Equivalence of Dataflow Graphs via Rewrite Rules
Using a Graph-to-Sequence Neural Model

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Abstract
In this work we target the problem of provably computing the equivalence between two programs represented as dataflow graphs. To this end, we formalize the problem of equivalence between two 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 the first 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 system outputs via inference a correct rewrite sequence for 96% of the 10,000 program pairs isolated for testing, using 30-term programs. And in all cases, the validity of the sequence produced and therefore the provable assertion of program equivalence is computable, in negligible time.

1 Introduction
The problem of program equivalence is summarized as determining whether two programs would always produce the same output for all possible inputs, and is a central problem in computing [19, 27, 48]. The problem ranges from undecidable, e.g. [21], up to trivial in cases of testing the equivalence of a program with itself.

We claim the problem of program equivalence cannot be efficiently mechanized by using a stochastic process to determine the equivalence between two program regions. Precisely, obtaining a binary answer yes/no to equivalence with a certain probability of confidence does not lead to a provable conclusion on equivalence [54]. This is a major limitation to the deployment of machine learning techniques for program equivalence. Such an approach might prove useful for e.g. filtering, to focus via another process on only a subset of likely equivalent programs; but it is not a suitable approach for provably correct automated program equivalence checking as is typically developed, e.g., [3, 28, 36].

To overcome the fundamental stochastic nature of neural networks, we use a very different approach to the problem of machine learning for program equivalence: instead of making the network produce a binary answer to the question of equivalence, we make the network produce a sequence of rewrite terms that make one program strictly equal to the other, if the input programs are equivalent. This way, the output of the network can be deterministically checked in negligible time. We represent programs as graphs, and successively apply the axiom-based graph rewrites produced by the network on one of the input programs, then ensure the resulting graph is identical to the other input graph via a simple simultaneous depth-first visit.

Our neural network approach allows for deterministically proving equivalence, entirely avoids false positives, and quickly invalidates incorrect answers produced by the network (no deterministic answer is provided in this case). 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 programs/-graphs structurally identical without violating their original semantics. We make the following contributions:
• We propose a machine learning system for program equivalence which ensures correctness for all non-equivalent programs input, and a deterministically checkable output for equivalent programs.
• We introduce pe-graph2seq, the first graph-to-sequence neural network system targeting program equivalence to the best of our knowledge. We provide the first implementation of such graph-to-sequence systems in the popular OpenNMT-py framework [29].
• 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 96% of the 10,000 test cases, for a typical inference time of 16ms per pair of programs. 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 formally defines the type of program representation and axioms of equivalence we manipulate in this work, and formalizes the equivalence problem addressed. Automatic sample generation is discussed in Sec. 4 before Sec. 5 which introduces pe-graph2seq, its
overall design principles and key components. A complete experimental evaluation of our system is detailed in Sec. 6. Related work is presented in Sec. 7 before concluding.

2 Motivation and Overview

Input program representation  Figs. 1a–1d show four examples of simple computations. For example, Fig. 1a models the expression $a(1b + 1c)$, one can imagine it to be the result of $a(db + dc)$ after e.g. constant-propagation of 1 to $d$. In the following we call these equivalently programs, sentences from a language, and graphs, the reader needs to be ready to jump between these equivalent representations. They are defined by a single root, have nodes which can be operations consuming the value of their immediate predecessor or terminal/input values, and a node produces a value that can be used by its immediate successors. In essence this is a classical dataflow representation of the computation [14], and what our system uses as input program representation.

Rewrite rules as axioms of equivalence  Consider the programs in Fig. 1a versus Fig. 1b. The multiplication of a value by 1 does not change the value, if we rely on an axiom of equivalence stating $1 * x = x$, $\forall x \in \mathbb{N}$. This axiom specifies a strict criterion of application: the node must be of type $\mathbb{N}$, the expression pattern must be $1 * x$, and a strict rewrite rule: replace a sub-graph $1 * x$ for any $x$ by the graph $x$. In other words, replacing $1 * b$ by $b$ in Fig. 1a is a semantics-preserving rewrite, from the axiom of equivalence. In this work we view the problem of program equivalence as finding a sequence of semantics-preserving rewrites, each from a precisely defined axiom of equivalence, that rewrites one program into the other. If one program can be rewritten by a sequence of individually-correct semantics-preserving transformations into another one, then not only are they equivalent under the set of axioms used, but the sequence forms the constructive and verifiable proof of equivalence.

An example  In this work we illustrate and experimentally evaluate our system using a rich linear algebra expression language because it exposes clearly (and intuitively) the various key concepts that must be handled: (1) operating on dataflow graphs as input, supporting transformations that can (2) delete or (3) create new nodes in the graph, and transformations that (4) manipulate entire subtrees. We also wanted a language with (5) multiple variable types, e.g. scalars, vectors and matrices and (6) a large number of different operators with (7) distinct axioms applicable for each. All of these are captured in the language we experiment with, see Sec. 3 for its formal definition.

When applying the axiom $A1 : 1 * x = x$, $\forall x \in \mathbb{N}$ on the program $P$ in Fig. 1a for its node $b$, we obtain an equivalent and yet syntactically different program, we have $P \equiv A1(b, P)$. Applying the same axiom $A1$ on $c$ in the resulting program leads to program $P'$ in Fig. 1b, and $P' \equiv P \equiv A1(c, A1(b, P))$. Precisely, in graph terms, Fig. 1b is the result of a sequence of two semantics-preserving node deletion operations, as defined in the axiom.

Consider now the axiom $A2 : x * (y + z) = x * y + x * z$, $\forall x, y, z \in \mathbb{N}$. This is the standard distributivity axiom on natural arithmetic. In terms of graph transformations, this is a complex rewrite: a new node is created (+), one node is moved (+ to the root), and edges are significantly modified. When this complex, but semantics-preserving, rewrite is applied to Fig. 1b, we obtain Fig. 1c, that is $P \equiv A2(\ast, A1(c, A1(b, P)))$.

Finally consider the axiom $A3 : x + y = y + x$, $\forall x, y \in \mathbb{N}$, the standard commutativity axiom for +. The graph transformation does not change the number of nodes nor edges, instead only alters two specific edges. Note that as the previous axioms, it also illustrates operations on sub-graphs: indeed $x$ and $y$ do not need to be input/terminal nodes, they can be any subgraph producing a value of the proper type. This is illustrated by applying on Fig. 1c to obtain Fig. 1d, that is the computation $ac + ab$. We have $P \equiv A3(\ast, A2(\ast, A1(c, A1(b, P))))$, a verifiable proof of equivalence under our axioms between the programs $a(1b + 1c)$ 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 $a(1b + 1c)$ to $ac + ab$, or the converse using the same (but reverted) sequence. Note also the non-unicity of a sequence: by possibly many ways a program can be rewritten into another one, for example the sequence $P \equiv A3(\ast, A1(c, A1(b, A2(\ast, P)))$ also correctly rewrites Fig. 1a into Fig. 1d. Conversely, a sequence may not exist: for example no sequence of the 3 above axioms allow to rewrite $a + b$ into $a * b$. 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.
The need for a verifiable procedure  A key motivation of our work is to enable in a safe and provably correct way the use of machine learning for program equivalence. For full automation of the process, we focus on ensuring correctness in case an equivalence result is computed by the system. That is, our system by design answers only with a probability of confidence that the two programs are not equivalent, but it produces a verifiable procedure to assess equivalence otherwise. We believe such an approach is key for a practical, automated deployment of neural networks for program equivalence: verifiably proving equivalence to ensure no false positive, while tolerating a moderate amount of false negative (i.e., missing that two programs were in fact equivalent).

Numerous practical applications of the kind of system we develop exist, even on the linear algebra language we demonstrate on: for example the automatic correction of exercises for students, where they typically need to prove equivalence between two formulas by successive application of other formulas/axioms. Languages like e.g. Matlab could use interactive checking of the equivalence between the expression being typed and the pre-existing library implementations (e.g., BLAS-based [22]) to use instead accelerated implementations when possible in real-time. But we have designed and evaluated our system in a robust enough way to be applicable to a wide variety of languages and problems, as long as they can be cast in the framework in Sec. 3. We discuss other uses cases and applications in Sec. 6.

