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Multi-link wavelets on hierarchical graphs

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ABSTRACT

Much of the recent progress in one- and two-dimensional signal processing can be attributed to the introduction of sparse representation techniques such as wavelets. Researchers have recently focused on extending the sparse representation to more complicated data, such as high-dimensional data and data on graphs. Some wavelet techniques applicable to trees as special cases of graph structures have been proposed that are very computationally efficient and easy to implement. However, a tree is too simple to model a data manifold accurately, in particular since a node has at most one parent. In this paper we propose a new efficient wavelet transform applicable to a directed acyclic graph (DAG), in which nodes are allowed to have multiple parents. Our method generalizes a Haar-like wavelet on an unweighted tree by using a redundant representation. In our method, we treat a DAG that has some nodes with signals we wish to analyze and the remaining nodes without signals. Nodes without signals are used to represent the underlying hierarchical structure of the data domain. We also describe a practical application to semi-supervised learning and show that our approach demonstrates an improvement over tree-based wavelets.

1. Introduction

The efficient representation of data is one of the key issues in various fields, such as signal processing, data mining, and machine learning. The appropriate representation is critical for performing data analyses effectively and efficiently. In recent years, many interesting applications involve data defined on topologically complicated domains, e.g., high-dimensional structures, irregularly sampled spaces, and nonlinear manifolds. The development of data representation methods applicable to such complicated data domains is an interesting problem.

The wavelet transform is known to be a powerful harmonic analysis tool for one- and two-dimensional signal processing, which can localize signals in both space and frequency [1]. Wavelets are widely used in various signal processing problems, including denoising, data compression, deblurring, and data analysis, because of their ability to sparsely approximate piece-wise smooth signals. Note that for two-dimensional signals (i.e., images), better representation techniques, such as curvelets [2], have also been proposed to achieve more sparsity than can wavelets.

The effectiveness of harmonic analysis techniques on low-dimensional spaces motivates the investigation of extensions to complicated domains. Such data can naturally be modeled as signals defined on the nodes of graphs. The graph Fourier transform, which provides a harmonic analysis of graph signals, is derived based on the graph Laplacian [3]. As a sparse representation method, several extensions of the wavelet transform, operating on a graph, have already been proposed [4–6]. Moreover, computationally efficient wavelet transform methods are proposed for data on a tree, which is a special case of graphs [7–11]. However, a tree has the strong constraint that each node has at most one parent.

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Two types of sparse representation exist: redundant ones and non-redundant ones. Sparse and redundant representations are widely used and are shown to be highly effective in low-dimensional data analysis [12]. For example, these techniques can compensate for the lack of the translation-invariance property of non-redundant representations in regular spaced samples (e.g., [13]). Sparse and redundant representations provide flexibility in representing signals by using overcomplete vectors. In this paper, we use a sparse and redundant representation to describe the extension of a tree-based wavelet transform.

We propose a new fast wavelet transform, which we call a multi-link wavelet transform (MLWT), applicable to a directed acyclic graph (DAG) by using a sparse and redundant representation. A DAG is permitted to have nodes with more than one parent, and thus is a generalization of a tree. The MLWT can be considered as an extension of a wavelet on an unweighted tree [7,8,10,11], and can be applicable to any DAG where the sum of weights of all edges connected to each node is one. DAGs (not trees) are used to represent data structures in many applications: for example, Hasse diagrams [14], gene ontology [15], a collection of tasks that have dependencies between them [16], and multi-path routing [17]. Since DAGs can represent more flexible hierarchical structures than trees, the proposed method is expected to be effective.

First, in Section 2, we present an outline of the problem. In Section 3, we then provide the MLWT algorithm and some of its properties. Experimental results of semi-supervised learning are presented in Section 4, and the last section gives some conclusions.

2. Problem outline

We consider a graph $G = (V, E)$ consisting of a set of nodes V and a set of edges $E \subseteq V \times V$. Signals $x[v] \in \mathbf{R}$ that we wish to analyze are defined for some nodes v in V, where $\mathbf{R}$ is the set of real numbers. Let V_s be the set of nodes having signals ($V_s \subseteq V$ holds). Nodes without signals, which is in $V \setminus V_s$, represent the underlying hierarchical structure of the data domain. As a simple example, we can treat an image as data on a graph with a regular two-dimensional lattice structure (in this case, $V_s = V$). Another example is a tree structure constructed by clustering, where each leaf node represents a data point (in this case, V_s is the set of leaf nodes), and each non-leaf node represents a cluster containing all of its lower-level nodes (e.g., [18]). Graphs can model rich geometrical structures, including high-dimensional, irregular, and non-Euclidean manifolds.

