# Kozax: Flexible and Scalable Genetic Programming in JAX

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#### Abstract

Genetic programming is an optimization algorithm inspired by natural selection which automatically evolves the structure of computer programs. The resulting computer programs are interpretable and efficient compared to black-box models with fixed structure. The fitness evaluation in genetic programming suffers from high computational requirements, limiting the performance on difficult problems. To reduce the runtime, many implementations of genetic programming require a specific data format, making the applicability limited to specific problem classes. Consequently, there is no efficient genetic programming framework that is usable for a wide range of tasks. To this end, we developed Kozax, a genetic programming framework that evolves symbolic expressions for arbitrary problems. We implemented Kozax using JAX, a framework for high-performance and scalable machine learning, which allows the fitness evaluation to scale efficiently to large populations or datasets on GPU. Furthermore, Kozax offers constant optimization, custom operator definition and simultaneous evolution of multiple trees. We demonstrate successful applications of Kozax to discover equations of natural laws, recover equations of hidden dynamic variables and evolve a control policy. Overall, Kozax provides a general, fast, and scalable library to optimize white-box solutions in the realm of scientific computing.

## 1 Introduction

Genetic programming (GP) is an evolutionary algorithm which automatically generates the structure of computer programs that map inputs to an output value [22]. GP does not require a fixed structure to be pre-selected for the solution, which allows the algorithm to flexibly discover general structures of solutions with less human bias. The computer programs are often represented by parse trees, consisting of functions and variables. GP discovers interpretable solutions that provide understanding about the data or model itself, and consequently GP has become one of the main pillars in the field of automated scientific discovery [46, 3]. In scientific discovery, GP has been used in (re-)discovery of natural laws [39, 25], symbolic regression of dynamical systems [3, 11], learning symbolic control policies [17, 44, 32] and evolving learning rules [19].

Most such GP applications are based on separate implementations, each individually tailored to a specific task. Ideally, one unifying framework would exist that allows users to apply GP to their target problem. However, a major issue in GP is the high computational requirements needed to perform the fitness evaluation [16], especially when applied to difficult problems or large datasets. This complicates the development of a GP framework that both generalizes to arbitrary problems and runs efficiently. Variations of GP have been proposed that are computationally more efficient, such as Cartesian GP [30] and linear GP [6], however these variants have limitations in turn, such as reduced interpretability and inefficient evolution. Another approach for reducing computation time, is to improve the parallelization of the evaluation of different candidate solutions. Due to the inherently parallel nature of evolutionary algorithms, candidate solutions can be evaluated independently [16]. Nonetheless, this remains difficult for GP, as the individual solutions in the population may have different structures and sizes.

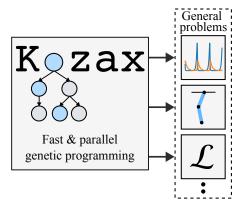


Figure 1: Kozax is a general framework for genetic programming, utilizing JAX for fast and parallelizable computation. It allows for highly flexible problem and fitness function specifications, making Kozax applicable to diverse and complex tasks, including symbolic regression of dynamical systems, control policy optimization and objective function evolution for training neural networks.

Feature	PySR	Kozax
JIT compilation	✓	✓
Custom operators	✓	$\checkmark$
Custom fitness function	✓	$\checkmark$
Pareto front	✓	$\checkmark$
SymPy interface	✓	$\checkmark$
Constant optimization	✓	$\checkmark$
Symbolic constraints	✓	_
Simplification during evolution	✓	_
Flexible tree definition	_	$\checkmark$
Different tree classes	_	$\checkmark$
Runs on GPU	_	$\checkmark$

Table 1: Comparison of algorithmic and software features between PySR and Kozax. A check mark indicates that this feature is included in the library, while a dash shows that this feature is currently missing. Data preprocessing functionality is excluded from this evaluation since this can be handled externally or included in the evaluation of the fitness function.

