

Goldenberry: EDA Visual Programming in Orange

Sergio Rojas-Galeano
Engineering School
District University of Bogota
Bogota, Colombia
srojas@udistrital.edu.co

Nestor Rodriguez
Engineering School
District University of Bogota
Bogota, Colombia
nearodriguezg@correo.udistrital.edu.co

ABSTRACT

Orange is an open-source component-based software framework, featuring visual and scripting interfaces for many machine learning algorithms. Currently it does not support Estimation of Distribution Algorithms (EDA) or other methods for black-box optimization. Here we introduce **Goldenberry**, an **Orange** toolbox of EDA visual components for stochastic search-based optimization. Its main purpose is to provide an user-friendly workbench for researchers and practitioners, building upon the versatile visual front-end of **Orange**, and the powerful reuse and glue principles of component-based software development. Architecture of the toolbox and implementation details are given, including description and working examples for the components included in its first release: **cGA**, **UMDA**, **PBIL**, **TILDA**, **UMDA_c**, **PBIL_c**, **BMDA**, **CostFunctionBuilder** and **BlackBoxTester**.

Goldenberry is open-source and freely available at:
<http://goldenberry.codeplex.com>.

Categories and Subject Descriptors

D.2.6 [Software]: Software Engineering—*Programming Environments*; I.2.8 [Computing Methodologies]: Artificial Intelligence—*Problem Solving, Control Methods and Search*

Keywords

Component-based evolutionary software systems; EDAs

1. INTRODUCTION

Visual environments for machine learning (e.g. Clementine or SPSS Modeler [9], Weka [7], RapidMiner [12]) provide graphical workbenches to conduct user-friendly data analysis. Instead of scripting commands in an imperative computer language, users are able to graphically sketch processing units and interactions that are needed to run said analysis. **Orange** is one of such open-source visual frameworks, originally proposed for functional genomic analysis [4]. It has been progressively enriched with additional visual

software components (*widgets*) for several machine learning tasks. It is known that many of these tasks can be casted as, or make use of, optimization problems in their underlying machinery (regression analysis, regularization, clustering, feature selection); however as far as we know, to this day **Orange** does not include a set of tools available to model explicit optimization problems within the context of machine learning analysis. The latter is precisely the motivation behind the software system we introduce in this paper: **Goldenberry**, a supplementary machine learning and evolutionary computation suite for **Orange**.

The software was built by taking advantage of three interesting features in **Orange**: (i) its versatile visual front-end; (ii) the powerful reuse and glue postulates of component-based software development in which it is based; and (iii) its conformity to the *open/closed* principle of object-oriented programming through an scripting interface to Python. We reasoned that such features would be advantageous for extending its functionality to the realm of optimization problems. Since our research group has been recently working on stochastic-search-based optimization, particularly in the field of Estimation of Distribution Algorithms (EDA [10, 15]), a decision was made to start off the project in its first stage by focusing on this kind of algorithms. As a result, the first release of **Goldenberry** comprises a set of EDA components (**cGA** [8], **UMDA** [13], **PBIL** [2], **TILDA** [17], **PBIL_c** [19], **UMDA_c** [6] and **BMDA** [14]) and a set of utility components (**CostFunctionBuilder** and **BlackBoxTester**) that we shall describe in the following sections. The second stage of the project is currently under development; it will comprise other black-box optimization techniques and also additional meta-heuristics and machine learning components.

The paper describes a general depiction of the software architecture, and provide working examples of its operation using standard benchmark and custom optimization problems. The latter was made possible by using the built-in cost functions or the free-text Python input mode from the **CostFunctionBuilder** component, which are convenient design features allowing this suite to be applied over a wide range of discrete and continuous optimization domains. **Goldenberry** is also open-source and is freely available at:

<http://goldenberry.codeplex.com>

For download instructions please refer to the Appendix.

2. THE SOFTWARE AT A GLANCE

Goldenberry was built as a suite of *widgets* for **Orange**. Widgets are visual elements that can be dragged onto the **Orange** visual programming board, also known as *canvas*.

