

Evolutionary Dataset Optimisation: learning algorithm quality through evolution

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Abstract

In this paper we propose a new method for learning how algorithms perform. Classically, algorithms are compared on a finite number of existing (or newly simulated) benchmark data sets based on some fixed metric. The algorithm(s) with the smallest value of this metric are chosen to be the ‘best performing’. We offer a new approach to flip this paradigm. We instead aim to gain a richer picture of the performance of an algorithm by generating artificial data through genetic evolution, the purpose of which is to create populations of datasets for which a particular algorithm performs well. These data sets can be studied to learn as to what attributes lead to a particular progress of a given algorithm.

Following a detailed description of the algorithm as well as a brief description of an open source implementation, a number of numeric experiments are presented to show the performance of the method.

1 Introduction

When a research problem manifests itself and an algorithm is developed to solve the problem, the investigator is presented with questions about the performance of their proposed method, and its relative performance to existing methods. The standard response to these situations is to fix some benchmark datasets and a common metric amongst the proposed method and its competitors. The algorithm is then assessed based on this metric. This paradigm has a number of problems:

1. How were these benchmark examples selected? In some domains and disciplines there are well-established benchmarks so literature can be reliable, in others less so.
2. In the case of the latter, a ‘new’ dataset is sometimes simulated to assess the algorithm. This begs the question as to how and why that simulation is created.
3. In disciplines where there are established benchmarks, there may still be underlying problems:
 - (i) Work by Torralba and Efros [13] showed that benchmark datasets used to train and evaluate object recognition models do not give a reliable measure for their performance when evaluated on other benchmark datasets.
 - (ii) The amount of learning one can gain as to the characteristics of data which lead to good (or bad) performance of an algorithm are constrained to the finite set of attributes present in the benchmark data chosen in the first place.

This work presents a novel approach that flips this paradigm on its head. Instead of fixing data and evaluating an algorithm on some metric, the proposed method will generate data for which the algorithm performs well (or poorly) through evolution. These datasets can then be studied to learn which attributes and characteristics lead to the success (or failure) of a given algorithm.

Evolutionary algorithms (EAs) have been applied successfully to solve a wide array of problems in recent history - particularly where the complexity of the problem or its domain are significant. These methods are highly adaptive and their population-based construction allows for the efficient solving of problems that are otherwise beyond the scope of traditional search and optimisation methods. It is clear that the domain of studying algorithm quality falls into this category of problems.