The space of equivalences  Intuitively, our approach to program equivalence is as follows. We can intellectually reason on a graph for equivalent programs where each node represents a distinct program in the language, and two nodes (i.e., two different programs) are connected by a directed edge iff the source node can be rewritten as the target node by the application of a single one of the pre-defined axioms for equivalence. The edge is labeled by the axiom used and the specific position in the source node’s program to which it needs to be applied to obtain the program in the target node. Then there will be one or more paths in this graph from the two nodes modeling the two input programs if they are equivalent (one can be rewritten into the other while preserving semantics); and no path if no such rewrite is possible, that is the programs would be not equivalent in our framework. Exposing a path between two nodes is sufficient to prove the equivalence of their associated programs.

This path is exactly a sequence of rewrite rules from one program to another. To test the correctness of an arbitrary sequence, i.e., verify if this path exists in the graph and assess equivalence if it does, one then needs to simply apply the proposed sequence to one of the input programs: verify at each step that the rewrite in the sequence is indeed applicable (by a simple check of the applicability of the axiom at this particular program point), and eventually ensure the rewritten program is identical to the other input one. This test can be computed in time mostly linear with the program size in our framework, and when successful it implements a constructive proof of equivalence between the two programs.

Pathfinding equivalence proofs  When formulating the program equivalence problem this way, we can then view its solution as learning how to build at least one feasible path between any two pairs of nodes in the above graph, when it can exist. We can see that by design, there is a lot of redundancy in this space: the same labeled path will occur between many different pairs of programs (e.g., those where only the variable symbols differ), and there are typically many paths between the same two (equivalent) programs. This creates opportunities for the system to learn program representation and path construction techniques more easily.

Our key contribution is the development of a deep learning framework that learns this procedure automatically. The neural network system we build is trained by randomly sampling this graph, with samples made of two nodes and a path between them when training on equivalent programs, and an empty path otherwise. We specifically learn a generalization of the problem of finding paths in this graph as follows. We represent input programs in a carefully-crafted normalized dataflow-like graph encoded as a gated graph neural network [11, 44], to enable structural, size-tolerant reasoning by the network on the inputs. It is combined with a global attention-based mechanism and a memory-based LSTM [24] decoder which can memorize graph changes for producing the rewrite sequence and enable path-size tolerant reasoning, while following the properties of the axioms for equivalence.

In a nutshell, we make the network learn a stochastic approximation of an iterative algorithm that would be able to construct a feasible path (when possible) between any two pairs of nodes in this equivalence graph, but trained simply by randomly sampling pairs of nodes and one carefully labeled path between them. This avoids entirely the need to craft smart exploration heuristics to make this path-finding problem feasible in practice. This is instead what we let the neural network learn automatically; and specifically why we implemented graph neural networks to solve this problem [44, 54]. We rely on the network to suggest a transformation path by inference, and then verify its validity in linear time.

System overview  In order to implement our approach, we need a simple-enough grammar for a language, in which we enumerate randomly valid sentences, and a set of axioms of equivalence between two sentential forms expressible as semantics-preserving rewrite rules from one to the other. The system takes as input two programs (i.e., sentences accepted by the language), and produces an ordered sequence of axioms along with their position of application (or node) that can be used to rewrite sequentially one input program into the other input program. This sequence is then checked for correctness using the axioms as reference. To train the
system, we generate pairs of equivalent programs by iterating the axioms with random probability on one program, thereby generating both a path to equivalence and the target program. Random programs are generated so as to respect the grammar defined. The training set is then appropriately selected from these random samples, as detailed in Sec. 6.

When the system outputs that two programs are equivalent, as provable reasoning (the rewrite sequence) is always produced, no false positive can ever occur. When the system fails to demonstrate equivalence, no provable conclusion is produced regarding the input programs however: we are left with only a (high) probability of non-equivalence.

A key of our approach is to introduce graph-to-sequence neural networks to quickly compute one or more possible rewrite sequences. The details of the network are covered in Sec. 5. In a nutshell, the key principle is to combine a memory-based neural network approach, e.g., using Long-Short Term Memory (LSTM) [24] neurons and a graph neural network design (which uses Gated Recurrent Units (GRUs) internally) [11] that matches our program graph representation. We use a sequence generation principle, using an attention mechanism to allow observation of program graph node information while generating the rewrite sequence. This enables the production of the rewrite sequence token-by-token, matching our axiom of equivalence design principle.

As presented in Sec. 5, we designed an efficient embedding of the program equivalence problem into a graph neural network (Node initialization) to facilitate the network’s ability to walk the program graphs and memorize structural changes being made by applying the axioms. To the best of our knowledge, this is the first graph-to-sequence system for program equivalence, which outputs verifiable proofs. Our system is fully implemented end-to-end in OpenNMT-py and is ready for artifact evaluation. As detailed in Sec. 4 we developed a very rigorous evaluation (test) set to ensure our system has developed some intelligence, which is fully confirmed in Sec. 6. As an extreme case, even if we would make a system that each time two programs are checked for equivalence, produces systematically all possible distinct rewrite sequences it has ever seen during training (up to 118k in our experiments), and we check all of these outputs for correctness and applicability for the input programs, this would still not exceed 60% of correct test cases for equivalent programs tested. We report a steady 95% or more using only a beam size of 10, that is asking the network to output only the 10 most likely rewrite sequences for the input programs.

3 Framework for Program Equivalence

We now present the formalism we use in this work to represent programs 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.

3.1 Program Representation

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. In particular, we do not restrict to tree-like structures nor acyclic graphs, as briefly discussed in Sec. 6.4.

Definition 3.1 (Program graph node). A node \( n \in N \) in the program 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 \( n_{\text{root}} \) of the graph, the only node without successor.

Definition 3.2 (Program 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 program graph connects the producer of a value \( (n_1) \) to a node consuming this value in the computation.

Definition 3.3 (Program graph). A program 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, \( G = (n_{\text{root}}, N, E) \). 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 program: scalars, vectors and matrices. We use the standard notation $a, \bar{a}, A$ 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 $*, /, +, -$ between scalar operands, and $\times, -$ between vectors and $+m, -m, *m$ for matrices. For $/,$ we also support their unary version for all types, e.g. $1/,$ for unary scalar inversion and $-um$ for unary matrix negation. For example $a^{-1 \times}$ computes to $1/a$. We also support multi-type operations, such as vector and matrix scaling by a scalar $s_m, s_m$. We support two specific unary matrix operations, transpose $t_m$ and matrix inversion as $-t_m$. Note every operator has a unique name in our language, driven by the type of its operand. This will facilitate the learning of the program embedding, avoiding the need to learn type propagation.

**Examples** Programs of the form $A(BCD)E^{-1}, \bar{a} + \bar{c}e^{-1} - 0e, (a + b) + (c(d/e)), (aA + bB)C^2$ 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 program 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 program 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 program 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 program 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 program graph $G$. We have $P = \langle G_P, M_a, M_e \rangle$ where for each node $n_i \in N^{G_P}$, $\{n\text{match}\} = M_a(n_i)$ returns the set of node values $n\text{match}$ 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 $M(n_i)$ and $M(n_j)$ to be matched in $G$. A pattern $G_P$ is matched in $G$ if (a) $\forall n_i \in G_P, \exists n_m = M(n_i) \in N^G$; (b) $\forall e_i \in E^{G_P}, \exists e_{M_a(n_i), M_a(n_j)} = M_e(n_i, n_j) \in E^G$; and (c) $\exists e_{M_a(n_i), M_a(n_j)} \in E^G \neq M_e(n_i, n_j)$.

