### Abstract

We target the problem of provably computing the equivalence between two complex expression trees. To this end, we formalize the problem of equivalence between two such programs as finding a set of semantics-preserving rewrite rules from one into the other, such that after the rewrite the two programs are structurally identical, and therefore trivially equivalent. We then develop a graph-to-sequence neural network system for program equivalence, trained to produce such rewrite sequences from a carefully crafted automatic example generation algorithm. We extensively evaluate our system on a rich multi-type linear algebra expression language, using arbitrary combinations of 100+ graph-rewriting axioms of equivalence. Our machine learning system guarantees correctness for all true negatives, and ensures 0 false positive by design. It outputs via inference a valid proof of equivalence for 93% of the 10,000 equivalent expression pairs isolated for testing, using up to 50-term expressions. In all cases, the validity of the sequence produced and therefore the provable assertion of program equivalence is always computable, in negligible time.

## 1 Introduction

Deep neural network systems have excelled at a variety of classification and reinforcement learning tasks [26]. However, their stochastic nature tends to hinder their deployment for automated program analysis: ensuring the correctness of the solution produced is often required, e.g., when determining the semantics equivalence between two programs (or symbolic expressions).

In this work we target the problem of automatically computing whether two input symbolic expressions are semantically equivalent [31], under a well-defined axiomatic system for equivalence using semantics-preserving rewrite rules [21]. Program equivalence is summarized as determining whether two programs would always produce the same outputs for all possible inputs, and is a central problem in computing [23, 31, 55]. The problem ranges from undecidable, e.g. [25], to trivial in cases of testing the equivalence of a program with itself. Our work directly studies the subset of programs represented by symbolic linear algebra expressions which include scalar, vector, and matrix types for both constants and variables, and 16 different operators with 147 distinct axioms of equivalence. For example, the expression using matrices, scalars, and a vector: \((A+B)I((a+(b−b))/a)\bar{v}−A\bar{v}\) can be proven equivalent to \(B\bar{v}\) by applying 10 axioms in sequence; our work generates the proof steps between these expressions.

While prior work has shown promises for deep networks to compute some forms of program equivalence [5, 62], the system typically outputs only a probability of equivalence, without any reasoning or insight that can be verified easily: false positive can be produced. Programs can be represented as a tree (or graph) of symbols, and deep networks for symbolic reasoning have been studied, e.g. to compute the derivative of a symbolic expression [38]. In this work, we take a significantly different approach to the problem of symbolic program reasoning with deep networks: we make the system produce the sequence of steps that lead to rewriting one program into another, that is the reasoning for (or proof of) equivalence between the two programs, instead of producing directly the result of this reasoning (e.g., a probability of equivalence, without explanation about the reasoning). In a nutshell, we approach expression equivalence as a theorem proving problem, in which all the axioms as well as tactics to compute a proof are all learned by example in a deep learning system, without any human insight.

We propose a method for generating training samples using probabilistic applications of production rules within a formal grammar, and then develop a graph-to-sequence [13, 40] neural network system for program equivalence, trained to learn and combine rewrite rules to rewrite one program into another. It can deterministically prove equivalence, entirely avoids false positives, and quickly invalidates incorrect answers produced by the network (no deterministic answer is provided in this case, only a probability of non-equivalence). In a nutshell, we develop the first graph-to-sequence neural network system to accelerate the search in the space of possible combinations of transformation rules (i.e., axioms of equivalence in the input language) to make two graphs representing symbolic expressions structurally identical without violating their original semantics. We propose a machine learning system for program equivalence which ensures correctness for all non-equivalent programs input (specificity = 100%), and a deterministically checkable output for equivalent programs (no false positives). We make the following contributions:

1. We design, implement and evaluate two competing approaches using graph-to-sequence neural network systems to generate proofs of equivalence. We provide
the first implementation of such graph-to-sequence systems in the popular OpenNMT-py framework \cite{opennmt-py}.

2. We present a complete implementation of our system operating on a rich language for multi-type linear algebra expressions. Our system provides a correct rewrite rule sequence between two equivalent programs for 93% of the 10,000 test cases. The correctness of the rewrite rule is deterministically checkable in all cases in negligible time.

The rest of the paper is organized as follows. Sec. 2 outlines the program equivalence problem we address, and motivates our proposed approach. Sec. 3 formalizes the equivalence problem addressed. Automatic sample generation is discussed in Sec. 4 before Sec. 5 which introduces our DNN system, its overall design principles and key components. A complete experimental evaluation of our system is detailed in Sec. 6. We present related work in Sec. 7 before concluding.

2 Motivation and Overview

Rewrite rules as axioms of equivalence In this work we represent programs with symbolic expressions made of variables (e.g., \(a, b, c\)), operators (e.g., \(+, \ast\)) and neutral/absorbing elements (e.g., \(1\)). We consider a rich linear algebra expression language, supporting three variable types (scalars as shown in P1-P4, vectors, and matrices) and 5 different variables per type; 16 operators including operators mixing different variable types such as vector-matrix product. We represent these programs as dataflow graphs \cite{graph2seq} with a single root node, that is to compute a single value.

P1 is equivalent to P2 if we consider the axiom \(A1: 1 \ast x = x, \forall x \in \mathbb{N}\). This axiom is also a clear rewrite rule: the LHS expression \(1 \ast x\) (with \(x \in \mathbb{N}\)) can be matched and replaced by the RHS expression \(x\) anywhere in the program without altering its semantics. An axiom, or equivalently here a graph rewrite rule, may be applied repeatedly to different subtrees. When applying \(A1\) on a specific location, the node \(b\) of P1, we obtain an equivalent and yet syntactically different program, we note \(P1 \equiv A1(b, P1)\). These equivalences can be composed, incrementally, to form a complex transformation: we have \(P1 \equiv A1(c, A1(b, P1))\). The result of these semantics-preserving transformations can be computed in sequence: first implement \(A1(b, P1)\) to obtain a new program \(P'\), then \(A1(c, P')\) to obtain \(P''\). To prove \(P1 \equiv P2\), we simply check \(P''\) is structurally identical to \(P2\), a linear time process.

To assess the validity of a transformation sequence \(S\) where \(P2 = S(P1)\), one simply needs to check for \(S\), in sequence, that each axiom is applicable at that program point, apply it to obtain a new temporary program, and repeat the process for each axiom in the complete sequence. If the sequence is verified to be valid, and \(S(P1)\) is structurally equivalent to \(P2\), then we have proved \(P1 \equiv P2\), and \(S\) forms the complete proof of equivalence between the two programs. Using \(A2: x \ast (y + z) = x \ast y + x \ast z, \forall x, y, z \in \mathbb{N}\) and \(A3: x + y = y + x, \forall x, y \in \mathbb{N}\), we have \(P1 \equiv P4 \equiv A3(+, A2(\ast, A1(c, A1(b, A2(+, P1))))\), a verifiable proof of equivalence under our axioms between the programs \((a \ast b + 1)\) and \((ac + ab)\), which involved structural changes including node deletion, creation and edge modification. Note the bidirectional nature of the process: one can rewrite from \((a \ast b + 1)\) to \((ac + ab)\), or the converse using the same (but reverted) sequence. Note also the non-uniquity of a sequence: by possibly many ways a program can be rewritten into another one, for example the sequence \(P4 \equiv A3(+, A1(c, A1(b, A2(+, P1)))\) also correctly rewrites \(P1\) into \(P4\). Conversely, a sequence may not exist: for example no sequence of the 3 above axioms allow to rewrite \(a + b\) into \(a \ast b\). We call these non-equivalent in our system, that is precisely if there is no sequence of axioms that can be applied to rewrite one program into the other. Our approach aims to compute some \(S\) for a pair of programs \(P1, P2\), so that \(S\) is verified correct when \(P1 \equiv P2\). Consequently, if \(P1 \not\equiv P2\), no sequence \(S\) produced can be verified correct: true negatives are trivially detected.

Pathfinding program equivalence proofs Intuitively, we can view the solution space as a graph, where every possible syntactically different program in the language is represented by its own vertex \(v_i\). And \(A(x, y) : v_i \rightarrow v_j\) iff \(A(x, y)\) an axiom and \(x, y\) a node in \(v_i\) such that \(A(x, y)\). Any two programs connected by a path in this graph are therefore semantically equivalent. Building \(S\) for \(P1 \equiv S(P2)\) amounts to exposing one path between \(P1\) and \(P2\) in this graph when it exists, the path forming the proof of equivalence. We build a deep learning graph-to-sequence system to learn a stochastic approximation of an iterative algorithm to construct such feasible path when possible, trained only by randomly sampling pairs of programs and one carefully labeled path between them. This avoids the need to craft smart
We now present the formalism we use in this work to represent symbolic expressions and their equivalences. We carefully co-designed this problem representation and the (graph) neural network approach to make the best use of machine learning via deep networks, as discussed in Sec. 5.

3 Framework for Program Equivalence

A key design aspect is to match the capability of the neural network to model the input as a walkable graph with the actual input program representation to be handled. We therefore model “programs” in a dataflow-like representation (i.e., a directed graph), using a single root/output node. Symbolic expressions computing a single result typically fit this representation. The following definitions are applicable to programs represented as dataflow graphs, albeit we specialize them to symbolic expressions.

Definition 3.1 (Expression graph node). A node \( n \in N \) in the expression graph models \( n \)-ary operations and input operands. A node produces a value which can be consumed by any of its immediate successors in the graph. When a node has no predecessor, it models an input value. The output value for the computation is produced by the unique root node \( n_{root} \) of the graph, the only node without successor.

