Extension of wavelets to networks

Mani Mehra

Department of Mathematics
Indian Institute of Technology Delhi (IITD)
1 Introduction to wavelets

2 Spectral graph wavelet

3 Adaptive spectral graph wavelet method on networks
Wavelets

A wavelet (due to Morlet and Grossmann in the early 1980s) is a mathematical function used to divide a given function or continuous-time signal into different scale components. They used the French word ondelette, meaning “small wave”. Soon it was transferred to English by translating “onde” into “wave”, giving “wavelet”.

Example

Left: Initial signal  
Middle: Fourier approximation with only 17 terms  
Right: Wavelet approximation with only 17 terms
Example

Left: **Signal**  Middle: **error in Fourier approximation**  Right: **error in wavelet approximation**
Multiresolution Analysis of $L_2(\mathbb{R})$

**Definition**

MRA is characterized by the following axioms

- $\{0\} \subset \cdots \subset V^{-1} \subset V^{0} \subset V^{1} \cdots \subset L_2(\mathbb{R})$
- $\bigcup_{j \in \mathbb{Z}} V^j = L_2(\mathbb{R})$
- $\bigcap_{j \in \mathbb{Z}} V^j = \{0\}$
- Invariance to dilations, i.e $f \in V^j$ iff $f(2(\cdot)) \in V^{j+1}$
- Invariance to translations, i.e
  \[ \{ \phi^0_k \text{ (scaling function)} = \phi(x - k) | k \in \mathbb{Z} \} \]
  is an orthonormal basis for $V^0$

Now the sequence $\phi^j_k(x) = 2^{j/2} \phi(2^j x - k)_{k \in \mathbb{Z}}$ is an orthonormal basis for $V^j$. 
Since \( \phi_0^0(x) = \phi(x) \in V^0 \subset V^1 \), so

\[
\phi(x) = \sum_{k=-\infty}^{\infty} h_k \phi_1^k(x).
\]

This is called dialation equation and for Daubechies compactly supported scaling function only finitely many \( h_k, k = 0, 1, \cdots D - 1 \) will be nonzero. Where \( D \) is even positive integer called the wavelet genus and \( h_0, h_1, \cdots, h_{D-1} \) are called low pass filter coefficients.
Define $\mathcal{W}^j = \{\psi^j_k \ (\text{wavelet}) \mid k \in \mathbb{Z}\}$ to be the complement of $\mathcal{V}^j$ in $\mathcal{V}^{j+1}$, where $\mathcal{V}^{j+1} = \mathcal{V}^j + \mathcal{W}^j$.

Now the sequence $\psi(x) \in \mathcal{W}^0$ (which is called mother wavelet) such that $\psi^j_k(x) = 2^j/2 \psi(2^j x - k)_{k \in \mathbb{Z}}$ is an orthonormal basis for $\mathcal{W}^j$. For, Daubechies compactly supported wavelet $\psi(x) \in \mathcal{W}^0 \subset \mathcal{V}^1$, therefore

$$\psi(x) = \sum_{k=0}^{D-1} g_k \phi^1_k(x).$$

This is called wavelet equation and $g_0, g_1, \cdots, g_{D-1}$ are called high pass filter coefficients connected by the relation $g_k = (-1)^k h_{D-1-k}, k = 0, 1, \cdots, D - 1$. 

Benasque, 2017
Why second generation wavelets?

- Second generation wavelet was developed by W. Swelden in 1996.
- Fast $O(N)$ transform.
- Dynamic grid adaption to the local irregularities of the solution.

