Kirchhoff Graph Uniformity

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Abstract

This article discusses Kirchhoff graph uniformity—that all edge vectors in a Kirchhoff graph have the same multiplicity. For a given Kirchhoff graph, an associated digraph is constructed. Based on these graphs, the equivalence of a linear-algebraic condition and a vector graph being Kirchhoff is proven. This condition is then used to show that 2-connected Kirchhoff graphs are uniform. Other Kirchhoff graphs need not be uniform.

Introduction

Consider a set $\mathcal{S} := \{\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_n\}$ of vectors in *any* vector space $\mathcal{V}$ over the *rationals*. For convenience, suppose that no vector in $\mathcal{S}$ is a scalar multiple of another vector in $\mathcal{S}$. Suppose that for some k where $1 < k < n$, the $\{\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_k\}$ are a basis for Span$(\mathcal{S})$ ($k = 0, 1$, and n are trivial cases), so that one can write $\boldsymbol{s}_{k+1}$, $\boldsymbol{s}_{k+2}, \ldots$, $\boldsymbol{s}_n$ in terms of this basis. Thus there is a coefficient matrix C such that $\boldsymbol{s}[C/-I] = 0$ where $\boldsymbol{s} = [\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_n]$ is a row vector of vectors and $[C/-I]$ is the $n \times (n-k)$ matrix with the C block over the negative of the $(n-k) \times (n-k)$ identity block. Let $N := [C/-I]$ and $R := [I|C]$; these are the null and row matrices for our set of vectors. In particular, the columns of N are a basis for Null(R), and the columns of R can be taken as representatives of the vectors $\{\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_n\}$ regardless of which vector space $\mathcal{V}$ we started with. That is, since $RN = 0$ and $\boldsymbol{s}N = 0$, the columns of R and the vectors in $\mathcal{S}$ have the same dependencies.

The mathematical issue now is whether or not one can construct a vector graph using the vectors $\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_n$ as edges, having a cycle basis corresponding to a basis for Null(R), and all of whose vertex cuts lie in Row(R). A cycle of edge vectors in the graph corresponds to vector addition in the vector space, $\mathcal{V}$. Vertices occur where the edge vectors meet in the cycles. Multiple copies of the *same* edge vector may lie on top of each other between two given vertices; this multiplicity (if greater than one) is represented by hash marks in Figure 1 and can be thought of as a weight on that edge. These weights (multiplicities) are the entries in the vertex cut

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vector for each vertex; a vertex cut entry is positive if the corresponding edge vector exists the vertex and negative if that edge vector enters the vertex. Such a vector graph, $\boldsymbol{G}$, if it exists, is a *Kirchhoff graph* (see the example on the left in Figure 1). Kirchhoff graphs were first defined and discussed by Fehribach (2009); their orthogonality is an extension of the classic result that the cycle space and the cut space of a (standard) graph are orthogonal complements (*cf. e.g.* Diestel (1997) or Bollobas (1998)).

Along with being a graphic representation of ortho-complementarity for Row(R) and Null(R), a Kirchhoff graphs can be used as a kind of circuit diagram for a reaction network. As discussed by Fehribach (2009), if R is row equivalent to the stoichiometric matrix of a chemical or other reaction network, then the Kirchhoff graph for R satisfies the Kirchhoff current and potential laws and is a diagram of all possible reaction pathways. Another interesting property of Kirchhoff graphs is that they frequently but not always have the same number of occurrences of each edge vector. This property is called uniformity; it has been studied by Reese (2018) and Reese *et al.* (2019). This article is a second look at uniformity using a smaller associated digraph (defined below) and a somewhat briefer presentation.

Definition: *Given a vector graph* $\boldsymbol{G}$, *with edge vectors* $\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_n$, *let* $\eta_i \in \mathbb{Z}^+$ *be the number of times the edge vector* $\boldsymbol{s}_i$ *occurs in* $\boldsymbol{G}$. *The graph* $\boldsymbol{G}$ *is* **uniform** *if and only if* $\eta_i = \eta$ *for some* $\eta \in \mathbb{Z}^+$ *independent of* i.

