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EDAspy: An extensible python package for estimation of distribution algorithms

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ABSTRACT

Estimation of distribution algorithms (EDAs) are a type of evolutionary algorithms where a probabilistic model is learned and sampled in each iteration. EDAspy provides different state-of-the-art implementations of EDAs including the recent semiparametric EDA. The implementations are modularly built, allowing for easy extension and the selection of different alternatives, as well as interoperability with new components. EDAspy is totally free and open-source under the MIT license.

1. Introduction

Estimation of distribution algorithms (EDAs) [1] are a type of evolutionary algorithms [2] in which traditional mutation and crossover operators are replaced by a probabilistic model that is iteratively learned and sampled during the optimization process. EDAs have been successfully applied to a wide range of tasks [3–6]. See [7] for a review on EDAs applied to solve machine learning tasks. In recent meetings within the field of EDAs [8] a need for establishing an EDA reference library has been identified. EDAspy is proposed to satisfy this need for the scientific community working on this topic.

In this paper we present a python package in which several EDA implementations are efficiently designed. The different optimizers are easily called and can be tuned in a user friendly mode. Each EDA variant is built using different available modules, which can be customly selected to build a new implementation. These variants can be easily extended and interoperate with new components.

2. Background

Algorithm 1 shows the pseudocode of the EDA baseline. Firstly, random population (G_0) with size N is sampled (line 1). Secondly, population G_{t-1} is evaluated (line 3) and ranked (line 4) according to a given cost function $g(\cdot)$. Thirdly, a probabilistic model is learned from a fraction α of the best individuals, i.e., the top $\lfloor \alpha N \rfloor$ solutions (line 5). Finally, a new population is sampled (line 6). These four steps are iterately repeated until the stopping criterion is met.

Depending on the complexity of the probabilistic model and the nature of the optimization problem, different EDA variants are identified in the literature.

Algorithm 1 Estimation of distribution algorithm

Input: Population size N, selection ratio α, cost function g
Output: Best individual $\boldsymbol{x}'$ and cost found $g(\boldsymbol{x}')$

1: $G_0 \leftarrow N$ individuals randomly sampled
2: **for** $t = 1, 2, \ldots$ until stopping criterion is met **do**
3: Evaluate G_{t-1} according to $g(\cdot)$
4: $G^S_{t-1} \leftarrow$ Select top $\lfloor \alpha N \rfloor$ individuals from G_{t-1}
5: $f_{t-1}(\cdot) \leftarrow$ Learn a probabilistic model from G^S_{t-1}
6: $G_t \leftarrow$ Sample N individuals from $f_{t-1}(\cdot)$
7: **end for**

Univariate approaches assume independence among the variables, and a probability distribution is fitted independently to each of them. EDAspy uses independent Gaussian distributions, kernel density estimation (KDE) or categorical probability distributions, depending on the EDA variant and the nature of the data.

Multivariate approaches contemplate dependencies between the variables using different probabilistic models. EDAspy uses multivariate Gaussians or different types of Bayesian networks (BNs) [9], corresponding to different EDA versions.

3. Software framework

Fig. 1 represents the high order representation of the previously mentioned modules in EDAspy. In general, an EDA implementation is applied to a cost function to be minimized, and some results are