(This situation arises e.g. in the tracking of storms or fronts for the simulation of global atmospheric dynamics.)
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Why general manifolds? (e.g. Sphere)

- Application of adaptive wavelet collocation method (AWCM) to the problems of geodesy, climatology, meteorology (Representative examples include forecasting the moisture and cloud water fields in numerical weather prediction).
- Many PDEs arise from mean curvature flow, surface diffusion flow and Willmore flow on the sphere.
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Why wavelets on manifolds? (e.g. spherical wavelets)

- Spherical triangular grids (quasi uniform triangulations) avoid the pole problem.
  Conventional grids–uniform longitude-latitude grid
- Problem- Singularity of coordinate system near the poles
- Solution-
  - Necessary to introduce auxiliary coordinate system.
  - Another solution is to avoid the introduction of the 'metric term' which are unbounded near the poles.
- To solve PDEs efficiently using adaptivity on general manifold by wavelet methods was an open problem till 2000.
- Past applications of wavelets to turbulence have been mainly restricted to flat geometries which severely limits for geophysical applications.
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Wavelet multiresolution analysis of $L_2(S)$

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MRA is characterized by the following axioms

- $\mathcal{V}^j \subset \mathcal{V}^{j+1}$ (subspaces are nested).
- $\bigcup_{j=-\infty}^{\infty} \mathcal{V}^j = L_2(S)$.
- Each $\mathcal{V}^j$ has a Riesz basis of scaling function $\{\phi_k^j | k \in \mathcal{K}^j\}$.

Define $\mathcal{W}^j = \{\psi_m^j (\text{wavelets}) | m \in \mathcal{M}^j\}$ to be the complement of $\mathcal{V}^j$ in $\mathcal{V}^{j+1}$, where $\mathcal{V}^{j+1} = \mathcal{V}^j \oplus \mathcal{W}^j$.

$$\phi_k^j = \sum_{l \in \mathcal{K}^{j+1}} h_{k,l}^j \phi_{l}^{j+1} \quad \text{(dilation equation)}$$

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Construction of spherical wavelets based on spherical triangular grids

The set of all vertices

\[ S^j = \{ p_k^j \in S : p_k^j = p_{2k}^{j+1} | k \in K^j \} \text{ and } M^j = K^{j+1} / K^j. \]

Level 0

Dyadic icosahedral triangulation of the sphere
Construction of spherical wavelets based on spherical triangular grids

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Dyadic icosahedronal triangulation of the sphere
Wavelet compression

\[ u^J(p) = \sum_{k \in K^0} c_k^J \phi_k^J(p) + \sum_{j=J_0}^{J-1} \sum_{m \in M^j} d_m^j \psi_m^j(p) \]

Test function

Wavelet locations \( x_k^J \) without compression at \( J = 6 \), \( \#K^6 = 40962 \)
Wavelet compression

\[ u^J(p) = \sum_{k \in \mathcal{K}} c_k^0 \phi^0_k(p) + \sum_{j=0}^{J-1} \left( \sum_{m \in \mathcal{M}^j} d^j_m \psi^j_m(p) + \sum_{m \in \mathcal{M}^j} d^j_m \psi^j_m(p) \right) \]

Test function

Wavelet locations \( x^J_k \) without compression at \( J = 6, \# \mathcal{K}^6 = 40962 \)

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Wavelet compression

\[ u^J_{\geq}(p) = \sum_{k \in \mathcal{K}^0} c^J_k \phi^J_k(p) + \sum_{j=J_0}^{J-1} \sum_{m \in \mathcal{M}^j_{\epsilon}} d^j_m \psi^j_m(p) + \text{Discarded term} \]

Test function

Wavelet locations \( x^J_k \) st \( J = 6, \epsilon = 10^{-5} \),
\[ N(\epsilon) = 8175 \text{ and ratio } \frac{\#\mathcal{K}^6}{N(\epsilon)} \approx 5 \]
Wavelet compression

\[ u^J(p) = \sum_{k \in \mathcal{K}^0} c_k \phi_k^J(p) + \sum_{j=J_0}^{J-1} \sum_{m \in \mathcal{M}_j} d_{m}^j \psi_m^j(p) \]

