What is a graph shift operator?

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Abstract

We consider the role of the graph shift operator in graph signal processing [3]. Typically, the graph shift operator is assumed to be given to us by default, often following some well-known rule that reflects the graph structure (the adjacency matrix, or the Laplacian, for instance). In this document, we seek to uncover what makes a graph shift operator 'tick,' by proposing a few useful invariants and properties that could prove useful in justifying the use of certain operators over others.

Familiarity with basic definitions in graph signal processing is assumed. This informal note reflects many authors who have considered the roles of locality, equivariance, and substructures in graph processing architectures [2, 4, 1], among others.

In graph signal processing, we consider finite graphs $G = (V, E)$ and signals on graphs $x : V \to \mathbb{R}$. Denote by $\mathbb{X}(G)$ the set of all graph signals, *i.e.*, $\mathbb{X}(G) = \{x : V \to \mathbb{R}\}$. Via identification with $\mathbb{R}^{|V|}$, we endow $\mathbb{X}(G)$ with the usual Hilbert space structure. It is typical to speak of a graph shift operator, which is merely a linear map $S : \mathbb{X}(G) \to \mathbb{X}(G)$ that operates in some local way. Typically, S is thought of as a matrix indexed by the pairs of nodes, so that for some $x \in \mathbb{X}(G)$ and any $v \in V$, S acts as follows:

$$[Sx]_v = \sum_{u \in N(v)} [S]_{vu}[x]_u. \tag{1}$$

That is to say, S takes linear combinations of the signal on the immediate neighborhood of each node. The typical idea is to say that S is some kind of model for basic diffusion on a graph, in a way that acts strictly locally and without regard to node ordering or other arbitrary choices.

This is not quite satisfying, though. Without demanding more structure, one can easily construct a whole gamut of shift operators that don't make much sense.

Example 1. (Triangle-weighted adjacency matrix) For a graph $G = (V, E)$, let $t(G, \Delta)$ be the homomorphism density of triangles in G (oft-computed as the trace of the cubed adjacency matrix divided by $(2|V|)!$). Define the triangle-weighted adjacency matrix as the operator $A_\Delta : \mathbb{X}(G) \to \mathbb{X}(G)$ with the following rule. For $u, v \in V$, define

$$[A_\Delta]_{uv} = \begin{cases} 1/t(G, \Delta) & (u, v) \in E \\ 0 & \text{otherwise.} \end{cases} \tag{2}$$

See that the triangle-weighted adjacency matrix is merely a scalar multiple of the typical adjacency matrix, where one merely divides by the density of triangles in the graph. In this sense, the shift operator A_Δ is purely local, as it acts in the same way as the adjacency matrix, *i.e.*, only over local neighborhoods. However, this is a ridiculous choice of shift operator! Looking at it, applying this rule in defining this shift operator yields different responses to *local* structures depending on the *global* structure of the graph. What is even worse is that this shift operator satisfies the basic properties such as permutation equivariance that are adored by graph signal processors.

Although this is a silly example, constructions such as this one indicate the need for more restrictive notions of "graph shift operator." Before proceeding, let us also highlight the issue of "locality." What follows is the most non-local linear map on the space of graph signals.

Example 2. (Global averaging shift) For any graph $G = (V, E)$, define the global average shift operator as the matrix $\frac{1}{|V|}J$, where J is the all-ones matrix.

For a more subtle example, let us consider the symmetric normalized adjacency matrix.

Example 3. (Symmetric normalized adjacency matrix) For a graph $G = (V, E)$, let A be the adjacency matrix, and D be the diagonal matrix of node degrees (assuming there are no isolated nodes). Define the symmetric normalized adjacency matrix $\tilde{A} : \mathbb{X}(G) \to \mathbb{X}(G)$ as the matrix $\tilde{A} = \sqrt{D^{-1}} A \sqrt{D^{-1}}$.

The symmetric normalized adjacency matrix is local in the sense that it does not depend on global features of the graph (such as triangle homomorphism densities), and it appears to perform local computations, but I would argue that this operator is less local than it seems. Observe that the computation at a given node can not be determined strictly by the structure of its one-hop neighborhood. This is due to the normalization by node degrees: since the degrees of nodes in the neighborhood of a given node depend on the structure of the two-hop neighborhood of that node, the symmetric normalized adjacency matrix actually depends on the two-hop neighborhood, even if it only uses signal values from the one-hop neighborhood.

Or even more blatantly, some authors use higher-order neighborhood adjacency matrices.