Definition 3.2 (Expression graph directed edge). A directed edge \( e_{n_1, n_2} : n_1 \rightarrow n_2 \) with \( n_1, n_2 \in N \) in the expression graph connects the producer of a value \( (n_1) \) to a node consuming this value in the computation.

Definition 3.3 (Expression graph). A expression graph \( G \) is a directed dataflow graph modeling the computation, made of nodes \( n \in N \) and edges \( e_{n_1, n_2} \in E \) as defined in Def. 3.1 and Def. 3.2. That is, \( G = (n_{root}, N, E) \). There is no dangling edge nor unconnected node in \( G \).
Language of linear algebra expressions  We developed a complex-enough language to evaluate carefully our work, that captures rich linear algebra expressions. Specifically, we support 3 types of data/variables in the expression: scalars, vectors and matrices. We use the standard notation $a, \ddot{a}, A$ for scalars, vectors and matrices. We evaluate using different variable names for each of the 3 types above, along with their identity and absorbing elements.

We also model a rich set of operators, mixing different unary and binary operations for each type. Specifically, we support $*, \sigma, \tau, \sigma / \tau$ between scalar operands, and $*, \sigma, \tau$ between vectors and $*, \sigma, \tau$ for matrices. For $\sigma / \tau$ we also support their unary version for all types, e.g. $\sigma^{-1}$, for unary scalar inversion and $\tau^{-1}$ for unary matrix negation. For example $a^{-1}$ computes to $1/a$. We also support multitype operations, such as vector and matrix scaling by a scalar $*, \sigma, \tau$. We support two specific unary matrix operations, transpose $\tau$ and matrix inversion as $\tau^{-1}$. Note every operator has a unique name in our language, driven by the type of its operand. This will facilitate the learning of the expression embedding, avoiding the need to learn type propagation.

Examples  Expressions of the form $A(BCD)E^{-1} \ddot{a} + b\ddot{c}^{-1} - 0\ddot{e}, (a+b) + (c(d/e)), (aA+bB)C^2$ etc. can be parsed trivially to our representation, one simply needs to be able to provide a unique name for each operand and operator type (possibly via some analysis, or simple language design principles), that is avoiding to overload the semantics of operators and operands. Note the semantics is never explicitly provided to our DNN approach, it is learned by examples. There will be no example of the form e.g. $a + A$, an invalid expression in our language.

We believe a sensible approach is to develop a clean, regular grammar for the language to be handled, as implicitly these are concepts the DNN will need to learn. We did so, using a classical LL(1) grammar description of our linear algebra language. This is not a requirement of our approach, as one can arrive to the desired input expression graph by any means necessary, but we believe making the reasoning on the language structure “easy” is an important design aspect.

3.2 Axioms of Equivalence
A central aspect of our approach is to view the problem of expression equivalence as finding a sequence of locally-correct rewrite rules that each preserve the semantics, thereby making incremental reasoning possible. We explicitly do not consider non-semantics-preserving axioms. A rich structure of alternate but equivalent ways to rewrite one expression to another makes the problem easier to sample and more amenable to machine learning. Semantics-preserving axioms enable incremental per-axiom reasoning, and enforce semantics preservation without overly complicated semantics analysis; while still manipulating a very rich space of transformations. To illustrate this we specifically design axioms that perform complex graph modifications, such as node deletion or creation, subtree manipulation, multi-node graph changes, etc.

A graph pattern can be viewed as a pattern-matching rule on graphs and its precise applicability criteria. It can also be viewed as a sentential form of the language grammar, e.g. $\text{ScalarVal PlusOp ScalarVal}$ is a pattern, if the grammar is well formed.

Definition 3.4 (Graph pattern). A graph pattern $P$ is an unambiguous structural description of a (sub-)graph $G_P$, which can be deterministically matched in any expression graph $G$. We have $P = \langle G_P, M_P, M_E \rangle$ where for each node $n_i \in N^{G_P}$, $\{n_{match}\} = M_{A}(n_i)$ returns the set of node values $n_{match}$ accepted to match $n_i$ on a graph $G$. For $n_i,n_j \in N^{G_P}$, $e_i = M_{e}(n_i,n_j)$ returns the set of edges between $M_{e}(n_i)$ and $M_{e}(n_j)$ to be matched in $G$. A pattern $P_G$ is matched in $G$ if (a) $\forall n_i \in G_P, \exists n_m = M_{n}(n_i) \in N^{G}$; (b) $\forall e_i \in E^{G_P}, \exists e_M = M_{e}(n_i,n_j) \in E^{G}$; and (c) $\forall e_{M}(n_i,n_j) \in E^{G} \not\in e_{M}(n_i,n_j)$.

Note when a graph pattern models a rewrite, $M_P$ and $M_E$ are adjusted accordingly to output the rewrite of a node $n \in N^{G_P}$ into its desired value, instead of the set of acceptable nodes from $n \in N^{G_P}$.

Definition 3.5 (Axiom of equivalence). An axiom $A$ is a semantics-preserving rewrite rule $G^' = A(n, G)$ that can arbitrarily modify a expression graph $G$, and produces another expression graph $G^'$ respecting Def. 3.3 with identical semantics to $G$. We note $A : \langle P_{match}, P_{replace} \rangle$ an axiom, where $P_{match}, P_{replace}$ are graph patterns as per Def. 3.4. The application of axiom $A$ to node $n$ in $G$ is written $A(n, G)$.

We can compose axioms to form a complex rewrite sequence.

Definition 3.6 (Semantics-preserving axiom composition). Given a sequence $S : A_1(n_1, A_2(n_2, ..., A_m(n_{m}, G)))$ of $m$ axioms applications. It is a semantics-preserving composition if for each $G_i = A_i(n_i, G_i) \in S, P_{match}$ succeeds on the subgraph with root $n_i$ in $G_i$, and $G_j$ is obtained by applying $P_{replace}$ to $n_i$.

Theorem 3.7 (Expression graph equivalence). Given a expression $G$. If $G^' = S(G)$ such that $S$ is a semantics-preserving sequence as per Def. 3.6, then $G \equiv G^'$, they are equivalent under the axiom system used in $S$.

This is a direct consequence of using only semantics-preserving axioms, each rewrite cannot individually alter the semantics, so such incremental composition does not. It leads to the formal problem we are addressing:

Corollary 3.8 (Expression graphs equivalence matching). Given two expression $G, G^'$. If there exist a semantics-preserving sequence $S$ such that $G^' = S(G)$, then $G \equiv G^'$.

Note here $\equiv$ means complete structural equivalence between the two graphs: they are identical in structure and
label/node values. Determining $G = G'$ amounts to visiting both graphs simultaneously e.g. in depth-first search from the root to ensure structural equivalence, and also verifying the same node labels appear in both at the same time. This is trivially implemented in linear time in the graph size.

**Language of linear algebra expressions** We have implemented a total of 102 different axioms for our language, made of the multi-type versions of the 13 core restructuring axioms described later in Table 1. They all follow established linear algebra properties. Note different data types have different axioms following typical linear algebra rules, e.g., matrix-multiplication does not commute, but scalar and vector multiplications do. Examples of axioms include $x(yz) → (xy)z$, $X - X → 0$, $-\overline{\overline{y}} - \overline{\overline{x}}$, or $X' → X$, an exhaustive list is displayed in the Supplementary Material.

In our experiments, we presume matrix and vector dimensions are appropriate for the given operation. Such dimension compatibility checks are simple to implement by e.g. introducing additional nodes in the program representation, but are not considered in our test language.

**Examples** We illustrate axiom-based rewrites using axioms presented in later Table 1. Note axiom names follow the structural changes applied. For example, we have $a + b ≡ b + a : \{a + b\} = \text{Commute}(\{+, (b + a)\})$. $a + b + c ≡ b + c + a : \{a + b + c\} = \text{Commute}(\{+, \text{Cancel}(\{+, \text{Noop}(\{+\}, \text{Cancel}(\{-\})), (c + b + (a - a)))\}))$. Such axioms are developed for scalars, matrices and vectors, and include complex rewrites such as distributivity rules and transpositions. A total of 102 axioms are used in our system.

### 3.3 Space of Equivalences

We now define the search space being explored in this work, i.e., the exact space of solutions on which the DNN system formally operates, and that we sample for training.

**Definition 3.9** (Graph of the space of equivalences) Given a language $L$. The directed graph of equivalences between expressions is $G_{\text{equiv}} = \langle N_{\text{equiv}}, E_{\text{equiv}} \rangle$ such that $∀ l ∈ L, n_i ∈ N_{\text{equiv}}$, and $e_{n_i,n_j} : n_i → n_j ∈ E_{\text{equiv}}$ iff $n_j ≡ A_i(x, n_i), ∀ A_i$ in the axiom system and $x$ a position in $n_i$ where $A_i$ is applicable.

In other words, the graph has one node per possible expression in the language $L$, and a single axiom application leads to connecting two nodes. We immediately note that $G_{\text{equiv}}$ is a (possibly infinite) multigraph, and contains circuits.

**Theorem 3.10** (Expression equivalence with pathfinding). Given two expressions $n_i, n_j ∈ N_{\text{equiv}}$. If there is any path from $n_i$ to $n_j$ in $G_{\text{equiv}}$, then $n_i ≡ n_j$.

The proof is a direct consequence of Def. 3.9. In this work, we randomly sample this exact graph to learn how to build paths between arbitrary expressions. As it is a multigraph, there will be possibly many different sequences modeled to prove the equivalence between two expressions. It is sufficient to expose one to prove equivalence.

