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Matrices over finite fields and their Kirchhoff graphs

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ABSTRACT

Given a stoichiometric matrix A with integer entries, we seek to visualize the information by a reaction network N, whose edges are labeled by the columns of A, such that all column dependencies are realized as cycles in N. Moreover, the vector edges of N are assigned integer multiplicities so that every vertex of N corresponds to a vector in the row space of A. A finite such N is called a Kirchhoff graph. We establish the existence of nontrivial Kirchhoff graphs over finite fields, but the general problem over the integers is still open.

1. Introduction

Kirchhoff's laws are well-studied for electrical networks with voltage and current sources, and edges marked by resistors; see, for example, [1]. Kirchhoff's voltage law states that the sum of voltages around any circuit of the network graph is zero, while Kirchhoff's current law can be formulated as the requirement that the sum of the currents along any cutset of the network graph is zero. Given a network, these requirements may be encoded by the circuit matrix, C, and cutset matrix, Q, of the network graph. The

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columns of C and Q are both indexed by the edges of the network graph and $CQ^T = 0$ over $\mathbb{Z}_2$. A network with positive resistors is known to be uniquely solvable if and only if the subset of edges of the network graph determined by the voltage sources does not contain a cycle, and the subset of edges determined by the current sources does not contain a cutset. It should be noted, however, that the network graph is typically not recoverable from the matrices C and Q.

This article studies the opposite problem, where rather than beginning with a network graph we now begin with a matrix. For example, an electrochemical reaction network can be encoded by an integer-valued matrix—the stoichiometric matrix—the columns of which correspond to reaction steps. In particular, this leads to the following question: given this matrix, what is a suitable graphic rendering of a network that properly visualizes the underlying chemical reactions? Although we cannot expect uniqueness, the goal is to prove existence of such a graph for any matrix.

Specifically, this article extends previous work on Kirchhoff graphs for matrices over the rationals to matrices over finite fields. Kirchhoff graphs were introduced by Fehribach [2] as a mathematically precise version of the reaction route graphs discussed by Fishtik, Datta et al. [3], [4] to represent electrochemical reaction networks. In the context of these networks, Kirchhoff graphs represent the orthocomplementarity of the row space and null space of the stoichiometric matrix for a given reaction network. As such, a chemical engineer can use a Kirchhoff graph in the way an electrical engineer uses a standard circuit diagram. This paper is presented in two primary sections: Section 2 considers Kirchhoff graphs for rational-valued matrices, whereas Section 3 studies Kirchhoff graphs for matrices over finite fields.

Section 2.1 begins with an electrochemical reaction network view of Kirchhoff graphs. Specifically, the details of how Kirchhoff graphs depict Kirchhoff's current and potential laws as applied to a sample network are explained through an illustrative example. Section 2 then continues, building upon the work of [2], [5] and [6], by presenting definitions, examples, and fundamental results on Kirchhoff graphs. Motivated by studying electrochemical networks, Section 2.2 abstracts the ideas presented in Section 2.1, and gives an example of how to construct a Kirchhoff graph for a rational-valued matrix. In the process, connections of Kirchhoff graphs with graph theory, linear algebra, and group theory are illustrated.

The definitions presented in Section 2.2 are mathematically equivalent to those of [5]; Section 3.1 now generalizes these to $\mathbb{Z}_p$-valued matrices and $\mathbb{Z}_p$-Kirchhoff graphs. The primary open mathematical problem in the study of Kirchhoff graphs is the conjecture of Fehribach that every rational-valued matrix has a Kirchhoff graph [2], [5]. While we do not answer this question for matrices over the rationals, Section 3.2 addresses this problem for $\mathbb{Z}_p$-valued matrices. Theorem 1 shows that for any integer-valued matrix A, there exists a nontrivial $\mathbb{Z}_p$-Kirchhoff graph for the matrix $A \pmod{p}$ for sufficiently large prime p. Moreover, nonzero $\mathbb{Z}_p$-Kirchhoff graphs are explicitly constructed for $\mathbb{Z}_p$-valued matrices with an entry-wise nonzero vector in the row space. Finally, Section 3.3 demon-