Note when a graph pattern models a rewrite, $M_a$ and $M_e$ are adjusted accordingly to output the rewrite of a node $n \in N^G$ 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 program graph $G$, and produces another program graph $G'$ respecting Def. 3.3 with identical semantics to $G$. We note $A = \langle P\text{match}, P\text{replace} \rangle$ an axiom, where $P\text{match}, P\text{replace}$ 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 $G_i = A_i(n_i, G_i) \in S, P_{A_i}^{\text{match}}$ succeeds on the sub-graph with root $n_i$ in $G_i$, and $G_j$ is obtained by applying $P_{A_i}^{\text{replace}}$ to $n_i$.

**Theorem 3.7** (Program graph equivalence). Given a program $G$. 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** (Program graphs equivalence matching). Given two programs $G, G'$. If there exist a semantics-preserving sequence $S$ such that $G' = S(G)$, then $G \equiv G'$.

Note here $=$ means complete structural equivalence between the two graphs: they are identical in structure and label/node values. Determining $G \equiv G'$ 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 4. 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 $x(yz) \rightarrow (xy)z$, $X - X \rightarrow O$, $-(\bar{x} - \bar{y}) \rightarrow \bar{y} - \bar{x}$, or $X^T \rightarrow X$, 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 rewritings using axioms presented in later Table 4. Note axiom names follow the structural changes applied. For example, we have $a + b \equiv b + a : \{a + b\} = \text{Commute}(+, \{b + a\})$. $a + b + c \equiv b + c + a : \{a + b + c\} = \text{Commute}(+, \text{Commute}((+), \{b + c + a\}))$. Note we refer to different nodes with the same symbol (e.g., $+$) subscripting them by their order in a DFS traversal of the program graph, starting from the unique root. We have $0 \equiv a - a : \{0\} = \text{Cancel}((-), \{a - a\})$. These can be combined in complex paths, e.g., $b + c \equiv x + b + (a - a) : \{b + c\} = \text{Commute}(+, \text{Noop}(+, \text{Cancel}((-), \{c + b + (a - a)\})))$. 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 $\mathcal{L}$. The directed graph of equivalences between programs is $G^{\text{equiv}} = (N^{\text{equiv}}, E^{\text{equiv}})$ such that $\forall l \in \mathcal{L}, n_l \in N^{\text{equiv}}$, and $\forall l, l' \in \mathcal{L}, n_l \rightarrow n_{l'} \in E^{\text{equiv}}$ iff $n_j \equiv A_i(x, n_i), \forall A_i$ 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 program in the language $\mathcal{L}$, 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** (Program equivalence with pathfinding). Given two programs $n_i, n_j \in N^{\text{equiv}}$. If there is any path from $n_i$ to $n_j$ in $G^{\text{equiv}}$, then $n_i \equiv n_j$.

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 programs. As it is a multigraph, there will be possibly many different sequences modeled to prove the equivalence between two programs. 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 programs, described by the sequence of axioms and program 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 programs and folding equivalent paths between nodes. When building e.g. a deterministic algorithm for pathfinding, such space size reduction would bring complexity benefits [9, 27]. 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.
The leaves obtained will form a sentence accepted by the language, i.e., a program [13].

In particular, we skew the pseudo-random generation so that (1) binary operations are more likely to be created than unary operations, and (2) 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 91%. The algorithm then subtracts a 23% probability for children at each level of the graph, so that the path length from the root to any leaf does not exceed 6. Note these probabilities and algorithm have been computed to match the size restrictions for our system evaluated in Sec. 6: handle programs with 30 nodes maximum, and sequences made of 5 axiom applications maximum.

We produce equivalent program samples by iterating pseudo-randomly the axioms on one randomly generated program to produce a rewrite sequence and the associated equivalent program. The process iterates through all nodes of a program graph, and at each node checks which axiom(s) can be applied. E.g., the \(+_o\) 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-graph2seq 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.

### 4.2 Final Experimental Dataset

After these generation algorithms are run, a final data preparation phase is done to prune the dataset for the learning phase. Any lexically equivalent program pair (if any) is removed. Importantly, we remove some cases with only 1 or 2 axioms being used once, to slightly bias the dataset to longer rewrite sequences. We also ensured a reasonable statistical distribution of the use of the various axioms.

| Rewrite Rule          | Example(s) | Samples using rule |
|-----------------------|------------|--------------------|
| Cancel                | (A \cdot A) \rightarrow O, (b/b) \rightarrow 1 | 13.0% |
| Noop                  | (v \cdot o) \rightarrow v          | 29.2% |
| Double                | A'' \rightarrow A, 1/1/x \rightarrow x       | 7.5%  |
| Commute               | (a + b) \rightarrow (b + a)        | 29.5% |
| DistributeLeft        | (a + b)c \rightarrow ac + bc        | 28.0% |
| DistributeRight       | a(b + c) \rightarrow ab + ac        | 19.6% |
| FactorLeft            | ab + ac \rightarrow a(b+c)         | 2.1%  |
| FactorRight           | ac + bc \rightarrow (a+b)c         | 3.1%  |
| AssociativeLeft       | a(bc) \rightarrow (ab)c           | 16.6% |
| AssociativeRight      | (ab)c \rightarrow a(bc)         | 16.2% |
| FlipLeft              | -(v \cdot w) \rightarrow w-v       | 9.7%  |
| FlipRight             | a/(b/c) \rightarrow a(c/b)        | 23.2% |
| Transpose             | (AB)^T \rightarrow B^2A^2         | 10.1% |

Table 1. Distribution of the set of 13 rewrite rule types in the final dataset. The totals add to more than 100% since a single program pair can require multiple rewrite rules for equivalence proof. In total, 102 axioms are used, when considering different data types and operators.

5 Deep Neural Networks for Program Equivalence

Prior work explored using graph neural networks (GNNs [33]) to find a program embedding usable for machine learning, e.g., [5]. GNNs for binary code equivalence checking, e.g., [54], as well as using a graph-to-sequence model with attention to analyze and generate human language, e.g., [11]. But to the best of our knowledge, our work is the first to use a graph-to-sequence approach to generate a verifiable rewrite rule sequence which proves two program graphs are equivalent. In this section we discuss the implementation details of these components.

5.1 pe-graph2seq Deep Neural Network

Fig. 2 overviews the entire system architecture including sample generation, the pe-graph2seq network, and the rewrite checker. Key design decisions are presented below.

**System components** The system in Fig. 2 is composed of the following blocks. **Node initialization** is the process in which the program graph is used to initialize the data structures used by the neural network with correct values, it is a direct procedure which sets up the network.

**Graph neural network** refers to a neural network that has weights which allow it to learn interrelations between network nodes based on edge connections for the problem set it is trained on.

**Global attention** [35] when used with a graph neural network allows the decoder to pay attention to certain nodes in the graph as it creates each token in the output sequence. For example, a node associated with scalar multiply might get extra attention when deciding that the axiom to apply is commutation.

**Token embedding** is a neural network layer in which tokens are assigned a learnable multidimensional embedding vector [37] which can then be processed by other neural network components.

**LSTM 2 layers** is referring to 2 layers of Long Short Term Memory (LSTM) neurons, each layer can have hundreds of neurons. An LSTM has 'long' memory in the sense that weights which define its behavior are learned from the training data so it has a long memory regarding all the training data it has seen. It has a 'short' memory in the sense that it is a recurrent neural network unit which can change state as the network processes output tokens. As such, a given
LSTM cell could change state when the Commute token is output so that the Commute axiom is not repeated.

**Token generator** is the final output portion of the network. It learns to output the correct token based on the current LSTM hidden states and the global attention from the graph neural network. As each token is output, it feeds back into the LSTM layer through the embedding layer to affect the next state of the LSTM.

**Graph neural network internal representation** The sample generation discussed in section A.1 provides input to the **Node Initialization** module in Fig. 2 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 floating point values which are used to create an embedding for the full meaning of the given node. Initially all of the 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 node in Fig. ?? would be initialized to 1.0. This is a one-hot encoding similar to that used in neural machine translation models [??]. 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 \( N + \text{depth} \) to 1.0; hence, the a node in Fig. ??, which is at level 2 in the graph, would set dimension \( N + 2 \) 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 grandchilden (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 3 by the solid circles in the lower left of the diagram.