Test function

Wavelet locations \( x_k^J \) without compression at \( J = 7 \),

\[ \# \mathcal{K}^7 = 163842 \]
Wavelet compression

\[ u_J^J(p) = \sum_{k \in K^0} c^J_k \phi^J_k(p) + \sum_{j=J_0}^{J-1} \sum_{m \in M^j} d^j_m \psi^j_m(p) + \text{Discarded term} \]

Test function

Wavelet locations \( x_k^J \) at \( J = 7 \), \( \epsilon = 10^{-5} \), \( N(\epsilon) = 20353 \) and ratio

\[ \frac{\# K^7}{N(\epsilon)} \approx 8 \]

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Wavelet compression

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Test function

Wavelet locations \( x_k^J \) without compression at \( J = 8 \),
\[ \#\mathcal{K}^8 = 655362 \]
Wavelet compression

\[ u_J^J(p) = \sum_{k \in K^0} c_k^0 \phi_k^0(p) + \sum_{j=J_0}^{J-1} \sum_{m \in M^i} d_m^j \psi_m^j(p) + \text{Discarded term} \]

Test function

Wavelet locations \( x_k^J \) at \( J = 8 \), \( \epsilon = 10^{-5} \), \( N(\epsilon) = 64231 \) and ratio \( \frac{\#K^8}{N(\epsilon)} \approx 10 \)

Given a manifold $X$ and a diffusion operator $T$ on $L^2(X)$ such that high powers of $T$ have low numerical rank, an MRA can be constructed for $L^2(X)$ which leads to the construction of diffusion wavelet.

Classes of operators which can be used for the construction of diffusion wavelet include approximation of second order differential operators.

A precision $\tau > 0$ is fixed and $X^J = \{x_1, x_2, \cdots, x_N\}$ is the discretization of $X$ using $N$ points.

$\Phi^J = \{\delta_k\}_{k \in X^J}$, $\delta_k$ is an $N \times 1$ vector having 1 at $k^{th}$ place and 0 otherwise, then space $\mathcal{V}^J$ is defined as:

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\]
$[T]^{\Phi_{J-1}}_{\Phi_J}$ is used to indicate the matrix representing the linear operator $T$ with respect to basis $\Phi^J$ in the domain and $\Phi^{J-1}$ in the range.
For the operator $T$ it is clear that

$$\cdots \subseteq \text{range}_\tau(T^{1+2+\cdots+2^j-1}) \subseteq \cdots \subseteq \text{range}_\tau(T) \subseteq \text{span}\{\Phi^j\} \subseteq \cdots \subseteq \mathcal{L}_2(X),$$

so that we have

$$\cdots \subseteq \mathcal{V}^{j-j} \subseteq \cdots \subseteq \mathcal{V}^{j-1} \subseteq \mathcal{V}^j \subseteq \cdots \subseteq \mathcal{L}_2(X),$$

which is analogous to the axiom (1) of MRA.

In the construction of diffusion wavelet the operator $T$ being the diffusion operator dilates the functions on which it is operated. Now the functions in $\mathcal{V}^j$ are obtained by applying the operator $T$ on the functions of the space $\mathcal{V}^{j+1}$, hence the functions of the space $\mathcal{V}^j$ are dilations of the functions in the space $\mathcal{V}^{j+1}$.

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For the operator $T$ it is clear that

$$\cdots \subseteq \text{range}_\tau(T^{1+2\cdots+2^j-1}) \subseteq \cdots \subseteq \text{range}_\tau(T) \subseteq \text{span}\{\Phi^J\} \subseteq \cdots \subseteq L_2(X),$$

so that we have

$$\cdots \subseteq \mathcal{V}^{J-j} \subseteq \cdots \subseteq \mathcal{V}^{J-1} \subseteq \mathcal{V}^J \subseteq \cdots \subseteq L_2(X),$$

which is analogous to the axiom (1) of MRA.