To discuss Kirchhoff graph uniformity, an associated digraph is defined: Given a vector graph $\boldsymbol{G}$, define a digraph D having the same vertex set V, but having a single directed edge between any two vertices that are connect by at least one edge vector. Let the direction of the digraph edge be the same as the corresponding edge vector in the vector graph. This digraph is similar to the one defined by Reese *et al.* (2019), but smaller since this earlier digraph was not simple, having a separate directed edge for each copy of a given edge vector between two specific vertices. This smaller digraph is computationally more efficient and more closely resembles the given vector graph.

As an example of a vector graph (that is indeed a Kirchhoff graph) and its corresponding digraph, consider the pair shown in Figure 1. In this example,

$$R = \begin{bmatrix} 1 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{bmatrix} \qquad N = \begin{bmatrix} 2 & 1 \\ 1 & 2 \\ -1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1}$$

and the vector edges in Figure 1 are drawn based on the columns of R. Each vertex cut vector lies in Row(R); for example the vertex cut for the vertex in the lower left corner of $\boldsymbol{G}$ is $[1, 1, 3, 3]$ which is the sum of the

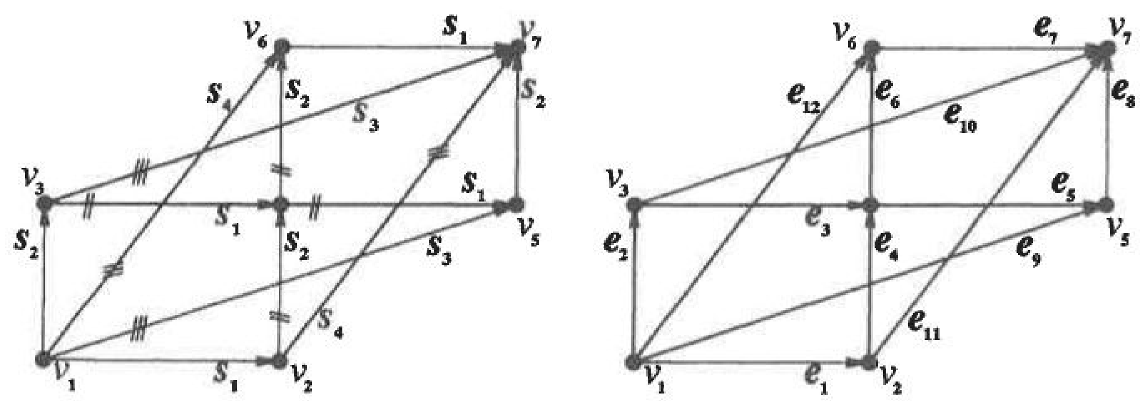

Figure 1: A Kirchhoff-Diagraph Pair. The Kirchhoff graph G on the left is generated by any set of vectors $S = \{s_1, s_2, s_3, s_4\}$ where the last two vectors depend on the first two vectors through a matrix C that is the upper 2×2 block of N and the right 2×2 block of R in (1). Hash marks indicate the number of copies of a given edge vector lying in parallel connecting the same two vertices. Here each edge vector corresponds to a column of R. The digraph D on the right corresponds to G, having the same vertices as G and a single, distinct edge e_j connecting two vertices if and only if there is at least one edge vector connecting those vertices in G.

two rows of R. Each cycle lies in Null(R); for example, each column of N corresponds to a triangle of edge vectors in G, and the cycle vector $[1, -1, -1, 1]^{\mathrm{T}}$ corresponds to multiple cycles in G. The latter cycle vector is the difference between the two columns of N.

Uniformity

Proving that certain Kirchhoff graphs are uniform depends on an linear-algebraic characterization for a Kirchhoff graph.

