Evolving Graphs by Graph Programming

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Abstract. Rule-based graph programming is a deep and rich topic. We present an approach to exploiting the power of graph programming as a representation and as an execution medium in an evolutionary algorithm (EGGP). We demonstrate this power in comparison with Cartesian Genetic Programming (CGP), showing that it is significantly more efficient in terms of fitness evaluations on some classic benchmark problems. We hypothesise that this is due to its ability to exploit the full graph structure, leading to a richer mutation set, and outline future work to test this hypothesis, and to exploit further the power of graph programming within an EA.

1 Introduction

Representation is crucial in computer science, and an important specific representation is the graph. Graphs are used in a wide range of applications and algorithms, see for example [4, 22, 5]. In evolutionary algorithms (EAs), graphs are used in some applications, but are usually encoded in a linear genome, with the genome undergoing mutation and crossover, and a later "genotype to phenotype mapping" used to decode the linear genome into a graph structure. For example in Cartesian Genetic Programming (CGP) [14, 12], the connections of feed forward networks are encoded in a linear genome. NEAT [24, 23] provides a linear encoding of ANNs which are seen as graph structures. Trees (a subset of more general graphs) are also used in EAs. Grammatical Evolution [15, 21] uses a linear genome of integers to indirectly encode programs. Genetic Programming [7, 6] is unusual for an EA: rather than using a linear genome, it typically directly manipulates abstract syntax trees. Poli [20, 19] uses a 'graph on a grid' representation: the underlying structure is a graph, but the nodes are constrained to lie on discrete grid points. MOIST [8] proposes using trees with multiple output nodes and sharing to extend traditional genetic programming to domains where problems have multiple, related outputs. Pereira et al [16] represent Turing machines as graphs encoded in a linear genome, and develop a crossover operator based on the structure of the underlying graph.

There are arguments for and against linear genomes representing graphs. Linear genomes are standard in EAs, and they can exploit the knowledge about

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evolutionary operators. However, they can hide the underlying structure of the problem, and can have biases in the effect of the evolutionary operators. There may be advantages in evolving graphs directly, rather than via linear genome encodings or 2D grid encodings, and defining mutation operators that respect the graph structure. Direct graph transformation has deep theoretical underpinnings, and has become increasingly accessible through efficient graph programming languages such as GP 2 [17, 2]. GP 2 enables high-level problem solving in the domain of graphs, freeing programmers from handling low-level data structures. It has a simple syntax whose basic computational units are graph transformation rules which can be graphically edited. Also, GP 2 comes with a concise operational semantics to facilitate formal reasoning on programs.

Here we exploit an extension to GP 2 [1] that has probabilistic elements to support EA applications. We perform experiments of evolving graphs directly, and compare the results with experiments previously done with CGP. Using graph transformations, we write evolutionary operators as graph transformation rules, and we calculate fitness in the same context. Our results indicate that direct evolution can be significantly more efficient (significantly fewer fitness function evaluations) than basic CGP, due to the increased number of mutations available, allowing more effective exploration of the search landscape.

The paper is organised as follows. In §2 we overview Graph Programming. In §3 we describe how we have incorporated an EA into graph programming (EGGP). In §4 we compare our EGGP setup with Cartesian Genetic Programming (CGP). In §5 we describe benchmark experiments, and in §6 provide the results, demonstrating that EGGP is significantly more efficient, in terms of fitness evaluations, than vanilla CGP. In §7 we draw conclusions and outline future work in examining the reasons for this improvement.

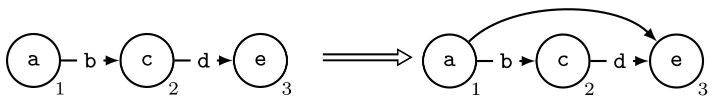
2 Graph Programming

This section is a (very) brief introduction to the graph programming language GP 2; see [18] for a detailed account of the syntax and semantics of the language. A graph program consists of declarations of *graph transformation rules* and a main command sequence controlling the application of the rules. Graphs are directed and may contain loops and parallel edges. The rules operate on *host graphs* whose nodes and edges are labelled with integers, character strings or lists of integers and strings. Variables in rules are of type `int`, `char`, `string`, `atom` or `list`, where `atom` is the union of `int` and `string`. Atoms are considered as lists of length one, hence integers and strings are also lists. For example, in Figure 1, the list variables `a`, `c` and `e` are used as edge labels while `b` and `d` serve as node labels. The small numbers attached to nodes are identifiers that specify the correspondence between the nodes in the left and the right graph of the rule.