In the construction of diffusion wavelet the operator $T$ being the diffusion operator dilates the functions on which it is operated. Now the functions in $\mathcal{V}^j$ are obtained by applying the operator $T$ on the functions of the space $\mathcal{V}^{j+1}$, hence the functions of the space $\mathcal{V}^j$ are dilations of the functions in the space $\mathcal{V}^{j+1}$.

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The detail spaces $\{W^j\}$s are constructed in such a way that
$V^j = V^{j-1} \oplus W^{j-1}$.

**Construction of the MRA can be visualized with following diagram**

- $V^J = \text{span}\{\Phi^J\}$
  - ($\Phi^J$ is the basis.)
- $V^{j-1} = \text{range}_r T$
  - ($\Phi^{j-1}$ is the basis.)
- $W^{j-1} = \text{range}_r (I - T)$
  - ($\Psi^{j-1}$ is the basis.)
The detail spaces $\{\mathcal{W}^j\}$s are constructed in such a way that

$$\mathcal{V}^j = \mathcal{V}^{j-1} \oplus \mathcal{W}^{j-1}.$$
Wavelet basis allowed to represent objects with singularities of complex structures with low number of degrees of freedom, a property that is particularly promising when thinking of an application to the numerical solutions of PDEs.

- Good approximation properties
- Efficient multiscale decompositions
- Compact support
- Vanishing moments
- Existence of fast wavelet transform
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The first attempts to use wavelet bases for numerical solution of PDEs go back to early 1990s. Despite the vast literature available, the wavelet theory for numerical solution of PDEs on general manifold is still in nascent stage. We have developed adaptive meshfree diffusion wavelet method for solving PDEs on the sphere and this method can be easily generalised onto general manifolds.


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Spectral graph wavelet constructed in 2011 by Hammond and others.

The wavelet is constructed on an arbitrary finite weighted graph $G = \{V, E, \omega\}$.

The adjacency matrix $A = \{a_{m,n}\}$ for the weighted graph $G$ has the entries

$$a_{m,n} = \begin{cases} \omega(e) & \text{if } e \in E \text{ connects vertices } m \text{ and } n \\ 0 & \text{otherwise.} \end{cases}$$

For a weighted graph, the degree of each vertex $m$, written as $d(m)$, is defined as the sum of weights of all the edges incident to it, i.e., $d(m) = \sum_{n} a_{m,n}$. A matrix $D$ is defined as a diagonal matrix with $d(m)$ as the diagonal entries.

A non normalized Laplacian for the graph is defined as $\mathcal{L} = D - A$. 

Benasque, 2017
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Extension of wavelets to networks
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- A non normalized Laplacian for the graph is defined as $\mathcal{L} = D - A$. 
For any $f \in \mathbb{R}^N$ defined on the vertices of the graph $G$, its graph Fourier transform $\hat{f}$ is defined by

$$\hat{f}(l) = \langle \chi_l, f \rangle = \sum_{n=1}^{N} \chi_l^*(n)f(n),$$

where $\{\chi_l, \quad l = 0, 1, 2, \ldots, N - 1\}$ are the eigenvectors corresponding to the eigenvalues $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \cdots \leq \lambda_{N-1}$ of the matrix $\mathcal{L}$ (like $e^{i\omega x}$ used in defining the Fourier transform of the function defined on $\mathbb{R}$ are eigenfunctions of the one–dimensional Laplacian operator $\frac{d^2}{dx^2}$).

The inverse graph Fourier transform is

$$f(n) = \sum_{l=0}^{N-1} \hat{f}(l) \chi_l(n).$$
To define **spectral graph wavelet transform**, initially a kernel function \( g : \mathbb{R}^+ \rightarrow \mathbb{R}^+ \) is chosen satisfying \( g(0) = 0 \) and \( \lim_{x \to \infty} g(x) = 0 \) (we will refer \( g \) as wavelet kernel).

