the spectral projector associated to the eigenvalue $\eta_i \in \mathbb{C}$.

In order to represent the low-frequency component of a function f on a directed graph, we introduce the scaling operator Φ .

The scaling operator at a scale $t \Phi_t$ is LSI w.r.t **P**. It can be expressed as follows:

$$\Phi_t = \sum_i h(t\omega_i) \mathbf{G}_i,$$

where $h : \mathbb{R} \to \mathbb{R}$ is a function acting as a low-pass filter.

 Φ_t thus acts as a linear low-pass graph filter on the function f. The scaling functions are given by $\phi_{t,n} = \Phi_t \delta_n$, that is the low-pass graph filter Φ acting on a Kronecker δ -function at vertex n.

5.2 Wavelet operator

Similarly to the scaling operator Φ , we are able to construct wavelet operators Ψ . The wavelet operator at a scale t, Ψ_t is expressed as follows:

$$\Psi_t = \sum_i g(t\omega_i) \mathbf{G}_i,$$

where $g: \mathbb{R} \to \mathbb{R}^+$ is a function acting as a band-pass filter.

 Ψ_t acts as a linear band pass graph filter on the function f. The wavelet functions are given by $\psi_{t,n} = \Psi_t \delta_n$.

5.3 Wavelet transform frame

Given a fixed set of scales $\{t_j\}_{j=1}^J$, the scaling and wavelet Φ and Ψ operators, we define the synthesis operator \mathbf{W} as

$$\mathbf{W}=ig(\Phi_J,\Psi_1,\cdots,\Psi_Jig)$$

where Ψ_j (resp. Φ_j) stands here and in the following for Ψ_{t_i} (resp. Φ_{t_j}).

From \mathbf{W} , we define the *analysis operator* $\bar{\mathbf{W}}$

$$\bar{\mathbf{W}} = \begin{pmatrix} \bar{\Phi}_J \\ \bar{\Psi}_1 \\ \vdots \\ \bar{\Psi}_J \end{pmatrix}$$

where $\bar{\Psi}_j$ (resp. $\bar{\Phi}_j$) are graph filters. $\bar{\Psi}_t$ (resp. $\bar{\Phi}_t$) are defined at a scale t as follows:

$$\bar{\Psi}_t = \sum_i \bar{g}(t\omega_i) \mathbf{G}_i.$$

$$\bar{\Phi}_t = \sum_i \bar{h}(t\omega_i) \mathbf{G}_i$$

 $\bar{\mathbf{W}}$ requires two conditions:

- 1. $\overline{\Phi}$ and $\overline{\Psi}$ need to be graph filters.
- 2. The filters should guarantee the perfect reconstruction condition, i.e.

$$\sum_{j=1}^{J} g(t_j \omega_i) \bar{g}(t_j \omega_i) + h(t_J \omega_i) \bar{h}(t_J \omega_i) = 1.$$

These two conditions yield:

 $\mathbf{W}\mathbf{\bar{W}} = \mathbf{I}.$

Following what is done in⁹ we can construct a frame with desirable filter properties h and g (for instance by using filters that combine so that they leave no Fourier modes be put at zero by their joint actions). This aspect is not detailed here and we focus in the following on the construction of diffusion wavelets.

6. DIFFUSION WAVELETS ON DIRECTED GRAPHS

In the previous section, we have set the elements to construct a multi-scale frame, based on the bi-orthogonal basis of the random walk operator \mathbf{P} for functions defined over directed graphs. Among these scaling frames at each scale, we can select a subset of basis elements representing the scaling space in a compact way. We thus can go further through the extension of the diffusion wavelets framework^{10,11,35} to the directed graph setting.

In this section, we review the concept and construction of the diffusion wavelets and we introduce the generalization of the diffusion wavelets to the directed graph setting.

6.1 Diffusion wavelets

Diffusion wavelets is a multi-scale representation allowing a fast multi-resolution analysis of functions on graphs, generalizing the multi-resolution analysis in the classical setting. More specifically, the diffusion wavelets framework allows the construction of well-localized scaling functions and wavelets from powers of a diffusion operator.