Besides carrying list expressions, nodes and edges can be *marked*. For example, in the program of Figure 3, blue and red node marks are used to prevent the rule `mutateEdge` from creating a cycle.

```
Main := link!

link(a,b,c,d,e:list)
```



```
where not edge(1,3)
```

Fig. 1: A GP 2 program computing the transitive closure of a graph.

The principal programming constructs in GP 2 are conditional graph-transformation rules labelled with expressions. The program in Figure 1 applies the single rule `link` *as long as possible* to a host graph. In general, any subprogram can be iterated with the postfix operator "`!`". Applying `link` amounts to non-deterministically selecting a subgraph of the host graph that matches `link`'s left graph, and adding to it an edge from node 1 to node 3 provided there is no such edge (with any label). The application condition `where not edge(1,3)` ensures that the program terminates and extends the host graph with a minimal number of edges. Rule matching is injective and involves instantiating variables with concrete values. We remark that GP 2's inherent non-determinism is useful as many graph problems are naturally multi-valued, for example the computation of a shortest path or a minimum spanning tree.

Given any graph G, the program in Figure 1 produces the smallest transitive graph that results from adding unlabelled edges to G. (A graph is *transitive* if for each directed path from a node v_1 to another node v_2, there is an edge from v_1 to v_2.) In general, the execution of a program on a host graph may result in different graphs, fail, or diverge. The *semantics* of a program P maps each host graph to the set of all possible outcomes [17]. GP 2 is computationally complete in that every computable function on graphs can be programmed [18]. Commands not used in this paper are the non-deterministic application of a set of rules and various branching commands.

While rule matching in GP 2 is non-deterministic, the refined language P-GP 2 (for *Probabilistic GP 2*) selects a match for a rule uniformly at random [1]. This language has been used to obtain the results described in the rest of this paper.

3 Evolving Graphs by Graph Programming (EGGP)

3.1 Representation

Our approach uses the following representation of individual solutions. An individual I over function set $F = \{f_1, f_2, ...f_n\}$ is a directed graph containing a set V_i of input nodes which have no outgoing edges and a set V_o of output nodes which have one outgoing edge and no incoming edges. Each non-input and non-output node is associated with some function in F. For simplicity we assume

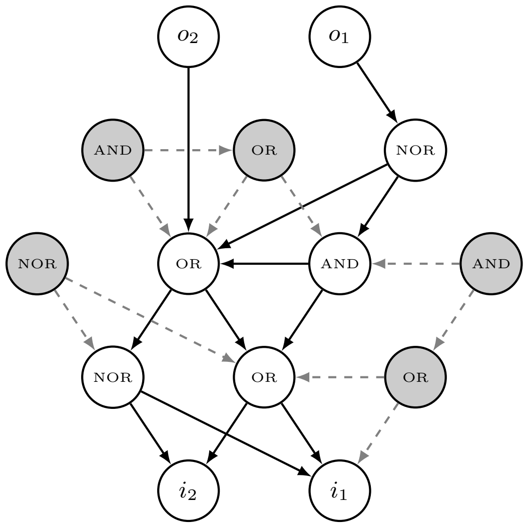


Fig. 2: An example EGGP Individual for a binary logic problem.

that all functions in F (and the fitness function) operate on a single domain. EGGP individuals are defined in Definition 1.

Further, for each function node v labelled with a function f of arity n, v has outgoing edges $e_1, ..., e_n$ such that for $i = 1, ..., n$, $a(e_i) = i$. Then a provides the order in which to pass v's inputs to f, resolving ambiguity for asymmetric functions. We assume acyclic graphs in this work, and hence an individual I represents a solution as a network, where each node computes a function on its inputs (which are given by its outgoing edges). We refer to acyclic EGGP individuals as being "feed-forward".

Definition 1 (EGGP Individual). *An EGGP Individual over function set F is a directed graph $I = \{V, E, s, t, l, a, V_i, V_o\}$ where V is a finite set of nodes and E is a finite set of edges. $s\colon E \to V$ is a function associating each edge with its source. $t\colon E \to V$ is a function associating each edge with its target. $V_i \subseteq V$ is a set of input nodes. Each node in V_i has no outgoing edges and is not associated with a function. $V_o \subseteq V$ is a set of output nodes. Each node in V_o has one outgoing edge, no incoming edges and is not associated with a function. $l\colon V \to F$ labels every "function node" that is not in $V_i \cup V_o$ with a function in F. $a\colon E \to \mathbb{Z}$ labels every edge with a positive integer.*

Such a representation may contain neutral material; nodes to which there is no path from any output and therefore do not contribute to the functionality of the solution. This is a direct encoding, and the conversion from genotype to phenotype is given by simply removing material which does not contribute to any output. We present an example individual in Figure 2. This individual is both feed-forward and satisfies the arities of its associated function set F = {OR, AND, NOR} This individual has two input nodes, labeled i_1 and i_2, and two

`Main` := `pickEdge`; `markOutput`!; `mutateEdge`; `unmark`!