The combination of the root node type and the edges connecting it to programs 1 and 2 allow the network to learn weights which allow the graph neural network to ’walk’ information from the graph of program 1 through the root node to the graph of program 2 as it creates the node embeddings necessary for rewrite rule generation. This is a novel feature of our network not used in prior work with GNNs on program analysis [5, 54].

**Graph neural network processing** After initialization, the graph neural network iterates in order to convert the initial node state into the embeddings needed for rewrite rule generation. For our problem size, we iterate the GNN 10 times. This process is shown in figure 3 with the dotted circles starting with the initial state on the bottom left and rising to the final state before input to the LSTM-based decoder. 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 \( l_{\text{in}[n]} \) of edges entering node \( n \), the edge types \( l_{\text{out}[n]} \) of edges exiting node \( n \), and the hidden states \( x_{\text{ne}[n]} \) of the neighbors of node \( n \):

\[
x_n(t + 1) = f(x_n(t), l_{\text{in}[n]}, x_{\text{ne}[n]}(t), l_{\text{out}[n]})
\]

Each of the edge types has a different weight matrix for learning, allowing aggregation of information into a given node related to its position and function in the full graph of the program. The root node initial state along with the special edge types connecting it to the graph trees of the programs are able to learn specific information regarding rewrite rules as demonstrated by our experimental results.

**Graph neural network output to decoder** Fig. 3 shows two ways that the final node values for the graph are used by the decoder to create the rewrite rules. First, the final root node value \( x_{\text{root}} \) is fed through a learnable bridge function to initialize the 2 layer LSTM of the decoder network. In this way, the aggregated information of the 2 programs seeds the generation of the rewrite rules. The LSTM layer updates 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 \( y_{j-1} \) [16]. Second, all nodes in the graph can be used by a learnable attention layer [7]. 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 \( P(y_j) \):

\[
P(y_j \mid y_{j-1}, y_{j-2}, ..., y_0, c_j) = g(h^d_j, y_{j-1}, c_j)
\]
the rewrite rule generation (i.e., after initialization of the decoder).

![Graph-to-sequence neural network data flow details.](image)

**Figure 3.** Graph-to-sequence neural network data flow details.

**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 [2, 16]. Beam search can be viewed as proposing multiple possible paths/rewrite sequences. 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. If no sequence is valid, the system answers the programs are likely not equivalent. We evaluate in Sec. 6 beam sizes ranging from 1 to 10, showing higher success with larger beams.

**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.

**6.1 Implementation Setup**

**System implementation** We developed the entire system presented in the OpenNMT-py system [29], adding on an available prior implementation of gated graph neural networks [33]. Specifically, we developed a general graph neural network encoder within OpenNMT-py, as well as our program graph initialization procedure.

For our training and evaluation experiments, we use systems with Intel Xeon 3.6GHz CPUs and 6GB GeForce GTX 1060 GPUs. OpenNMT-py supports automatic CUDA acceleration of training and inference for our system.

**Training, validation and test sets creation** For evaluation of our system, we generate sample programs pairs and rewrite rule sequences as discussed in Sec. 4. For the initial evaluations, we generate 100,000 total unique samples, separated into 80,000 cases for training, 10,000 for validation of the model during the training process, and 10,000 cases withheld for testing of the selected model. As every tuple $(P_1, P_2, S)$ in the main dataset is unique, i.e., there is never twice the same pair of programs with the same rewrite sequence, the test set cannot intersect with the training set.

We ensured numerous stringent properties on our test set. >99.5% of the test set cases use at least one input program that does not appear in the training set. 69.07% of the test set use a rewrite rule sequence that appears in the training set: we ensured about 30% of the ground truth rewrite sequences in the test set do not even occur in the training set. This proportion has been selected to ensure we verify the system has learned how to reason on programs (e.g., two different pairs of programs may use the same rewrite rule, e.g. $(a + b, b + a)$ and $(c + d, d + c)$, we verify this generalization is learned); and to verify the system can compute new paths/sequences (showing generalization of the concept of incremental application of axioms).

Note that there are 118,278 unique RW sequences in the training data, so, as an example, if we allowed a beam search size of 118,278 instead of 10, and if the network learned to naively output all 118,278 RW sequences from the training data it would fail on 50.93% of the test data, well below our 95.5% score. Clearly the network is adding intelligence to the problem.

For our more complex language evaluations, we maintain 10,000 cases for the validation and test sets, but increase the training cases to as many as 500,000, which approaches the memory limits of the systems we train on.

**Training procedure and parameters** Our initial investigations with small models are done with 50,000 epochs and a batch size of 32. Hence, when training with 80,000 training samples each sample is trained on 20 times. Our full language trains 400,000 samples for 250,000 epochs on a batch size of 32, hence again each is trained on 20 times. During training, the majority of our testing runs the validation set on the model every 10,000 epochs and saves a model for test data processing every 50,000 epochs. Although we used a validation set for tracking the evolution of the learning quality, we did not use early stopping criteria.

**Evaluation procedure** Our evaluation consists of multiple scoring methods. As a model is learning proper matrix weights during training on the training samples, we track the typical current per-token prediction accuracy as the model learns to predict the correct rewrite rule sequences (optionally including the Not_equal token). Similarly, when the validation is evaluated, the token accuracy for the predicted outputs is reported.

However for our test dataset evaluation, we instead of course report the accuracy of the model to output a correct rewrite sequence with beam sizes of 1, 2, 5, or 10. When testing, a ground truth sequence between the two programs is
available. The model may or may not produce a sequence that matches exactly this test sample ground truth sequence. We call it a match when the model produced the ground truth, and a correct sequence when it is a verified correct proof, even when it does not match the ground truth.

6.2 Language Complexity and Performance
As discussed in later Sec. 6.3, we iterated numerous possible designs and approaches to figure out the best-working system for this network. In particular, we evaluated simpler approaches before reaching the complexity of our final design, to ensure a more complex approach was needed.

Table 2 shows the result of 12 different experiments and designs. 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 reach 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 \(<<1\)ms.

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 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 contrasted: 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.

Our best result (golden model) with the full language has 9545/10000 exact matches with beam width 10, and 9623/10000 correct proofs of equivalence (i.e., 78 of the 455 cases without an exact match still have a legal rewrite rule sequence produced).

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 \(AB \neq BA\) given no verifiable equivalence sequence was produced, but that provably \(ab = ba\) indeed. We also verified that \(A^n(B + C - C) = AB\), and that \(AB\bar{a} - AB\bar{w} = A\bar{b} - A\bar{w}\) which would be a much faster implementation. The system correctly suggests that \(AB\bar{a} - BA\bar{w} \neq A\bar{b} - A\bar{w}\). We ensured that \(A'(AA)^{-1}A \neq A'(AA^{-1})A\), from a typo we once made when typing the computation of an orthonormal sub-space. We also verified that indeed \(AB + AC + aD - aD = A(B + C)\).

In essence, the network has learned each axiom, its valid applicability criteria, and how to sequence them to form a complex rewrite; being trained only from simple pairs of random programs and a sequence describing a labeled path between them in the equivalence space. It learned a generalization of programs, and in particular how to associate tokens for operators to specific axioms whichever their position in the input program. It has also learned how to find a short path in the equivalence graph to build a valid rewrite sequence between the two input programs provided, probably the hardest task of all.

6.3 Additional Results
In order to design the system, we explored parts of the design space quickly and performed several single training run comparisons between 2 options. Numerous results are reported in Suppl. material B, in Table 3. They were influential on our final system design. In many cases one model was clearly better than the alternative, driving our design choices.