**Corollary 3.11** (Semantics-preserving rewrite sequence). Any directed path in $G_{\text{equiv}}$ is a semantics-preserving rewrite sequence between the expressions, described by the sequence of axioms and expression position labeling the edges in this path. This sequence forms the proof of equivalence.

We believe that ensuring there are possibly (usually) many ways to compute a proof of equivalence in our specific framework is key to enable the DNN approach to learn automatically the pathfinding algorithm for building such proofs. Other more compact representations of this space of equivalences are clearly possible, including by folding nodes in the equivalence graph for structurally-similar expressions and folding equivalent paths between nodes. When building e.g. a deterministic algorithm for pathfinding, such space size reduction would bring complexity benefits [11, 31]. We believe that for the efficient deployment of graph-to-sequence systems, exposing significant redundancy in the space facilitates the learning process. We also alleviate the need to reason on the properties of this space to find an efficient traversal heuristic.

### 4 Samples Generation

The careful creation of our training dataset is key: as we let the DNN learn by example only what the axioms are and when they are applicable in the structure of a program, we must carefully sample the space of equivalences to ensure appropriate distributions of the examples. We produce a final dataset of tuples $(P_1, P_2, S)$, a pair of input programs and a possible rewrite rule sequence that proves the pair equivalent. Duplicates are removed such that all samples have a unique $P_1$. From this dataset, we create 1,000,000 training samples, 10,000 validation samples, and 10,000 test samples. We outline below its generation principles; extensive details and the algorithms used are presented in section B.1.

**Random sample generation** Deep learning typically requires large training sets to be effectively deployed, hence we developed a process to automate sample generation. We specifically use randomized program generation algorithms that are inspired by a given language grammar. By randomly choosing between production rules, one can build random parse trees by simply iterating the grammar. The leaves obtained will form a sentence accepted by the language, i.e., a program [15]. We limit to programs of 50 nodes in the program tree (or AST), with a maximal tree depth of 7. We
assert that our random production rule procedure has a non-zero probability of producing any program allowed by the grammar for our datasets.

We produce equivalent program samples by pseudo-randomly applying axioms on one randomly generated program to produce a rewrite sequence and the associated equivalent program. Given a randomly selected node in the program graph, our process checks which axiom(s) can be applied. E.g., the \( +_m \) operator may have the Commute axiom category applied, or it may have the Transpose axiom category applied, which affects the operator’s children.

**Final experimental dataset: AxiomStep10** To train our network to produce one axiom step at a time, as described in Sec. 2, AxiomStep10 has a single axiom in each output sequence \( S \). For a complete proof \( S : A_1(A_2(\ldots)\) in a \((P_1, P_2, S)\) we generated made of \( N \) axioms, we then create \( N \) training samples.

**Datasets to study generalizability and robustness** In order to study our model’s ability to generalize, we have created alternate datasets on which to train and test models which are summarized in table 2. WholeProof10 will help us contrast learning approaches. This dataset has the complete proof sequence \( S \) made of \( N \geq 1 \) axioms as reference output for a program pair, while for AxiomStep10, \( N = 1 \). Models trained on WholeProof\( X \) must maintain internal state representing the graph transformations that the axioms create.

They are not “iterative”: a single inference is expected to produce the complete proof; in contrast to AxiomStep10 for which a single axiom of the sequence is produced at each inference step. Training long output sequences can benefit from complex training approaches such as Professor forcing [37], but we will show that our AxiomStep10 model generalizes well with our sequence model training approach.

**Table 2. Datasets used for studies in experiments.**

| Dataset            | AST depth | AST #nodes | Proof length | Iterative |
|--------------------|-----------|------------|--------------|-----------|
| AxiomStep10        | 2-7       | 2-50       | 1-10         | Yes       |
| AxiomStep5         | 2-6       | 2-25       | 1-5          | Yes       |
| WholeProof10       | 2-7       | 2-50       | 1-10         | No        |
| WholeProof5        | 2-6       | 2-25       | 1-5          | No        |

**Complexity of equivalence space** Figure 3 provides a view of the complexity of the equivalence problem we tackle. The distribution of the dataset per proof length is displayed in the right chart; the left chart shows by size of bubble the number of test samples with a given number of semantics-preserving axioms that may be implemented as the first step of the proof and the proof length needed.

There is a large number of proofs possible in our system, as detailed in Appendix B.3. For example, for proofs of length 5, about 340,000 proofs made only of legal applications of axioms can be performed on the average sample in our dataset. Since many programs have multiple possible proofs, about 10,000 different programs can be produced, only one of which is the target to prove, i.e., randomly drawing a valid 5 axiom proof on a program known to be 5 axiom steps from the target has roughly a 1 in 10,000 chance of being a correct proof of equivalence between the two programs.
5 Deep Neural Networks for Program Equivalence

Fig. 2 overviews the entire system architecture including sample generation, the pe-graph2axiom network, and the rewrite checker. Key design decisions are presented below.

Graph neural network The sample generation discussed in section 4 provides input to the Node Initialization module in Fig. 2 to create the initial state of our graph neural network [13]. For each node in the program graph, a node will be initialized in our graph neural network with a value that encodes the AST level and language token of the program node. To interconnect the edges we support 9 edge types and their reverse edges which allows information to move in any direction necessary: 1) left child of binary op, 2) right child of binary op, 3) child of unary op, 4) root node to program 1, 5) root node to program 2, 6-9) there are 4 edge types for the node grandchildren (LL, LR, RL, RR). The node states and edge adjacency matrix represent the initial graph neural network state.

After initialization, the graph neural network iterates 10 times in order to convert the initial node state into the embeddings needed for rewrite rule generation. Given an initial hidden state for node \( n \) of \( x_n(0) \), \( x_n(t + 1) \) is computed with a learnable function \( f \) which combines the current hidden state \( x_n(0) \), the edge types \( l_{in}[n] \) of edges entering node \( n \), the edge types \( l_{out}[n] \) of edges exiting node \( n \), and the hidden states \( x_{ne}[n] \) of the neighbors of node \( n \): \( x_n(t + 1) = f(x_n(t), l_{in}[n], x_{ne}[n](t), l_{out}[n]). \)

Each edge type has a different weight matrix for learning, allowing aggregation of information into a given node related to its function in the full graph of the program. The root node’s initial state along with the edge types connecting it to the program graph trees allow it to aggregate and transfer specific information regarding rewrite rules as demonstrated by our experimental results. This is a novel feature of our network not used in prior work with GNNs on program analysis [4, 62].

Graph neural network output to decoder After stepping the GGNN, the final node values are used by the decoder in two ways to create rewrite rules. First, the final root node value \( x_{root}(10) \) is fed through a learnable bridge function to initialize the LSTMs of the decoder. In this way, the aggregated information of the 2 programs seeds the generation of rewrite rules. The LSTMs update as each output token \( y_j \) is generated with a learnable function based on the current decoder hidden state \( h^d_j \) at decoder step \( j \) and the previous output token \( y_{j-1} \) [18]. Second, all nodes in the graph can be used by an attention layer [8]. The attention layer creates a context vector \( c_j \) which can be used by a learnable function \( g \) when computing the probability for generating the \( j \)th output token \( P(y_j) : P(y_j \mid y_{j-1}, y_{j-2}, ..., y_0, c_j) = g(h^d_j, y_{j-1}, c_j). \)

Because pe-graph2axiom has a robust output verification, we make use of beam search to track up to 10 likely candidates for proofs of equivalence.

By using the root node only for seeding the initial hidden state \( h^d_0 \) of the decoder, the weights associated with its connections to the program graphs for \( P_1 \) and \( P_2 \) learn to represent the information necessary for the rewrite rule sequence. In parallel, after the graph neural network iterations complete, the final embedding for all the nodes in the graphs for \( P_1 \) and \( P_2 \) are only used by the attention network, so their final embedding represents information useful during rewrite rule generation.

Intermediate program generation pe-graph2axiom applies the axiom and program node chosen by the neural network token generator to the input program to create an intermediate program \( P' \) on the path from \( P_1 \) to \( P_2 \). If this program is equal to \( P_2 \), then our axiom path is complete, otherwise the new pair \( P', P_2 \) is inferred to determine the next axiom step.

Incremental versus non-incremental sequence production The models we train on the AxiomStep5, WholeProof10, and WholeProof5 datasets have the same neural network hyperparameters as the AxiomStep10 data model. However, the models for WholeProof10 and WholeProof5 are trained to output the entire sequence of axioms needed to prove the 2 programs identical, hence these models do not make use of the intermediate program generation and instead have a component which checks whether the full sequence of axioms legally transforms \( P_1 \) into \( P_2 \). We encode the path to the AST node an which to apply an axiom using 'left' and 'right' tokens which specify the path from the current program root node. This encoding is sufficient for the iterative model and necessary to allow the non-iterative model to identify nodes which may not have been in the initial AST for \( P_1 \). The non-iterative models must learn a representation in the LSTM network to allow them to track AST transformations as they are generated.

6 Experimental Results

We now present extensive experimental results, and compare the quality of several neural network approaches to address the problem of program equivalence. We have proceeded incrementally for fine-tuning the final system design, and report on several of these design points below.

We focus our experiments below on 4 key questions: 1) Is performance related to input program size? 2) Is performance related to proof length? 3) Is the incremental, per-axiom approach more generalizable than producing the full sequence in a single inference step? And 4) Is performance consistent across a range of datasets, including human-written examples?
**Implementation setup**  We developed the neural network system presented in the OpenNMT-py system [34], adding on a new encoder based on a prior implementation of gated graph neural networks [40]. For our training and evaluation experiments, we use systems with Intel Xeon 3.6GHz CPUs and 6GB GeForce GTX 1060 GPUs. During training, we save a model snapshot every 50,000 iterations and score the accuracy the model achieved on the validation dataset. Graphs showing that validation accuracy plateaus at 200,000 to 300,000 iterations are provided in section E. We run each model twice and evaluate the test set using the saved model which achieved the highest validation score.