Definitions: *Let n^* be the number of directed edges in D. Let $S = [s_{ij}]$ be the* **assignment matrix** *for a given vector graph G: the i-th directed edge e_i in the digraph D is assigned s_{ij} copies of the j-th edge vector s_j in G when e_i and s_j connect the same edge vector. Let $T = [t_{ij}]$ be the* **characteristic matrix***: $t_{ij} = 1$ if the i-th directed edge in D and the j-th edge vector in G connect the same vertices; $t_{ij} = 0$ otherwise. So S and T are both $n \times n^*$ matrices, and T has a 0 whenever S has a 0 entry, and 1 as an entry whenever S has a nonzero entry. Let P be the* **incidence matrix** *for D: the ij-th entry of P is 1 if e_j exits vertex v_i, -1 if e_j enters vertex v_i, and 0 otherwise.*

REMARK: With these definitions, PS is the **incidence matrix** for G.

In the example above,

$$P = \begin{array}{c|cccccccccccc|} & e_1 & e_2 & e_3 & e_4 & e_5 & e_6 & e_7 & e_8 & e_9 & e_{10} & e_{11} & e_{12} \\ \hline v_1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ v_2 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ v_3 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ v_4 & 0 & 0 & -1 & -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_5 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 0 \\ v_6 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & -1 \\ v_7 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & -1 & -1 & 0 \end{array}$$

and

$$S = \begin{array}{c|cccc|} & s_1 & s_2 & s_3 & s_4 \\ \hline e_1 & 1 & 0 & 0 & 0 \\ e_2 & 0 & 1 & 0 & 0 \\ e_3 & 2 & 0 & 0 & 0 \\ e_4 & 0 & 2 & 0 & 0 \\ e_5 & 2 & 0 & 0 & 0 \\ e_6 & 0 & 2 & 0 & 0 \\ e_7 & 1 & 0 & 0 & 0 \\ e_8 & 0 & 1 & 0 & 0 \\ e_9 & 0 & 0 & 3 & 0 \\ e_{10} & 0 & 0 & 3 & 0 \\ e_{11} & 0 & 0 & 0 & 3 \\ e_{12} & 0 & 0 & 0 & 3 \end{array} .$$

The following theorem gives a linear-algebric characterization for when a graph is Kirchhoff. It is similar to Theorem 1 of Reese *et al.* (2019), but involves smaller matrices.

Theorem: *A vector graph $\boldsymbol{G}$ is Kirchhoff if and only if*

$$T^{\mathrm{T}}\mathrm{Null}(P) = \mathrm{Null}(PS) \ . \tag{2}$$

PROOF: Because PS is the incidence matrix for the vector graph, there is automatically a cycle basis for $\boldsymbol{G}$ corresponding to a basis for $\mathrm{Null}(PS)$. Given a vertex $v \in V(\boldsymbol{G}) = V(D)$, let $\boldsymbol{\lambda}(v)$ $[\lambda(v)]$ be the vertex cut or incidence vector for v in $\boldsymbol{G}$ $[D]$, respectively. Similarly, if $c \in \mathcal{C}(\boldsymbol{G}) = \mathcal{C}(D)$, let $\boldsymbol{\chi}(c)$ $[\chi(c)]$ be the cycle vector for c in $\boldsymbol{G}$ $[D]$, respectively.

$(\Leftarrow)$ Suppose that (2) holds. Let $v \in V(\boldsymbol{G}) = V(D)$, and $c \in \mathcal{C}(\boldsymbol{G}) = \mathcal{C}(D)$.

Then[1]

- $\lambda(v) \in \text{row}(P) \quad \Rightarrow \quad \boldsymbol{\lambda}(v) = \lambda(v)S \in \text{Row}(PS)$
- $(\chi(c))^{\text{T}} \in \text{Null}(P) \quad \Rightarrow$
  $(\boldsymbol{\chi}(c))^{\text{T}} = (\chi(c)T)^{\text{T}} = T^{\text{T}}(\chi(c))^{\text{T}} \in T^{\text{T}}\text{Null}(P) = \text{Null}(PS)$

Thus $\boldsymbol{\lambda}(v) \perp \boldsymbol{\chi}(c) \ \forall \ v, c$.