6.2 Notations

Here we define notations required for the construction of diffusion wavelets. Two notations are defined, one for the representation of linear operators as matrices and another one for the representation of sets of vectors as matrices with each columns corresponding to a vector. The same notations were used in^{10,31} except that we here adopt a column vector convention whereas a row vector convention was used in.^{10,31}

Let V_0 be the space of signals on a graph $G = (\mathcal{V}, \mathcal{E})$. If **L** is a linear operator on V_0 , $[\mathbf{L}]_{B_1}^{B_2}$ denotes the matrix representing the linear operator **L** with respect to the basis B_1 in the domain and B_2 in the range. If B_1, B_2, B_3, B_4 are arbitrary bases, the representation of an operator **L** in different bases verify

$$[\mathbf{L}]_{B_1}^{B_2} = [\mathbf{I}]_{B_4}^{B_2} [\mathbf{L}]_{B_3}^{B_4} [\mathbf{I}]_{B_1}^{B_3}.$$
(6)

Furthermore, if B_1 or B_2 are linearly independent sets of vectors that do not span the whole space, then we will still use the notation $[\mathbf{L}]_{B_1}^{B_2}$, but in that case it will represent the *restriction* of the operator \mathbf{L} to the domain and range subspaces spanned by B_1 and B_2 .

A set of vectors X represented on a basis B will be written as a matrix $[X]_B$, with each column corresponding to a vector in X. The columns of $[X]_B$ are the coordinates of the vectors of X in the basis B_2 . When the set of vectors forms a basis B_1 , its representation on a basis B_2 , $[B_1]_{B_2}$ verifies $[B_1]_{B_2} = [\mathbf{I}]_{B_1}^{B_2}$. We will also abuse this notation if B_2 spans a subspace of the space spanned by B_1 . If B_1 and B_2 are two bases, the representations of X in B_1 and B_2 are related as follows: $[X]_{B_2} = [\mathbf{I}]_{B_1}^{B_2}[X]_{B_1}$.

6.2.1 Construction of Diffusion Wavelets

The construction of diffusion wavelets starts with a *diffusion operator* \mathbf{T} defined on the directed graph G. In the diffusion wavelet framework of Coifman and Maggioni, the graph is assumed undirected and they suggest using the reversible random walk operator \mathbf{P} as the diffusion operator. More generally, any operator \mathbf{T} can be used as long as it can be interpreted as a dilation operator when applied to localized functions on the graph. In classical signal processing terms, \mathbf{T} needs to behave like a low-pass filter. For a directed graph G, a sensible choice with respect to the Fourier analysis we propose is to use a low-pass graph filter. More precisely, this is a graph filter as defined in section 2 using the random walk \mathbf{P} as the reference operator and with a low-pass frequency response with respect to the definition of frequency we propose in section 4.

Assuming an ordering of vertices in \mathcal{V} , **T** is initially represented on the canonical basis $\Phi_0 = {\{\delta_k\}_{k \in \mathcal{V}}}$ of V_0 where δ_k is the Kronecker δ -function at vertex $k \in \mathcal{V}$, i.e $\delta_j = 1$ if j = k and $\delta_j = 0$ otherwise. With our notations, $[\mathbf{T}]_{\Phi_0}^{\Phi_0}$ is the matrix representing the linear operator **T** with respect to the basis Φ_0 in the domain and Φ_0 in the range.

The columns of $[\mathbf{T}]_{\Phi_0}^{\Phi_0}$, can also be viewed as a set of functions $\widetilde{\Phi}_1 = {\{\widetilde{\phi}_{1,k}\}_{k\in\mathcal{V}}}$ represented in the basis Φ_0 . These correspond to the application of \mathbf{T} to Dirac functions: $[\widetilde{\phi}_{1,k}]_{\Phi_0} = [\mathbf{T}]_{\Phi_0}^{\Phi_0} \delta_k$.

Due to the low-pass property of \mathbf{T} , each of the $\tilde{\phi}_{1,k}$ is a function localized around vertex k whose support extends to its close neighbors. In terms of the diffusion wavelets construction, these can therefore be interpreted as *scaling functions* at scale 1. Because of their support covering a small neighborhood around vertices, these functions $\phi_{1,k}$ can generally be well approximated by a linear combination of the other functions $\tilde{\phi}_{1,l}$ with $l \neq k$. The next step in the construction is to select a subset $\{\tilde{\phi}_{1,k}, k \in \mathcal{I}_1\}$ such that all $\tilde{\phi}_{1,k}$ are well-enough approximated by linear combinations of the functions in the subset. This can be seen as the equivalent of the decimation of a set of scaling functions in the classical discrete wavelet transform. Coifman and Maggioni used a greedy approach to build the set \mathcal{I}_1 iteratively by using a modified Gram-Schmidt orthogonalization procedure.¹⁰

The subset $\{\phi_{1,k}, k \in \mathcal{I}_1\}$ spans a subspace V_1 which is the first approximation subspace of the multi-resolution analysis. We will thus denote $\{\phi_{1,k}, k \in \mathcal{I}_1\}$ as Φ_1 , where Φ_1 is by definition a basis of V_1 that is generally not orthogonal. The vectors in Φ_1 are the *scaling functions* at scale 1.