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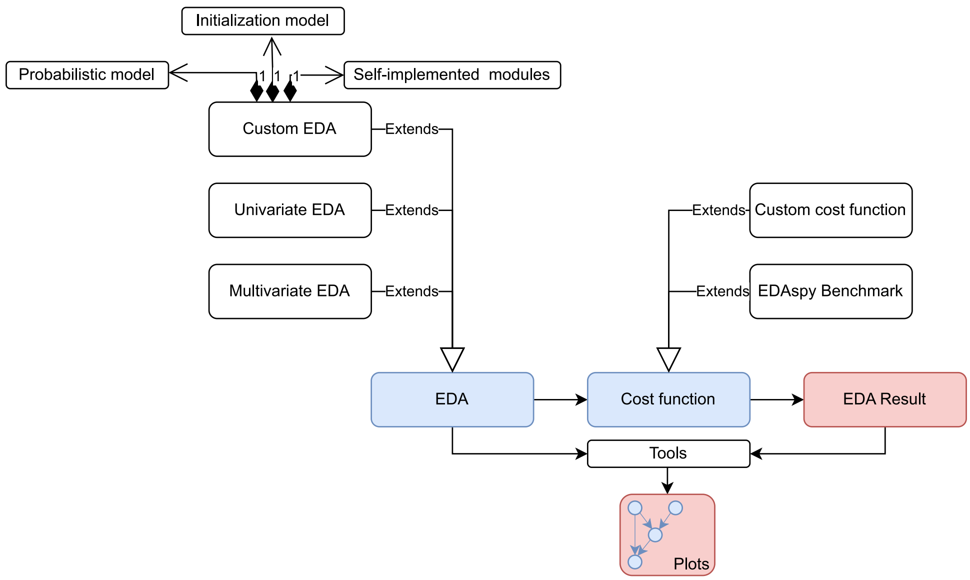


Fig. 1. High order organization of the EDAspy library.

found. There are several EDA implementations available in the library organized in univariate and multivariate modules, but it is also possible to build a customizable implementation by integrating the already available components with other modules (optionally) in the EDA object. Regarding the cost function, there are several benchmarks implemented. In addition, a custom cost function can be used. Once the optimizer has converged, several information and plots can be extracted from the execution.

Moreover, although the library has been built modular in order to allow the integration with new custom implementations, the EDA optimizer can be easily extended and built from scratch by the user without using *Custom EDA* module facilities.

`EDAspy` is organized in different modules:

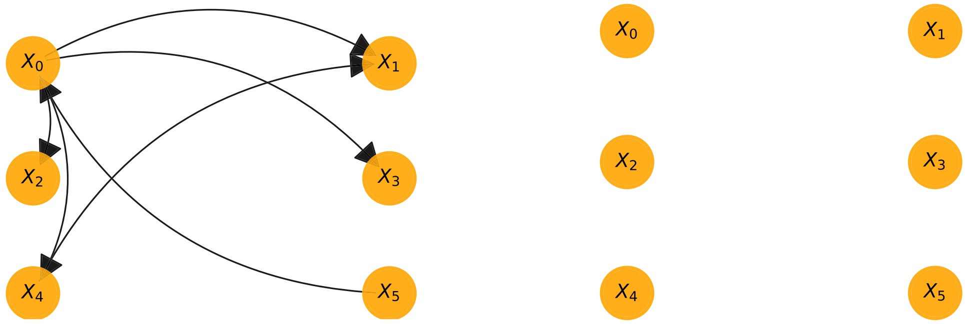
- **Benchmarks**. Different test functions for benchmarking and comparing the different optimizers are included. Toy discrete functions such as OneMax [10] and benchmark suites such as IEEE CEC 2014 [11] are included.
- **Univariate**. The following univariate approaches in which no dependencies between variables are considered: univariate marginal distribution algorithm (UMDA) for (i) binary [12] (UMDA_B), (ii) categorical (UMDA_D), and (iii) continuous optimization [13] (UMDA_C); (iv) kernel EDA [14] (u_KEDA); and (v) population-based incremental learning algorithm [15] (PBIL).
- **Multivariate**. The following multivariate approaches in which dependencies between variables are considered: (i) estimation of Bayesian network algorithm [1] (EBNA), (ii) estimation of multivariate normal algorithm [1] (EMNA), (iii) estimation of Gaussian network algorithm [16] (EGNA), (iv) semiparametric EDA [17] (SPEDA), and (v) multivariate kernel density EDA [17] (m_KEDA), (vi) Bayesian optimization algorithm (BOA) [18] in which a discrete BN, a multivariate Gaussian distribution, a Gaussian BN, a semiparametric BN, a kernel density estimated BN, and a discrete BN are iteratively learned, respectively.
- **Custom**: this module includes the different components to build a custom EDA variant and is divided into probabilistic and initialization models.
  - **Probabilistic model**. The following components are implemented for learning and sampling. Regarding univariate probabilistic models, (i) binary, (ii) discrete, (iii) Gaussian, and (iv) KDE models are considered. Regarding Bayesian networks, (v) Gaussian, (vi) semiparametric, (vii) KDE, and (viii) discrete models are available. Other models include (ix) multivariate Gaussian.
  - **Initialization model**. Uniform sampling meeting landscape user defined bounds, Latin hypercube sampling [19] and initialization from a given dataset are available to build the first population of the EDA.
  - **Self-implemented modules**. This includes modules implemented by users that can be integrated into the library.
- **Plotting tools**. The tools for graphically representing the probabilistic model embedded by the EDA are included in this module. Fig. 2 shows an example of two different probabilistic models. Panel (a) represents a Gaussian BN, in which dependencies between variables are considered, while panel (b) represent a univariate model, in which no dependencies are considered.