($\Rightarrow$) Now suppose $\boldsymbol{\lambda}(v)(\boldsymbol{\chi}(c))^{\text{T}} = 0 \ \forall \ v \in V(\boldsymbol{G}),\ c \in \mathcal{C}(\boldsymbol{G})$. That $\boldsymbol{G}$ is Kirchhoff implies that $(\boldsymbol{\chi}(c))^{\text{T}} \in \text{Null}(PS)$. At the same time, $(\boldsymbol{\chi}(c))^{\text{T}} = (\chi(c)T)^{\text{T}} = T^{\text{T}}(\chi(c))^{\text{T}} \in T^{\text{T}}\text{Null}(P)$. So vectors are in $\text{Null}(PS)$ if and only if they are also in $T^{\text{T}}\text{Null}(P)$. □

Definition: *Let $H := T^TS$; so H is a diagonal matrix with $H_{jj} = \eta_j$, the number of times the vector $\boldsymbol{s}_j$ appears in $\boldsymbol{G}$.*

Lemma: *If $\boldsymbol{G}$ is Kirchhoff, then $\boldsymbol{v} \in \text{Null}(PS)$ implies $H\boldsymbol{v} \in \text{Null}(PS)$.*

PROOF: $v \in \text{Null}(PS) \Rightarrow PS\boldsymbol{v} = 0 \Rightarrow S\boldsymbol{v} \in \text{Null}(P) \Rightarrow$
$$H\boldsymbol{v} = T^{\text{T}}S\boldsymbol{v} \in T^{\text{T}}\text{Null}(P) = \text{Null}(PS).$$ □

The next theorem deals with the case where the null space is one-dimensional and the Kirchhoff graph is a single cycle. This result follows from Proposition 2.3 in Fehribach (2015) and was discussed in detail by Reese *et al.* (2019). To deal with more-general Kirchhoff graphs such as the one in Figure 1, the next section introduces the concept of 2-connectedness for a vector graph.

Theorem: *Suppose that* $\text{Null}(PS) = \text{Span}(\boldsymbol{b})$ *with* $\boldsymbol{b} = [b_1, b_2, \ldots b_n]^{\text{T}}$. *If $b_j \neq 0$, then $\eta_j = \eta$, independent of j. Hence each edge vector appears η times provided that the corresponding entry in $\boldsymbol{b}$ is nonzero.*

PROOF: Since $\boldsymbol{b} \in \text{Null}(PS)$, by the previous Lemma, $H\boldsymbol{b} \in \text{Null}(PS)$. Since $\text{Null}(PS)$ is spanned by a single vector $\boldsymbol{b}$, $H\boldsymbol{b} = \eta\boldsymbol{b}$ for some η. But then η is an eigenvalue for the diagonal matrix H, implying that $\eta_j b_j = \eta b_j$. Thus $\eta_j = \eta$ provided that $b_j \neq 0$. □

2-Connectedness

The previous theorem can be generalized to other Kirchhoff graphs when there are nontrivial cycles that weave there way through the vector graph.

[1] $\text{Row}(X)$ is the row space of the matrix X; $\text{row}(X)$ is the set of rows of X.

The exact sense of "nontrivial" needed here is 2-connected:

Definition: *A vector graph* $\boldsymbol{G}$ *is* **2-connected** *if and only if for any pair of vector edges* $\boldsymbol{s}_i$ *and* $\boldsymbol{s}_j$*, there exists a cycle* c *such that the cycle vector* $\boldsymbol{\chi}(c)$ *is nonzero with respect to both* $\boldsymbol{s}_i$ *and* $\boldsymbol{s}_j$*.*

This definition and its implications were first discussed by Reese *et al.* (2019). The name for this concept (2-connected) comes from the fact that one must remove *all* copies of at least two edge vectors in order to disconnect a 2-connected vector graph.