Previous attempts have been made to parallelize the fitness evaluation of GP on GPU. These ideas cover parallelizing the data points for each candidate [16], or distributing subpopulations over different GPUs [1, 35], but in the end this still requires evaluation of subsets of candidate solutions sequentially. JAX [5] offers vectorization of mathematical computation on CPU and GPU. Evosax [27], EvoX [18] and EvoJAX [42] provide implementations of genetic algorithms, evolution strategies, differential evolution in JAX with high parallelization. Although these algorithms assume a fixed solution structure and can therefore easily be parallelized, it still shows the potential of JAX to reduce the computation time of GP.

In this paper we introduce Kozax<sup>1</sup>, a JAX-based framework for GP to evolve symbolic expressions, named in honour of John R. Koza, the founder of GP. By representing the parse trees as matrices, the fitness evaluation is parallelized on CPU and GPU, showing reduced computation times when evaluating large populations or datasets. Like other libraries for GP, Kozax can be used for symbolic regression of laws and dynamical systems. However, Kozax also has many additional features (Table 1), and gives users much freedom to define the desired functionality for which symbolic expressions should be discovered, for example for control tasks or objective function optimization. Our results show that Kozax competes with other libraries on symbolic regression problems both in speed and performance, but can handle a larger range of complex problems. Overall, Kozax demonstrates to be a scalable, general implementation of the GP framework and more.

## 2 Related Work

Genetic programming (GP) was introduced by Koza in [22], including many applications such as symbolic regression [22], robot movement optimization [24], planning, solving equations and finding a control strategy [23]. More recently, new tools have been developed that focus on symbolic regression using GP, either for dynamical systems or natural laws, including Eureqa [3, 39], DEAP [14], Operon [9] and PySR [12]. Another relevant method for symbolic regression is SINDy [7], which seeks expressions for dynamical systems through sparse regression. This method has seen great successes, and has been further developed to extend to partially observed data [20], control problems [8] and learn robust ensembles [13]. Other applications of GP include control policy optimization [17, 44, 32], evolving learning rules [19] and objective functions [37].

However, most GP frameworks were developed for specific applications, as there is still a lack of a unifying framework for GP. HeuristicLab [45] attempted to provide GP software that allows users to tune the fitness evaluation to their problems, but the software was limited by high computational requirements. More broadly used GP libraries, such as Eureqa and PySR, apply tricks like partitioning and the finite difference method to the input data to improve

 $<sup>^{1} \</sup>verb|https://github.com/sdevries0/Kozax|$ 

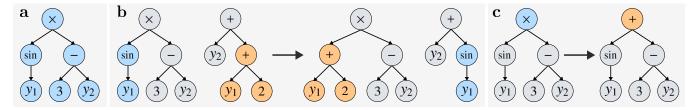


Figure 2: Overview of trees and reproduction in genetic programming. (a) An example of the parse tree representation used in genetic programming. (b) An example of crossover on a pair of trees, where the blue and orange subtrees are swapped. (c) An example of mutation on a tree, where the operator in blue is replaced with the new operator in orange.

the convergence to correct solutions. This requires the data to be provided in a specific format, focusing strictly on symbolic regression problems. Therefore, these libraries cannot be applied, without utilizing external methods, to other tasks involving numerical integration of differential equations or evaluating control policies in different environments.

The specific data format required in Eureqa and PySR helps to reduce the runtime of fitness evaluation, which is typically the most time consuming process of GP. Parallelization of the fitness evaluation also improves the computation speed of GP. Previous work parallelized the evaluation of a single tree on many data points [16]. However, this setup still requires the evaluation of different trees to be performed sequentially. A different approach is to evolve and evaluate different subpopulations on different processing nodes [1, 35], which shows a linear relation between runtime and the number of subpopulations. To parallelize the evaluation of many solutions, general GP interpreters on GPU were developed [26, 38, 10], showing large speed improvements. Still computational overhead remains, because each tree on a GPU thread has to be compiled by the interpreter.