**Evaluation procedure and neural network alternatives**  The benefits of key components of our neural network model are studied in table 3. The bidirectional RNN model is similar to state-of-the-art sequence-to-sequence models used for program repair [18]. The results for the graph-to-sequence model without attention show the benefit of providing the node information during the axiom generation process.

| Model description                      | Beam width |
|----------------------------------------|------------|
| Bidirectional RNN seq-to-seq with attention | 48 62 71 75 |
| Graph-to-sequence w/o attention         | 73 81 87 90 |
| pe-graph2axiom model                   | 76 84 90 93 |

Our final design was influenced by explorations we performed on varied models, datasets, and hyperparameters such as LSTM layers and graph neural network parameters. In relation to the model’s ability to learn a representation of the proof sequence, we note that our GGN initialization using the root node connection to the decoder outperforms the embedding learned by a bidirectional RNN model. Also, we found that averaging the embedding of all graph nodes had about 10% lower accuracy than using the more specific root node information. Numerous additional results are reported in Suppl. material E.

**Generalizing across different datasets**  We specifically look at the generalization potential for our models by studying their success rate as a function of the input program complexity, represented as the AST depth, in Table 4, and as a function of the output complexity, represented by the proof length in Table 5, all using the same input program, of the maximal number of nodes in an input program graph (the Program length, directly influencing the size of the graph network), and the Rewrite rule length, which contains the description of paths from the root node to the position of application of an axiom, this is directly related to the maximal graph height, itself determined by the maximal program size. Details on each row are provided in Supplementary Material.

We specifically compare against a sequence-to-sequence (S2S) approach, to quantify the gains brought by employing graph-to-sequence (G2S). When the space is small enough, S2S still performs well, especially using aggressive beam search. We recall that by design of our system testing the correctness of one sequence is trivial and deterministic, so one can easily use large beam sizes without any correctness impact nor major performance penalty during inference. For example, inference of beam 1 is about 15ms for our most complex networks, but beam 10 only takes 16ms. Checking correctness is << 1ms.

Table 6 shows the result of 12 different experiments and designs specifically for the WholeProof5 models. In particular, we incrementally increase the problem complexity from rows 1 to 10, increasing the number of Operators that can be used in any input program, of Axioms used in the rewrite sequence, of Operands in any input program, of the maximal number of nodes in an input program graph (the Program length, directly influencing the size of the graph network), and the Rewrite rule length, which contains the description of paths from the root node to the position of application of an axiom, this is directly related to the maximal graph height, itself determined by the maximal program size. Details on each row are provided in Supplementary Material.

### Table 4. Performance vs. AST size: counts and percentage pass rates.

| AST depth | Testset Count | Model trained on AxiomStep5 | Model trained on AxiomStep10 |
|-----------|--------------|----------------------------|-----------------------------|
|           | AS5          | AS10                       | AS5                        | AS10                        |
| 2-6       | 10000        | 6865                       | 99                         | 93                          |
| 7         | 0            | 3135                       | n/a                        | 86                          |
| All       | 10000        | 10000                      | 99                         | 90                          |

### Table 6. WholeProof Models: Language Complexity and Performance

Table 6 shows the result of 12 different experiments and designs specifically for the WholeProof5 models. In particular, we incrementally increase the problem complexity from rows 1 to 10, increasing the number of Operators that can be used in any input program, of Axioms used in the rewrite sequence, of Operands in any input program, of the maximal number of nodes in an input program graph (the Program length, directly influencing the size of the graph network), and the Rewrite rule length, which contains the description of paths from the root node to the position of application of an axiom, this is directly related to the maximal graph height, itself determined by the maximal program size. Details on each row are provided in Supplementary Material.

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Contrasting rows 2 and 3 displays the merits of the G2S approach for our problem: on this simple problem, in fact G2S gets near-perfect accuracy already. Progressively increasing the complexity of the search space, till row 9 and 10, displays...
Table 5. Performance vs. proof length: percentage pass rates.

| Axiom Count in | Model trained on WholeProof5 (WP5) | Model trained on WholeProof10 (WP10) | Model trained on AxiomStep5 (AS5) | Model trained on AxiomStep10 (AS10) |
|----------------|------------------------------------|-------------------------------------|-----------------------------------|------------------------------------|
| Proof          | WP5 WP10 AS5 AS10                  | WP5 WP10 AS5 AS10                   | WP5 WP10 AS5 AS10                 | WP5 WP10 AS5 AS10                 |
| 1-5            | 95 89 44 44                          | 94 93 44 44                        | 99 97 99 98                      | 99 98 99 98                      |
| 6              | 14 4                                    | 72 5                               | 81 88                            | 90 93                            |
| 7              | 0 1                                    | 63 2                               | 67 81                            | 83 87                            |
| 8              | 0 0                                    | 54 1                               | 54 75                            | 73 82                            |
| 9              | 0 0                                    | 47 0                               | 35 64                            | 63 74                            |
| 10             | 0 0                                    | 34 0                               | 24 57                            | 46 66                            |
| All            | 95 66 44 27                            | 94 84 44 27                        | 99 87 99 90                      | 99 93 99 93                      |

Table 6. Results for various language complexities studied, on non-incremental models (WholeProof).

| ID | Description | # Operators | # Axioms | # Operators | # Axioms | Program length | Rewrite rule length | Graph2seq(S2S) or seq2seq(G2S) | Training set size | Percent matching with beam width 1 | Percent matching with beam width 10 |
|----|-------------|-------------|----------|-------------|----------|----------------|---------------------|---------------------------|-----------------|--------------------------|-------------------------|
| 1  | Rewrite sequence is only single Commute, uses sequence-to-sequence model | 2 | 1 | 10 | 3-19 | S2S | 80,000 | 90.8% | 96.2% |
| 2  | Rewrite sequence is exactly 2 Commutes, uses sequence-to-sequence model | 2 | 1 | 10 | 5-24 | S2S | 80,000 | 98.3% | 96.5% |
| 3  | Rewrite sequence exactly 2 Commutes | 2 | 1 | 10 | 5-24 | S2S | 80,000 | 98.9% | 99.9% |
| 4  | Rewrite sequence exactly 3 Commutes | 2 | 1 | 10 | 7-45 | S2S | 80,000 | 94.1% | 99.9% |
| 5  | Rewrite sequence 1 to 3 Commutes | 2 | 1 | 10 | 3-45 | S2S | 180,000 | 97.1% | 99.2% |
| 6  | Commute, Noop, Cancel, DistributeLeft, DistributeRight | 2 | 5 | 12 | 3-45 | S2S | 180,000 | 93.1% | 97.4% |
| 7  | Scalars, Vectors, and Matrices | 16 | 5 | 20 | 3-30 | S2S | 250,000 | 83.3% | 95.6% |
| 8  | Axioms | 16 | 13 | 20 | 3-30 | S2S | 400,000 | 85.5% | 99.5% |
| 9  | Axioms | 16 | 13 | 20 | 3-30 | S2S | 500,000 | 79.8% | 93.8% |
| 10 | Rewrite sequence or Not_equal | 16 | 13 | 20 | 3-30 | S2S | 400,000 | 59.8% | 81.1% |
| 11 | Test sequence-to-sequence | 16 | 13 | 20 | 3-30 | S2S | 400,000 | 83.8% | 94.7% |
| 12 | Add loop axioms | 18 | 15 | 20 | 3-30 | S2S | 400,000 | 90.0% | 97.1% |

A slow but steady decrease in quality, while still maintaining excellent scores near or above 95% with beam 10. To reassess the limits of a sequence-to-sequence approach, row 9 and 11 can be constrained: they operate on the same search space, but S2S peaks at 81% accuracy, while G2S reaches 95%.

Row 10 displays the result when learning using also samples of non-equivalent programs, using the “empty path” symbol Not_equal. We evaluated this system to measure the impact of training on only equivalent programs vs. also sampling pairs of unconnected nodes in the equivalences graph. We recall that by design, if no rewrite rule produced is verified as correct, our system outputs the programs are not equivalent. In other words, whichever the sequence(s) produced by the network, if the two input programs are non-equivalent, the system will always output they are not equivalent: no equivalence sequence produced can be verified as correct. So training on only equivalent programs is clearly sensible for such system; furthermore as shown in row 10 vs. 9, even increasing the training set size, training using non-equivalent programs seem to lower the performance slightly.

Human written test expressions from Khan academy exercises
Unfortunately there is a dearth of existing large reference datasets for equivalence of linear algebra expressions, which justified our careful dataset creation approach in Sec. 4 and their upcoming public release. However numerous math exercises involve exactly this problem, and can provide small but human-written datasets. We solve all of the matrix expression equivalence programs from 2 relevant Khan academy modules designed to test student’s knowledge of matrix algebra [33]. Our AxiomStep10 model is able to correctly prove all 15 equivalent pairs from the modules with beam width 1 and wider. With a beam width of 10, the WholeProof10 model proved 12. An example problem solvable by AxiomStep10 but not WholeProof10 is: \( c(A + B) = cB + cA \) which can be proven by applying the rewrite rules NeutralOp, DistributeRight, and Commute to the proper nodes. The WholeProof10 model mostly fails because it was not trained on how to apply repeated transformations at the same point in the AST. This suggests AxiomStep10 has generalized well to these hand-written problems.