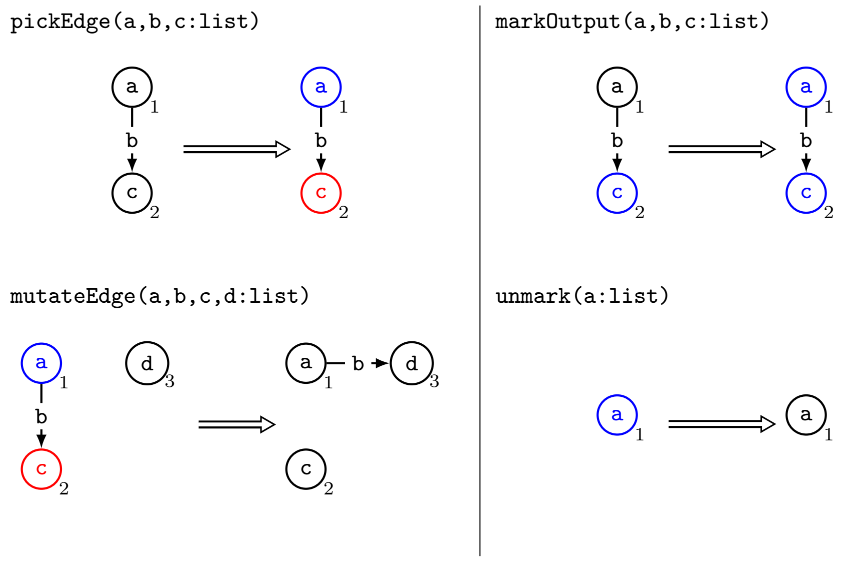


Fig. 3: Mutating an edge of an EGGP individual while preserving feed-forwardness using a graph program.

output nodes, labeled o_1 and o_2. Neutral material, which does not contribute to the phenotype of the individual, is coloured gray. Edge labels are omitted for visual clarity, and is unambiguous for this example as all of the functions in F are symmetrical.

3.2 Atomic Mutations

We describe two point mutations for an EGGP individual that appear maximally simplistic; changing the function associated with a node and changing a single input to a node.

As we assume that individuals are feed-forward in this work we require a mutation that respects this constraint. A point mutation of a node's input edge while maintaining feed-forwardness is shown in Figure 3. Firstly an edge to mutate is chosen and marked, with uniform probability, with `pickEdge` and then all nodes which have a path to the source of the chosen edge are marked using `markOutput!`. The edge is then mutated to target some unmarked node, chosen with uniform probability, using `mutateEdge`, and clearly there cannot be a cycle introduced as the earlier steps of the mutation have not marked that node and therefore that node does not have a path to the source of the chosen edge. Finally, we unmark all marked nodes using the `unmark` rule. Using the given mutation, we are able to mutate an individual while respecting feed-forwardness without

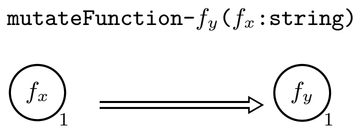


Fig. 4: Mutating the function of an EGGP individual's node to some function f_y. f_x is the existing function of the node being mutated, and an equivalent rule can be constructed for each function in the function set.

applying any restraints to the individual or the mutation, by transforming the individual using a graph program.

A point mutation of a node's function is shown in Figure 4. Here node 1 has its function updated to some function $f_y \in F$. This operator clearly preserves feed-forwardness as it introduces no new edges. In this work we deal with function sets with fixed, common arities. However, this may not always be desirable, for example when attempting symbolic regression over a function set containing both addition and sin operators. In the C-based library for Cartesian Genetic Programming this is overcome by simply using the first few inputs for lower arity functions [26], but in EGGP this would prevent some feed-forward preserving mutations when a node appears to contribute to the input of another but in truth does not. Although we do not address this issue in this work, we propose that it would be possible to add and delete input edges when mutating a node's function to maintain correct function arities, while also maintaining feed-forwardness when adding those new input edges in a similar manner to the algorithm for edge mutations given in Figure 3.