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Furthermore, widgets provide a set of input/output interfaces that encapsulate related services; many widgets collaborate to perform a given task. “Programming” in the canvas amounts to manually wiring up the appropriate interfaces between widgets. An example of a **Goldenberry** program to optimize a cost function using three different **EDA** widgets is shown in Figure 1. In that program, widgets are the components or processing units needed to perform the optimization task. Rather than depicting a *dataflow* between these components, connections represent provision and consumption of services encapsulated as objects, which are associated with each input/output interface. For instance, in this program the **cGA**, **PBIL** and **UMDA** widgets require a function to be optimized that is provided by the **CostFunctionBuilder** widget through three instances of the **CostFunction** object, one per **EDA**, each in charge of keeping statistics of the number of function evaluations and running times. The **EDA** components are responsible of setting up the parameters of their corresponding algorithm and of providing a ready-to-use **Optimizer** that is in turn, consumed by the **BlackBoxTester**. The latter is in fact responsible of orchestrating the execution of these **Optimizers**, that is, of running each **EDA** algorithm (whose parameters, including cost function, must have been already defined and provided in their output interfaces before execution begins) and also of collecting and visualizing the final results. Parameter settings and data presentation are embodied within the graphical user interface of the widgets, as we shall depict in Section 5 and 6 (also Figure 6 to Figure 11). Intuitively, this programming paradigm is very much the same as building a hardware apparatus: the user first gather, connect and set-up the required units before switching-on the resulting device.

3. ARCHITECTURAL VIEW

3.1 General design considerations

The following software patterns were taken into account during the conception of **Goldenberry**:

- A *layering* pattern [3] was applied in order to decouple the algorithmic logic of the components from their user interface (widgets); thereby all the implemented algorithms can be used and integrated in plain Python scripts or using the command-line.
- A *template method* pattern [5] was used by identifying commonalities of the different **EDA** approaches. In this way a generic abstraction of an **EDA** procedure was defined; concrete details of implementation were deferred to each particular algorithm. A unified **EDA** framework was achieved.
- A *responsibility splitting* pattern [1] was utilised in **EDA** optimisers so as to separate the search metaheuristic from the probability estimation technique. Therefore probability models were made reusable among multiple **EDAs** (those included in this and future releases).
- A *dynamic binding* [1] together with an *interpreter* pattern [5] were applied in order to allow the user to provide customised cost functions at runtime, in the form of Python-like scripts.

The application of such patterns guided the resulting design of the software, as described in the remainder of this section.

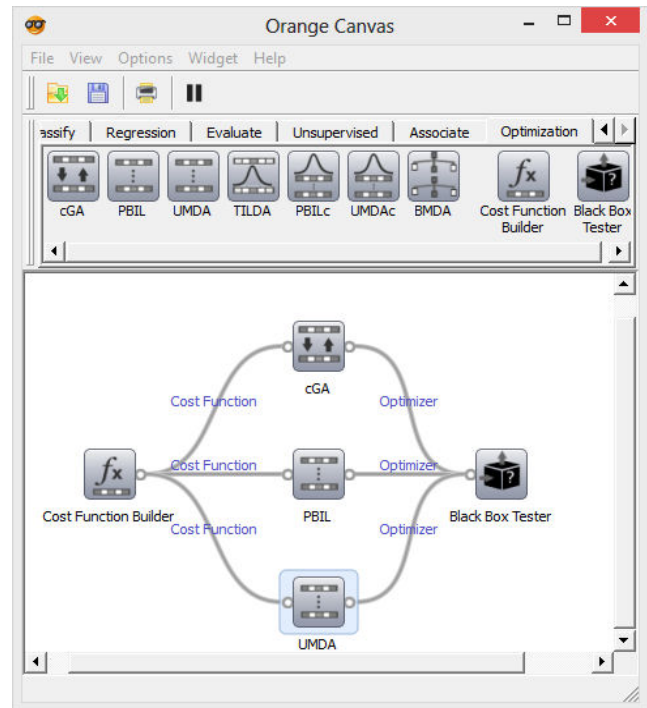


Figure 1: A Goldenberry program in the Orange canvas.

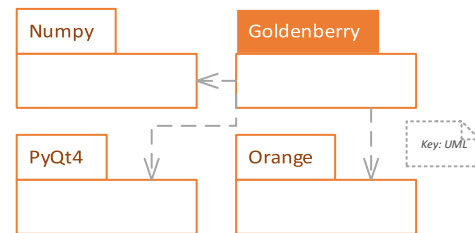


Figure 2: The context diagram of Goldenberry.