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 the test data, which, as expected, is much lower than the accuracy rates of 92.4% with a graph-to-sequence based classifier on our full language. It also does not produce any verifiable output, contrary to our system.
Table 2. Description and results for various language complexities studied.

| ID   | Description                                                                 | # Operators | # Axioms | # Operands | Program length | Rewrite rules length | Graph2seq (G2S) or seq2seq (S2S) | 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          | 1-5                  | S2S                              | 80,000           | 90.0%                           | 96.2%                           |
| 2    | Rewrite sequence is exactly 2 Commutes, uses sequence-to-sequence model      | 2           | 1         | 10         | 5-24          | 3-10                 | S2S                              | 80,000           | 80.3%                           | 96.5%                           |
| 3    | Rewrite sequence exactly 2 Commutes                                         | 2           | 1         | 10         | 5-24          | 3-10                 | G2S                              | 80,000           | 98.9%                           | 99.8%                           |
| 4    | Rewrite sequence exactly 3 Commutes                                         | 2           | 1         | 10         | 7-45          | 5-15                 | G2S                              | 80,000           | 91.4%                           | 99.0%                           |
| 5    | Rewrite sequence 1 to 3 Commutes                                            | 2           | 1         | 10         | 3-45          | 1-15                 | G2S                              | 180,000          | 97.1%                           | 99.2%                           |
| 7    | Commute, Noop, Cancel, Distribute Left, Distribute Right                    | 4           | 5         | 12         | 3-45          | 1-15                 | G2S                              | 180,000          | 93.1%                           | 97.4%                           |
| 8    | Scalars, Vectors, and Matrices                                              | 16          | 5         | 20         | 3-30          | 1-25                 | G2S                              | 250,000          | 88.3%                           | 95.6%                           |
| 9    | 13 Axioms                                                                    | 16          | 13        | 20         | 3-30          | 1-25                 | G2S                              | 400,000          | 85.5%                           | 95.5%                           |
| 10   | Rewrite sequence or Not_equal                                                | 16          | 13        | 20         | 3-30          | 1-25                 | G2S                              | 500,000          | 79.8%                           | 93.8%                           |
| 11   | Test sequence-to-sequence                                                   | 16          | 13        | 20         | 3-30          | 1-25                 | S2S                              | 400,000          | 59.8%                           | 81.1%                           |
| 12   | Add loop axioms                                                              | 18          | 15        | 20         | 3-30          | 1-25                 | G2S                              | 400,000          | 83.8%                           | 94.7%                           |

**Evolution of learning quality** Fig. 4 is for a model trained on 250,000 samples from our full language to generate rewrite rule sequences. The highest test accuracy on beam width 10 is 93.78%, with the model from iteration 150K. As shown in the figure, the training accuracy continues to increase even as the validation and test accuracies plateau. In order to address this, our final model trains on 400,000 training samples (near the disk space limit available for our testing). That model achieved a test accuracy of 95.45%.

**Figure 4.** Results for network training for rewrite rule generation on 250,000 training samples. The training and validation accuracy are per token of the rewrite sequence; the test accuracy is the score for accurately generating the full sequence with various beam widths.

**6.4 Extensions and Discussions**

**Complex control-flow graph** Given the apparent robustness of our approach to increasingly complex search spaces, we conducted a preliminary study with a node that introduces a cycle in the graph: a loop node (i.e., a back-edge from a node to a leaf). In Table 2, row 12 displays the results. The 2 new operators are used in Fig. 6 in Suppl. material. The ‘DoX’ operator will execute the subgraph some number of times X. The ‘DoHalf’ operator will execute the subgraph half of X times. Such nodes would model recursive domain decomposition for example, however we restrained from inserting the concept of loop and loop iterators in the language.

The new operator results 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 DoX(g(y)) = DoHalf(g(g(y))) (where y is the variable reused each iteration), and Dox states the reverse. In the results for ID12, 1,412 of the 10,000 test cases involve a loop axiom in the ground truth rewrite rules. Of those cases, 1,351 are matched by the trained network (95.7%). Additional developments and experiments are needed to ensure we can efficiently manipulate large, complex control-flow graphs, but these results are particularly encouraging.

**Discussions** We have specifically designed our system and its evaluation on a rich language that captures structural changes and properties of a large variety of problems, by
modeling input programs as a specific dataflow-like graph. Our results suggest the applicability of this approach to a wide range of problems that can be modeled as finding an (axiom-based) rewrite sequence from one graph to another, a general problem of which program equivalence is only an instance. We evaluated complex graphs including ones containing cycles, however we recall we limited the input graphs to 30 nodes maximum, for the system to complete training in reasonable time. Increasing massively the input program size, e.g., to thousands of nodes, would require larger graph networks to accommodate them, and this puts high stress on the scalability of the training procedure.

Progresses in deep learning frameworks implementation, and/or using other popular systems such as TensorFlow+XLA [1] could possibly significantly accelerate the training time of our experiments and allow the handling of larger problems. Note we did not do any specific effort to optimize the training time in our system.

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 [12] which supports the formal framework for equivalence we describe in this paper, to (Approximate Probabilistic) Model Checking [15, 18, 23], where a program equivalence system can also be built, e.g. [17, 39, 45, 51]. Our contribution is not in the formal definition of program equivalence we presented, semantics-preserving rewrite systems have been studied, e.g. [34, 43, 50]. 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. [20, 23, 38]. 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.

Static program equivalence Algorithms for static program equivalence have been developed, e.g. [3, 9, 25, 49]. These approaches typically restrict to demonstrating the equivalence of different schedules of the operations, possibly dynamically [8]. In this work we target graph-modifying rewrites (and therefore which alter the operation count). Barthou et al. [3, 9] 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 [28]. Mansky and Gunter used the TRANS language [26] to represent transformations. The correctness proof implemented in the verification framework [36] is verified by the Isabelle [41] proof assistant. Other works also include translation validation [30, 40].

Program analysis with machine learning Numerous prior work has employed (deep) machine learning for program analysis, e.g. [4, 6, 10, 31, 42, 47]. code2vec [6] teaches a method for creating a useful embedding vector that summarizes the semantic meaning of a snippet of code. Program repair approaches, e.g. [16, 47] 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. [52] learns to extract the rules for Tomita grammars [46] 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 [44, 53] 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 [11]. 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 [5]. Their work achieves 84% accuracy on correcting variable misuse cases and provides insights to useful edge types. Structure2vec [54] uses a graph neural network to detect binary code similarity. Structure2vec uses a graph neural network to learn an embedding from a 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 [32] 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-graph2seq, the first graph-to-sequence neural network system generating quickly verifiable program equivalence proofs. Evaluated on a rich language for linear algebra expressions, our system outputs
proofs when input programs are equivalent which are verified correct in 96% of cases. In addition, the system always outputs non-equivalence for non-equivalent programs by design.

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. We demonstrated our approach on a carefully crafted linear algebra language, to expose clearly the various difficulties the system overcame, such as node deletion or subtree manipulation. We believe this has laid the foundations on how to build such deep learning systems for program equivalence in other languages.

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References

[1] Martin Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, et al. 2016. Tensorflow: Large-scale machine learning on heterogeneous distributed systems. arXiv preprint arXiv:1603.04467 (2016).

[2] Umair Z Ahmed, Pawan Kumar, Amey Karkare, Purushottam Kar, and Sumit Gulwani. 2018. Compilation error repair: for the student programs, from the student programs. In Proceedings of the 40th International Conference on Software Engineering: Software Engineering Education and Training. ACM, 78–87.

[3] Christophe Alias and Denis Barthou. 2004. On the recognition of algorithm templates. Electronic Notes in Theoretical Computer Science 82, 2 (2004), 395–409.

[4] Miltiadis Allamanis, Earl T. Barr, Premkumar Devanbu, and Charles Sutton. 2018. A Survey of Machine Learning for Big Code and Naturalness. ACM Comput. Surv. 51, 4, Article 81 (July 2018), 37 pages. https://doi.org/10.1145/3212695

[5] Miltiadis Allamanis, Marc Brockschmidt, and Mahmoud Khademi. 2018. Learning to Represent Programs with Graphs. In 6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 - May 3, 2018, Conference Track Proceedings. https://openreview.net/forum?id=BJOFETxR-

[6] Uri Alon, Meital Zilberstein, Omer Levy, and Eran Yahav. 2019. Code2Vec: Learning Distributed Representations of Code. Proc. ACM Program. Lang. 3, POPL, Article 40 (Jan. 2019), 29 pages. https://doi.org/10.1145/3290353

[7] Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. 2014. Neural machine translation by jointly learning to align and translate. arXiv preprint arXiv:1409.0473 (2014).