Example 4. (K-hop adjacency matrix) For a graph $G = (V, E)$ and integer $K \geq 0$, let A_K be the shift operator such that for all $v, u \in V$,

$$[A_K]_{vu} = \mathbb{1}(u \text{ in } K\text{-hop neighborhood of } v). \tag{3}$$

The K-hop adjacency matrix is clearly not local in the 1-hop sense, but is kind of local in the sense that it does not necessarily depend on global graph structure. Should this even be considered a graph shift operator? Let's find out!

1 A milieu of motifs

We will now develop the basic machinery to help characterize the local properties of graph shift operators. Let $G = (V, E)$ be a graph.

1.1 Rooted balls

For any integer $K \geq 0$, and any node $v \in V$, the *rooted K-ball* centered at v is the graph $G_K(v) = (N^K(v), E \cap N^K(v) \times N^K(v))$ with v marked as the root, *i.e.*, the induced subgraph of the K-hop neighborhood of v.

For two graphs $G = (V, E), G' = (V', E')$ and some $K \geq 0$, if there exists a map $\phi : V \to V'$ such that, for all $v \in V$, the rooted balls $G_K(v)$ and $G'_K(\phi(v))$ are isomorphic to each other, we say that ϕ is a K-morphism in the sense of rooted balls. If the two graphs have associated signals, $x \in \mathbb{X}(G), x' \in \mathbb{X}(G')$, then we also demand that the signal structure is preserved by K-morphisms as well, *i.e.*, for any rooted K-ball in G, the corresponding rooted K-ball in G' under the map ϕ has the same signal on it.

1.2 Rooted trees

For any integer $K \geq 0$, and any node $v \in V$, the *rooted K-tree* centered at v is a less descriptive object than the rooted K-ball centered at v. It is constructed in the following way: define $U_0 = \{v\}$. Then, for $k < K$ and any $u \in U_k$, let the children of u be given by the neighbors of u in G, excluding u itself. Let U_{k+1} be comprised of all children of nodes in U_k, and $F_k \subseteq U_k \times U_{k+1}$ the set of directed edges that satisfy the parent-child relationship stated above. Finally, put $U = \coprod_{k=0}^{K} U_k$, and $F = \coprod_{k=0}^{K-1} F_k$, where $\coprod$ denotes the disjoint union.[1] Denote the tree constructed in this way by $T_k(v) = (U, F)$.

We define a similar notion of K-morphism for rooted trees. For two graphs $G = (V, E), G' = (V', E')$ and some $K \geq 0$, if there exists a map $\phi : V \to V'$ such that, for all $v \in V$, the rooted balls $T_K(v)$ and $T'_K(\phi(v))$ are isomorphic to each other, we say that ϕ is a K-morphism in the sense of rooted trees. If the two graphs have associated signals, $x \in \mathbb{X}(G), x' \in \mathbb{X}(G')$, then we also demand that the signal structure is preserved by K-morphisms as well.

One can check that if $\phi : V \to V'$ is a K-morphism in the sense of rooted balls, then it is also a K-morphism in the sense of rooted trees, but not vice-versa. This is what was meant by "the rooted K-tree is a less descriptive object than the rooted K-ball."

We illustrate the notion of "rooted ball" and "rooted tree" in Fig. 1.

[1] We use the *disjoint union*, as there may be repeated copies of the same node.