3.3 Evolutionary Algorithm

Crossover between EGGP individuals is not obvious as there is no apparent relationship between the nodes and edges of any two individual solutions. It might be possible to use historical markers, as used in the graph-based neuroevolution algorithm NEAT [24], or some other approach, but this is not attempted in this work. Without a crossover operator, it is natural to consider single-survivor evolutionary algorithms. As we intend to benchmark against Cartesian Genetic Programming in §5, we propose the use of the evolutionary algorithm most commonly used with it, the $1 + \lambda$ evolutionary algorithm shown in Figure 5. This algorithm is an extended form of Random Hill Climbing, where in each generation λ new individuals are generated by mutating the sole surviving parent from the previous generation. Additionally, we allow a new individual with equal fitness to its parent to replace its parent in the next generation, facilitating the phenomena of "neutral drift". Propagating changes in the genotype which result in neutral changes in the phenotype is known to positively influence the performance of CGP [13] and we see no obvious reason why this would not also be the case in EGGP.

```
procedure $1 + \lambda$(maxGenerations, $\lambda$)
    $parent \leftarrow generateindividual$
    $parentScore \leftarrow evaluate(parent)$
    $generation \leftarrow 0$
    while solution not found and $generation \leq maxGenerations$ do
        $newParent \leftarrow parent$
        for $i = 0$ to $\lambda$ do
            $child \leftarrow mutate(parent)$
            $childScore \leftarrow evaluate(child)$
            if $childScore \leq parentScore$ then
                $newParent \leftarrow child$
                $parentScore \leftarrow childScore$
        $parent \leftarrow newParent$
        $generation \leftarrow generation + 1$
```

Fig. 5: The $1 + \lambda$ evolutionary algorithm with neutral drift enabled.

3.4 Parameters

Use of the EGGP representation and the $1 + \lambda$ algorithm is parameterised by the following items:

- m_r: the mutation rate. Nodes and edges have no particular order in EGGP, and the order in which feed-forward edges are mutated may influence the availability of future mutations. We therefore opt to generate the number of node mutations and edge mutations to apply to the individual using binomial distributions (simulating one probabilistic mutation for each node or edge) and then distribute these mutations across the individual at random.
- λ: the number of individuals to generate in each generation of the $1 + \lambda$ algorithm.
- F: A function set. The maximum arity of functions in F is used to specify the number of input edges associated with each function node.
- n: the number of function nodes to use in each individual.
- p: the number of inputs that each individual should have to interface with the fitness function ($|V_i| = p$).
- q: the number of outputs that each individual should have to interface with the fitness function ($|V_o| = q$).
- A fitness function used to evaluate each individual.

4 Relation to Cartesian Genetic Programming

4.1 Cartesian Genetic Programming

Cartesian Genetic Programming (CGP) is a type of evolutionary algorithm in which individuals are represented as linear sequences of genes corresponding to a directed acyclic graph. Each gene is an integer representing either (1) where a node gets its inputs from or (2) the function of a node. These nodes are ordered so

	Node 1			Node 2			Node 3			Output
Genotype:	0	0	1	1	0	2	0	1	0	2

Phenotype:

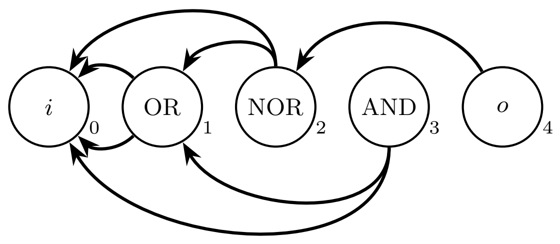


Fig. 6: The genotype-phenotype mapping of a simple CGP individual consisting of 1 input, 3 nodes and 1 output and arity 2. Each node is represented by 3 genes; the first 2 describe the indices of the node's inputs (starting at index 0 for the individual's input i) and the third describing the node's function. Function indices 0, 1 and 2 correspond to AND, OR and NOR respectively. The final gene describes the index of the node used by the individual's output o. .

that all input connections must respect that ordering, preventing cycles. When evolving over a function set where each function takes 2 inputs, there are 3 genes for each node in the individual; 2 representing each of the node's inputs, and 1 representing the node's function. Outputs are represented as single genes describing the node in the individual which corresponds to that output. These connection genes (nodes' input genes and the singular output genes) point to other nodes based on their index in the ordering.

An example genotype-phenotype mapping is given in Figure 6. Here an individual consisting of 3 nodes over a function set of arity 2, 1 input and 1 output is represented by 10 genes. These genes decode into the shown directed acyclic graph. In CGP individuals may be seen as a grid of n_r rows and n_c columns; a node in a certain column may use any node from any row in an earlier column as an input. Hence the total $n = n_r \times n_c$ nodes are ordered under a $\leq$ operator. The example shown in Figure 6 is a single row instance of CGP.