[8] Wenlei Bao, Sriram Krishnamoorthi, Louis-Noël Pouchet, Fabrice Rastello, and Ponnuswamy Sadayappan. 2016. Polychexam: Dynamic verification of iteration space transformations on affine programs. In ACM SIGPLAN Notices, Vol. 51. ACM, 539–554.

[9] Denis Barthou, Paul Feautrier, and Xavier Redon. 2002. On the equivalence of two systems of affine recurrence equations. In Euro-Par 2002 Parallel Processing.

[10] Rohan Bavishi, Michael Pradel, and Koushik Sen. 2017. Context2Name: A Deep Learning-Based Approach to Infer Natural Variable Names from Usage Contexts. http://tubiblio.ulb.tu-darmstadt.de/101419/

[11] Daniel Beck, Gholamreza Haffari, and Trevor Cohn. 2018. Graph-to-Sequence Learning using Gated Graph Neural Networks. In Proceedings of the 56th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers). Association for Computational Linguistics, 273–283. http://aclweb.org/anthology/P18-1026

[12] Yves Bertot and Pierre Castéran. 2013. Interactive theorem proving and program development: Coq’Art: the calculus of inductive constructions. Springer Science & Business Media.

[13] Pavel Bielik, Veselin Raychev, and Martin Vechte. 2016. PHOG: Probabilistic Model for Code. In Proceedings of The 33rd International Conference on Machine Learning (Proceedings of Machine Learning Research), Maria Florina Balcan and Qian Lin (Eds.), Vol. 48. PMLR, New York, New York, USA, 2933–2942. http://proceedings.mlr.press/v48/bielik16.pdf

[14] Joseph Tobin Buck and Edward A Lee. 1993. Scheduling dynamic datagraphs with bounded memory using the token flow model. In 1993 IEEE international conference on acoustics, speech, and signal processing, Vol. 1. IEEE, 429–432.

[15] Jerry R Burch, Edmund M Clarke, Kenneth L McMillan, David L Dill, and Lain-Junn Hwang. 1992. Symbolic model checking: 1020 states and beyond. Information and computation 98, 2 (1992), 142–170.

[16] Zimin Chen, Steve Komnarchus, Michele Tufano, Louis-Noel Pouchet, Denis Poshyvanyk, and Martin Monperrus. 2019. SequenceR: Sequence-to-Sequence Learning for End-to-End Program Repair. IEEE Transactions on Software Engineering (2019). https://doi.org/10.1109/TSE.2019.2940179

[17] Edmund Clarke, Daniel Kroening, and Karen Voray. 2003. Behavioral consistency of C and Verilog programs using bounded model checking. In Proceedings 2003. Design Automation Conference (IEEE Cat. No. 03CH37451). IEEE, 368–371.

[18] Edmund M Clarke, Orna Grumberg, and David E Long. 1994. Model checking and abstraction. ACM transactions on Programming Languages and Systems (TOPLAS) 16, 5 (1994), 1512–1542.

[19] Benny Govlin and Ofer Strichman. 2008. Inference rules for proving the equivalence of recursive procedures. Acta Informatica 45, 6 (2008), 403–439.

[20] Vihvah Gogate and Pedro Domingos. 2012. Probabilistic theorem proving. arXiv preprint arXiv:1202.3724 (2012).

[21] Robert Goldblatt and Marcel Jackson. 2012. Well-structured program equivalence is highly undecidable. ACM Transactions on Computational Logic (TOCL) 13, 3 (2012), 26.

[22] Kazushige Goto and Robert Van De Geijn. 2008. High-performance implementation of the level-3 BLAS. ACM Trans. Math. Softw. 35, 1 (2008), 4–1.

[23] Thomas Hérault, Richard Lassaigne, Frédéric Magniette, and Sylvain Peyronnet. 2004. Approximate probabilistic model checking. In International Workshop on Verification, Model Checking, and Abstract Interpretation. Springer, 73–84.

[24] Sepp Hochreiter and Jürgen Schmidhuber. 1997. Long short-term memory. Neural computation 9, 8 (1997), 1735–1780.

[25] Guillaume Iooss, Christophe Alias, and Sanjay Rajopadhye. 2014. On program equivalence with reductions. In International Static Analysis Symposium. Springer, 168–183.

[26] Sara Kalvala, Richard Warburton, and David Lacey. 2009. Program transformations using temporal logic side conditions. ACM Trans. on Programming Languages and Systems (TOPLAS) 31, 4 (2009), 14.

[27] Donald M Kaplan. 1969. Regular expressions and the equivalence of programs. J. Comput. System Sci. 3, 4 (1969), 361–386.

[28] Chandan Karfa, Kunal Banerjee, Dipankar Sarkar, and Chittaranjan Mandal. 2013. Verification of loop and arithmetic transformations of array-intensive behaviors. IEEE Trans. on Computer-Aided Design of Integrated Circuits and Systems 32, 11 (2013), 1787–1800.