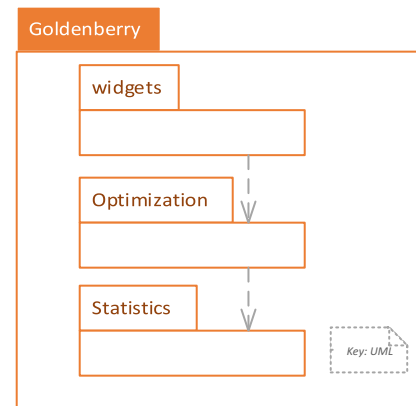


Figure 3: The three basic modules in Goldenberry.

such as cGA, TILDA, PBIL and UMDA (discrete and continuous-domain variants for the last two), and also a bivariate algorithm, the BMDA. The latter extends the base class with an additional method `build_graph()` to model pairwise dependencies between problem variables. This assortment of algorithms was chosen so as to incorporate techniques using both univariate and bivariate probability distribution approaches. In the first release of the software we emphasised in univariate versions due to their algorithmic simplicity; nonetheless, future releases will build upon these algorithms and contemplate higher-order EDAs using tree-based, Bayes and dependency networks techniques.

For illustration purposes, we shall now outline some of the Python scripts implementing these classes. Firstly, let us recall the *Population-Based Incremental Algorithm* (PBIL) [2]. The aim of this algorithm is to discover a real-valued probability vector from which a population of competent binary candidate solutions can be sampled. The algorithm starts-off with a random-valued vector; then, the vector is iteratively sampled in order to refine the model using the most promising solutions from the sample and an *incremental learning* re-estimation rule, until the vector converges to a fixed distribution. Our rendering of this procedure is shown in Algorithm 1, where a vectorized operation mode was assumed.

Algorithm 1 PBIL

Requires: Cost function $\text{fitness}(\cdot)$, binomial distribution model $\mathcal{B}(\theta)$ with parameters $\theta \in \mathbb{R}^d$, learning rate $0 \leq \eta \leq 1$

Outputs: Solution $\mathbf{s} \in \mathbb{R}^d$

Initialize θ and \mathbf{s} with random values in $[0, 1]^d$

repeat until convergence

 Sample n candidates from model: $P \sim \mathcal{B}(\theta)$

 Assess fitness of candidate population: $\mathbf{f} = \text{fitness}(P)$

 Choose m candidates: $S = \{\mathbf{x}_i \in P : f_i \in \text{top-}m\text{-ranked}\}$

 Re-estimate model: $\theta = (1 - \eta)\theta + \eta \frac{1}{m} \sum_i \mathbf{x}_i$, $\mathbf{x}_i \in S$

 Update solution: $\mathbf{s} = \text{argmax}(\text{fitness}(\mathbf{s}), \text{fitness}(S^{\text{top}}))$

In Goldenberry, the PBIL widget defines a class `Pbil` which overrides the `initialization()` and `estimate()` methods according to the previous algorithm. Thus, PBIL is fully implemented as the following class script (notice that the `average` vectorized auxiliary operation from the NumPy library (`np`) is used):

```
class Pbil(GbBaseEda):
    def initialize(self):
        self.distr=Binomial(self.var_size)

    def estimate(self, top_ranked, best):
        self.distr.p=self.distr.p*(1-self.learning_rate)
        + self.learning_rate * np.average(top_ranked)
```

The small size of the script is due to the fact that many algorithmic details have been inherited from the parent class, `GbBaseEda`, because they are common to most of other EDAs. For example, the parent class defines the initialization of parameters such as `sample_size`, `pop_size` (size of the population), `selection_rate` (percentage of top-ranked selected candidates), and `max_evals` (limit on the number of cost function evaluations allowed on an entire search). Other common features such as the `sample()` method (which delegates this task to the respective probability model), the

`get_top_ranked()` method to select the most promising candidates from the sample, and the `search()` method itself, are defined in this abstract class. Its script is partially shown below.

```
class GbBaseEda(GbBaseOptimizer):
    ...
    def sample(self, sample_size, top_ranked, best):
        return self.distr.sample(sample_size)

    def get_top_ranked(self, candidates):
        fits = self.cost_func(candidates)
        index = np.argsort(fits)
        [:(self.cand_size*self.selection_rate/100):-1]
        return candidates[index],
            bSolution(candidates[index[0]],fits[index[0]])
    ...
    def search(self):
        if not self.ready():
            raise Exception("Optimizer not ready.")
        best = GbSolution(None, float('-Inf'))
        top_ranked = None
        while not self.done():
            candidates=self.sample(self.sample_size,
                                    top_ranked, best)
            top_ranked, winner =
                self.get_top_ranked(candidates)
            self.estimate(top_ranked, best)
            if best.cost < winner.cost:
                best = winner
            self.iters += 1
        return best

@abc.abstractmethod
def estimate(self, candidates, best):
    raise NotImplementedError()
```

It can be seen in the previous code that the implementation of `estimate()`, the estimation of distribution method, is deferred to the specific EDA class, as it was the case of the PBIL component.

