EC-KitY: Evolutionary Computation Tool Kit in Python with Seamless Machine Learning Integration

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Abstract

\textbf{EC-KitY} is a comprehensive Python library for doing evolutionary computation (EC), licensed under the BSD 3-Clause License, and compatible with \texttt{scikit-learn}. Designed with modern software engineering and machine learning integration in mind, \textbf{EC-KitY} can support all popular EC paradigms, including genetic algorithms, genetic programming, coevolution, evolutionary multi-objective optimization, and more. This paper provides an overview of the package, including the ease of setting up an EC experiment, the architecture, the main features, and a comparison with other libraries.

\textit{Keywords:} Evolutionary Algorithms, Evolutionary Computation, Genetic Programming, Machine Learning, \texttt{scikit-learn}

1. Introduction

In Evolutionary Computation (EC)—or Evolutionary Algorithms (EAs)—core concepts from evolutionary biology—inheritance, random variation, and selection—are harnessed in algorithms that are applied to complex computational problems. As discussed by Sipper et al. \cite{Sipper2021}, EAs present several important benefits over popular machine learning (ML) methods, including: less reliance on the existence of a known or discoverable gradient within the search space; ability to handle design problems, where the objective is to design new entities from scratch; fewer required a priori assumptions about the problem at hand; seamless integration of human expert knowledge; ability to solve problems where human expertise is very limited; support of interpretable solution representations; support of multiple objectives.
Importantly, these strengths often dovetail with weak points of ML algorithms, which has resulted in an increasing number of works that fruitfully combine the fields of EC and ML or deep learning (DL). For example, Sipper and Moore \cite{2} “converted” a selection method in EC to a random forest ensemble producer; Lapid and Sipper \cite{3} used EC to evolve activation functions for DL-based image classifiers; Lapid et al. \cite{4} designed an evolutionary algorithm for generating adversarial instances in deep convolutional neural networks; Livne et al. \cite{5} utilized EC and DL to create accurate and interpretable context-aware recommender systems. Major conferences in the field of EC now regularly address the combining of EC and ML, e.g., GECCO, arguably the major EC event, devotes two entire tracks and three workshops to the blending of evolution and learning. There are a number of good surveys on evolutionary machine learning: Telikani et al. \cite{6}, Al-Sahaf et al. \cite{7}, and Zhang et al. \cite{8}.

EC is thus a popular family of potent algorithms that complements ML and DL to the benefit of all fields concerned. Further, there is a large and growing community of EC+ML practitioners. We have used several EC open-source software packages over the years and have identified a large “hole” in the software landscape—there is a lacuna in the form of an EC package that is:

1. A comprehensive toolkit for running evolutionary algorithms.
2. Written in Python.
3. Can work with or without scikit-learn (aka sklearn), the most popular ML library for Python. To wit, the package should support both sklearn and standalone (non-sklearn) modes.
4. Designed with modern software engineering in mind.
5. Designed to support all popular EC paradigms: genetic algorithms (GAs), genetic programming (GP), evolution strategies (ES), coevolution, multi-objective, etc’.

While there are several EC Python packages, none fulfill all five requirements. Some are not written in Python, some are badly documented, some do not support multiple EC paradigms, and so forth. Importantly for the ML community, most tools do not intermesh with extant ML tools. Indeed, we have personally had experience with the hardships of combining EC tools with scikit-learn when doing evolutionary machine learning. We hope that by adhering to the above five pillars EC-KitY will be deemed useful by a large community.
2. **EC-KitY**

2.1. Setting up an evolutionary experiment

**EC-KitY** is available at [github.com/ec-kity/ec-kity/](https://github.com/ec-kity/ec-kity/), along with examples, tutorials, Google Colab notebooks, and more. Installing it is simply done by:

```
pip install eckity
```

As noted, **EC-KitY** can work both in standalone, non-sklearn mode, and in sklearn mode. In the following code examples, we use both modes for solving a symbolic regression problem, where the goal is to seek regressors of arbitrary complexity, i.e., beyond linear or polynomial ones [9].

We begin with the standalone mode, demonstrating how the user can run an EA with a mere three lines of code:

```
from eckity.algorithms.simple_evolution import SimpleEvolution
from eckity.subpopulation import Subpopulation
from examples.treegp.non_sklearn_mode.symbolic_regression.sym_reg_evaluator
    import SymbolicRegressionEvaluator

algo = SimpleEvolution(Subpopulation(SymbolicRegressionEvaluator()))
algo.evolve()
print('algo.execute(x=2, y=3, z=4):', algo.execute(x=2, y=3, z=4))
```

An algorithm can operate on a single Subpopulation (as in the case of SimpleEvolution), two Subpopulations (e.g., in a coevolutionary setup), or $n > 2$ Subpopulations (e.g., island model). Each Subpopulation may have its own evaluation function, which is why in the above example the SymbolicRegressionEvaluator is a parameter of Subpopulation. There are additional parameters of Subpopulation (e.g., genetic operators), and the algorithm (e.g., breeder and statistics). In the example, these parameters received the default values. The default function set is \([\text{add, sub, mul, div}]\), the default terminal set is \(['x', 'y', 'z', 0, 1, -1]\), and there are additional parameters, as defined in the API [10]. Below we show examples that demonstrate, among others, the use of non-default values.