7 Related Work

Theorem provers
The problem of equivalence as we formulated may be solved by other (smart) brute-force approaches, where a problem is solved by pathfinding. This ranges from theorem proving systems like Coq [14] which supports the formal framework for equivalence we describe in this paper, to (Approximate Probabilistic) Model Checking [17, 20, 27], where a program equivalence system can also be built, e.g. [19, 46, 52, 58]. Our contribution is not in the formal definition of program equivalence we presented, semantics-preserving rewrite systems have been studied,
e.g. [41, 50, 57]. But understanding why this particular formalism was well suited to deep learning graph-to-sequence systems was key. The merits of stochastic search to accelerate such systems has been demonstrated, e.g. [24, 27, 45]. The novelty of our approach is to develop carefully crafted graph-to-sequence neural networks to automatically learn an efficient pathfinding heuristic for this problem. Our approach is potentially applicable in these areas too, however training scalability can become a challenge if increasing the input representation size excessively. Theorem provers using deep learning have recently started to be investigated, Aygun et al. [7] developed a graph neural network system for automatic proof generation. Wu et al. [60] explores the ability of theorem provers using GNNs, TreeLSTMs, and BagOfWords architectures to generalize and solve proofs with lengths up to 7 axioms and found that GNNs performed the best of the architectures studied when more complex proofs were required. While our model works in a slightly different problem space, we study the ability of our models to generalize on proofs with lengths up to 10, with 14 different rewrite rules acting on 147 distinct axioms. These frameworks could also be used to prove equivalence between symbolic expressions, as theorem provers.

Static program equivalence  Algorithms for static program equivalence have been developed, e.g. [2, 11, 29, 56]. These approaches typically restrict to demonstrating the equivalence of different schedules of the operations, possibly dynamically [10]. In this work we target graph-modifying rewrites (and therefore which alter the operation count). Barthou et al. [2, 11] have developed techniques to recognize algorithm templates in programs. These approaches are restricted to static/affine transformed programs. Karfa et al. also designed a method that works for a subset of affine programs using array data dependence graphs (ADDGs) to represent input and transforming behaviors. Operator-level equivalence checking provides the capability to normalize expressions and establish matching relations under algebraic transformations [32]. Mansky and Gunter used the TRANS language [30] to represent transformations. The correctness proof implemented in the verification framework [43] is verified by the Isabelle [48] proof assistant. Other works also include translation validation [35, 47].

Program analysis with machine learning Numerous prior work has employed (deep) machine learning for program analysis, e.g. [3, 5, 12, 36, 49, 54]. code2vec [5] teaches a method for creating a useful embedding vector that summarizes the semantic meaning of a snippet of code. Program repair approaches, e.g. [18, 54] are deployed to automatically repair bugs in a program. Output accuracies of up to 20% on the test set is reported, using sequence-to-sequence models. Wang et al. [59] learns to extract the rules for Tomita grammars [53] with recurrent neural networks. The learned network weights are processed to create a verifiable deterministic finite automata (DFA) representation of the learned grammar. This work demonstrates that deterministic grammars can be learned with RNNs, which we rely on.

Graph Neural Networks Graph neural networks [51, 61] use machine learning to analyze a set of nodes and edges for patterns related to a target problem. Using a graph-to-sequence network with attention has been analyzed for natural language processing [13]. Allamanis et al. use graph neural networks to analyze code sequences and add edge types representing LastUse, ComputedFrom, and LastWrite to improve the system’s ability to reason about the code [4]. Their work achieves 84% accuracy on correcting variable misuse cases and provides insights to useful edge types. Structure2vec [62] uses a graph neural network to detect binary code similarity. Structure2vec uses a graph neural network to learn an embedding from an annotated control flow graph (ACFG) of a program. This learning process targets the embedding so that equivalent programs will have equivalent embeddings, reporting precision scores of 84% and 85% on various test datasets for correctly predicting program equivalence. It only outputs a probability of equivalence, and not a verifiable proof, which is sufficient in their context.

The G2SKGE model [39] has a similar graph network structure which uses a node embedding (which they refer to as an information fusion mechanism) in order to predict relationships between nodes. This technique of using a neural network to understand and predict node interrelationships is common to our approach.

8 Conclusion
In this work, we presented pe-graph2axiom, the first graph-to-sequence neural network system to generate verifiable axiomatic proofs (via rewrite rules) for equivalence for a class of symbolic programs. Evaluated on a rich language for linear algebra expressions, this system produces correct proofs of up to 10 axioms in length in 93% of the 10,000 equivalent cases evaluated. We believe the performance of our approach comes in part from using graph neural networks for what they aim to excel at: learning efficient heuristics to quickly find paths in a graph; and the observation that program equivalence can be cast as a path-based solution that is efficiently found by such networks.

Acknowledgments
This work was supported in part by the U.S. National Science Foundation award CCF-1750399.

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A Appendix

Supplementary Materials:
Learning Axioms to Compute Verifiable Symbolic Expression Equivalence Proofs using Graph-to-Sequence Networks

Document Overview
This document supplements the submission Proving Equivalence Between Complex Expressions Using Graph-to-Sequence Neural Models. We have provided below numerous additional information for completeness. We also provide access to anonymized software artifacts to replicate our results. Our supplementary materials are organized as follows:

- Appendix B of this document presents the dataset generation approach we developed.
- Appendix C of this document presents exhaustively the language for complex linear algebra expressions we evaluate on, including the list of all 147 axioms of equivalence we learned.
- Appendix D of this document presents additional details about the neural network architectures we developed.
- Appendix E of this document presents complementary experimental results and additional in-depth details on results presented in the main paper body.

B Dataset generation

B.1 Generation of Examples

Machine learning benefits from large training sets, so in order to produce this data, we created algorithms that would generate programs meeting a given language grammar along with target programs which could be reached by applying a rewrite rule to the given operation as such dimension checks are simple to implement and are not considered in our procedure. Note the token syntax here is exactly the one used by our system, and is strictly semantically equivalent to the mathematical notations used to describe these operations, e.g. $I_2$ is 1.

- Scalar operations: $+s -s *s /s$ is $ns$, where $ns$ is the unary reciprocal and $ns$ is the unary negation.

- Matrix operations: $+m -m *m im nm tm$, where $im$ is matrix inversion, $nm$ negates the matrix, and $tm$ is matrix transpose.
- Vector operations: $+v -v *s nv$, where $nv$ is the unary negation.
- Scalars: $a b c d e 0 1$
- Matrices: $A B C D E O I$, where $O$ is the empty matrix and $I$ is the identity matrix.
- Vectors: $v w x y z o$, where $o$ is the empty vector.

Summary: 16 operations, 20 terminal symbols

Initially, GenPl is called with GenPl("$+s -s *s /s +s -s *s /s +s -s *s /s +s -s *s /s is ns +m -m *m +m -m *m +m -m *m +m +v -v *v +v -v *v +v -v *v nv$,0.94)" In this initial call binary operations are repeated so that they are more likely to be created than unary operations, and the initial probability that a child of the created graph node will itself be an operation (as opposed to a terminal symbol) is set to 94%. Since the algorithm subtracts a 19% probability for children at each level of the graph, trees are limited to 7 levels.

Algorithm 1 starts execution by randomly selecting an operation from the set provided as input. When GenPl is called recursively, the operation set is limited such that the operation produces the correct type as output (scalar, matrix, or vector). Lines 3 through 15 of the algorithm show an example case where the $*s$ operation is processed. This operation requires scalar operands. If the probability of children at this level is met, then GenPl is called recursively with only scalar operands available, otherwise a random scalar operand is chosen.

The text for algorithm 1 does not show the process for all operations. Certain operations, such as $*v$, have a variety of operand types that can be chosen. The $+v$ operand is a multiplication which produces a vector. As such, $Av$ (matrix times vector), $bv$ (scalar times vector), or $vc$ (vector times scalar) are all valid options and will be chosen randomly.

After generating a program which follows the grammar rules of our language, algorithm 2 will produce a new program along with a set of rewrite rules which transform the source program to the target program.

Algorithm 2 receives as input the source program (or subprogram) along with the path to the current root node of the source program. If the source program is a terminal symbol, the algorithm returns with no action taken. Otherwise, the program starts with an operation and the algorithm proceeds to process options for transforming the given operation. For our wholeproof01 and wholeproof05 datasets, algorithm 2 is only called once, simplifying the possible node order and proof complexity. For the axiomstep10 and axiomstep5 datasets, algorithm 2 is called multiple times, allowing for the possibility that after a path is chosen for one axiom any node can be accessed for the next axiom (including the same node).