Now let us complete the illustration by mentioning another well-known EDA, the *Compact Genetic Algorithm* (cGA) [8]. The algorithm is similar in fashion to PBIL, the main difference being that it operates in a *compact* mode, that is, instead of estimating the distribution from a batch of many candidates (population), the algorithm works by sampling two candidates at a time and using them to incrementally build the estimation. The pseudo-code of this procedure is thus shown in Algorithm 2, which again is our rendition of the original, written in vectorized operation mode.

Algorithm 2 cGA

Requires: Cost function $\text{fitness}(\cdot)$, binomial distribution model $\mathcal{B}(\theta)$ with parameters $\theta \in \mathbb{R}^d$

Outputs: Solution $\mathbf{s} \in \mathbb{R}^d$

Initialize θ and \mathbf{s} with random values in $[0, 1]$

repeat until convergence

repeat n times

 Sample 2 candidates from model: $\{\mathbf{x}_1, \mathbf{x}_2\} \sim \mathcal{B}(\theta)$

 Rank them: $\{\mathbf{w}, \mathbf{l}\} = \text{compete}(\text{fitness}(\mathbf{x}_1), \text{fitness}(\mathbf{x}_2))$

 Re-estimate model with winner and loser: $\theta = \theta + \frac{1}{n}(\mathbf{w} - \mathbf{l})$

 Update solution: $\mathbf{s} = \text{argmax}(\text{fitness}(\mathbf{s}), \text{fitness}(\mathbf{w}))$

```
class Cga(GbBaseEda):
    def initialize(self):
        self.distr=Binomial(self.var_size)
        self.learning_rate=1.0/float(self.pop_size)
        self.sample_size=2

    def estimate(self, (winner, loser), best):
        self.distr.p =
            np.minimum(np.ones((1, self.var_size)),
                np.maximum(np.zeros((1, self.var_size)),
                    self.distr.p +
(winner.params-loser.params)*self.learning_rate))

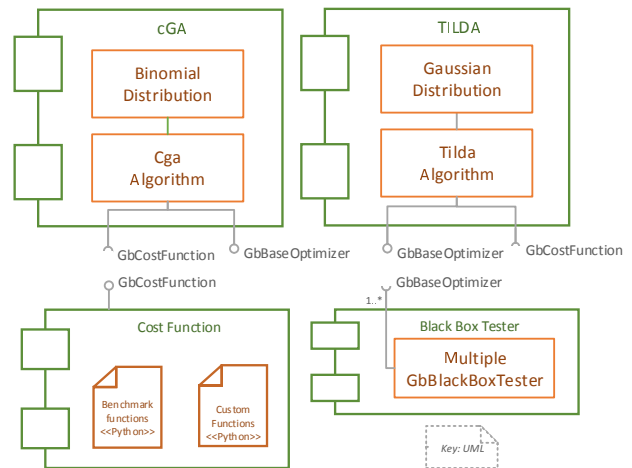
    def get_top_ranked(self, candidates):
        costs = self.cost_func(candidates)
        maxindx = np.argmax(costs)
        winner = GbSolution(candidates[maxindx],
            costs[maxindx])
        loser = GbSolution(candidates[not maxindx],
            costs[not maxindx])
        return (winner, loser), winner
```

4.3 Statistics classes

5. COMPONENTS VIEW

5.1 The EDA components

These components are at the end of the day deployed as widgets in the **Orange** canvas, under a new toolbar named “Optimization” (see again Figure 1). The user interface of these widgets consists of a setup/results window. In there, parameters settings are applied to the **EDA** component and optimization results are displayed in an output text box after execution of the algorithm. An example of the user interface for the **cGA** widget, applied to solve the classical **OneMax** problem with 100 variables, using a population size of 30, and 1000 maximum number of evaluations, is shown in Figure 6.