Theorem: *Every 2-connected Kirchhoff graph is uniform.*

PROOF: First suppose that the upper block C in the matrix N has no zero entries. Let $\boldsymbol{b}_j$ denote the j-th column of N; By the Lemma above, $\boldsymbol{b}_j \in \text{Null}(PS)$ implies

$$H\boldsymbol{b}_j = \gamma_1\boldsymbol{b}_1 + \gamma_2\boldsymbol{b}_2 + \ldots + \gamma_k\boldsymbol{b}_k$$

for some $\gamma_j \in \mathbb{Q}$. Since H is a diagonal matrix, and because of the lower identity block in N, one can go entry by entry through $\boldsymbol{b}_j$ to find that $\gamma_i = 0$ for $i \neq j$, implying that

$$H\boldsymbol{b}_j = \gamma_j\boldsymbol{b}_j$$

for all $1 \leq j \leq k$, which makes γ_j an eigenvalue of H and unless the i-th entry in $\boldsymbol{b}_j$ is zero, then all of the corresponding entries on the diagonal of H must be the same. But this must be true for each j. Again, because of the block structure of N and the lack of zeros in C, all of the entries on the diagonal of H must be the same. Hence $H = \eta I$.

Now suppose that the upper block C has at least some zero entries. The argument above again works to force all of the entries of H to be the same, unless the block C itself has a block structure as shown in (3),

$$\left[\begin{array}{c|c} C_1 & 0 \\ \hline 0 & C_2 \end{array}\right] \tag{3}$$

possibly after relabelling the edge vectors and vertices. In this case, each block can have a separate η value, and the Kirchhoff graph can have disconnected subgraphs.

Finally suppose that N has an upper block in the form of (3). Then there is a bases for Null(R) (and hence for the cycle space for our Kirchhoff graph) corresponding to the columns of N. This implies that our Kirchhoff graph is *not* 2-connected. □

There is a simple example of a Kirchhoff graph that is not uniform,

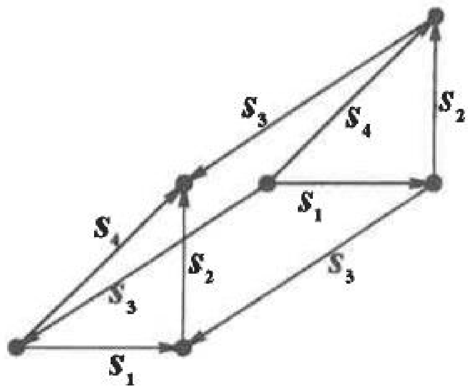

Figure 2: Tent Kirchhoff graph. There are two copies of s_1, s_2 and s_4, but three copies of s_3.

and thus of course not 2-connected: Suppose that

$$R = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \qquad N = \begin{bmatrix} 1 \\ 1 \\ 0 \\ -1 \end{bmatrix}$$

Notice that in this example, the null space is 1-dimensional, and R has essentially the block structure described in (3) (the third and fourth edge vectors would need to be relabeled to achieve exactly that structure). One Kirchhoff graph for this combination of R and N is shown in Figure 2.

Conclusion

The discussion above proves the uniformity of 2-connected Kirchhoff graphs using an approach similar to that of Reese *et al.* (2019). The main advantage to the current approach is that the digraph used here is smaller (has fewer edges) than the one used in Reese *et al.* (2019), and it more closely resembles the original Kirchhoff graph G (see example in Figure 1). Indeed the desired digraph D can be obtained from G by using the same vertices (G and D have the same vertex set V), dropping the weights or edge-vector multiplicities, and reinterpreting the now single edge vectors between vertices as the directed edges of D. That the current digraph D has fewer edges than the one in Reese *et al.* (2019) can also have computational advantages.

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