4.2 Comparison to EGGP

Here we demonstrate that EGGP provides a richer representation than CGP:

- For a fixed number of nodes n and function set F, any CGP individual can be represented as an EGGP individual, whereas the converse may not always hold when the number of rows in a CGP individual is greater than one.
- Any order-preserving CGP mutation can be represented as a feed-forward preserving mutation in EGGP, whereas some feed-forward preserving mutations may not be order-preserving nor valid in the CGP framework.

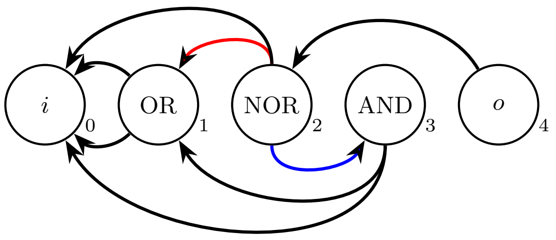


Fig. 7: A feed-forward preserving edge mutation. An edge (red) directed from node 2 to node 1 is replaced with an edge (blue) directed to node 3. This mutation produces a valid circuit but is impossible in CGP as it does not preserve order.

Firstly, consider the genotype-phenotype decoding of a CGP individual. Here we have clearly defined sets of input, output and function nodes. Additionally each function node is associated with some function from the function set, and there are ordered input connections (edges) from each function node to its inputs. Clearly this decoded individual can be treated as an EGGP individual fitting Definition 1. Conversely, consider the case where $n_r > 1$. Then there is the trivial counter example of an EGGP individual with a solution depth greater than n_c (as $n > n_c$) which clearly cannot be expressed as a CGP individual limited to depth n_c.

We now consider mutations available over a CGP individual in comparison to those for an EGGP individual where feed-forward preserving mutations are used. Clearly, as each order preserving mutation is feed-forward preserving, any valid mutation for the CGP individual is available for its EGGP equivalent. However, consider the example shown in Figure 7. Here a feed-forward mutation, connecting node 3 to node 4 is available in the EGGP setting but is not order preserving so is impossible in the CGP setting. Additionally, the semantic change that has occurred here, where an active node has been inserted between two adjacent active nodes is a type of phenotype growth that is impossible in CGP. Hence every mutation available in CGP is available in EGGP for an equivalent individual but the converse may not be true.

Therefore the landscape described by EGGP over the same function set and number of nodes is a generalisation of that described by CGP, with all individual solutions and viable mutations available, alongside further individual solutions and mutations that were previously unavailable.

4.3 Ordered EGGP (O-EGGP)

To demonstrate whether any differences in performance between EGGP and CGP arise from the freedom of mutation using feed-forward preserving, rather

Digital Circuit	**Number of Inputs**	**Number of Outputs**
1-bit adder (1-Add)	3	2
2-bit adder (2-Add)	5	3
3-bit adder (3-Add)	7	4
2-bit multiplier (2-Mul)	4	4
3-bit multiplier (3-Mul)	6	6
3:8-bit de-multiplexer (DeMux)	6	6
4×1-bit comparator (Comp)	4	18
3-bit Even Parity (3-EP)	3	1
4-bit Even Parity (4-EP)	4	1
5-bit Even Parity (5-EP)	5	1
6-bit Even Parity (6-EP)	6	1
7-bit Even Parity (7-EP)	7	1

Table 1: Digital Circuit benchmark problems.

than order-preserving, input mutations, we compare performance against an ordered variant of EGGP, called Ordered EGGP.

Each node in an O-EGGP individual is associated with an order in an analogous manner to CGP. Node function mutations from EGGP are used, but input mutations are order-preserving rather than feed-forward preserving. Hence the same set of mutation operators, with the same probability distribution over their outcomes, is available for equivalent O-EGGP and CGP individuals. This approach simulates the landscape and search process of CGP under identical conditions, so should produce identical results to an equivalent CGP implementation. By also benchmarking O-EGGP we demonstrate that it is EGGP's free graphical representation and the associated more general ability to mutate input connections with respect to preserving feed-forwardness that yields higher quality results.