The screenshot shows a software interface titled "cGA". It has two main sections. The top section, labeled "Parameters", contains four input fields: "Name" with the value "cGA", "Variables" with "100", "# Candidates" with "30", and "Max Evals." with "1000". Below these are two large buttons: "Apply" (grey) and "Run" (blue). The bottom section, labeled "Result", displays the output of the algorithm. It starts with a long binary string "Best: [1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.]" followed by several statistics: "cost:99.0", "#evals:932", "#argmin:4", "argmax:667", "min val:41.0", "max val:99.0", "mean:81.178111588", and "stdev:15.5864759758". There are scroll bars on the right side of the "Result" panel.

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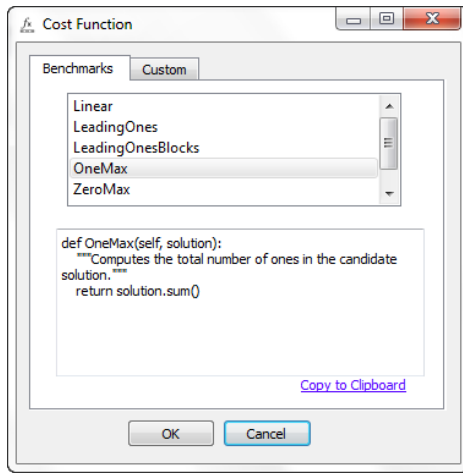
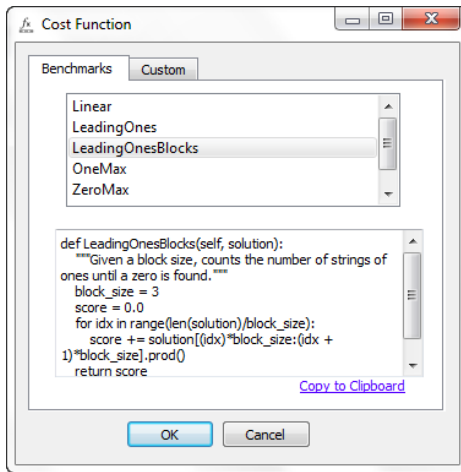
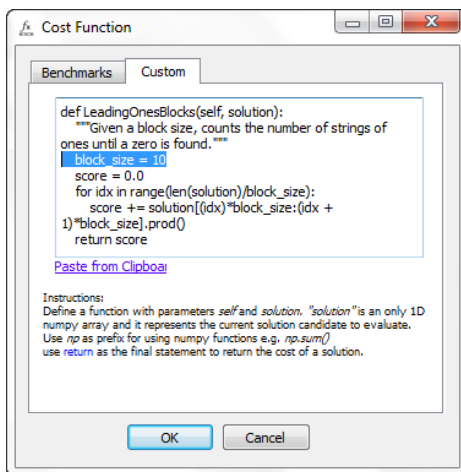


Figure 7: The benchmark input mode of the CostFunctionBuilder component. Here the well-known Onemax problem is chosen.



(a)



(b)

Figure 8: How to customize a built-in benchmark function: (a) A benchmark function is chosen and its code is copied into the clipboard; (b) the code is pasted in the “Custom” tab and edited as required.

5.2 The Cost Function Builder component

This component enables the user to define the cost function for the optimization problem. It provides two input modes to setup such a function. In the first mode, a set of ready-to-use built-in benchmark functions are listed to the user as it is illustrated in Figure 7. This mode appears on the “Benchmarks” tab of the **CostFunctionBuilder** user interface. The user chooses a function name, and then the Python script implementing the function is shown in the underlying text box; the box is read-only, so the code can not be edited but can be copied into the clipboard. The benchmark functions were taken from those suggested in [11].

The second mode consists of a free-text input box for writing up any customized cost function in the Python language. This mode appears on the “Custom” tab of the **CostFunctionBuilder** user interface. Custom functions must be written complying with the following Python-style signature:

```
def yourcustomfunctionname(self, solution):
    ...
    return computedcostofsolution
```

An arbitrary routine to evaluate the given **solution** (a NumPy 1D vector array with the values of that solution to the problem variables) must be defined in order to compute its associated cost. For example, if the user wants to define a customized version of the benchmarks built-in functions, he or she may copy to the clipboard its original code, then paste it in the “Custom” tab and make the necessary adjustments (see Figure 8). Alternatively the user may write up his cost function code from scratch, to meet his particular problem needs. We remark that this is a non-intrusive input mode, meaning that the user-written-code is bind to the **Goldenberry** components in run time; no additional intervention has to be done in the source code of the software. We anticipate this feature would extend the usability of the **EDA** components to a wide range of discrete and continuous optimization problem domains.