In [32], linear and Cartesian GP were implemented in JAX, allowing for parallelization of the fitness evaluation of all candidate solutions, as well as parallelization of the reproduction stage. Their implementation, however, was solely focused on learning control policies and does not allow users to apply the library to their own problems. NEAT is another direction in evolutionary computing that evolves the structure of small neural networks [40]. Similar to GP, the applicability of NEAT is limited by computational bottlenecks [47]. Ref. [47] showed that with tensorization of the NEAT algorithm, JAX can be used to parallelize fitness evaluation and significantly reduce the runtime of the algorithm compared to existing implementations. Still, NEAT specializes in optimizing the structure of neural networks for control tasks, while GP is a more general algorithm.

We developed Kozax with the intention to introduce a GP framework that provides both applicability to arbitrary problems and efficient fitness evaluation. Implemented in JAX, Kozax vectorizes the population, allowing for full parallelization of fitness evaluation, initialization and reproduction, therefore no longer requiring compilation of trees to executable programs. Consequently, Kozax can run on either CPU and GPU, where the latter allows Kozax to scale the fitness evaluation to large datasets or populations. Furthermore, the functionality for fitness evaluation is not embedded in Kozax, therefore the fitness function can be adjusted by users for their problems of interest. This flexibility makes Kozax a general library for GP, while not sacrificing computational efficiency.

# 3 Genetic programming

GP is a variant of evolutionary algorithms that evolves the structure of computer programs [22]. In Kozax, we focus on evolving symbolic expressions represented by parse trees, a subset of computer programs. Parse trees consist of mathematical operators as interior nodes and variables and constants as the leaf nodes. Parse trees are executed recursively, where child nodes have to be computed before their parent node. An example of the parse tree representation is presented in Figure 2a.

In GP, a population of solutions is optimized on a specified task through stochastic optimization. See Algorithm 1 for an overview of the GP algorithm. To evaluate the fitness of a candidate solution, it is transformed into a executable program and tested on a problem. The performance of a candidate solution is expressed by a fitness score, computed with a fitness function. The fitness scores are used to select individuals for reproduction, where fitter individuals produce more offspring.

### Algorithm 1 Genetic programming algorithm

**Input** Number of generations G, population size N, elite percentage E, fitness function F

```
1: initialize population P with size N
 2: for g in G do
        evaluate each individual in P on F
 3:
        offspring O \longleftarrow \emptyset
 4:
        append fittest E of P to O
 5:
        while size(O) < N do
 6:
           select parents p from P
 7:
           children c = reproduce(p)
 8:
           append c to O
 9:
        end while
10:
        P \longleftarrow O
11:
12: end for
13: return fittest individual in P
```

In every generation a new population is evolved, consisting of new solutions that are generated by reproducing existing solutions with crossover and mutation. In crossover, the genotype of two individuals is combined to produce new solutions. In both parents a random node is selected, after which these nodes and the corresponding subtrees are swapped. An example of the crossover operator is shown in Figure 2b. Mutation is applied to a single individual to generate one offspring. Many aspects of trees can be mutated, for example changing, deleting or adding operators, replacing subtrees or changing variables or constants. Figure 2c shows an example of mutation, in which an operator is changed to a different type of operator.

## 4 Kozax

Kozax is a GP library for general and efficient problem optimization, implemented in JAX [5]. In this section, the major features of Kozax are described in more detail. Afterwards, we will explain the vectorized representation of solutions adopted in Kozax, and how this representation allows for parallelization of fitness evaluation.

#### 4.1 Features

Table 1 shows a comparison between the most important features in PySR [12] and Kozax. PySR provided an extensive comparison with other frameworks for GP and symbolic regression [12]. PySR has some features that are currently not present in Kozax, such as placing constraints on symbolic operators that improve interpretability and reduce the search space. In the remainder of this section, the major features present in both libraries are described, followed by the advantages of the features exclusively available in Kozax.