5 Benchmarking

To benchmark EGGP we compare against basic CGP and O-EGGP for a set of Digital Circuit problems taken from [28], which are used in comparisons between CGP and its Embedded variant ECGP. We produce our own CGP benchmark results, which are roughly in line with those available in [28], by using the C-based CGP library [26]. The set of Digital Circuit problems studied is given in Table 1; we study bit adders, bit multipliers and even-parity circuits of various sizes alongside a 3:8-Bit de-multiplexer and a 4×1-Bit comparator (see [28] for details). As many of these circuits are typically constructed manually using XOR gates, we use the function set $\{\mathrm{AND}, \mathrm{OR}, \mathrm{NAND}, \mathrm{NOR}\}$ to artificially increase the difficulty of these problems. We use the number of incorrect bits produced by a candidate solution in comparison to the full truth table of the given problem as the fitness function.

Each algorithm is run 100 times, with a maximum generation cap of 20,000,000; every run in each case successfully produced a result with the exception of the 3-Mul for CGP, which produced a correct solution in 99% of cases. In all 3 benchmarks, 100 nodes are used for each individual. Following conventional wisdom for CGP, we use a mutation rate of 4% for CGP and O-EGGP benchmarks. Additionally, a single row of nodes is used in each of these cases ($n_r = 1$). However, from our observations EGGP works better with a lower mutation rate, so for EGGP benchmarks we use 1%. An investigation of how mutation rate influences the performance in EGGP is left for future work. The $1 + \lambda$ algorithm is used in all 3 cases, with $\lambda = 4$. Due to time constraints, O-EGGP is only benchmarked on easier problems; 1-Add, 2-Add, 2-Mul, DeMux, 3-EP, 4-EP and 5-EP. We argue that if the results from these benchmarks are in line with the CGP benchmark results we may extrapolate that O-EGGP is indeed simulating CGP. In this case the two distinguishing factors between the EGGP and CGP benchmarks are the use of mutation operator (feed-forward preserving vs. order preserving) and mutation rate (1% vs. 4%).

To provide comparisons, we use the following metrics; median number of evaluations (ME), median absolute deviation (MAD; median of the absolute deviation from the evaluation median ME), and interquartile range (IQR). The number of evaluations taken for each run is calculated as the number of generations used multiplied by the total population size ($1 + \lambda = 5$). The hypotheses we investigate for these benchmarks are:

1. EGGP performs significantly better than CGP on the same problems under similar conditions. This hypothesis, if validated, would demonstrate the value of our approach.
2. O-EGGP does not perform significantly better or worse than CGP on the same problems under identical conditions. This hypothesis, if validated, would indicate that the possible factors influencing EGGP's greater performance for the first hypothesis would be reduced to the use of the feed-forward mutation operator and the mutation rate.

6 Results

Here we present results from our benchmarking experiments. Digital circuit results for EGGP and CGP are given in Table 2; results for O-EGGP on a smaller benchmark suite are given in Table 3.

To test for statistical significance we use the two-tailed Mann-Whitney U test [10], which (essentially) tests the null hypothesis that two distributions have the same medians (the non-parametric analogue of the t-test applicable only to normally distributed data). In the case where we get a statistically significant result ($p < 0.05$), we also calculate the effect size, using the non-parametric Vargha-Delaney A Test [27].

	EGGP			**CGP**				
Problem	ME	MAD	IQR	ME	MAD	IQR	p	A
1-Add	5,723	3,020	7,123	6,018	3,312	7,768	0.62	–
2-Add	74,633	32,863	66,018	180,760	88,558	198,595	10^{-15}	**0.82**
3-Add	275,180	114,838	298,250	2,161,378	957,035	1,837,942	10^{-31}	**0.97**
2-Mul	14,118	5,553	12,955	10,178	5,258	14,459	0.018	0.60
3-Mul	1,241,880	437,210	829,223	15,816,940	7,948,870	19,987,744	10^{-34}	**0.99**
DeMux	16,763	4,710	9,210	20,890	6,845	14,063	0.013	0.60
Comp	262,660	84,248	174,185	1,148,823	425,758	1,012,149	10^{-31}	**0.97**
3-EP	2,755	1,558	4,836	4,365	2,530	5,345	0.038	0.58
4-EP	13,920	5,803	11,629	22,690	11,835	24,340	10^{-6}	0.69
5-EP	34,368	15,190	30,054	106,735	55,615	126,063	10^{-18}	**0.86**
6-EP	83,053	33,273	66,611	485,920	248,150	535,793	10^{-3}	**0.97**
7-EP	197,575	61,405	131,215	1,828,495	843,655	1,860,773	10^{-33}	**0.99**

Table 2: Results from Digital Circuit benchmarks for CGP and EGGP. The p value is from the two-tailed Mann-Whitney U test. Where $p < 0.05$, the effect size from the Vargha-Delaney A test is shown; large effect sizes ($A > 0.71$) are shown in **bold**. The values for CGP on the 3-Mul problem include the single failed run.