[29] Guillaume Klein, Yoon Kim, Tunyan Deng, Jean Senellart, and Alexander M. Rush. 2017. OpenNMT: Open-Source Toolkit for Neural Machine Translation. In Proc. ACL. https://doi.org/10.18653/v1/P17-4012
[30] Sudipta Kundu, Zachary Tatlock, and Sorin Lerner. 2009. Proving
optimizations correct using parameterized program equivalence. ACM SIGPLAN Notices 44, 6 (2009), 327–337.
[31] Jeremy Lacomis, Pengcheng Yin, Edward J. Schwartz, Miltiadis Allamanis, Claire Le Goues, Graham Neubig, and Bogdan Vasilescu. 2019. DIRE: A Neural Approach to Decompiled Identifier Naming. In International Conference on Automated Software Engineering (ASE ’19).
[32] W. Li, X. Zhang, Y. Wang, Z. Yan, and R. Peng. 2019. Graph2Seq: Fusion Embedding Learning for Knowledge Graph Completion. IEEE Access 7 (2019), 157960–157971. https://doi.org/10.1109/ACCESS.2019.2950230
[33] Yujia Li, Richard Zemel, Marc Brockschmidt, and Daniel Tarlow. 2016. Gated Graph Sequence Neural Networks. In Proceedings of ICLR’16 (proceedings of iclr’16 ed.). https://www.microsoft.com/en-us/research/publication/gated-graph-sequence-neural-networks/
[34] Dorel Lucanu and Vlad Rusu. 2015. Program equivalence by circular reasoning. Formal Aspects of Computing 27, 4 (2015), 701–726.
[35] Thang Luong, Hieu Pham, and Christopher D. Manning. 2015. Effective Approaches to Attention-based Neural Machine Translation. In Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing. Association for Computational Linguistics, Lisbon, Portugal, 1412–1421. https://doi.org/10.18653/v1/D15-1166
[36] William Mansky and Elsa Gunter. 2010. A framework for formal verification of compiler optimizations. In Interactive Theorem Proving. Springer.
[37] Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg S Corrado, and Jeff Dean. 2013. Distributed Representations of Words and Phrases and their Compositionality. In Advances in Neural Information Processing Systems 26. C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K. Q. Weinberger (Eds.). Curran Associates, Inc., 3111–3119.
[38] Andrzej S Murawski and Joel Ouaknine. 2005. On probabilistic program equivalence and refinement. In International Conference on Concurrency Theory. Springer, 156–170.
[39] Kedar S Namjoshi and Robert P Kurshan. 2000. Syntactic program transformations for automatic abstraction. In International Conference on Computer Aided Verification. Springer, 435–449.
[40] George C. Necula. 2000. Translation validation for an optimizing compiler. ACM SIGPLAN Notices 35, 5 (2000), 83–94.
[41] Lawrence C. Paulson. [n. d.]. Isabelle Page. https://www.cl.cam.ac.uk/research/hvg/Isabelle.
[42] Veselin Raychev, Martin Vechev, and Andreas Krause. 2015. Predicting Program Properties from “Big Code”. In Proceedings of the 42Nd Annual ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages (POPL ’15). ACM, New York, NY, USA, 111–124. https://doi.org/10.1145/2676726.2677009
[43] Uday S Reddy. 1989. Rewriting techniques for program synthesis. In International Conference on Rewriting Techniques and Applications. Springer, 388–403.
[44] Franco Scaletti, Marco Gori, Ah Chung Tsoi, Markus Hagenbuchner, and Gabriele Monfardini. 2009. The Graph Neural Network Model. IEEE Transactions on Neural Networks 20 (2009), 61–80.
[45] Bernhard Steffen. 1991. Data flow analysis as model checking. In International Symposium on Theoretical Aspects of Computer Software. Springer, 346–364.
[46] M. Tomita. 1982. Dynamic Construction of Finite Automata from examples using Hill-climbing. In Proceedings of the Fourth Annual Conference of the Cognitive Science Society. Ann Arbor, Michigan, 105–108.
[47] Michele Tufano, Cody Watson, Gabriele Bavota, Massimiliano Di Penta, Martin White, and Denys Poshyvanyk. 2019. An Empirical Study on Learning Bug-Fixing Patches in the Wild via Neural Machine Translation. ACM Trans. Softw. Eng. Methodol. 28, 4, Article 19 (Sept. 2019), 29 pages. https://doi.org/10.1145/3340544
[48] Sven Verdoolaege, Gerda Janssens, and Maurice Bruynooghe. 2009. Equivalence checking of static affine programs using widening to handle recurrences. In Computer aided verification. Springer, 599–613.
[49] Sven Verdoolaege, Gerda Janssens, and Maurice Bruynooghe. 2012. Equivalence checking of static affine programs using widening to handle recurrences. ACM Trans. on Programming Languages and Systems (TOPLAS) 34, 3 (2012), 11.
[50] Eelco Visser. 2004. Program transformation with Stratego/XT. In Domain-specific program generation. Springer, 216–238.
[51] Willem Visser, Klaus Havelund, Guillaume Brat, Seunghoon Park, and Flavio Lerda. 2003. Model checking programs. Automated software engineering 10, 2 (2003), 203–232.
[52] Qinglong Wang, Kaixuan Zhang, Alexander G. Ororbia, II, Xinyu Xing, Xue Liu, and C. Lee Giles. 2018. An Empirical Evaluation of Rule Extraction from Recurrent Neural Networks. Neural Comput. 30, 9 (Sept. 2018), 2568–2591. https://doi.org/10.1162/neco_a_01111
[53] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and Philip S. Yu. 2019. A Comprehensive Survey on Graph Neural Networks. CoRR abs/1901.00596 (2019). arXiv:1901.00596 http://arxiv.org/abs/1901.00596
[54] Xiaojun Xu, Chang Liu, Qian Feng, Heng Yin, Le Song, and Dawn Song. 2017. Neural Network-based Graph Embedding for Cross-Platform Binary Code Similarity Detection. In Proceedings of the 2017 ACM SIGSAC Conference on Computer and Communications Security (CCS ’17). ACM, New York, NY, USA, 363–376. https://doi.org/10.1145/3133956.3134018
A Appendix

Figure 2 overviews the entire system architecture including sample generation, the pe-graph2seq network, and the rewrite checker. In this section we will discuss the implementation details of these components.

A.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 given axiom set. By creating this process, we could create as large and varied a dataset as our machine learning approach required.

Algorithm 1 provides an overview of the full program generation algorithm. For this generation process, we define a set of operations and operands on scalars, matrices, and vectors. For our process, we presume matrix and vector dimensions are appropriate for 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:

- **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.

Initially, GenSrc is called with GenSrc("+s -s *s /s is ns, where is the unary reciprocal and ns is the unary negation.  
- Matrix operations: +m -m *m im nm tm, where im matrix inversion, nm negates the matrix, and tm is matrix transpose.  
- Vector operations: +v -v *v nv, where nv is the unary negation.  
- Scalars: +v -v *v +m -m *m im nm tm +v -v *v +v -v *v nv", 0.91). 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 91%. Since the algorithm subtracts a 23% probability for children at each level of the graph, at most 6 levels will be created by this algorithm (i.e., the path length from the root to any leaf does not exceed 6).

Algorithm 1 starts execution by randomly selecting an operation from the set provided as input. When GenSrc 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 GenSrc 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, Ao (matrix times vector), bo (scalar times vector), or vo (vector times scalar) are all valid options and will be chosen randomly.

| Algorithm 1: GenSrc |
|---------------------|
| **Result:** Prefix notation of computation with parenthesis |
| **Input:** Ops, P |
| **Output:** (op L R) or (op L) |
| op = select randomly from Ops |
| // Create subtree for chosen op |
| if op == "*s" then |
| if random < P then |
| L = GenSrc("+s -s *s /s +s -s *s /s is ns", P-0.23) |
| else |
| L = select random scalar operand |
| end |
| if random < P then |
| R = GenSrc("+s -s *s /s +s -s *s /s is ns", P-0.23) |
| else |
| R = select random scalar operand |
| end |
| return (op L R) |

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.

As shown on line 10 of the algorithm, when the operation and children meet the conditions necessary for a rewrite rule (in this case Noop), the rule is applied with some probability (in this case 50%). Note that before processing a node, the left and right operands are further analyzed to determine their operators and operands as well (or if the child is a terminal). Processing the left and right operands allows for complex axioms to be applied, such as distribution or factorization. When a rule is applied, the rewrite rule is added to the rewrite rule sequence and a new target program is generated for any remaining subtrees. When creating the rewrite rules for subtrees, the path variable is updated as
rewrites are done. In the case of Noop, the current node is being updated, so the path is not changed. But in the case of the Commute rule, the return would be generated with \((op \text{ GenTgt}(R, \text{path.}"\text{left }") \text{ GenTgt}(L, \text{path.}"\text{right }"))\) which creates rewrite rules for the prior right and left operands of the \(op\) and updates the path used to the new node positions. With some probability, illegal rewrites can be done; for example, commuting a subtraction operation or mutating an operation into another. In that case, the GenTgt process continues to create a target program, but transform_sequence is set to Not_equal.

Algorithm 2: GenTgt

| Result: Second program and transform_sequence |
|-----------------------------------------------|
| **Input:** :ProgA, path                        |
| **Output:** :ProgB                             |

1. if terminal symbol then  
2. return ProgA  
3. end  
4. \(op = \text{find operator of ProgA}\)  
5. \(L = \text{find left operand of ProgA}\)  
6. \(R = \text{find right operand of ProgA}\)  
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 \((\text{op == }"+v" \text{ and } (L == "o" \text{ or } R == "o")) \text{ or } (\text{op == }"-v" \text{ and } R == "o"))\) then  
11. append path."Noop " to transform_sequence  
12. // Eliminate unnecessary operator and 0 vector  
13. if \(L == "o"\) then  
14. return GenTgt(R, path)  
15. else  
16. return GenTgt(L, path)  
17. end  
18. end

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 source and target program pair total to 60 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 5 or less, that there are 5 or fewer rewrite rules applied and that the rewrite rule token list is 25 or fewer (including left/right identifiers for location). Also, the pruning insures that there are no lexically equivalent programs in the process and removes some of the 1 and 2 rewrite rule cases to bias the dataset to longer rewrite sequences. Table 1 details the distribution of rewrite rules created by the full process. Section D details all axioms when variable types and operators are considered.

A.2 Rewrite checking

The rewrite checker 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 rewrite checking, we begin with a program 1 and a sequence of rewrite rules. We follow the path given by the rewrite rule sequence, check that a node can legally accept a rule, apply the rule, and process the remaining rewrite sequence on the adjusted program. If a rule cannot legally be applied, program 1 is not proven equal to program 2. If all rules can be legally applied in sequence to program 1, the program is compared lexically to program 2 and if they match then equivalence has been proven.

B Details on Experimental Results

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 2. Language IDs 1 through 5 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 4 and 5.