First of all, Kozax and PySR make use of just-in-time (JIT) compilation to minimize computational overhead and improve the computation speed. In PySR, compilation is used to combine multiple operators into a single compiled operator, which speeds up fitness evaluation. In Kozax, the fitness evaluation and reproduction functionality are compiled, resulting in large speed improvements, as the complete population is evaluated and evolved in parallel. Both libraries allow users to define custom operators and fitness functions, which remains compatible with JIT compilation.

Furthermore, both PySR and Kozax keep track of the best solutions in a Pareto front throughout evolution. The Pareto front stores the best solution in terms of fitness at every complexity level, and finally includes solutions only when the fitness is improved over less complex solutions. One feature only present in PySR is that the best solutions from earlier generations are randomly reintroduced at later stages in evolution. In Kozax, the Pareto front is solely used for keeping track of the best solutions. Both libraries use a SymPy interface [29] to represent the individual solutions. In Kozax, the discovered expressions after evolution, but PySR also applies simplification throughout the optimization process.

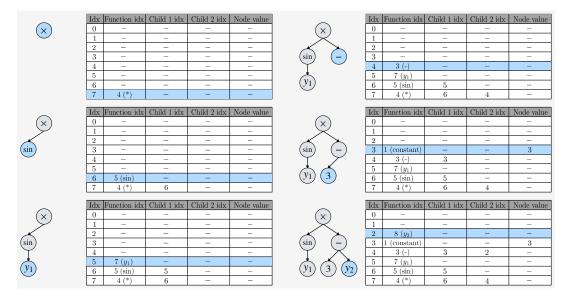


Figure 3: **Step-by-step mapping of a tree to a matrix.** The node added in the tree and the corresponding row in the matrix are marked blue at every step. The references to child nodes are added to the relevant rows once the child node itself has been added to the tree.

An important improvement of the standard GP algorithm is to integrate an external method for optimization of the constants in individual solutions [43]. In PySR, the Broyden–Fletcher–Goldfarb –Shanno (BFGS) algorithm is utilized for constant optimization by default. Kozax provides gradient-based optimization, based on automatic differentiation in JAX, and a simple version of a genetic algorithm to optimize constants. Kozax offers these two methods for constant optimization, as either method may be more effective for balancing computation time and performance in specific tasks. To reduce the computational load, users can specify the number of solutions to apply constant optimization to. When using gradient-based optimization, the number of epochs for each optimized solution can be defined, and when using genetic algorithms, both the number of iterations and the population size are tunable. These factors together result in the number of constant optimization steps.

One feature that differentiates Kozax from PySR and other GP implementations, is the ability for users to completely define the functionality for which trees are evolved. This includes when a tree is evaluated in the fitness evaluation, what its inputs are and where the output of a tree is used. A related feature is the ability to optimize multiple trees in Kozax, with an option to provide different operator and variable sets for individual trees. These two options allow Kozax to be applied to problems other than standard symbolic regression tasks, such as control policy optimization or inferring equations of hidden variables without requiring external methods.

PySR parallelizes the fitness evaluation over multiple CPU cores, which is also available in Kozax. However, a large advantage of Kozax over PySR is the ability to run the algorithm on GPU, and even distribute over multiple GPUs nodes. On GPU, Kozax scales the fitness evaluation to large populations or datasets efficiently, where Kozax and PySR obtain high computation time on CPU. Altogether, these features make Kozax a general, high-performing and scalable GP library.

### 4.2 Tree representation

Kozax implements the GP algorithm using JAX [5]. Typical applications of GP include symbolic regression, policy optimization and other problems that benefit from interpretable solutions. As these are challenging problems, being able to evaluate large populations efficiently is advantageous. JAX offers features for faster computation, high scalability and high-performance machine learning, like vectorization of functions, just-in-time compilation and automatic differentiation. Accordingly, Kozax makes use of these features to improve runtime, scale to large populations and evolve accurate solutions.