As shown on line 10 of the algorithm, when the operation and children meet the conditions necessary for a rewrite rule
### Algorithm 2: GenP2

**Result:** Second program and transform_sequence

**Input:** \(P_1, \text{path}\)

**Output:** \(P_2\)

1. **if** terminal symbol **then**
   2. return \(P_1\)
   3. **end**

4. \(op = \text{find operator of } P_1\)
5. \(L = \text{find left operand of } P_1\)
6. \(R = \text{find right operand of } P_1\)
7. \(Lop, LL, LR = \text{operator and operands of left child}\)
8. \(Rop, RL, RR = \text{operator and operands of right child}\)
9. // Randomly apply transform if allowed
10. **if** random < 0.5 and ((\(op == \text{"+v"} \land L = \text{"o"}) \lor (\(op == \text{"-v"} \land R = \text{"o"})\)) **then**
    11. append path. "NeutralOp " to transform_sequence
12. // Eliminate unnecessary operator and 0 vector
13. **if** \(L = \text{"o"}\) **then**
    14. return GenP2(R, path)
    15. **else**
    16. return GenP2(L, path)
    17. **end**
18. **end**

### Algorithm 1: GenP1

**Result:** Prefix notation of computation with parenthesis

**Input:** \(\text{Ops, } P\)

**Output:** \((op \; L \; R)\) or \((op \; L)\)

1. \(op = \text{select randomly from } \text{Ops}\)
2. // Create subtree for chosen \(op\)
3. **if** \(op == \text{"s"}\) **then**
   4. **if** random < \(P\) **then**
      5. \(L = \text{GenP1}(*s \; s /s +s -s \; s/s is ns*,P-0.19)\)
   6. **else**
      7. \(L = \text{select random scalar operand}\)
   **end**
7. **if** random < \(P\) **then**
   8. \(R = \text{GenP1}(*s \; s /s +s -s \; s/s is ns*,P-0.19)\)
   9. **else**
      10. \(R = \text{select random scalar operand}\)
   **end**
11. return \((op \; L \; R)\)
12. **end**
13. // Other ops may have more complex options for children types.
14. // (For example, "m" may have a matrix multiplied by a scalar or matrix)
15. ...

After these generation algorithms are run, a final data preparation process is done which prunes the data set for the learning algorithm. The pruning used on our final data set insures that the \((P_1, P_2)\) program pair total to 100 tokens or fewer (where a token is an operation or terminal), that the graph is such that every node is reachable from the root with a path of length 6 or less, and that there are 10 or fewer rewrite rules applied. But within these restrictions, we assert that our random production rule procedure has a non-zero probability of producing any program allowed by the grammar. Also, the pruning insures that there are no lexically equivalent programs in the process and removes some of the cases with fewer than 10 rewrite rules generated to bias the dataset to longer rewrite sequences. Table 1 details the distribution of rewrite rules created by the full process. Section C details all axioms when variable types and operators are considered.

We produce equivalent program samples by pseudo-randomly applying axioms on one randomly generated program to produce a rewrite sequence and the associated equivalent program. Given a randomly selected node in the program graph, our process checks which axiom(s) can be applied. E.g., the \(+m\) operator can have the Commute axiom applied, or depending on subtrees it may be allowed to have the Factorleft axiom applied, as discussed in Sec. 6. Generally we choose to apply or not an operator with 50% probability, so that pe-graph2axiom is forced to rely on analysis of the two programs to determine whether an operator is applied instead of learning a bias due to the local node features.
B.2 Intermediate program generation

The intermediate program generation algorithm is very similar to algorithm 2. For program generation of the target program, algorithm 2 will check that a node can legally apply a given rule, apply the rule with some probability, record the action, and process the remaining program. For intermediate program generation, we begin with a P1 and a rewrite rule. We follow the path provided to identify the node, check that a node can legally accept a rule, apply the rule, and return the adjusted program. If a rule cannot legally be applied, P1 is not successfully transformed. If a rule can be legally applied to P1, the program is compared lexically to P2 and if they match then equivalence has been proven.

B.3 Complexity of Proving Equivalence

Table 7 shows the complexity of the solution space for our problem for proofs from our AxiomStep10 test dataset up to length 7 (deterministically computing all possible programs requires too many resources for longer proof lengths). The ‘All possible nodes and axioms’ row includes the total number of proofs of a given length available to our problem space. The entry 5933 for a single axiom represents that for an AST depth of 7 we have 43 axioms which can be applied to all 63 possible operator nodes and 104 axioms which can be applied to the 31 nodes which possibly have child operator nodes themselves: 63 * 43 + 31 * 104 = 5933. Subsequent columns can select repeatedly from the same set growing as 5933^2 to 5933^7. The ‘sample node + axiom group’ row is based on our 10,000 sample test dataset and represents the possible selection of any of the 14 axiom groups being applied to any node in the program. The ‘sample node + legal axiom’ row represents only legal node plus legal axiom group being applied and effectively represents the total number of programs derivable from the start program in the test dataset. The final row ‘Sample derivable unique programs’ represents the total number of programs derived from legal node and axiom sequences which are lexically unique.

C Language and Axioms for Complex Linear Algebra Expressions

We now provide the complete description of the input language for multi-type linear algebra expressions we use to evaluate our work, and the complete list of all axioms that are used to compute equivalence between programs.

Variable types We model programs made of scalars, vectors and matrices. We limit programs to contain no more than 5 distinct variable names of each type in a program:
• Scalar variables are noted a, b, ..., e.
• Vector variables are noted a, w, ..., z.
• Matrix variables are noted A, B, ..., E.

Note we also explicitly distinguish the neutral and absorbing elements for scalars and matrices, e.g., 1 = 1_M. This enables the creation of simplification of expressions as a program equivalence problem, e.g. if A + B = (B + A) = 0_M, this enables the creation of simplification of expressions as a program equivalence problem.

Unary operators We model 6 distinct unary operators, all applicable to any variable of the appropriate type:
• is(a) = a⁻¹ is the unary reciprocal for scalars, is(A) = A⁻¹ is matrix inverse.
• ns(a) = −a is unary negation for scalars, ns(v) = −v for vectors, ns(M) = −M for matrices.
• tM(M) = Mᵀ is matrix transposition.

Binary operators We model 10 distinct binary operators that operate on two values. 7 operators require the same type for both operands, while 3 enable multi-type operands (e.g., scaling a matrix by a scalar). Note we do not consider potential vector/matrix size compatibility criterion for these operators, in fact we do not represent vector or matrix sizes at all in our language, for simplicity.
• +s(a, b) = a + b, the addition on scalars, along with −s(a, b) = a − b, +s(a, b) = a * b and /s(a, b) = a/b.
• *v(v, w) = v · w, the dot product between two vectors, producing a scalar.
• +m(A, B) = A + B, the addition on matrices, along with −m(A, B) = A − B, and *m(A, B) = AB the product of matrices.
• *m(a, A) = aA and *m(A, a) = Aa are used to represent scaling a matrix by a scalar.
• *v(v, A) = aA represents a vector-matrix product.
• *v(a, v) = a⁻¹ and *v(v, a) = a⁻¹v represent scaling a vector by a scalar.

List of axioms of equivalence Tables 8-9 show the full 147 axioms supported by our rewrite rules. Many rewrite rules can be applied to all 3 variable types as well as multiple operator types.
| Rewrite Rule   | ID | Example(s)          |
|---------------|----|---------------------|
| Cancel        | 1  | (a - a) → 0         |
|               | 2  | (b/b) → 1           |
|               | 3  | (A - A) → O         |
|               | 4  | (A * A⁻¹) → I       |
|               | 5  | (A⁻¹ + A) → I       |
|               | 6  | (v - v) → o         |
| NeutralOp     | 7  | (a + 0) → a         |
|               | 8  | (0 + a) → a         |
|               | 9  | (a - 0) → a         |
|               | 10 | (a * 1) → a         |
|               | 11 | (1 * a) → a         |
|               | 12 | (a / 1) → a         |
|               | 13 | (A + O) → A         |
|               | 14 | (O + A) → A         |
|               | 15 | (A - O) → A         |
|               | 16 | (I * A) → A         |
|               | 17 | (v + o) → v         |
|               | 18 | (o + v) → v         |
|               | 19 | (v - o) → v         |
| DoubleOp      | 20 | (a - a) → 0         |
|               | 21 | (a⁻¹⁻¹) → a         |
|               | 22 | -(-a) → a           |
|               | 23 | (a⁻¹⁻¹⁻¹) → a       |
|               | 24 | -(a⁻¹ - a) → A      |
|               | 25 | (A⁻¹⁻¹⁻¹⁻¹) → A     |
|               | 26 | (A⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻¹⁻� |
## Table 9. Full axiom count when all type options and other supported permutations are included (part 2 of 2)
D Details on neural network model

Figure 4 overviews the entire pe-graph2axiom architecture including sample generation, the graph-to-sequence network, the intermediate program generation, and lexical equivalence checker. In this section we will discuss the implementation details of these components.

Graph neural network internal representation The sample generation discussed in section 4 provides input to the Node Initialization module in Fig. 4 to create the initial state of our graph neural network. For each node in the program graph, a node will be initialized in our graph neural network. Each node has a hidden state represented by a vector of 256 floating point values which are used to create an embedding for the full meaning of the given node. Initially all 256 dimensions of the hidden states of the nodes are set to zero except for 2. Given N tokens in our input program language, one of the dimensions from 1 through N of a node will be set based on the token at the program position that the node represents. For example, if the scalar variable a is assigned to be token 3 in our language, then the a nodes of Fig. 5 recalled below would have their 3rd dimension initialized to 1.0. This is a one-hot encoding similar to that used in neural machine translation models which leverage Word2vec [44].

The second non-zero dimension in our node initialization indicates the tree depth, with the root for the program being at depth 1. We set the dimension N+depth to 1.0; hence, the a nodes in Fig. 5, which vary from level 2 or 3 in the graph, would set dimension N + 2 or N + 3 to 1. In addition to nodes correlating to all tokens in both input programs, we initialize a root node for program comparison which has edges connecting to the root nodes of both programs. The root node does not represent a token from the language, but it is initialized with a 1.0 in a hidden state dimension reserved for its identification.

For a graph neural network, the edge connections between nodes are a crucial part of the setup. In particular, to match the formulation of our problem, we must ease the ability of the network to walk the input program graphs. We therefore designed a unified graph input, where both program graphs are unified in a single graph using a single connecting root node; and where additional edges are inserted to make the graph fully walkable.