Comparing EGGP to CGP in Table 2, we find no significant improvement of EGGP over CGP for small problems (1-Add, 2-Mul). Indeed, for 2-Mul CGP significantly outperforms EGGP ($p < 0.05$), albeit with a small effect size (0.56 < A < 0.64). As the problems get larger and harder we find significant ($p < 0.05$) improvement of EGGP over CGP in all cases. The effect size is small (0.56 < A < 0.64) for the 3:8-Bit De-Mux and 3-Bit Even Parity, and medium (0.64 < A < 0.71) for 4-EP. We find highly significant ($p < 0.001$) improvements along with large effect sizes (0.71 < A) on all other problems, including the most difficult problems: 3-Add, 3-Mul, 4 × 1-Bit Comparator and 7-Bit Even Parity. So there is a clear progression of increasing improvement with problem difficulty.

We visualise some highly significant results as box-plots, with raw data overlayed and jittered, in Figure 8. For each of the named problems, it can be clearly seen that EGGP's interquartile range shares no overlap with CGP's, highlighting the significance of the improvement made. Overall, we see these results to validate our first hypothesis that EGGP performs significantly better than CGP when addressing the same harder problems, although we note that no significant improvement is made for simpler problems.

When comparing O-EGGP to CGP in Table 3, we find no significant difference between either approach on any of the problems in the smaller benchmark set. The results show similar numbers of median evaluations (ME) in each case, and produce p values indicating no significant difference between the samples.

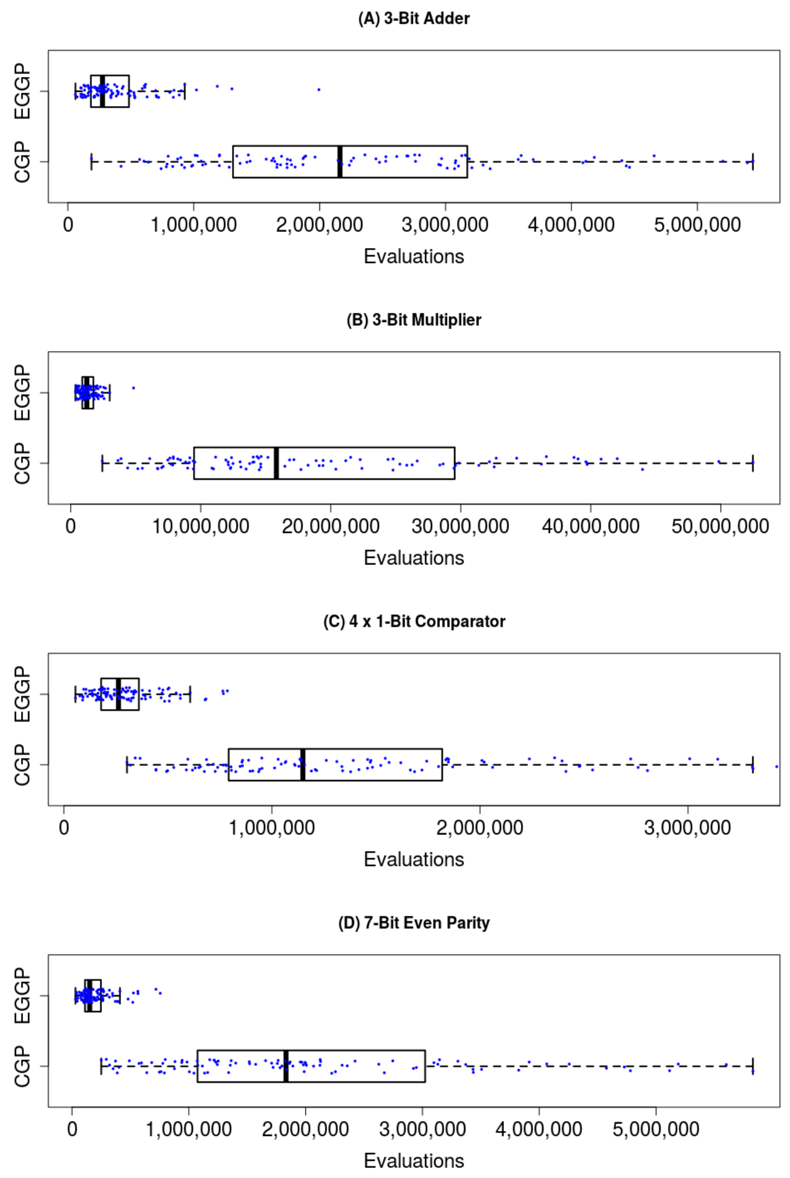


Fig. 8: Box-plots with data overlayed for the following highly significant results; (A) 3-Bit Adder, (B) 3-Bit Multiplier, (C) 4 x 1-Bit Comparator and (D) 7-Bit Even Parity. Overlayed data is jittered for visual clarity.

