Rule-Based Linear Operators and Rule-Algebras

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Abstract

Linear operators are fundamental in control theory, quantum physics and the theory of Markov chains. Inspired by the analogy between quantum physics and stochastic processes that has been popularized in recent years, this paper introduces rule-algebras in an attempt to reach for the theoretical physicists' tool chest, for example to analyse complex networks and stochastic graph transformation in general.

1 Encapsulating Rule-Based Modelling into Linear Algebra

The idea of the paper can be wrapped up in a single sentence: *We propose to use linear operators on the* $\mathbb{R}$*-vector space* $\mathfrak{G}_{\mathbb{R}}$ *that is spanned by the set of isomorphism classes of finite graphs as semantic domain to reason about quantitative aspects of graph transformation.* In particular, we do not focus on any one of the algebraic approaches [1, 2] *a priori.*

The Rule-Algebra of Finite Graphs

We start with a quick review of the relevant aspects of graph rewriting [1], using as an example the rule that replaces a pair of edges with the same target node by a pair of edges with the same source node while keeping everything else unchanged.

$$\boxed{\cdot \rightarrow \cdot \leftarrow \cdot} \quad \rightharpoonup \quad \boxed{\cdot \leftarrow \cdot \rightarrow \cdot}$$

There are a finite number of ways in which the rule can be applied to rewrite a given graph. For example, there are two ways to rewrite the graph $\cdot \leftrightarrows \cdot \rightleftarrows \cdot \leftarrow \cdot$ to $\cdot \leftleftarrows \cdot \rightrightarrows \cdot \leftarrow \cdot$ and two ways to rewrite the graph $\cdot \leftrightarrows \cdot \rightleftarrows \cdot \leftarrow \cdot$ to $\cdot \leftrightarrows \cdot \leftleftarrows \cdot \rightarrow \cdot$.

Generally and formally, for each partial map $\theta\colon L_\theta \rightharpoonup R_\theta$ between finite directed multigraphs and each monomorphism $f\colon L_\theta \rightarrowtail G$, there is an up to isomorphism unique result of rewriting [2], denoted by $\theta_f(G)$. Since there are only finitely many monomorphisms $f\colon L_\theta \rightarrowtail R_\theta$, we can define the linear operator A_θ for θ on $\mathfrak{G}_{\mathbb{R}}$ via $A_\theta \left|[G]_\cong\right\rangle := \sum_{f\colon L_\theta \rightarrowtail G} \left|[\theta_f(G)]_\cong\right\rangle$, where $|[G]_\cong\rangle$ is the basis vector of the isomorphism class $[G]_\cong$. Thus, certain linear operators on $\mathfrak{G}_{\mathbb{R}}$ are *rule-based*, i.e. are of the form A_θ for some partial map $\theta\colon L_\theta \rightharpoonup R_\theta$. Fixing single pushout rewriting [2] as rewriting formalism gives the following fundamental result:

▶ **Theorem 1.1** (Rule-Algebra). *Rule-based operators are the basis of a unital algebra.*

The proof idea is that the identity is $A_{\varnothing \rightharpoonup \varnothing}$ and that for a pair of rules θ and ϕ, there are only a finite number of ways $(i = 1, \cdots, n)$ in which they can depend causally on each other, each captured by a combined rule ψ_i such that $A_\theta A_\phi = \sum_{i=1}^{n} A_{\psi_i}$ (see also Equation (1)).

Discrete Graph Rewriting and the Heisenberg-Weyl Algebra

Consider the two rules for creation and deletion of a node, i.e., the partial maps $\cdot \rightharpoonup \varnothing$ and $\varnothing \rightharpoonup \cdot$, respectively. Restricting $\mathfrak{G}_{\mathbb{R}}$ to the subspace $\mathfrak{G}^0_{\mathbb{R}} \subset \mathfrak{G}_{\mathbb{R}}$ spanned by the basis vectors $|[n\cdot]_\cong\rangle$ (where $n\cdot$ is an n-vertex graph), the rules $\cdot \rightharpoonup \varnothing$ and $\varnothing \rightharpoonup \cdot$ have respective

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linear operators $A_{\cdot\rightharpoonup\varnothing}$ and $A_{\varnothing\rightharpoonup\cdot}$, acting as $A_{\cdot\rightharpoonup\varnothing}|[n\cdot]_{\cong}\rangle = n|[(n-1)\cdot]_{\cong}\rangle$ and $A_{\varnothing\rightharpoonup\cdot}|[n\cdot]_{\cong}\rangle = |[(n+1)\cdot]_{\cong}\rangle$ on each basis vector $|[n\cdot]_{\cong}\rangle$.