In our full model, we support 9 edge types and their reverse edges. The edge types are: 1) left child of binary op, 2) right child of binary op, 3) child of unary op, 4) root node to program 1, 5) root node to program 2, 6-9) there are 4 edge types for the four node grandchildren (LL, LR, RL, RR). After the node hidden states and edge adjacency matrix are initialized, the network is ready to begin processing. This initial state is indicated in figure 6 by the solid circles in the lower left of the diagram.

Beam search A typical approach when using sequence-to-sequence systems is to enable beam search, the process of asking for multiple answers to the same question to the network. It is particularly relevant when creating outputs which can be automatically checked [1, 18]. Beam search can be viewed as proposing multiple possible axioms to apply. Given the stochastic nature of generation model, a beam width of n can be thought of as creating the n most likely sequences given the training data the model as learned on. Each proposal can be checked for validity, the first valid one is outputted by the system, demonstrating equivalence. Our system builds on the neural network beam search provided by OpenNMT to create a ‘system beam search’ of variable width. In particular, we set the OpenNMT network beam search to 3, which constrains the token generator to produce 3 possible axiom/node proposals for a given pair of input programs. Using these 3 proposals, when our system beam width is 10, we build up to 10 intermediate programs that are being processed in the search for a proof. To illustrate with a system beam width of 5, after P1 and P2 are provided to the neural network, 3 possible intermediate programs may be created (so long as all axioms are legal and don’t produce duplicates). After those 3 intermediates are processed, 9 possible new intermediates are created, all of which are checked for lexical equivalence with P2, but only 5 of which are fed back into the neural network for further axiom generation. This process is continued for up to 12 axioms at which point the system concludes an equivalence proof cannot be found.
and the programs are likely not equivalent. We evaluate in Sec. 6 beam sizes ranging from 1 to 10, showing higher success with larger beams.

### E Details on Experimental Results

#### E.1 Complementary Results and Observations

Table 10 describes part of our neural network hyperparameter tuning showing that our golden model has as high a result as other variations explored. Note that the validation token accuracy is not too high (it’s not above 90%) despite the ability to predict full correct proofs with over 93% accuracy. This is because the training dataset can have multiple examples of axioms given similar input programs. For example, proving \((a+b)(c+d) = (b+a)(d+c)\) requires commuting the left and right subexpressions. The training dataset could have similar programs which are sometimes transformed first with a right Commute and then a left or vice-versa. Given this data, the network would learn to apply one or the other (it would not get trained to use associativity for these program pairs for example), hence the actual output given may or may not match the validation target axiom. We will discuss this further in section E.2.

#### Training convergence

Since our model trains on axiomatic proofs which may vary in order (allowing 2 or 3 options to be correct and occur in the training set), we see our training and token accuracies plateau below 90% during training for AxiomStep10 as shown in Figure 7. Full testset proof accuracies for beam width 10 exceed 90%, but also plateau along with the training and validation results. This result differs from our WholeProof10 training, which achieves training and validation accuracies above 96% because the expected axiom sequence is more predictable, but as we have seen less generalized.

As another observation on generalization and overfitting, we note that figure 7 shows a slight separation between the training and validation accuracies starting at around iteration 180,000. While the training accuracy rises slowly, validation accuracy plateaus, indicating slight overfitting on the training data. Yet our model continues to slowly increase in quality, with the model snapshot that scores best on both validation and test accuracies occurring at iteration 300,000. This is our golden model, with 93.1% of P1 to P2 proofs accurately found using beam width 10.
Testing simpler models  In addition to the sequence-to-sequence and graph-to-sequence models, we explored a feed-forward equal/not equal classifier on a simple version of our language. That model uses an autoencoder on the program to find an embedding of the program and then a classifier based on the program embeddings found. It achieves a 73% accuracy on identifying equivalent pairs in the test data, which, as expected, is much lower than the full proof rate of 93% achieved with a graph-to-sequence proof generator on our full language. This simple experiment highlights the importance of a system which prevents the false positives which a classifier might have by creating a verifiable proof.

We explore initial language generation using a simple language in order to assess feasibility of different approaches. For fine tuning network parameters and architectural features, we add more complexity to the language as shown in table 11. Language IDs 1 through 3 are all based on a simple grammar which only allows the "+" or "−" operators on scalar variables labeled a through j. The only axiom is Commute, which can be applied on up to 3 nodes in language IDs 2 and 3. Language ID 4 adds the scalar constants 0 and 1, scalar operations "*" and "/", and 4 more axioms. We perform a fair amount of network development on this model in an effort to maintain high accuracy rates. Language ID also 4 expands the operands to 3 types and hence the number of operators also increases. To speed up model evaluation, we reduced the program length for IDs 5, 6, and 7, allowing us to train larger data sets for more epochs. ID 7 is a forward looking-model which makes a minor increment to the language to support the analysis of loop rolling and unrolling, discussed further in section E.3. ID 8 is the WholeProof5 model in relation to these early experiments.

We designed our datasets in section 4 with the goal of using the varied models to understand the generalizability of pe-graph2axiom and to show that our model is not over-fitting on training data. For these next experiments, all results of for beam width 10, which provides for a neural-network directed search of up to 10 axiomatic proofs of equivalence for each program pair. Recall that our most complex dataset is AxiomStep10 which includes (P1, P2, S) samples requiring up to 10 rewrite rules, P1 and P2 can have up to 50 AST nodes each, and an AST depth of up to 7. AxiomStep5 has samples requiring up to 5 rewrite rules, P1 and P2 can have up to 25 AST nodes each, and an AST depth of up to 6. Tables 12 and 13 (repeated from main paper below) demonstrate the ability of a model trained on AxiomStep5 to perform well on the larger distribution of programs from AxiomStep10, implying that the model has generalized well to our program equivalence problem and that pe-graph2axiom does not overfit its response to merely the training set distribution.

Table 13 illustrates the ability of a model trained on AxiomStep5 (i.e., limited to proofs of length 5) to perform well when evaluated on the more complex AxiomStep10, which includes proofs of unseen length of up to 10. The robustness to the input program complexity is illustrated with the 86% pass rate on AST depth 7, for the model trained on AxiomStep5 which never saw programs of depth 7 during training.

As an indication of the breadth of equivalent programs represented by AxiomStep10 relative to WholeProof10, table 14 shows the full detail of models trained on all 4 datasets when tested on test data from all 4 datasets. AxiomStep10, while training on our broadest dataset in which axioms can be applied to nodes repeatedly and in variable order, achieves a 93% average success rate. 72% of the proofs of length 6 from the WholeProof10 testset were solved by the model trained on WholeProof10, but only 5% of such proofs from AxiomStep10 were, suggesting the method of generating AxiomStep pairs covers the problem space more thoroughly.

The complete result for the WholeProof10 model on the WholeProof10 dataset was 8,388 out of 10,000 program pairs had a correct proof found; of those, 8,350 were the exact proof created during P1, P2 generation, implying that WholeProof10, while performing well on its own testset distribution, is not learning to generalize to alternative proof paths.

Manual verifications  We conducted a series of manual verifications of the system used to produce all the above results. First, we are happy to confirm that most likely AB ≠ BA given no verifiable equivalence sequence was produced, but that provably ab = ba indeed. We also verified that

\[ A^T (B + C - C) = AB, \]

and that

\[ AB\bar{u} - AB\bar{w} = AB(\bar{v} - \bar{w}) \]

which would be a much faster implementation. The system correctly suggests that

\[ AB\bar{u} - BA\bar{w} ≠ AB(\bar{v} - \bar{w}). \]

We ensured that

\[ A^T(\text{AA}^T)^{-1}A ≠ A^T(\text{AA}^{-1})^T A, \]

from a typo we once made when typing the computation of an orthonormal sub-space. We also verified that indeed

\[ AB + AC + aD - aD = A(B + C). \]

Generalizing variable types  We explored the ability of the model to understand variable typing by training a model with the AxiomStep10 distribution but with no samples that included the scalar variable 'e' and scalar multiplication '*'. This removed about 50% of the training set, as longer programs were often included both tokens. When tested with the unaltered AxiomStep10 test set and beam width 10, test samples that included a scalar variable not 'e' and...
Table 11. Results for various language complexities studied, on non-incremental models (WholeProof).

Table 12. Generalizing to longer P1 inputs. Percentage pass rates for equivalence proofs with P1 having increasing program graph nodes. The model trained with the AxiomStep5 dataset had no training examples more than 25 program graph nodes yet it performs relatively well on these more complex problems. The furthest right column shows the pe-graph2axiom model results on the most complex dataset.

Table 13. Performance vs. AST size: counts and percentage pass rates.