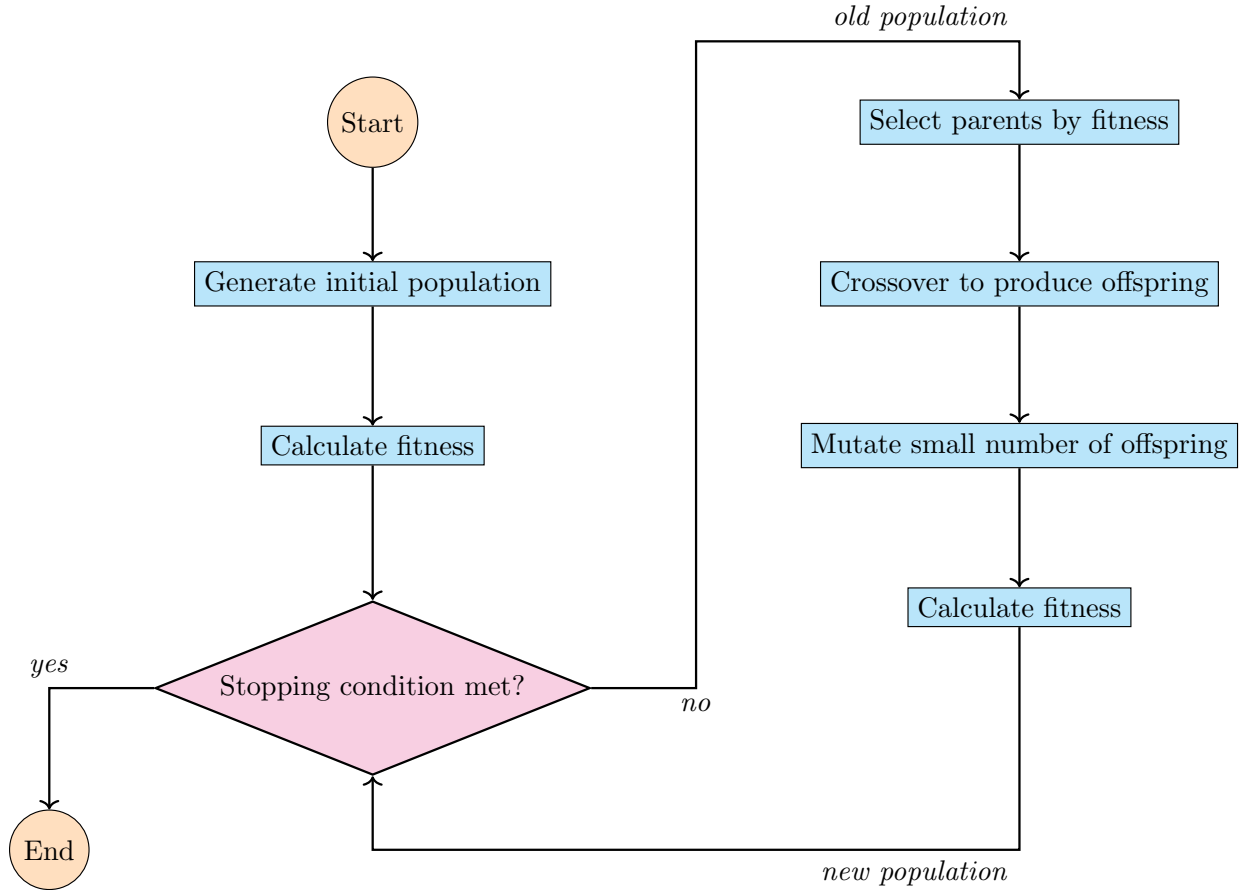


Figure 1: A general schematic for an evolutionary algorithm.

The use of EAs to generate artificial data is not a new concept; these methods are used in the automated testing of software to achieve maximal coverage and to support structural tests [5, 7, 10]. Such methods also have a long history in the parameter optimisation of algorithms, and recently in the automated design of convolutional neural networks [11, 12].

2 The evolutionary algorithm

2.1 Structure

On the surface, the EDO method is built as an evolutionary algorithm which follows a traditional (generic) schema with some additional features that keep the objective of artificial data generation in mind. With that, there are a number of parameters passed to the algorithm, including several that are not typical:

- A real-valued fitness function, $f : X \rightarrow \mathbb{R}$, which acts on a dataset to return a single fitness score.
- A population size, $N \in \mathbb{N}$.
- Limits on the number of rows a dataset can have, $R \in \{(r_{\min}, r_{\max}) \in \mathbb{N}^2 \mid r_{\min} \leq r_{\max}\}$.
- Limits on the number of columns a dataset can have

$$C := (C_1, \dots, C_{|\mathcal{P}|}) \text{ where } C_j \in \{(c_{\min}, c_{\max}) \in (\mathbb{N} \cup \{\infty\})^2 \mid c_{\min} \leq c_{\max}\}$$

for each $j = 1, \dots, |\mathcal{P}|$. That is, C is defined as a tuple detailing the minimum and maximum number of columns a dataset can have for each distribution passed in \mathcal{P} .

- A set of probability distribution families, \mathcal{P} . Each family in this set has some parameter limits which form a part of the overall search space. For instance, the normal distribution family, denoted by $N(\mu, \sigma^2)$, would have limits on values for the mean, μ , and the standard deviation, σ .
- A probability vector to sample distributions from \mathcal{P} , $w = (w_1, \dots, w_{|\mathcal{P}|})$ such that $\sum_{i=1}^{|\mathcal{P}|} w_i = 1$ and $w_i \in [0, 1]$, $\forall i = 1, \dots, |\mathcal{P}|$.
- A maximum number of iterations, $M \in \mathbb{N}$.
- Two selection parameters: one to indicate the proportion of the fittest individuals to carry forward, $b \in [0, 1]$, and to allow for a small proportion of “lucky” individuals in the next generation, $l \in [0, 1]$.
- A mutation probability, $p_m \in [0, 1]$, used to indicate the intensity and likelihood of the mutation a new individual might undergo.
- A shrink factor, $s \in [0, 1]$. The relative size of a component of the search space to be retained after adjustment.

The concepts discussed in this section form the mechanisms of the evolutionary dataset optimisation algorithm. To use the algorithm practically, these components have been implemented in Python as a library built on the scientific Python stack [6, 9]. The library is fully tested and documented (at <https://edo.readthedocs.io>) and is freely available online under the MIT license [3]. The EDO implementation was developed to be consistent with the best practices of open source software development.

The statement of the EDO algorithm is deliberately vague. This is, in part, because of the customisable nature of its build but also to lay out its general structure from a high level perspective. Lower level

Algorithm 1: The evolutionary dataset optimisation algorithm

Data: $f, N, R, C, \mathcal{P}, w, M, b, l, p_m, s$

Result: A full history of the populations and their fitnesses.

begin

 create initial population of individuals

 find fitness of each individual

 record population and its fitness

while *current iteration less than the maximum* **and** *stopping condition not met* **do**

 select parents based on fitness and selection proportions

 use parents to create new population through crossover and mutation

 find fitness of each individual

 update population and fitness histories

if *adjusting the mutation probability* **then**

 | update mutation probability

end

if *using a shrink factor* **then**

 | shrink the mutation space based on parents

end

end

end

Algorithm 2: Creating a new population

Data: parents, $N, R, C, \mathcal{P}, w, p_m$

Result: A new population of size N

begin

 add parents to the new population

while *the size of the new population is less than N* **do**

 sample two parents at random

 create an offspring by crossing over the two parents

 mutate the offspring according to the mutation probability

 add the mutated offspring to the population

end

end

discussion is provided below where additional algorithms for the individual creation, evolutionary operator and shrinkage processes are given along with diagrams (where appropriate).