Regarding the multivariate EDA implementations, some of the probabilistic models are interfaced to `PyBNesian` library [20], which uses `C++` to speed up the back-end computations. All the algebraic computations in `EDAspy` are computed using `numpy` library [21], employing `C` to speed up the back-end computations. Moreover, the parallelization of the optimizer is available by using `multiprocessing` library [22,23], and can be optionally activated in all the EDA implementations.

4. Related work

Although there are several libraries in which different evolutionary algorithms are available, to the best of our knowledge we have not found comparable published libraries with different EDA implementations in `python`. However, here we list some libraries in which some EDA implementations are available.

- `mateda` [24] is a `matlab` library which allows building multivariate EDAs based on undirected probabilistic models and Bayesian networks. The purpose of the library is different from `EDAspy`. It offers a framework to build a multivariate EDA algorithm by modules, in which different components can be integrated. `mateda` implements categorical and Gaussian Bayesian networks, multivariate Gaussian distributions, Markov networks and mixtures of Gaussian distributions as probabilistic models. However, semiparametric and KDE Bayesian networks are missed, and the implementations for univariate approaches are omitted. Moreover, the last released version of `mateda` was in 2020.



(a) Gaussian BN structure (b) Univariate Gaussian structure

Fig. 2. Probabilistic models graphical representations.

Table 1
Summary of functionalities implemented in each library. Note that X^x denotes that the implementation is expected to be released in the near future.

	`EDAspy`	`mateda`	`inspyred`	`LEAP`
Language	`python`	`matlab`	`python`	`python`
UMDA$_C$	X		X	
UMDA$_D$	X			
UMDA$_B$	X			
u_KEDA	X			
PBIL	X			X^x
BOA	X			X^x
EMNA	X	X		
EGNA	X	X		
SPEDA	X			
m_KEDA	X			
EBNA	X	X		
Custom	X	X		

- `inspyred` [25] is a `python` library which implements general evolutionary algorithms such as genetic algorithms, evolutionary strategies, differential evolution and multi-objective genetic algorithms, among others. UMDA$_C$ is the only EDA implemented.
- `LEAP` [26] is a `python` library built for evolutionary computation and incorporates useful visualization modules. Regarding EDAs, the population-based incremental learning algorithm (PBIL) [15] and Bayesian optimization algorithm (BOA) [18] are expected to be available in future releases.

Table 1 summarizes the main differences between the listed libraries. Regarding univariate approaches, `inspyred` implements UMDA$_C$ and `LEAP` plans to integrate PBIL approaches in the near future, compared to the five implemented variants in `EDAspy`. Regarding multivariate approaches, `LEAP` will incorporate BOA approach, which is also implemented in `EDAspy`. The most competitive library is `mateda`, which overlaps with some of the implemented multivariate approaches. It also allows for building a custom EDA version with some additional probabilistic models. However, `mateda` is implemented in `matlab` and seems to be no longer updated.

5. Performance analysis

In this section we compare the performance of different continuous domain optimizers implemented in EDAspy. For the evaluation three different cost functions (to be minimized) have been selected from the benchmark suite in `EDAspy`: CEC14_3, CEC14_4 and CEC14_8, where the former is unimodal and the rest are multimodal functions.