	O-EGGP			
Problem	ME	MAD	IQR	p
1-Add	6,253	3,610	9036	0.66
2-Add	193,753	109,420	239,133	0.95
2-Mul	13,930	7,905	19,104	0.12
DeMux	21,406	5,115	10,065	0.66
3-EP	3,903	2,315	4,831	0.64
4-EP	23,360	11,893	21,865	0.84
5-EP	121,820	51,150	107,868	0.56

Table 3: Results from Digital Circuit benchmarks for O-EGGP on a smaller benchmark suite. The p value is from the two-tailed Mann-Whitney significance test comparing against CGP; no result is statistically significant ($\alpha = 0.05$).

We believe that these findings support our hypothesis that O-EGGP does not perform significantly better or worse than CGP on identical problems under identical conditions. As O-EGGP theoretically simulates CGP, this indicates that we can consider the differences between the runs of EGGP and O-EGGP, namely feed-forward preserving mutations and mutation rate, as the major contributors to the differences in performance shown in Table 2.

Further, we suggest that the significant differences in results would not be resolved by tuning the mutation rate parameter. Therefore we turn our attention to the feed-forward preserving input mutation operator. As shown in Figure 7, feed-forward preserving mutations may insert nodes between nodes that would be considered adjacent in the CGP framework. This allows a subgraph of the solution to grow and change in previously unavailable manners. Performing functionally equivalent mutations with order preserving input mutations might require the construction of an entirely new subgraph in the neutral component of the individual which is then activated. We propose that the former mutation is more likely to occur than the sequence of mutations required to achieve the latter. Therefore where those unavailable mutations are "good" mutations in the sense of the fitness function, better performance will be achieved by using them directly. A future investigation into the quality of the neighborhood when using the feed-forward preserving mutation would clarify this hypothesis.

Additionally, this ability to insert material from anywhere in the individual that preserves feed-forwardness allows various neutral drifts to occur in the active component, even between nodes that would be considered adjacent in the CGP framework. For example, a connection using node x as input could be replaced by the semantically equivalent AND(x, x), for the function set used here. The insertion of that AND gate would then allow new mutations in the active component; for example changing its function, or mutating one of its inputs. Similar neutral mutations exist in this domain, such as the insertion of double negations using NAND gates. Additionally, the reverses of these transformations are also possible, freeing up genetic material to be used elsewhere. How useful these neutral mutations in the active component are is left for future work.

7 Conclusion and Future Work

We have proposed graphs as a fundamental representation for evolutionary algorithms and in particular the use of rule-based graph programming as a means to perform mutations. We have developed an algorithm, Evolving Graphs by Graph Programming, and demonstrated significantly improved performance on a suite of classic benchmark problems in comparison to CGP. We have demonstrated an ordered variant of EGGP, O-EGGP, that simulates and produces similar results to CGP, to support our hypothesis that the feed-forward preserving input mutation leads to improved performance. We believe this sets a clear precedent for future work on evolutionary algorithms using graphs as a fundamental representation and graph programming as a mechanism for transforming them.

There are a number of directions in which this work may be built upon. Further investigation into the value of the feed-forward preserving mutation operator and how the phenotype is able to change under it is necessary. If our hypothesis that neutral mutations in the active component are useful is confirmed, it may then be possible to force similar neutral mutations by encoding equivalence laws for a given domain as graph programming mutations, such as logical equivalence laws for circuits [11] or the ZX-calculus's equivalence rules for quantum graphs [3]. Additionally, a study of whether strict adherence to function arities for function sets with varying arities is helpful, as discussed in §3.2, may be worthwhile. In the present work we have avoided crossover operators, but a thorough investigation into how graphs can be usefully recombined would be of interest. Existing ideas such as history-based crossover [23] and subgraph swapping [16, 9] offer potential inspiration. We note the possibility of transferring the active component of one individual into the neutral component of another to be reabsorbed via future mutations (in a manner analogous to horizontal gene transfer in bacteria [25]), a mechanism made possible by the lack of constraint on our representation.

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