In order to define the next scales of scaling functions, we consider the restriction of the diffusion operator to V_1 . The latter can be represented in Φ_1 as

$$[\mathbf{T}]_{\Phi_1}^{\Phi_1} = [\mathbf{I}]_{\Phi_0}^{\Phi_1} [\mathbf{T}]_{\Phi_0}^{\Phi_0} [\mathbf{I}]_{\Phi_1}^{\Phi_0}$$

where $[\mathbf{I}]_{\Phi_0}^{\Phi_1}$ represents the restriction of the signal space V_0 to V_1 (with bases Φ_0 and Φ_1) and $[\mathbf{I}]_{\Phi_0}^{\Phi_1}$ represents the embedding of V_1 in V_0 .

The next approximation space $V_2 \subset V_1$ and its basis Φ_2 can be obtained in the same way as the definition of V_1 and its basis Φ_1 except that we now consider the operator \mathbf{T}^2 restricted to V_1 instead of \mathbf{T} in V_0 . The columns of $[\mathbf{T}^2]_{\Phi_1}^{\Phi_1} = ([\mathbf{T}]_{\Phi_1}^{\Phi_1})^2$ can be interpreted as scaling functions at scale 2, $\tilde{\Phi}_2 = \{\tilde{\phi}_{2,k}\}$, represented in the basis Φ_1 . From these functions we extract a subset $\Phi_2 = \{\tilde{\phi}_{2,k}, k \in \mathcal{I}_2\}$ such that any function in $\tilde{\Phi}_2$ is well-approximated by a linear combination of functions of Φ_2 .

After j iterations of this procedure we have defined j approximation subspaces $V_j \subset V_{j-1} \subset \cdots \subset V_1$ with corresponding bases $\Phi_j, \Phi_{j-1}, \ldots, \Phi_1$. At each step the basis Φ_j is defined by its representation in the basis Φ_{j-1} based on the restriction of the operator \mathbf{T}^{2^j} to V_{j-1} . In order to represent these functions in the original basis Φ_0 of V_0 we can use

$$[\Phi_{j}]_{\Phi_{0}} = [\mathbf{I}]_{\Phi_{j}}^{\Phi_{0}} = [\mathbf{I}]_{\Phi_{0}}^{\Phi_{0}} [\mathbf{I}]_{\Phi_{1}}^{\Phi_{0}} \cdots [\mathbf{I}]_{\Phi_{j-1}}^{\Phi_{j-2}} [\mathbf{I}]_{\Phi_{j}}^{\Phi_{j-1}}.$$
(7)

Since every function in Φ_0 is defined on V_0 , so is every function on Φ_j . Hence any function in the approximation space V_j can be extended naturally to the whole space V_0 .

Regarding the construction of the wavelets, the wavelet bases Ψ_j for the subspaces W_j are built similarly to the scaling functions by selecting a subset of the columns of $[I_{V_j} - \Phi_{j+1} \Phi_{j+1}^{\dagger}]_{\Phi_j}^{\Phi_j}$ which is the orthogonal projector on the complement of V_{j+1} into V_j . The wavelets capture the detail lost from going from V_j to V_{j+1} .

6.3 A generalization using more arbitrary scaling operators

We propose a generalization of the diffusion wavelet framework that enables it to be combined for instance with the wavelet construction presented in section 5. The idea is merely to replace the powers of **T** as multiresolution scaling operators by more arbitrary low-pass filters. More precisely, where the operator $\mathbf{T}^{2^{j}}$ is used to define the approximation space V_{j+1} in section 6.2.1, we propose to use instead a low-pass graph filter \mathbf{H}_{j} . If the graph filters \mathbf{H}_{j} correspond to the scaling operators of section 5.1 with appropriately increasing scales, this approach provides a way to reduce the redundancy of the sets of scaling functions. Similarly, the same approach could be used to reduce the redundancy of the wavelet functions defined in section 5.2.

7. EXAMPLE

In this section, we illustrate the proposed multi-resolution construction on directed graphs, in the case of the directed ring graph. We compare the orthogonal and bi-orthogonal construction of scaling functions and wavelets.