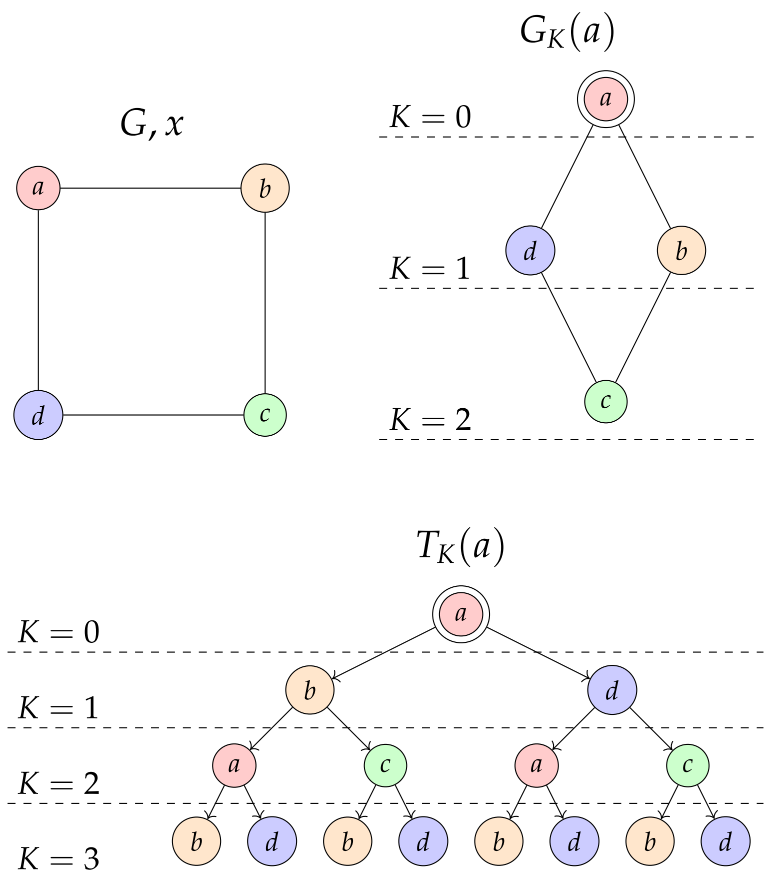

Figure 1: Rooted balls and rooted trees. **(Top left)** A graph G with associated graph signal x denoted by the node coloring. **(Top right)** Rooted K-balls with signal centered at node a for $K = 0, 1, 2$. Observe that $G_K(a) \cong G_{K+1}(a)$ for all $K \geq 2$. **(Bottom)** Rooted K-trees with signal centered at node a for $K = 0, 1, 2, 3$.

2 Permutation/Morphism Equivariance

Two key features of graph shift operators that are often appealed to are as follows: locality and symmetry. In the examples given in the introduction, we showed how a graph shift operator could be symmetric, and even appear to act locally, but still use global information, and how a graph shift operator could use higher-order neighborhoods than expected. We wish to characterize classes of graph shift operators based on the machinery of K-morphisms in the sense of either rooted balls or rooted trees. Let us start with a basic definition.

Definition 1. (Graph shift operator) A graph shift operator S is a rule that assigns to any graph G a corresponding linear map $S(G) : \mathbb{X}(G) \to \mathbb{X}(G)$.

This is the most generic definition for a (linear) graph shift operator: it makes no demands on equivariance, locality, or any other related property. All that is required is for it to be a linear map from the space of graph signals to the space of graph signals.[2] If one is so inclined, one might start thinking of graph shift operators as functors from some suitably defined category of graphs to a category of endomorphisms of graph signals that preserves the right kinds of structures, but this is not necessary for our purposes.

We now define properties of graph shift operators with the hope of narrowing down to something that feels right. We begin with the usual property of permutation equivariance.

Property 1. (Permutation equivariance) Let two graphs $G = (V, E)$ and $G' = (V', E')$ with associated signals $x \in \mathbb{X}(G)$ and $x' \in \mathbb{X}(G')$ be given arbitrarily. A graph shift operator S is said to be permutation equivariant if for any such graphs, if there exists a signal-preserving isomorphism $\phi : V \to V'$, then $[S(G)x]_v = [S(G')x']_{\phi(v)}$ for all $v \in V'$. Denote the set of all permutation equivariant shift operators by PERM.

Most graph shift operators one would think of satisfy this property, unless something strange such as using node numberings is done. Shift operators such as the global averaging shift operator satisfy this as well. We now refine this definition to take locality into account, starting with rooted balls and extending it to rooted trees.

Property 2. (Ball-equivariance) Let two graphs $G = (V, E)$ and $G' = (V', E')$ with associated signals $x \in \mathbb{X}(G)$ and $x' \in \mathbb{X}(G')$ be given arbitrarily. A graph shift operator S is said to be K-ball equivariant if for any such graphs, if a map $\phi : V \to V'$ is a K-morphism in the sense of rooted balls, then $[S(G)x]_v = [S(G')x']_{\phi(v)}$ for all $v \in V'$. Denote the set of all K-ball equivariant shift operators by $\mathsf{BALL}(K)$.

If a shift operator is such that this property always holds for a pair of graphs with a K-morphism where K is sufficiently large but not fixed,[3] we say that it is ∞-ball equivariant, and denote the set of such operators by $\mathsf{BALL}(\infty)$.

[2] One could also call such a map an *endomorphism*.

[3] That is, K is allowed to vary based on the graphs at hand

Property 3. (Tree-equivariance) Let two graphs $G = (V, E)$ and $G' = (V', E')$ with associated signals $x \in \mathbb{X}(G)$ and $x' \in \mathbb{X}(G')$ be given arbitrarily. A graph shift operator S is said to be K-tree equivariant if for any such graphs, if $\phi : V \to V'$ is a K-morphism in the sense of rooted trees, then $[S(G)x]_v = [S(G')x']_{\phi(v)}$ for all $v \in V'$. Denote the set of all K-tree equivariant shift operators by $\mathsf{TREE}(K)$.