*$_s$ were proven equal 90% of the time; test samples that included 'e' and *$_s$ were also proven equal 90% of the time. For beam width 1 the proof success rates were 72% and 70% for without and with 'e', implying that the heavily biased
Table 14. Generalizing to longer proofs. Percentage pass rates for equivalence proofs of increasing axiom counts when testing each of 4 datasets on models trained using each of 4 datasets.

| Axiom Count in Proof | Model trained on WholeProof5 (WP5) | Model trained on WholeProof10 (WP10) | Model trained on AxiomStep5 (AS5) | Model trained on AxiomStep10 (AS10) |
|----------------------|-------------------------------------|-------------------------------------|-----------------------------------|-------------------------------------|
|                      | WP5 | WP10 | AS5 | AS10 | WP5 | WP10 | AS5 | AS10 | WP5 | WP10 | AS5 | AS10 | WP5 | WP10 | AS5 | AS10 |
| 1                    | 100 | 100 | 100 | 99   | 100 | 100 | 100 | 100  | 100 | 100 | 100 | 100  | 100 | 100 | 100 | 100  |
| 2                    | 99  | 98  | 66  | 64   | 99  | 98  | 66  | 63   | 100 | 99  | 99  | 99   | 100 | 99  | 99  | 99   |
| 3                    | 98  | 94  | 34  | 33   | 97  | 95  | 33  | 33   | 100 | 98  | 99  | 98   | 100 | 99  | 99  | 99   |
| 4                    | 93  | 84  | 16  | 15   | 90  | 88  | 16  | 15   | 98  | 95  | 98  | 97   | 99  | 98  | 98  | 98   |
| 5                    | 84  | 70  | 8   | 7    | 84  | 82  | 8   | 7    | 96  | 91  | 96  | 95   | 97  | 95  | 96  | 96   |
| 6                    | 14  | 4   | 72  | 5    | 81  | 88  | 90  | 93   |
| 7                    | 0   | 1   | 63  | 2    | 67  | 81  | 83  | 87   |
| 8                    | 0   | 0   | 54  | 1    | 54  | 75  | 73  | 82   |
| 9                    | 0   | 0   | 47  | 0    | 35  | 64  | 63  | 74   |
| 10                   | 0   | 0   | 34  | 0    | 24  | 57  | 46  | 66   |
| All                  | 95  | 66  | 44  | 27   | 94  | 84  | 44  | 27   | 99  | 87  | 99  | 90   | 99  | 93  | 99  | 93   |

The results in table 15 relate to the value of our approach in relation to reinforcement learning models for proof generation [22] [9]. To make an analogy with reinforcement learning, in our training, the world ‘state’ is presented as a P1, P2 pair and the system must learn to produce an axiom at a location which performs an ‘action’ on the ‘state’ of P1 in a predictable way. Unlike reinforcement learning, we do not produce a reward function and our system cannot learn from a poor reward produced by an incorrect axiom. However, we have demonstrated that our system, as it is presented with a wide distribution of (P1, P2, S) tuples to train on, learns a probability distribution of possibly correct axioms to produce for a given program pair. There may be value in combining our graph-neural-network within a reinforcement learning framework that used a hindsight mechanism [6] to learn from every attempted axiom, but it is not immediately obvious that our approach of learning only from examples of successful equivalence proofs would be improved.

Table 15. Learning multiple output options. When considering scalar expressions that can be proven equivalent by commuting the left and right subexpressions, such as \((a+b)(c+d) = (b+a)(d+c)\), pe-graph2axiom learns that either the left or right commute can occur first. The columns show counts for axioms and locations proposed by the token generator with beam width of 3 when given 120 different scalar expression pairs.

| Beam position | Commute left child | Commute right child | Commute root | DistributeLeft root |
|---------------|--------------------|---------------------|--------------|---------------------|
| First         | 49                 | 35                  | 36           | 0                   |
| Second        | 58                 | 59                  | 3            | 0                   |
| Third         | 13                 | 26                  | 45           | 36                  |
| Any of top 3  | 120                | 120                 | 84           | 36                  |
performed several single training run comparisons between 2 options, as shown in Table 16.

In cases where 2 options were similar, we chose the model which ran faster, or run the models a second time to get a more precise evaluation, or use our experience based on prior experiments to select an option.

Table 16. Example explorations as a single feature or parameter is changed. Each comparison is a distinct experiment, as the entire network and language used was being varied.

| Options compared                           | Match beam 1 | Match beam 10 |
|--------------------------------------------|--------------|---------------|
| 1 layer LSTM vs 2 layer LSTM               | 198          | 1380          |
| 2 layer LSTM vs 3 layer LSTM               | 5020         | 9457          |
| 3 layer LSTM                               | 4358         | 8728          |
| No edges to grandchild nodes vs Edges to grandchild nodes | 9244         | 9728          |
| No edges to grandchild nodes vs Edges to grandchild nodes | 9284         | 9774          |
| Encoder->Decoder only root node vs Encoder->Decoder avg all nodes | 8616         | 9472          |
| Encoder->Decoder avg all nodes            | 7828         | 9292          |

Experiments such as these informed our final network architecture. For example, in pe-graph2axiom, we include 4 edges with learnable weight matrices from a node to its grandchildren because such edges were found to improve results on multiple runs. Li et al. [39] discusses the importance of selecting the optimal process for aggregating the graph information hence we explore that issue for our network. Our approach uses the root comparison node to create aggregate the graph information for the decoder as it performs better than a node averaging.

Including Not_equal option Table 17 analyzes the challenge related to a model which only predicts Equal or Not_equal for program pairs along with various options which produce rewrite rules which can be checked for correctness. In all 4 output cases shown, 2 programs are provided as input. These programs use an earlier version of our language model with 16 operators, 13 core axioms, and 20 operands generated with a distribution similar to WholeProof5.

Table 17. Table showing alternate options for handling not equal programs

| Network output Description | Actual | Predicted Rules or Eq | Correct Rewrite Rules |
|----------------------------|--------|-----------------------|-----------------------|
| Eq or NotEq, Beam width 1  | Eq     | 5.4%                  | 94.6%                 | N/A                   |
|                            | NotEq  | 90.4%                 | 9.6%                  | N/A                   |
| Rules or NotEq, Beam width 1 | Eq     | 6.6%                  | 93.4%                 | 70.7%                 |
|                            | NotEq  | 90.9%                 | 9.1%                  | N/A                   |
| Rules only, Beam width 1   | Eq     | N/A                   | 100%                  | 87.8%                 |
|                            | NotEq  | N/A                   | N/A                   | N/A                   |
| Rules only, Beam width 10  | Eq     | N/A                   | 100%                  | 96.2%                 |
|                            | NotEq  | N/A                   | N/A                   | N/A                   |

For the first output case, the output sequence to produce is either Equal or Not_equal. Given a false positive rate of 9.6%, these results demonstrate the importance of producing a verifiable proof of equivalence when using machine learning for automated equivalence checking. For the second output case, the model can produce either Not_equal or a rewrite rule sequence which can be checked for correctness. The source programs for the first and second case are identical: 250,000 equivalent program pairs and 250,000 non-equivalent program pairs. In the second case, the false positive rate from the network is 9.1% (rules predicted for Not_equal programs), but the model only produces correct rewrite rules between actual equivalent programs in 70.7% of the cases.

One challenge with a model that produce rules or Not_equal is that beam widths beyond 1 are less usable. Consider that with a beam width of 1, if the network predicts Not_equal then the checker would conclude the programs are not equal (which is correct for 90.9% of the actually not equal programs). With a beam width of 10, there would be more proposed rewrite rules for equal programs to test with, but if 1 of the 10 proposals is Not_equal, should the checker conclude they are not equal? Or should the the checker only consider the most likely prediction (beam width 1) when checking for non-equivalence? The third and fourth network output cases provide an answer. For these 2 cases, the training set is 400,000 equivalent program pairs - none are non-equivalent. 250,000 of these pairs are identical to the equivalent programs in the first 2 cases, and 150,000 are new but were produced using the same random generation process. Note that by requiring the network to focus only on creating rewrite rules, beam width 1 is able to create correct rewrite rules for 87.8% of the equivalent programs. And now, since we’ve remove the confusion of the Not_equal prediction option, beam width 10 can be used to produce 10 possible rewrite rule sequences and in 96.2% of the cases these rules are correct. Hence, we propose the preferred use model for pe-graph2axiom is to always use the model which is trained for rule generation with beam width 10 and rely on our rule checker to prevent false positives. From the 10 rewrite rule proposals, non-equivalent programs will never have a correct rewrite rule sequence produced, hence we guarantee there are no false positives.

E.3 An Example of Back-Edge in the Program Graph

Figure 8 shows an example of DoX and DoHalf. The new operators result in 2 new edges in our graph representation (along with 2 new back-edges): there is a 'loopbody' edge type from the loop operator node to the start of the subgraph, and there is a 'loopfeedback' edge type from the variable which is written to each loop iteration. These 2 edge types are shown in the figure. The new Dohalf axiom intuitively
states that $\text{DoX}(g(y)) = \text{DoHalf}(g(g(y)))$ (where $y$ is the variable reused each iteration), and $\text{DoX}$ states the reverse.

\begin{figure}[h]
\centering
\begin{subfigure}{0.4\textwidth}
\centering
\begin{tikzpicture}
  \node (a) {$a$} ;
  \node (b) [below right of=a] {$b$} ;
  \node (c) [below left of=a] {$c$} ;
  \node (d) [above of=a] {$a/b$} ;
  \draw (a) -- (b) ;
  \draw (a) -- (c) ;
  \draw (d) -- (a) ;
\end{tikzpicture}
\caption{$\text{DoX}(b) = (a + b)/c$}
\end{subfigure}
\begin{subfigure}{0.4\textwidth}
\centering
\begin{tikzpicture}
  \node (a) {$a$} ;
  \node (b) [below left of=a] {$b$} ;
  \node (c) [above right of=a] {$c$} ;
  \node (d) [above of=a] {$a/c$} ;
  \node (e) [above of=b] {$a/(a+b)/c$} ;
  \draw (a) -- (b) ;
  \draw (a) -- (c) ;
  \draw (d) -- (a) ;
  \draw (e) -- (b) ;
\end{tikzpicture}
\caption{$\text{DoHalf}(b) = (a + (a + b)/c)/c$}
\end{subfigure}
\caption{Adding loop constructs creates cycles in the program graph.}
\end{figure}