7.1 Multiresolution on the directed ring graph

We consider the directed ring graph $C = (V_C, E_C)$ where V_C is the vertex set E_C , the edge set and $|V_C| = n$. This graph has an adjacency matrix **C**. The random walk operator on C is $\mathbf{P} = \mathbf{C}$. The matrix **P** is diagonalizable with $\mathbf{P} = \mathbf{DFT}_n \mathbf{ADFT}_n^*$. \mathbf{DFT}_n is the discrete Fourier transform matrix and $\mathbf{A} = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$, the eigenvalue matrix where $\lambda_k = e^{-2i\pi k/n}$. The Markov chain characterized by the random walk operator **P** is periodic. By this periodicity property, we are not able to obtain a unique limiting distribution π , necessary condition for our framework.

In order to break the periodicity of the random walk on this very specific graph, we consider a lazy random walk by adding self loops on the vertices of C. Formally, that amounts to consider $\tilde{\mathbf{P}} = \frac{1}{2}(\mathbf{I} + \mathbf{P})$. This choice of adding self loops has no impact on the Fourier basis but only on the eigenvalues where $\tilde{\lambda}_k = \frac{1}{2}(1 + \lambda_k)$, for all k, where $\tilde{\mathbf{A}} = \text{diag}(\tilde{\lambda}_1, \dots, \tilde{\lambda}_n)$ is the eigenvalue matrix of $\tilde{\mathbf{P}}$.

The associated frequency ω_k yields:

$$\omega_k = 1 - \Re(\widetilde{\lambda}_k) = \frac{1}{2}(1 - \cos\frac{2k\pi}{n})$$

We are able to construct the low pass graph filter \mathbf{H} as defined in the previous sections.

$$\mathbf{H} = \mathbf{DFT}_n h(\mathbf{\Omega}) \mathbf{DFT}_n^*.$$

where $\mathbf{\Omega} = \operatorname{diag}(\omega_1, \cdots, \omega_n)$ and $h : \mathbb{R} \to [0, 1]$ a function such that $h(\omega_k) = \cos \frac{2k\pi}{n}$ for all k.

We are able to apply the diffusion wavelet framework in the orthogonal and bi-orthogonal version, starting from the graph filter **H** on directed ring graph. The number of scales of the multi-resolution is equal to 10. We consider the powers $\mathbf{H}^{2^{j}}$.

We illustrate the two constructions by comparing the scaling functions and the wavelets at different scales. The figure 1 shows some bi-orthogonal scaling functions and wavelets at the scale 1, 3 and 6 over 10, localized at different vertices. They look like what is expected for scaling functions (low-pass aggregation functions) and wavelets (localized oscillating functions).

The figure 2 shows the orthogonal scaling functions and wavelets also at the scale 1,3 and 6. At each scale, we represent 3 or 4 scaling and wavelets functions, selected w.r.t the highest ℓ^2 -norm.

We note that at each scale, the support of bi-orthogonal scaling functions appear to be the same size whatever the vertex it is localized around, while for orthogonal scaling functions the support changes and some functions oscillate. This is due to the orthogonalization procedure. As the orthogonalization process proceeds, the scaling functions newly created become a linear combination of an increasing number of the columns previously selected. This yields to an extension of the support of the scaling functions unlike to the bi-orthogonal ones. Although the orthogonal scaling and wavelets basis have more advantages in a numerical perspective (they are more stable than bi-orthogonal ones), they show some shortcomings in terms of spatial and frequency localization.



Figure 1. Bi-orthogonal scaling and wavelets functions at different scales.



Figure 2. Orthogonal scaling and wavelets functions at different scales.

8. CONCLUSION

We have presented a general framework for constructing a multi-resolution analysis for functions defined over directed graphs. By constructing a frequency analysis on directed graphs from the Dirichlet energy of the random walk's eigenfunctions, we can consider random walk's eigenfunctions as Fourier basis for functions on directed graphs. This Fourier basis has the feature for not being orthogonal. Using this random walk Fourier basis, we have been able to build scaling and wavelets operators in the frequency domain and the directed graph wavelets (plus the last scaling function) form a frame. We also have been able to extend the diffusion wavelet framework to the directed graph setting, and we have illustrated the orthogonal and bi-orthogonal constructions on a directed ring graph. We show by relaxing the orthogonal requirement to bi-orthogonal, we obtain scaling and wavelets functions better localized and smaller support.

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