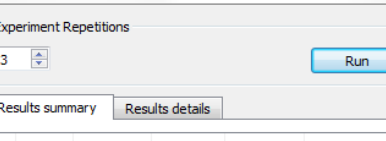
5.3 The Black-Box Tester component

This component was designed to allow the user to run and compare execution of different algorithms or algorithm configurations over the same cost function, in one experiment with several repetitions. The number of repetitions is set as an input parameter for this component. Another interesting functionality of the **BlackBoxTester** is that it is able to collect outputs of all the optimizer components provided as inputs, and display summarized statistics, and also details of the different runs and repetitions. The user interface of the widget associated to this component will be used to display results for the working experiments reported in the next section.

6. GOLDENBERRY AT WORK

In this section we show how to use the developed components to solve optimization problems defined as minimization of a cost function. We carried out experiments using benchmark and customized cost functions. Other uses in machine learning can be also envisioned (see for example the discussion in Section 7).

The results of these experiments are shown next. It is worth to remark that previous to deployment, additional val-



Black Box Tester

Experiment Repetitions

3

Run

Results summary Results details

	Name	Cost(max)	Cost(avg)	#Evals(avg)	Time[s](avg)
1	UMDA	100.0	100.0	500.0	0.00633335...
2	cGA	100.0	99.3333...	961.3333...	0.04299998...
3	PBIL	100.0	100.0	970.0	0.01733326...

Copy to Clipboard

The screenshot shows the "Black Box Tester" application window. At the top, there's a title bar with standard Windows icons. Below it, the "Experiment Repetitions" section has a spinner set to 3 and a blue "Run" button. The main area contains two tabs: "Results summary" (selected) and "Results details". Under "Results summary", there is a table with 9 rows of results.

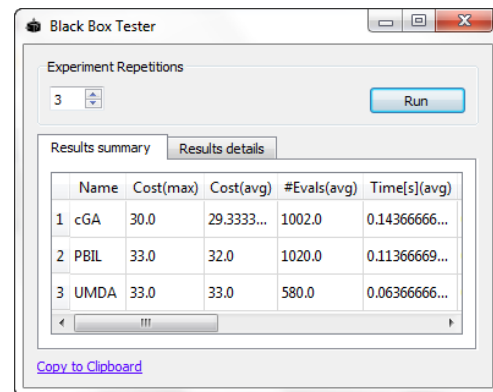
Name	Best	Cost	#Evals	Time[s]
1 PBIL	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	100.0	960	0.0249...
2 PBIL	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	100.0	960	0.0149...
3 PBIL	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	100.0	990	0.0120...
4 cGA	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	100.0	964	0.0409...
5 cGA	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	99.0	1002	0.0460...
6 cGA	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	99.0	918	0.0420...
7 UMDA	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	100.0	480	0.0060...
8 UMDA	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	100.0	510	0.0060...
9 UMDA	[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. ...]	100.0	510	0.0069...

At the bottom of the table, there are navigation arrows (back, forward) and a status indicator consisting of three exclamation marks (!!!).

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Two problems were chosen from the built-in benchmark library of functions: **Onemax** and **LeadingOnesBlock**. Results for the **Onemax** experiment are reported in Figure 9. Figure 9(a) shows the following aggregate results per EDA algorithm: maximum cost found in all experiment repetitions; average cost over all repetitions; average number of cost function evaluations per repetition; and average CPU time per repetition (in seconds). Other statistics can be dis-

For the **LeadingOnesBlock** experiment, results are similarly self-explained, as reported in Figure 10.