One of the major problems in signal processing on graphs is the estimation of unknown true signals $x[v]$ from given observations. An example is learning, which involves estimating the missing signals $x[v]$ by using the observed signal values. Another example is denoising, which involves recovering clean signals $x[v]$ from the noisy version $y[v] = x[v] + n[v]$ contaminated with additive noise $n[v]$. In many cases, it can be assumed that the true signals are highly related to the structure of the graph. For instance, it can be considered that when two nodes v and v' are connected with an edge, the corresponding signals $x[v]$ and $x[v']$ tend to be sufficiently close. It is important to represent true signals $x[v]$ effectively by using the properties of the graph structure to improve the performance of signal processing.

Let $N = |V_s|$ and let $\boldsymbol{x} \in \mathbf{R}^N$ be a vector representing the signal values $\{x[v]\colon\ v \in V_s\}$. An orthogonal wavelet transform of $\boldsymbol{x}$ is given by $\boldsymbol{\alpha} = U^T \boldsymbol{x}$, where $U \in \mathbf{R}^{N \times N}$ is an orthogonal matrix ($UU^T = U^T U = I$; I is the identity matrix), and $\boldsymbol{\alpha} \in \mathbf{R}^N$ is referred to as a coefficient vector. Each of the N columns of U is a fundamental element that describes a feature of the signals, which is called a basis vector (or atom), and $\boldsymbol{x}$ can be represented as linear combination of basis vectors with weights $\boldsymbol{\alpha}$: $\boldsymbol{x} = U\boldsymbol{\alpha}$.

Gavish et al. [10] proposed a Haar-like orthogonal wavelet transform (OWT) for a tree. An example of a basis of the OWT is shown in Fig. 1(a). In this example, all $N = 5$ leaves have the corresponding signals and the five filters, h_v and $g_{v,u}$, form the basis U. The OWT is applicable to any tree, but not a DAG in which at least one node has plural parents.

To capture the important features of the signals effectively, the representation that captures a large part of the signals with only a few coefficients is required. However, an intrinsic weakness of orthogonal wavelet transforms is: their limited expressiveness, which is caused by the limited number of basis vectors (only N vectors).

We consider a new wavelet transform applicable to a DAG. The possibility that an orthogonal wavelet transform applicable to such DAGs may be limited in expressiveness as well as complicated and time-consuming brings us to redundant representation modeling. In redundant representation, a vector $\boldsymbol{x}$ is expressed as $\boldsymbol{x} = \Phi\boldsymbol{\alpha}$, where $\Phi \in \mathbf{R}^{N \times S}$ is a matrix that has S linearly dependent columns ($S > N$), called frame vectors. Using such a redundant wavelet enables effective representation of a wider variety of signal types. Fig. 1(b) shows an example of a frame of the MLWT with $N = 5$ and $S = 7$. Note that if a given DAG is a tree, then the MLWT is equivalent to the OWT.

3. Multi-link wavelets

Let us consider a DAG $G = (V, E)$. If $(v, u) \in E$, then v is called a parent of u and u is called a child of v. Let $P[u]$ be the set of all parents of u, i.e., $P[u] = \{v\colon\ (v, u) \in E\}$, and $C[v]$ be the set of all children of v, i.e., $C[v] = \{u\colon\ (v, u) \in E\}$. We call a node without any child the lowest level node. Let $\mathcal{L}_0$ be the set of lowest level nodes and $\mathcal{L}_j$ $(j = 1, 2, \ldots)$ be $\mathcal{L}_j = \{v \notin \Delta_{j-1}\colon\ C[v] \subseteq \Delta_{j-1}\}$ where $\Delta_{j-1} = \bigcup_{k=0}^{j-1} \mathcal{L}_k$, that is, $v \in \mathcal{L}_j$ if and only if any child of v is an element of Δ_{j-1} but v is not an element of Δ_{j-1}. We call the index j such that $v \in \mathcal{L}_j$ the level of v. Let J be a natural number satisfying $\mathcal{L}_J \neq \phi$ and $\mathcal{L}_{J+1} = \phi$ (ϕ: the empty set). Note that $V = \Delta_J = \bigcup_{k=0}^{J} \mathcal{L}_k$ and the union is disjoint, i.e., $\mathcal{L}_j \cap \mathcal{L}_{j'} = \phi$ for any