Parallelization of different tree structures in GP is not trivial, as the trees in a population have varying structures. To this end, the trees are represented as matrices with a fixed size in Kozax. In cartesian and linear GP, the matrix

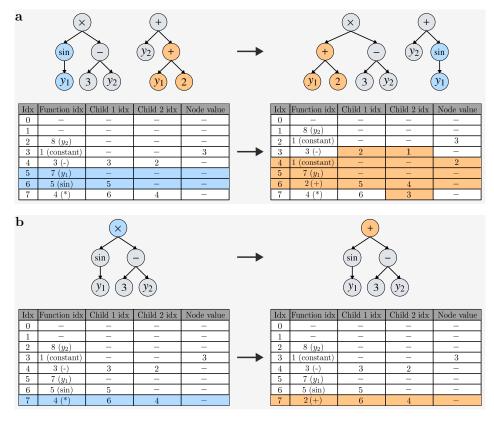


Figure 4: **Evolution of new trees in Kozax.** (a) Crossover applied to a pair of trees, producing two new trees. A random node is selected in both trees and the corresponding subtrees are swapped, indicated by the blue and orange subtrees. The matrix shows the representation of the left tree before and after crossover, where the blue and orange rows correspond to the removed and added subtrees respectively. The orange cells in the child index columns indicate a change in the reference to a child node. (b) Mutation is applied to a tree to evolve a new tree. In this example, the root node changes from a multiplication to an addition. The matrix representation is shown before and after mutation in blue and orange respectively.

representation is more natural [32], but we opted for the standard form of GP with parse trees, as it is a more general algorithm. Figure 3 presents a step-by-step mapping of a tree to a corresponding matrix. Figure 3 is purely illustrative, as mapping to matrix form produces computational overhead and therefore matrix representation is adopted at every step in evolution. Each row in the matrix represents a node in the tree, limiting the number of nodes in a tree to the matrix size. A row defines a node with an integer representing the function of the node, the node indices of the children of this node and the computed value of the node, which is set to 0 before execution. Before initialization, Kozax maps the set of operators and variables to unique indices, which cover the possible values a node can have. Constants are represented with a function index set to 1, and the value of the constant is directly stored in the solution column. Empty rows are represented by a 0 and nodes without children do not have references to other nodes.

The matrix is defined with the root node as the last row, as solving the tree requires that the values of child nodes are computed before the parent node will be executed. During evaluation, the computed value of a node is stored in the final column, which are available to nodes higher in the tree. To compute the value of a certain node, the corresponding function is executed with the value of the child nodes as inputs, as well as the values of the input variables. If the function represents a constant, it will store the value of the constant. If the function represents a variable, it will store the relevant value from the provided input variables. If the function represents an operator, it will compute the value given the inputs and store this. An empty node will return 0, but is never referred to by other nodes. The final outcome of the tree is obtained by returning the stored value of the last row.

With this representation, all trees can be evaluated simultaneously. Kozax also performs initialization and

Table 2: Hyperparameters used in each experiment. CO steps refers to the number of constant optimization steps performed at each generation. The LV equations represent the Lotka-Volterra dynamics.

Experiment	Generations	Population size	CO steps	Operators
Kepler's third law	100	1000	25000	$+, -, \times, \div$ , power
Newton's law of universal gravitation	100	1000	25000	$+, -, \times, \div, \text{power}$
Bode's law	100	1000	25000	$+, -, \times, \div$ , power
Fully observable LV equations	100	1000	25000	$+, -, \times, \div, \text{power}$
Partially observable LV equations	100	2000	100000	+, -, ×
Acrobot	50	1000	1000	$+, -, \times, \div$ , power, sin, cos
Objective function	50	1000	0	$+, -, \times, \div$ , power, log, exp

reproduction in matrix space, therefore these stages are also vectorized to further reduce computation speed. Unlike grammar evolution [34] or Cartesian GP [30] that make use of matrices or grid-like structures, Kozax adheres to the tree hierarchy in standard GP throughout evolution. This means that the matrices have to be adjusted accordingly when trees are evolved. Figure 4a shows how crossover is applied in matrix space. Old rows resembling a subtree in the current tree are replaced with rows representing a subtree from the other parent. Additionally, index references have to be updates because the size of the subtree may change. In mutation, a single row is adapted to match the mutated node, as shown in Figure 4b. For other mutation types, similar functionality is implemented to evolve matrices.