The above code takes 4 minutes to run in Google Colab; by adding a simple early-termination condition (as in the last example below) runtime can be reduced to 9 seconds.
Here is an example of an evolved GP tree:

```
add
  add
    z
    z
  add
    z
    y
  add
    x
    y
```

The evolved tree’s fitness (mean absolute error) is 9.41e-15. The code’s output was:

```
algo.execute(x=2, y=3, z=4): 20
```

Running an EA in sklearn mode is just as simple (again, a symbolic-regression problem):

```
from sklearn.datasets import make_regression
from sklearn.metrics import mean_absolute_error
from sklearn.model_selection import train_test_split

from eckity.algorithms.simple_evolution import SimpleEvolution
from eckity.creators.gp_creators.full import FullCreator
from eckity.genetic_encodings.gp.tree.utils import create_terminal_set
from eckity.sklearn_compatible.regression_evaluator import RegressionEvaluator
from eckity.sklearn_compatible.sk_regressor import SKRegressor
from eckity.subpopulation import Subpopulation

X, y = make_regression(n_samples=100, n_features=3)
terminal_set = create_terminal_set(X)
algo = SimpleEvolution(Subpopulation(creators=FullCreator(terminal_set=terminal_set),
                                      evaluator=RegressionEvaluator()))
regressor = SKRegressor(algo)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)
regressor.fit(X_train, y_train)
print('MAE on test set:',
      mean_absolute_error(y_test, regressor.predict(X_test)))
```

In this example, we wrap the algorithm as a sklearn regressor and execute it from sklearn. The toolkit repository contains examples of more-advanced ways in which EC-KitY interacts with sklearn, including grid search and pipeline.

Running this code in Google Colab took 14 minutes without an early-termination condition, and the output was:

```
MAE on test set: 0.07
```
The user may wish to specify additional components of the EA rather than rely on default values; this can be readily achieved through the relevant constructor, e.g.:

```python
algo = SimpleEvolution(
    Subpopulation(creators=
        RampedHalfAndHalfCreator(init_depth=(2, 4),
        terminal_set=terminal_set,
        function_set=function_set,
        bloat_weight=0.0001),
    population_size=200,
    evaluator=SymbolicRegressionEvaluator(),
    higher_is_better=False,
    elitism_rate=0.05,
    operators_sequence=[
        SubtreeCrossover(probability=0.9, arity=2),
        SubtreeMutation(probability=0.2, arity=1),
        ERCMutation(probability=0.05, arity=1)
    ],
    breeder=SimpleBreeder(),
    max_workers=4,
    max_generation=500,
    statistics=BestAverageWorstStatistics(),
    termination_checker=
        ThresholdFromTargetTerminationChecker(optimal=0, threshold=0.001)
)
```

Detailed API, tutorials, and several use cases are available at [10].

### 2.2. Architecture

As previously noted, we plan for EC-KitY to support all main EC paradigms, including genetic algorithms, genetic programming, evolution strategies, coevolution, and evolutionary multi-objective optimization. To support this plethora of algorithms and genetic operators, we based our design on ECJ, likely the most comprehensive EC package to date, which has been in use and under development for over two decades [11]. We did, however, veer away from ECJ on a crucial point: Statistics can be drawn from any operation using event hooks, thus improving the decoupling and the separation of concerns.

The architecture of EC-KitY is depicted in Figure[1]. The Algorithm class serves as the entry point to EC-KitY. It contains all the needed information for an experiment and acts on the population using the Breeder class. Several classes extend the Operator class (these are denoted by a small triangle); they emit events that can be intercepted by Statistics. The same EC-KitY code can be used both in standalone mode (Figure[1] left) and in sklearn mode.
Figure 1: The general architecture of EC-KitY (left), and the added components for sklearn mode (right).

(EC-KitY) is designed to be easily extended: it is heavily over-architected, with many hooks that facilitate system modification and enhancement. The architecture supports the following features: execution in the cloud or in a cluster, multiple statistics, multithreaded evaluation, replicability standards (all of which have already been implemented), as well as checkpointing and logging facilities (under active development).

3. Comparison with Other Packages

Through considerable hands-on experience with EC open-source software over many years, and through additional extensive research, we have identified the following eight tools, whose major features are compared in Table 1, along with EC-KitY: gplearn, geatpy, DEAP, Platypus, ECJ, Jenetics, KEEL, and HeuristicLab.

Only two packages are written in Python and are also sklearn-compatible: geatpy and gplearn. However, as shown in Table 1, they lack many important features that EC-KitY possesses.