Equipping $\mathfrak{G}^0_{\mathbb{R}}$ with the inner product $\langle [m\cdot]_{\cong}|[n\cdot]_{\cong}\rangle := m!\,\delta_{m,n}$, we obtain an important result as a direct consequence of the definitions:

▶ **Theorem 1.2.** *The algebra defined via the representation $a^{\dagger} \mapsto A_{\varnothing\rightharpoonup\cdot}$ and $a \mapsto A_{\cdot\rightharpoonup\varnothing}$ has commutator $[a, a^{\dagger}] = 1$ where $1 \mapsto A_{\varnothing\rightharpoonup\varnothing}$; this is the Heisenberg-Weyl algebra.*

As an important corollary, any linear operator in this representation may be realized as a linear combination of the *normal ordered* linear operators $A^{\dagger^m} A^n = A_{n\cdot\rightharpoonup m\cdot}$ where $A^{\dagger} = A_{\varnothing\rightharpoonup\cdot}$ and $A = A_{\cdot\rightharpoonup\varnothing}$. Thus, the $A_{n\cdot\rightharpoonup m\cdot}$ form a basis of the space of the linear operators on $\mathfrak{G}^0_{\mathbb{R}}$. For example, the composition of two such operators can be expressed as a linear combination of normal-ordered products of $A^{\dagger}$ and A, namely

$$A_{n_2\cdot\rightharpoonup m_2\cdot} A_{n_1\cdot\rightharpoonup m_1\cdot} = \sum_{p=0}^{min(m_1,n_2)} p!\binom{m_1}{p}\binom{n_2}{p} A_{(n_1+n_2-p)\cdot\rightharpoonup(m_1+m_2-p)\cdot}\,. \tag{1}$$

The pre-factors $p!\binom{m_1}{p}\binom{n_2}{p}$ can naturally be interpreted as the number of overlaps of the right hand side of $n_1\cdot \rightharpoonup m_1\cdot$ with the left hand side of $n_2\cdot \rightharpoonup m_2\cdot$ in p vertices.

Inner Products and Expectation Values

By equipping $\mathfrak{G}_{\mathbb{R}}$ with inner product $\langle [G]_{\cong}|[H]_{\cong}\rangle := f([G]_{\cong})\delta_{[G]_{\cong},[H]_{\cong}}$ (for a strictly positive function[1] f) and introducing the *projection dual vector* $\langle| := \sum_{[G]_{\cong}} \frac{1}{f([G]_{\cong})}|[G]_{\cong}\rangle$ – hence $\langle|[G]_{\cong}\rangle = 1$ for all $|[G]_{\cong}\rangle$ – we may define the *expectation values* $\langle\theta\rangle_G := \langle|A_{\theta}|[G]_{\cong}\rangle$ for any rule $\theta\colon L \rightharpoonup R$ and graph G. For example, the number of matches of a subgraph L in a graph G is given by $\langle|A_{L\rightharpoonup L}|[G]_{\cong}\rangle$, i.e. the linear operators associated to identity rules $L \rightharpoonup L$ are natural *counting observables* on $\mathfrak{G}_{\mathbb{R}}$.

2 Conclusion

Rule-based algebra aims for the linear algebraic core of graph transformation. We have shown that the rule-algebra of discrete graph rewriting is the Heisenberg-Weyl algebra (Theorem 1.2). A theoretical question is whether other rule-algebras of graph rewriting can be characterized in a similar fashion. Concerning applications, we plan to use rule-algebras to implement efficient algorithms for stochastic model checking. We are confident that rule-algebras are useful in coping with the unavoidably complicated combinatorics of graph transformation, and that they are a promising first step towards algebraic combinatorics.

References

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[1] For example, choosing $f([n\cdot]_{\cong}) = n!$ gives the inner product of the subspace $\mathfrak{G}^0_{\mathbb{R}}$ from Theorem 1.2.