The dramatic increase in performance of the graph neural network for 2 Commute languages is shown by comparing IDs 2 and 3. Language ID 7 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 8 expands the operands to 3 types and hence the number of operators also increase. To account for memory footprint concerns due growing complexity in our model, we reduce the maximum program size with ID 8. This reduction also allows us to train larger data sets for more epochs. ID 9 is our full language using our golden model which we focus on throughout this paper. ID 10 explores the use model where the model trains to produce a Not_equal token when the input programs are not identical. The discussion for table 5 will explore the use model in relation to non-equivalent programs in depth. ID 11 demonstrates on the full model the disadvantage of using a sequence-to-sequence model for this problem. ID 12 is a forward looking-model which makes a minor increment to the language to support the analysis of loop rolling and unrolling.

Exploration of alternate designs In order to design the system, we explored parts of the design space quickly and performed several single training run comparisons between 2 options, as shown in Table 3. 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.
Experiments such as these informed our final network architecture. For example, in pe-graph2seq, 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. [32] 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. Also clearly shown in these results is the improvement a graph neural network can provide over the tuned sequence-to-sequence model provided as part of the OpenNMT system. A sequence-to-sequence model cannot easily learn the full grammar of the language and the correct nature of the program as input.

Including Not_equal option Table 5 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 and programs use our full language model with 16 operators, 13 core axioms (102 total), and 20 operands.

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 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-graph2seq 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. Equivalent programs (within the random distribution we analyzed) will have a 96.2% chance of being proven equivalent.

C An Example of Back-Edge in the Program Graph

Figure 6 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 DoX(g(y)) = DoHalf(g(g(y))) (where y is the variable reused each iteration), and DoX states the reverse.

![Diagram](image)

**Figure 6.** Adding loop constructs creates cycles in the program graph.

## D Full axiom list

Tables 7, 8, 9, and 10 show the full 102 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  | (v - v) → o |
| Noop         | 5  | (a + 0) → a |
|              | 6  | (0 + a) → a |
|              | 7  | (a - 0) → a |
|              | 8  | (a * 1) → a |
|              | 9  | (1 * a) → a |
|              | 10 | (a / 1) → a |
|              | 11 | (A + O) → A |
|              | 12 | (O + A) → A |
|              | 13 | (A - O) → A |
|              | 14 | (A * I) → A |
|              | 15 | (I * A) → A |
|              | 16 | (v + o) → v |
|              | 17 | (o + v) → v |
|              | 18 | (v - o) → v |
| Double       | 19 | -(a) → a    |
|              | 20 | (a^-1) → a  |
|              | 21 | -(~A) → A   |
|              | 22 | (A^-1) → A  |
|              | 23 | (A^t) → A   |
|              | 24 | -(~v) → v   |

**Figure 7.** Full axiom count when all type options and other supported permutations are included (part 1 of 4)
| Rewrite Rule    | ID | Example(s) | ID | Example(s) |
|----------------|----|------------|----|------------|
| **Commute**    | 25 | (a + b) → (b + a) | 51 | ab + ac → a(b+c) |
|                | 26 | (a * b) → (b * a) | 52 | ab - ac → a(b+c) |
|                | 27 | (A + B) → (B + A) | 53 | AB + AC → A(B+C) |
|                | 28 | (v + w) → (w + v) | 54 | AB - AC → A(B-C) |
|                | 29 | (v * a) → (a * v) | 55 | Av + Aw → A(v+w) |
|                | 30 | (a * v) → (v * a) | 56 | Av - Aw → A(v-w) |
| **DistributeLeft** | 31 | (a + b)c → ac + bc | 57 | Aa + Ab → A(a+b) |
|                | 32 | (a - b)c → ac - bc | 58 | Aa - Ab → A(a-b) |
|                | 33 | (a + b)/c → a/c + b/c | 59 | va + vb → v(a+b) |
|                | 34 | (a - b)/c → a/c - b/c | 60 | va - vb → v(a-b) |
|                | 35 | (v + w)a → va + wa | 61 | ac + bc → (a+b)c |
|                | 36 | (v - w)a → va - wa | 62 | ac - bc → (a-b)c |
|                | 37 | (A + B)C → AC + BC | 63 | a/c + b/c → (a+b)/c |
|                | 38 | (A - B)C → AC - BC | 64 | a/c - b/c → (a-b)/c |
|                | 39 | (A + B)v → Av + Bv | 65 | AC + BC → (A+B)C |
|                | 40 | (A - B)v → Av - Bv | 66 | AC - BC → (A-B)C |
|                | 41 | (A + B)a → Aa + Ba | 67 | Av + Bv → (A+B)v |
|                | 42 | (A - B)a → Aa - Ba | 68 | Av - Bv → (A-B)v |
| **DistributeRight** | 43 | a(b + c) → ab + ac | 69 | Aa + Ba → (A+B)a |
|                | 44 | a(b - c) → ab - ac | 70 | Aa - Ba → (A-B)a |
|                | 45 | a(v + w) → av + av | 71 | va + wa → (v+w)a |
|                | 46 | a(v - w) → av - av | 72 | va - wa → (v-w)a |
|                | 47 | A(B + C) → AB + AC | 73 | a+(b+c) → (a+b)+c |
|                | 48 | A(B - C) → AB - AC | 74 | a(bc) → (ab)c |
|                | 49 | a(B + C) → aB + aC | 75 | A+(B+C) → (A+B)+C |
|                | 50 | a(B - C) → aB - aC | 76 | A(BC) → (AB)C |
| **FactorLeft**  | 51 | ab + ac → a(b+c) | 77 | A(ba) → (AB)a |
|                | 52 | ab - ac → a(b+c) | 78 | v+(w+x) → (v+w)+x |
| **FactorRight** | 53 | AB + AC → A(B+C) | 79 | |
|                | 54 | AB - AC → A(B-C) | 80 | |
|                | 55 | Av + Aw → A(v+w) | 81 | |
|                | 56 | Av - Aw → A(v-w) | 82 | |
|                | 57 | Aa + Ab → A(a+b) | 83 | |
|                | 58 | Aa - Ab → A(a-b) | 84 | |
|                | 59 | va + vb → v(a+b) | 85 | |
|                | 60 | va - vb → v(a-b) | 86 | |

**Figure 8.** Full axiom count when all type options and other supported permutations are included (part 2 of 4)

**Figure 9.** Full axiom count when all type options and other supported permutations are included (part 3 of 4)
| Rewrite Rule     | ID | Example(s)                                  |
|------------------|----|---------------------------------------------|
| AssociativeRight | 79 | (a+b)+c → a+(b+c)                            |
|                  | 80 | (ab)c → a(bc)                               |
|                  | 81 | (A+B)+C → A+(B+C)                           |
|                  | 82 | (AB)C → A(BC)                              |
|                  | 83 | (AB)a → A(Ba)                              |
|                  | 84 | (v+w)+x → v+(w+x)                           |
| FlipLeft         | 85 | -(a - b) → b-a                             |
|                  | 86 | (a/b)^{-1} → b/a                           |
|                  | 87 | -(A - B) → (B - A)                         |
|                  | 88 | -(a - w) → (w - v)                         |
| FlipRight        | 89 | a/(b/c) → a(c/b)                            |
|                  | 90 | a/(b^{-1}) → ab                            |
|                  | 91 | -a-(b-c) → a+(c-b)                         |
|                  | 92 | a-(b) → a+b                                |
|                  | 93 | A-(B-C) → A+(C-B)                          |
|                  | 94 | A-(B) → A+B                                |
|                  | 95 | v-(w-x) → v+(x-w)                          |
|                  | 96 | v-(w) → v+w                                |
| Transpose        | 97 | (AB) → (B'A')^t                            |
|                  | 98 | (A + B) → (A' + B')^t                      |
|                  | 99 | (A - B) → (A' - B')^t                      |
|                  | 100| (AB)^t → B'A^t                             |
|                  | 101| (A + B)^t → A' + B'^t                      |
|                  | 102| (A - B)^t → A' - B'^t                      |

**Figure 10.** Full axiom count when all type options and other supported permutations are included (part 4 of 4)