Then, for the given wavelet kernel \( g \), the wavelet operator \( T_g = g(\mathcal{L}) \) acts on a given function \( f \) by modulating each Fourier mode as

\[
\hat{T}_g f(l) = g(\lambda_l) \hat{f}(l),
\]

which implies

\[
(T_g f)(m) = \sum_{l=0}^{N-1} g(\lambda_l) \hat{f}(l) \chi_l(m).
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The wavelet operator at scale \( t \) is then defined by \( T_g^t = g(t\mathcal{L}) \).

The **spectral graph wavelets** are defined as

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\psi_n^t = T_g^t \delta_n.
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The wavelet coefficients of a function $f$ are obtained by taking the inner product of that function with these wavelets, as

$$\mathcal{W}_f(t, n) = \langle \psi_n^t, f \rangle \ \text{(Spectral graph wavelet transform (SGWT))}.$$ 

Spectral graph scaling functions are determined by a single real valued function $h : \mathbb{R}^+ \to \mathbb{R}$ which satisfies $h(0) > 0$ and $\lim_{x \to \infty} h(x) = 0$ (we will refer $h$ as scaling function kernel).

$$\phi_n = h(\mathcal{L})\delta_n.$$ 

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The naive way of computing SGST and SGWT requires explicit computation of entire set of eigenvalues and eigenfunctions of the Laplacian operator $\mathcal{L}$. This approach is computationally inefficient for large graphs.

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$d^j_k$ for different value of $j$ for

$$f(x) = - \tanh \left( \frac{x + x_0}{2\nu} \right) + e^{-64^2(x-x_0)^2}, \quad x_0 = \frac{1}{3}, \quad \nu = 10^{-3}, \quad (J = 4).$$

$f(x) = x$, if $0 < x < 0.5$ and $x - 1$ otherwise.
Functions and the corresponding adaptive node arrangements using SGW with $R = 0.1$ and $M = 4$. 
In 1952, A. M. Turing settled the basis for explaining biological patterns using two interacting chemicals, which under certain conditions, can generate stable patterns from an initial near-homogeneity. This phenomenon has now been shown to occur in chemistry and biology.

The Turing patterns are governed by a system of nonlinear reaction-diffusion equations. We solve the following system:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= D \delta \nabla^2 u + \alpha u (1 - r_1 v^2) + v (1 - r_2 u), \\
\frac{\partial u}{\partial t} &= \delta \nabla^2 v + \beta v \left( 1 + \frac{\alpha r_1}{\beta} uv \right) + u (\gamma + r_2 v).
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At initial state, i.e., at \( t = 0 \) we consider \( u = v = 0 \), except on a narrow band.
**Turing patterns on the sphere**

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\frac{\partial v}{\partial t} &= \delta \nabla^2 v + \beta v \left(1 + \frac{\alpha r_1}{\beta} uv\right) + u(\gamma + r_2 v).
\end{align*}
\]

- At initial state, i.e., at \( t = 0 \) we consider \( u = v = 0 \), except on a narrow band.
The stable patterns can be either stripes or spots, depending on the parameters $r_1$ and $r_2$. The parameter $r_1$ favours stripes while $r_2$ favours spots.

We fix the parameters

\[ D = 0.516, \delta = 0.0045, \alpha = 0.899, \beta = -0.91 \text{ and } \gamma = -\alpha. \]

As case 1, we take $r_1 = 3.5, r_2 = 0$.

As case 2, we take $r_1 = 0.002, r_2 = 0.2$. 
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Solution ($u$ component) and dynamically adapted node arrangement for case 1 at $t = 0$ and $t = 18$. 
Solution ($u$ component) and dynamically adapted node arrangement for case 1 at $t = 50$ and $t = 1000$. 

[Images of plots showing the solution at different times]
Solution \((u\text{ component})\) and dynamically adapted node arrangement for case 2 at \(t = 250\) and \(t = 1000\).