Section 4 reviewed some existing software for EDAs in different programming languages. In this section we also compare the result found by the UMDA$_C$ approach implemented in `inspyred`. Although `mateda` and `LEAP` were also reviewed, the former is implemented in a different programming language, and thus it is not fair to be compared in terms of CPU time, and the latter does not currently include any of the implemented approaches.

All the optimizers have been configured equally in order to perform a fair comparison. Hyper-parameters and a more extended tutorial can be found in the original documentation.[1]

Since a statistical study is out of the scope of the paper (see [17] for a more complete analysis), we show a runtime and final solutions analysis of the different variants for continuous optimization in `EDAspy`.

Fig. 3 shows the mean best cost found after 5 independent executions. It is generally observed how in the three functions the best approaches are SPEDA, m_KEDA and EGNA, which find the minimal costs in the benchmarks. Previous analyses have shown that m_KEDA, SPEDA and EGNA approaches are able to achieve statistically significant improvements in terms of quality of solutions [17]. In the case of the UMDA$_C$ implementation from `inspyred` library, a slightly worse result is found in all the three benchmarks compared to the implementation provided in `EDAspy`.

Fig. 4 shows the mean CPU times of all the tested algorithms after 5 independent executions. Note that all the tested approaches have been configured in the same environment, that is, the number of function evaluations and hardware. It is observed that generally the higher the complexity of the probabilistic model embedded, the longer the CPU time required. However, PBIL is one of the slowest approaches in the comparison for CEC14_3. In this case, the multivariate version of KEDA is the most expensive algorithm in terms of CPU time, followed by SPEDA and EGNA. In the case of the UMDA$_C$ implementation from `inspyred` library, our implementation seems to be more efficient implemented in terms of CPU time consumption, keeping a good performance in terms of results found (Fig. 3).

6. Illustrative examples

The following examples are available in the original documentation[1], where different EDAs are applied to different tasks:

- Using UMDA$_C$ for continuous optimization. UMDA$_C$ is tested on a IEEE CEC 2014 benchmark.
- Using SPEDA for continuous optimization. SPEDA is tested on a provided benchmark and several convergence plots are shown.
- Using EGNA for continuous optimization. SPEDA is tested on a provided benchmark and the plotting tools module is used to graphically show the probabilistic model embedded into the EDA approach.

[1] https://github.com/VicentePerezSoloviev/EDAspy/blob/master/notebooks/CPU%20time%20analysis.ipynb.

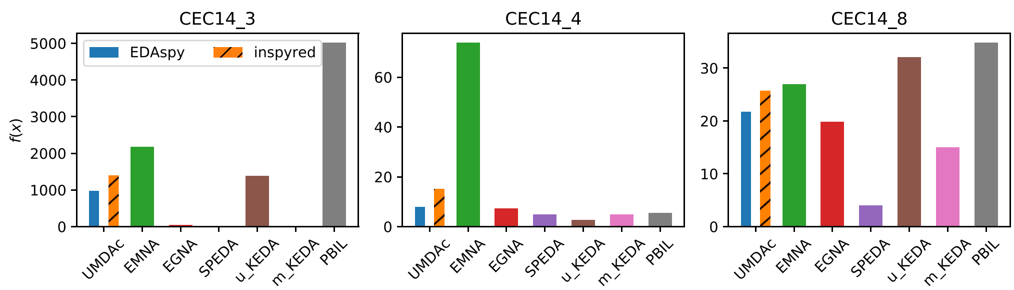


Fig. 3. Best cost found analysis of some EDA variants for continuous optimization. $UMDA_C$, EMNA, EGNA, SPEDA, univariate KEDA (u_KEDA), multivariate KEDA (m_KEDA) and PBIL are shown.