If a shift operator is such that this property always holds for a pair of graphs with a K-morphism where K is sufficiently large but not fixed,[4] we say that it is ∞-tree equivariant, and denote the set of such operators by $\mathsf{TREE}(\infty)$.

With this taxonomy of graph shift operators, we can now organize them based on how these properties relate to one another.

Proposition 1. *The following holds for all $K \geq 0$.*

1. $\mathsf{TREE}(K) \subseteq \mathsf{BALL}(K) \subseteq \mathsf{PERM}$
2. $\mathsf{BALL}(\infty) = \mathsf{TREE}(\infty) = \mathsf{PERM}$
3. $\mathsf{BALL}(K) \subseteq \mathsf{BALL}(K+1)$
4. $\mathsf{TREE}(K) \subseteq \mathsf{TREE}(K+1)$

We will not go through the trouble of proving this in detail, but a brief explanation is offered below.

1. Since K-morphisms in the sense of rooted balls are also K-morphisms in the sense of rooted trees, we have $\mathsf{TREE}(K) \subseteq \mathsf{BALL}(K)$. Graph isomorphisms are special types of K-morphisms in the sense of rooted balls, so $\mathsf{BALL}(K) \subseteq \mathsf{PERM}$.

2. It is clear from the above argument that $\mathsf{TREE}(\infty) \subseteq \mathsf{BALL}(\infty) \subseteq \mathsf{PERM}$. Observe that graph isomorphisms are K-morphisms in the sense of rooted trees for K equal to the maximum of the diameters of the two graphs in question, so that $\mathsf{PERM} \subseteq \mathsf{TREE}(\infty)$.

3. Clearly, $K+1$-morphisms in the sense of rooted balls are also K-morphisms in the sense of rooted balls.

4. Clearly, $K+1$-morphisms in the sense of rooted trees are also K-morphisms in the sense of rooted trees.

[4] Once again, this means that K is allowed to vary based on the graphs at hand

Shift	LOCAL(K)	TREE(K)	BALL(K)	PERM
A	$K = 1$	$K = 1$	$K = 1$	✓
A_Δ	$K = 1$	✗	✗	✓
$\tilde{A}$	$K = 1$	$K = 2$	$K = 2$	✓
A_K	$K = K$	✗	$K = K$	✓
$\frac{1}{\lvert V\rvert}J$	✗	✗	✗	✓

Table 1: Properties of shift operators

3 What does this mean for locality?

One common definition of a graph shift operator that one sees in the literature is: a matrix whose sparsity pattern matches that of the graph it represents. By no means! This reduces the rich combinatorial structure of a graph down to nothing more than a sparse matrix. We define another property of a shift operator to think about locality.

Property 4. (Locality) A graph shift operator S is said to be K-local if for any graph $G = (V, E)$, and any $v, u \in V$, $[S(G)]_{vu} \neq 0$ only if u is in the K-hop neighborhood of v. Denote the set of all K-local shift operators by $\mathsf{LOCAL}(K)$.

For instance, $\mathsf{LOCAL}(0)$ consists of diagonal matrices, and $\mathsf{LOCAL}(1)$ consists of matrices that match the sparsity pattern of the graph. Since rooted balls and rooted trees are inherently local objects, one would suspect that they are related to the property of locality.

Proposition 2. $\mathsf{BALL}(K) \subseteq \mathsf{LOCAL}(K)$ *for all* $K \geq 0$. *Therefore, it also holds that* $\mathsf{TREE}(K) \subseteq \mathsf{LOCAL}(K)$.

With this final classification settled, we categorize some of our example shift operators according to these properties in Table 1.

One reason that locality is so useful is that it gives us an idea of how graph filters behave when constructed from a graph shift operator. Since a graph filter is just a matrix polynomial, and matrix polynomial have matrix multiplication as their basic building block, we make the following simple claim.

Proposition 3. *(Locality of composition) Let* $K, L \geq 0$ *be given, and let* S, S' *be graph shift operators. Then, for any property* $\mathsf{P}(K) \in \{\mathsf{LOCAL}(K), \mathsf{TREE}(K), \mathsf{BALL}(K)\}$, *if* $S \in \mathsf{P}(K)$ *and* $S' \in \mathsf{P}(L)$, *then* $(SS') \in \mathsf{P}(K + L)$, *where*

$$(SS')(G) := S(G)S'(G) \tag{4}$$

is defined via composition of linear maps (matrix multiplication). Moreover, if $S, S' \in \mathsf{PERM}$, *then* $(SS') \in \mathsf{PERM}$.

References

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