4. Concluding Remarks

The EC-KitY library is under active development. Presently, we plan to add a variety of evolutionary algorithms, individual types, genetic operators,
Table 1: Feature comparison of **EC-KitY** with extant software packages. ✔: feature exists, (✔): feature planned soon, ∃: feature mostly lacking, ✗: feature completely lacking.

| Feature                          | EC-KitY | geatpy | gplearn | DEAP | Platypus | ECJ | Jenetics | XEEL | HeuristicLab |
|---------------------------------|---------|--------|---------|------|----------|-----|----------|------|--------------|
| Language                        | Python  | Python | Python  | Python| Python   | Java| Java     | Java | Java         |
| sklearn-compatible              | ✔       | ✔      | ✔       | ✔    | ✔        | ✔   | ✔        | ✔    | ✔            |
| SE Design                       | ✔       | ✗      | ✗       | ✗    | ✗        | ✔   | ✗        | ✔    | ✗            |
| GA representations              | ✔       | ✔      | ✔       | ✔    | ✔        | ✔   | ✔        | ✔    | ✔            |
| GP representations              | ✔       | ✔      | ✗       | ✔    | ✔        | ✔   | ✔        | ✔    | ✔            |
| User-defined operators          | ✔       | ✗      | ✗       | ✔    | ✔        | ✔   | ✔        | ✔    | ✔            |
| User-defined representation     | ✔       | ✗      | ✗       | ✔    | ✔        | ✔   | ✔        | ✔    | ✔            |
| Coevolution                     | ✔       | ✗      | ✗       | ✔    | ✔        | ✔   | ✔        | ✔    | ✗            |
| Multiobjective                  | ✔       | ✔      | ✔       | ✔    | ✔        | ✔   | ✔        | ✔    | ✗            |
| Statistics                      | ✔       | ✔      | ✔       | ✔    | ✔        | ✔   | ✔        | ✔    | ✗            |
| Documentation                   | ✔       | ✔      | ✔       | ✔    | ✔        | ✔   | ✔        | ✔    | ✔            |
| API                             | ✔       | ✔      | ✔       | ✗    | ✔        | ✔   | ✔        | ✔    | ✗            |
| Latest version                  | 2022    | 2022   | 2019    | 2019 | 2020     | 2019| 2022     | 2015 | 2022         |

and tests. We are also working on extending and enhancing the documentation. We wish to broaden both the user and developer communities by implementing more sample use cases from different domains and by encouraging developers to contribute.

We recently taught a course in which 48 students worked in groups of two or three, submitting a total of 22 projects that used **EC-KitY** to solve a diverse array of complex problems, including evolving Flappy Bird agents, evolving blackjack strategies, evolving Super Mario agents, evolving chess players, and solving problems such as maximum clique and vehicle routing. **EC-KitY** proved quite up to the tasks.

Given the popularity and diverse applicability of evolutionary algorithms, we hope that **EC-KitY** finds multitudinous and beneficial uses.

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Required Metadata

Current code version

| C1 | Current code version | v0.3.0 |
| C2 | Permanent link to code/repository used for this code version | https://github.com/EC-KitY/EC-KitY |
| C3 | Permanent link to Reproducible Capsule | https://codeocean.com/capsule/8740191/tree |
| C4 | Legal Code License | BSD 3-Clause License |
| C5 | Code versioning system used | git |
| C6 | Software code languages, tools, and services used | Python |
| C7 | Compilation requirements, operating environments & dependencies | numpy (>= 1.14.6), pandas (>= 0.25.0), overrides (>= 6.1.0). For sklearn mode: scikit-learn (>= 0.24.2) |
| C8 | Link to developer documentation/-manual | API—https://api.eckity.org/eckity.html
Tutorials—https://github.com/EC-KitY/EC-KitY/wiki/Tutorials
Examples—https://github.com/EC-KitY/EC-KitY/tree/main/examples |
| C9 | Support email for questions | sipper@bgu.ac.il |

Table 2: Code metadata

Current executable software version

[18] A. Elyasaf, M. Sipper, Software review: The HeuristicLab framework, Genetic Programming and Evolvable Machines 15 (2014) 215–218.
| S1 | Current software version | v0.3.0 |
|----|--------------------------|--------|
| S2 | Permanent link to executables of this version | https://pypi.org/project/eckity |
| S3 | Permanent link to Reproducible Capsule | https://codeocean.com/capsule/8740191/tree |
| S4 | Legal Software License | BSD 3-Clause License |
| S5 | Computing platforms/Operating Systems | Cross-platform |
| S6 | Installation requirements & dependencies | numpy (>= 1.14.6), pandas (>= 0.25.0), overrides (>= 6.1.0). For sklearn mode: scikit-learn (>= 0.24.2) |
| S7 | Link to user manual | API—https://api.eckity.org/eckity.html Tutorials—https://github.com/EC-KitY/EC-KitY/wiki Tutorials Examples—https://github.com/EC-KitY/EC-KitY/tree/main/examples |
| S8 | Support email for questions | sipper@bgu.ac.il |

Table 3: Software metadata