## 5 Results

## 5.1 Experiments

We tested Kozax in six experiments, both to demonstrate its ability to find accurate solutions and the variety of problems that can be studied. PySR showed to outperform other GP libraries in their paper [12], therefore we chose PySR as a competitive baseline for Kozax. Experiments and hyperparameters used in each experiment are presented in Table 2. The number of generations and population size are used in both Kozax and PySR, but the number of constant optimization steps is only relevant in Kozax. In each experiment, except for evolving the loss function, the genetic algorithm is used for constant optimization. The experiments include symbolic regression of laws and dynamic systems, optimizing a symbolic control policy and evolving a loss function. The two libraries are evaluated on ten different seeds, which influence both the data generation and the initial population. Both Kozax and PySR return a Pareto front, containing the best solution at every complexity level that was discovered throughout evolution. The results are reported as the fraction of runs in which a successful solution was included in the Pareto front, where the determination of a successful solution are explained in the experiments respectively. Results are shown in Table 3. The raw data and code to reproduce the results are available at https://github.com/sdevries0/kozax\_paper.

### 5.1.1 Law discovery

The first three experiments entail symbolic regression of Kepler's third law [21], Newton's law of universal gravitation [33] and Bode's law [4]. To accomplish the task, the correct equation structure and parameters should be discovered that represent each law. A symbolic expression receives the inputs corresponding to each law, which are mapped to a predicted value. The fitness function is computed as the absolute mean error between the predictions and the targets. PySR generated the datasets for each law based on the original papers or given realistic ranges for the variables [12].

Both libraries are able to evolve the correct expressions in the majority of the runs, although Kozax failed to evolve the correct equation for Kepler's third law in one run. Overall, both libraries quickly find correct equation structures and parameter values for these laws.

Table 3: Results of PySR and Kozax on a set of experiments. Each task was run with 10 different seeds, changing the initial population and data generation. The fraction shows the number of runs in which an accurate solution was evolved. A dash means that an experiment was not possible to conduct given the library without involving external methods.

Experiment	Evaluation method	PySR	Kozax
Kepler's third law	Regression	10/10	9/10
Newton's law of universal gravitation	Regression	10/10	10/10
Bode's law	Regression	10/10	10/10
Fully observable Lotka-Volterra equations	Finite difference	10/10	10/10
Partially observable Lotka-Volterra equations	Numerical integration	-	7/10
Acrobot	Control loop simulation	-	10/10
Loss function	Train neural network	-	10/10

#### 5.1.2 Symbolic regression of dynamical systems

The next experiment is symbolic regression of the Lotka-Volterra equations [15], a dynamical system governing the population of preys and predators. As methods such as PySR and SINDy make use of the finite difference method, we opted to use this method in Kozax as well. One trajectory of the Lotka-Volterra dynamics is integrated, given a randomly sampled initial condition. Afterwards, the true derivative of the state is computed for every time step. Symbolic regression is then performed with the states as the inputs and the derivatives as the target outputs. The fitness function is again the mean absolute error between the predicted and true derivatives. A successful solution recovers the equations for both variables, including the correct coefficients. PySR and Kozax are able to successfully rediscover the equations of both the prey and the predator in all runs.

The finite difference method allows symbolic regression of dynamical systems with PySR. However, this only works when all dimensions of the system are observed. In the fifth experiment, only the prey is observed in the Lotka-Volterra model, which requires GP to find two equations and integrate them as a system of ordinary differential equations. The evolved equations are integrated from the true initial condition, and the fitness is computed as the mean absolute error between the predicted and true prey populations, plus an additional penalty when either population is negative at any timepoint. This is not possible in PySR without involving external methods, but in Kozax the fitness function can be adjusted to integrate differential equations with latent variables. Kozax recovers the equations of both the prey and predator populations in eight out of ten runs.