Black Box Tester

Experiment Repetitions

3

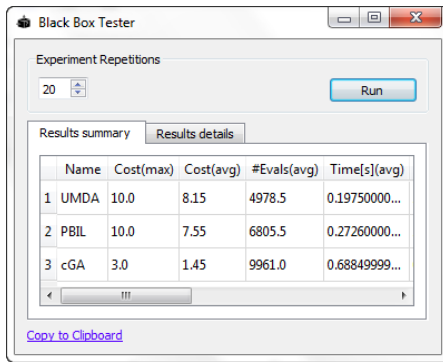
Run

Results summary Results details

	Name	Best	Cost	#Evals	Time[s]
1	PBIL	[1. 1. 1. 1. 1. 1. 1. 1. ...	31.0	1020	0.1150...
2	PBIL	[1. 1. 1. 1. 1. 1. 1. 1. ...	33.0	1020	0.1140...
3	PBIL	[1. 1. 1. 1. 1. 1. 1. 1. ...	32.0	1020	0.1119...
4	cGA	[1. 1. 1. 1. 1. 1. 1. 1. ...	30.0	1002	0.1469...
5	cGA	[1. 1. 1. 1. 1. 1. 1. 1. ...	28.0	1002	0.1419...
6	cGA	[1. 1. 1. 1. 1. 1. 1. 1. ...	30.0	1002	0.1420...
7	UMDA	[1. 1. 1. 1. 1. 1. 1. 1. ...	33.0	600	0.0639...
8	UMDA	[1. 1. 1. 1. 1. 1. 1. 1. ...	33.0	540	0.0640...
9	UMDA	[1. 1. 1. 1. 1. 1. 1. 1. ...	33.0	600	0.0629...

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In this experiment we used the same **Goldenberry** program of Figure 1 to carry out optimization of the customized cost function defined in Figure 8, that is, the same **LeadingOnesBlock** problem this time with a `block_size` value of 10. Similarly to the other experiments, results are shown in Figure 11.



The screenshot shows a window titled "Black Box Tester". Inside, there's a section for "Experiment Repetitions" with a value of 20 and a "Run" button. Below that is a "Results summary" tab. A table displays the results for three experiments: UMDA, PBIL, and cGA. The table has columns for Name, Cost(max), Cost(avg), #Evals(avg), and Time[s](avg). At the bottom, there is a "Copy to Clipboard" link.

Name	Cost(max)	Cost(avg)	#Evals(avg)	Time[s](avg)
1 UMDA	10.0	8.15	4978.5	0.19750000...
2 PBIL	10.0	7.55	6805.5	0.27260000...
3 cGA	3.0	1.45	9961.0	0.68849999...

Figure 11: Results of custom function experiment.

7. CONCLUSIONS

It is our belief that user-friendly, open-source visual tools may have a big potential benefit in tasks carried out daily by data mining analysts. The **Orange** platform is a fantastic effort complying with these premises by combining a powerful visual programming approach with the reuse and glue principles of component-based software. The **Goldenberry** initiative is a modest contribution intended to extend the application domain of **Orange** to the field of black-box and metaheuristics optimization. In this first release we developed a number of **EDA**-based software components featuring a non-intrusive, runtime-binding interface to allow users to define tailor-made discrete and continuous optimization problems.

As it was mentioned in the introduction, it is anticipated that these components can be used independently as function optimizers, as it is reported in this paper, or as part of higher-level data mining machines. Let us illustrate the point with the task of feature selection. The aim there is to select an optimal subset of relevant variables for a classification problem; the relevant found subset can be further analysed by experts for specific purposes (in biology for example, features may represent over-expressed gene activity due to an illness condition). In the so-called *wrapper* scheme of the problem [18] the classifier is enabled to incorporate the selection mechanism during the learning stage: a weighted kernel classifier, for example, may use an **UMDA** component to define relevance coefficients for the variables and then use them as input for the kernel machine (that is the approach taken in [16]). Currently these type of mechanisms are hidden in the current implementation of classifier or clustering components of **Orange**. Thus, by providing interfaces to black-box optimizers we hope to extend applicability to this type of tasks, giving researchers a flexible workbench to design new component-based machine learning techniques. Novel components complying with the design principles described in this paper will be needed though (e.g. component-based genetic algorithms, kernel machines, etc.), and that would be matter of the next **Goldenberry** release.

8. ACKNOWLEDGEMENTS

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Appendix. Download and installation

Goldenberry is hosted publicly under a GPL license in Codeplex (<http://goldenberry.codeplex.com>). To install the software follow these steps:

1. Download and install Orange 2.6.1 from: <http://orange.biolab.si/download/>.
2. Get the latest **Goldenberry** release from the Downloads tab in <http://goldenberry.codeplex.com> (the download link is located to the left side of the screen).
3. Follow the installation instructions in the release notes just below the download link.
4. Open the **Orange** application and look for the “Optimization” toolbar in the canvas (as shown in Figure 1).