Collaborator

- Günter Leugering (FAU Erlangen)
- Ankita Shukla (IIT Delhi)
Mathematical solutions of PDEs on network–like structure modelling many real life phenomenon (i.e. water wave propagation in open channels) exhibit singularities and these singularities are of physical relevance.

To discover all the features of the solution we need a large set of node points but this will increase the computational as well as storage cost.

In some cases the set required to capture all the features of the solution may exceed the practical limitations.

To deal with these problems we work on an adaptive node arrangement which will keep on modifying according to numerical solution of the PDE on networks evolves with time.
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Adaptive mesh refinement (AMR) is the most typical technique used for adaptivity. In AMR the entire computational domain is covered with a coarse Cartesian grid. Individual grid cells are selected for refinement in moving from one step of the numerical algorithm to the next step based on a posteriori criterion.

These methods are, no doubt, computationally efficient but the theory proving their advantages over their corresponding non-adaptive counterparts is not well developed. In particular, the rate of convergence of the adaptive algorithm, which describes the trade-off between the accuracy and complexity of the approximation is not clearly understood.

One of the important property of wavelet is that the wavelet coefficients $d^j_k$ decrease rapidly for smooth functions. Moreover, if a function has a discontinuity in one of its derivatives then the wavelet coefficients will decrease slowly only near the point of discontinuity and maintain fast decay where the function is smooth.
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This property of wavelet makes it suitable to detect where in the numerical solution of a PDEs on large networks the singularities are located.

The selection of appropriate basis functions in wavelet based adaptive methods is similar to the selection of the grid cells in AMR, therefore one could expect similar performances from both the approaches.

The advantage with wavelet based adaptive methods is that sound theoretical results exist which can answer the fundamental questions such as rate of convergence of the adaptive method.
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Topology of network

For our numerical computation, we have taken the following wavelet kernel

\[
g(\lambda) = \begin{cases} 
\lambda^2 & \text{for } \lambda < 1 \\
-5 + 11\lambda - 6\lambda^2 + \lambda^3 & 1 \leq \lambda \leq 2 \\
4\lambda^{-2} & \text{for } \lambda > 2.
\end{cases}
\]
The wavelet kernels are plotted in figure against different $\lambda$ using $t_1 = 8.80$, $t_2 = 2.57$, $t_3 = .75$ and $t_4 = .22$ for the star shaped network.

The wavelet scales $t_j$ are selected to be logarithmically equispaced between the minimum ($t_J$) and maximum ($t_1$) scales. All the properties (1, 2 and 3) of $g$ are satisfied as it could be observed from above figure.
The wavelet functions for $J = 4$ at $t_1 = 8.80$, $t_2 = 2.57$, $t_3 = .75$ and $t_4 = .22$. The space localization is apparent from the figure as $t_j \to 0$. 
Introduction to wavelets
Spectral graph wavelet
Adaptive spectral graph wavelet method on networks

Standard adaptation technique

$X^c$ Interpolation $X^J$

FWT

Scaling and wavelet coefficients

Adaptive node arrangement
Modified adaptation technique

\( X^{J_0} \) → FWT → Scaling and wavelet coefficients

\( X^{J_0+1} \) → Stopping criterion

- No → Adaptive node arrangement
- Yes → Further processing

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There is some sort of similarity in diffusion and spectral graph wavelet, for example, both require a diffusion operator for their construction.

The largest difference between the two is that the diffusion wavelet is designed to be orthonormal whereas the spectral graph wavelet is not. The orthogonalising technique in the construction of diffusion wavelet complicates the construction procedure. On the other hand the approach used for the spectral graph wavelet is much simpler.

Spectral graph wavelet is constructed for defining wavelet transform for data defined on the vertices of a weighted graph.

Weighted graphs provide a flexible generalisation of regular grid domains. This particular weighted graph wavelet motivated us to try spectral graph wavelet method for numerical solution of PDEs on network-like structure.
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Thank you very much for attention!