#### 5.1.3 Symbolic control policy optimization

In this experiment, a symbolic control policy was evolved to solve the acrobot swing-up task [41]. The fitness function is a sparse reward function, returning the first time point at which the swing-up was satisfied. The proposed policies return continuous values, but these values are mapped to [-1, 1] given the sign of the policy's output. A policy observes the sine and cosine of the angles of the first and second link, and the angular velocities of the two links. The acrobot task is simulated for a fixed number of time steps using Gymnax [28], a JAX implementation of Gym's control environments. A successful evolutionary run entails that a solution is discovered that solves the acrobot swing up within the specified number of time steps.

PySR could discover a symbolic policy by distilling a pre-trained black-box policy, however the accuracy heavily depends on the quality of the teacher policy, and information might be lost in the distillation stage. Therefore, it is advantageous to optimize a symbolic policy through direct interaction with the control environment. In Kozax, it is possible to evaluate solutions on control tasks directly, and Table 3 shows that Kozax evolves successful policies in all runs, while PySR is not compatible with the task.

#### 5.1.4 Evolving an objective function

Learning the objective function is a direction within the field of meta-learning that can improve convergence speed and robustness [2]. Previously, GP has been used to learn a symbolic expression for the loss function in various

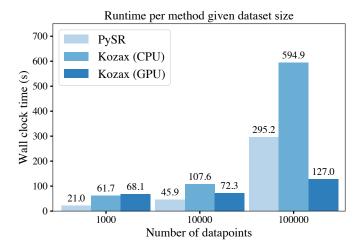


Figure 5: Runtime analysis of PySR and Kozax. The wall clock runtime is measured for PySR and Kozax to complete a fixed number of generations, given different dataset sizes. The runtime of Kozax is measured when running either on CPU and GPU. The wall clock time shows the average over three runs.

problems [37]. In the final experiment, a neural network is trained with backpropagation on the binary XOR classification problem using the evolved loss function. The input data consists of uniform samples between zero and one in two dimensions, and the target is zero when both dimensions of the input are either smaller than 0.5 or larger than 0.5, and one otherwise.

The loss function is tested on different batches of data and weight initializations of the neural network to prevent overfitting of the loss function. Each instance of a neural network is randomly initialized with two hidden layers, each with 16 hidden neurons. The activation functions of the two hidden layers are tanh, and the final layer applies a sigmoid to produce logits. The neural networks are trained for a 500 epochs, using an Adam optimizer with a learning rate of 0.01. The evolved loss function is applied to individual pairs of neural network predictions and targets, after which the loss is computed by averaing over the complete batch. After training, the final neural network is applied to unseen data, and the test accuracy is computed given the predicted labels. The test accuracy is used as the fitness of the proposed loss function.

During objective function optimization, the target outputs for fitness evaluation are not available. Therefore, PySR is incompatible with the task in this experiment. However, the fitness evaluation in Kozax can be adjusted to learn the objective function to train neural networks. Table 3 shows that Kozax discovers a loss function that enables the neural network to reach a test accuracy of at least 95%.

## 5.2 Runtime analysis

The results show that Kozax competes with PySR on the symbolic regression tasks in terms of performance, and that Kozax can handle a wider range of tasks. However, another important aspect of Kozax is the computational efficiency. In Figure 5, the average wall clock time of PySR and Kozax is presented on a symbolic regression task. The task was repeated with different datasets, where the number of data points that have to be evaluated by each candidate solution increases. As Kozax can be deployed on both CPU<sup>2</sup> and GPU<sup>3</sup>, the runtime is measured for each device. Note that the accuracy of the found solutions does not matter in this experiment, and that the wall clock time was measured given a fixed number of generations and population size.