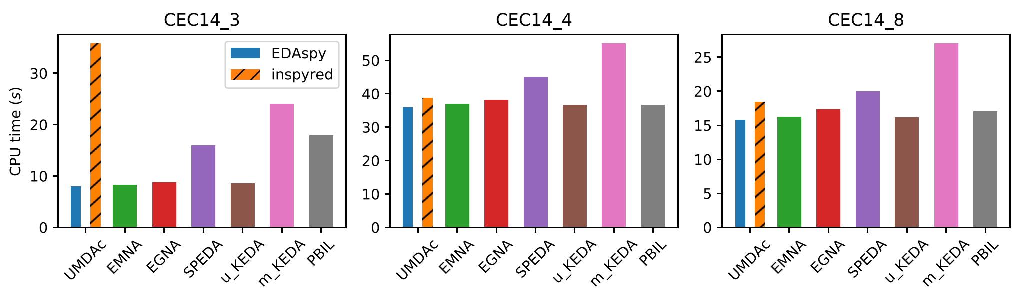


Fig. 4. CPU runtime analysis of some EDA variants for continuous optimization. $UMDA_C$, EMNA, EGNA, SPEDA, univariate KEDA (u_KEDA), multivariate KEDA (m_KEDA) and PBIL are shown.

Table A.2
Software metadata.

N	Software metadata description	Software metadata information
S1	Current software version	1.1.4
S2	Permanent link to executables of this version	https://github.com/VicentePerezSoloviev/EDAspy/releases/tag/1.1.3
S3	Legal software license	MIT License
S4	Computing platform/Operating system	Linux, OS X, Windows
S5	Installation requirements & dependencies	python 3.8–3.11, pybnesian, numpy, pandas, scikit_learn, scipy, pgmpy pyarrow, multiprocessing
S6	Link to user manual	https://edaspy.readthedocs.io/en/latest/
S7	Support email for questions	vicente.perez.soloviev@gmail.com

- Using EMNA for continuous optimization. EMNA is tested on a IEEE CEC 2014 benchmark.
- Using $UMDA_D$ for feature selection in a toy example. Given a dataset and a forecasting model, $UMDA_D$ is used to select the best subset of variables that optimizes the accuracy of the prediction.
- Categorical optimization using EBNA and $UMDA_D$. A categorical cost function is designed and optimized by EBNA and $UMDA_D$ approaches.
- Building my own EDA implementation. A tutorial on how to customize an EDA implementation is provided.
- CPU time analysis. All the continuous domain EDA variants are tested against the same IEEE CEC 2014 benchmark.

7. Conclusions

In this paper we present the first `python` library entirely dedicated to EDA implementations. `EDAspy` has been shown to be easy to use, and to integrate with custom implementations. Therefore, we hope that `EDAspy` can speed up the development of research on EDAs and their applications.

In addition to maintaining the code and solving bugs found by `EDAspy` users, future work would include adding more visualization tools for the optimization process and the implementation of other EDA variants.

CRediT authorship contribution statement

Vicente P. Soloviev: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Project administration, Methodology, Investigation, Formal analysis, Conceptualization. **Pedro Larrañaga:** Writing – review & editing. **Concha Bielza:** Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix. Required metadata

A.1. Current executable software version

See Table A.2.

Table A.3
Code metadata.

N	Software metadata description	Software metadata information
C1	Current code version	1.1.4
C2	Permanent link to code/repository used of this code version	https://github.com/VicentePerezSoloviev/EDAspy
C3	Legal software license	MIT License
C4	Code versioning system used	git
C5	Software code languages, tools, and services used	python 3.8–3.11
C6	Compilation requirements, operating environments & dependencies	Compatible python pybnesian, numpy, pandas, scikit_learn, scipy, pgmpy, pyarrow, multiprocessing
C7	Link to developer documentation/manual	https://edaspy.readthedocs.io/en/latest/
C8	Support email for questions	vicente.perez.soloviev@gmail.com

A.2. Current code version

See Table A.3.

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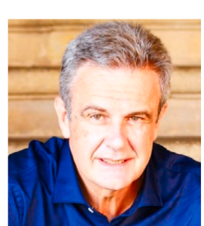

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