Figure 5 shows that PySR is faster than Kozax on CPU for each dataset size. Kozax requires more time for the just-in-time compilation, which explains the relatively large difference in runtime between PySR and Kozax for 1000 data points. The difference decreases relatively for larger datasets, as the compilation time is a smaller fraction of the total runtime. When the dataset contains 1000 items, both PySR and Kozax on CPU are faster than Kozax on GPU. However, when the number of data points increases to 10000, Kozax on GPU is slightly faster than Kozax on

<sup>&</sup>lt;sup>2</sup>AMD Genoa 9654, 64 cores

<sup>&</sup>lt;sup>3</sup>NVIDIA A100

CPU, and the difference compared to PySR becomes smaller. The difference in runtime becomes significantly large when the number of data points grows to 100000, where Kozax on GPU shows a speed up of more than factor 2 compared to PySR. The wall clock time of Kozax on GPU increases only slightly when more data points have to be evaluated. Kozax demonstrates to be extremely scalable when confronted with large datasets or population sizes because it can be deployed on GPU.

## 6 Discussion

In this paper, we introduced Kozax, a library for genetic programming (GP) built on JAX. By representing trees as matrices, while following the standard GP algorithm, Kozax parallelizes the evaluation of trees with different structures. This way, the fitness evaluation is sped up compared to evaluating candidate solutions sequentially. Additionally, Kozax runs op GPU, therefore the fitness evaluation scales efficiently to large populations or datasets.

GP has shown promising performance in several domains, such as symbolic regression [3, 12] and symbolic policy optimization [17, 44]. Most GP libraries are designed specifically for a certain class of problems, however a general framework that can handle arbitrary problem classes was still missing. We developed Kozax to give users much freedom in their problem definition. In the results, we showed that Kozax performs competitively compared to PySR on symbolic regression tasks. Yet, Kozax can also be applied to evolve control problems and objective functions, which is impossible with PySR without using external methods. Besides the scalability, another advantage of Kozax is that it flexibly learns trees for desired functionality.

As demonstrated, the matrix representation of trees in Kozax improves the computation speed of fitness evaluation and reproduction. The representation of the solution space has resemblances to related algorithms like grammar evolution [34], Cartesian GP [30] and linear GP [6]. In Kozax, the matrices implicitly adhere to the hierarchical tree structure in the standard GP algorithm. A big advantages of Kozax is that only rows with active nodes can be changes during evolution, while grammar evolution, Cartesian GP and linear GP suffer from the inefficiency that inactive nodes are changed during evolution. To our knowledge, Kozax is the first implementation that uses a matrix representation for the standard GP algorithm.

Although Kozax demonstrated efficient evolution of accurate solutions, there are still features that could further improve the applicability of Kozax to complex problems. PySR showed that integrating simplification of expressions throughout evolution and adding constraints of symbolic functions improve the interpretability of the discovered expressions [12]. Another improvement would be allow for higher-dimensional inputs and outputs in the trees, which relates to strongly typed GP [31]. Processing higher-dimensional inputs would enable Kozax to be applied to visual data or vector operations. Being able to evolve a tree with multiple outputs allows to learn the same functionality for multiple variables, which could for example evolve compact neural network structures. Extending GP with automatically defined functions (ADF) supports learning useful building blocks that may be included repeatedly in other trees. Especially when evolving multiple trees simultaneously, it would be efficient to reuse functionality in different trees. The additional value of ADFs increases even more when operators with more than two inputs could be evaluated in Kozax, as complex functions structure can be evolved.

In fields such as scientific discovery [46] and explainable artificial intelligence [36], it is beneficial to have interpretable white-box models. As GP automatically generates interpretable computer programs, it is a fundamental approach to optimize white-box models. By utilizing GP, the resulting models may provide knowledge about the underlying system, as seen in symbolic regression, or transparency in decision with symbolic control policies. With the development of Kozax, we hope to contribute to the creation of trustworthy artificial intelligence.

# 7 Acknowledgements

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