Note that there are no defined processes for how to stop the algorithm or adjust the mutation probability, p_m . These form two key areas of potential customisation since such conditions can be specific to the problem domain. With that, as is detailed in the Python implementation, a user may define their stopping condition or p_m -adjustment to be any reasonable function. Some examples include:

- These should be real-world examples used in other EA with references.
- Stopping when the difference in the variance of the current and last population fitnesses is below some tolerance.
- Halving the mutation probability every 100 iterations.

2.2 Individuals

Evolutionary algorithms operate on succeeding populations of individuals often coined as “generations”. Typically, an individual would be encoded as a bit string of a fixed length and treated as a chromosome-like object to be manipulated. In EDO, as the objective is to generate datasets, there is no encoding process. Instead, the datasets are manipulated directly so that the biological operators can behave and be interpreted in a more meaningful way.

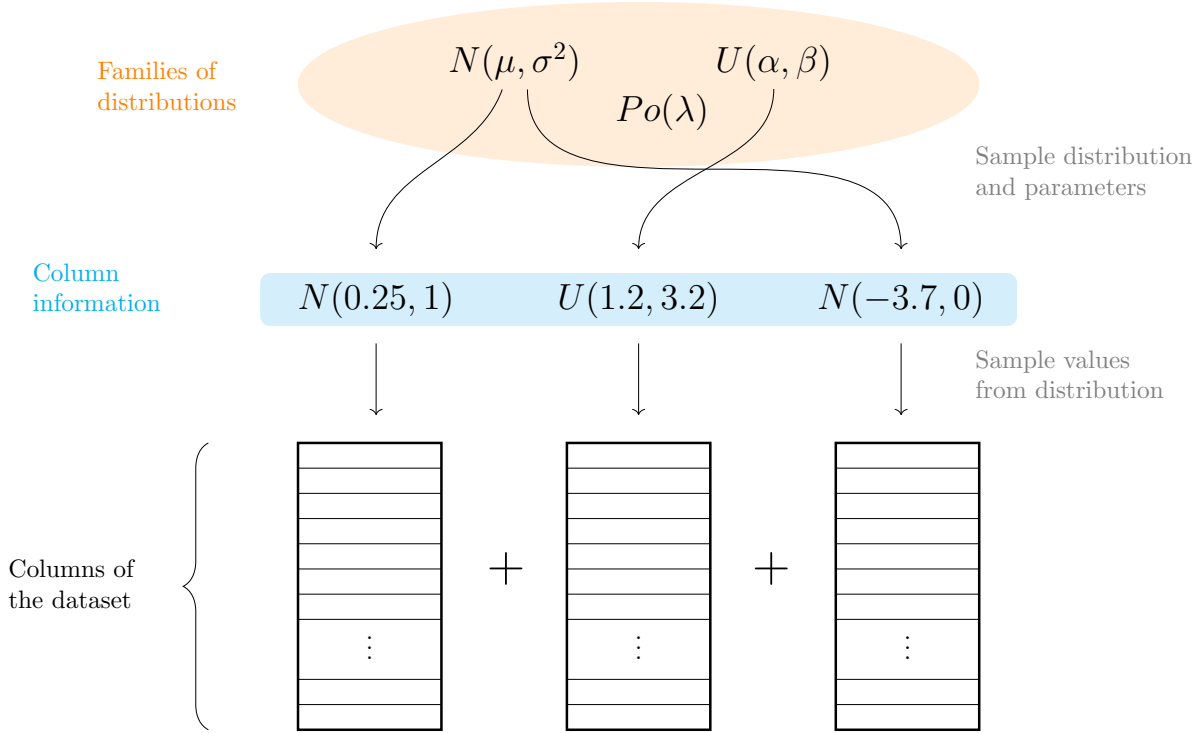


Figure 2: An example of how an individual is first created.

In a sense, a dataset is treated similarly to a classical bit string as the primary components (loci) of the dataset are considered to be its columns. As is seen in Figure 2, an individual's creation is defined by the random generation of its columns. A set of instructions on how to sample new values for that column are recorded in the form of a probability distribution. These distributions are sampled from a pool of distribution families which is passed to the evolutionary algorithm along with the other parameters.

Obviously, users and interpreters of EDO should not be so quick to assume that these pairs of distributions and columns are typical of their partner. That is, that the columns are a reliable representative of the distribution associated with them, or vice versa. A caveat to this statement: this is particularly true of “shorter” datasets with a small number of rows, whereas confidence in the pair could be given more liberally for “longer” datasets. In the case of the latter, the column metadata can become more useful for casually analysing the data which is generated. In any case, however, more direct and sophisticated methods should be employed to understand the structure and characteristics of the data before formal conclusions are made.

Algorithm 3: Creating an individual

Data: R, C, \mathcal{P}, w

Result: An individual defined by a dataset and some metadata

```
begin
  sample a number of rows and columns
  create an empty dataset
  for each column in the dataset do
    sample a distribution from  $\mathcal{P}$ 
    create an instance of the distribution
    fill in the column by sampling from this instance
    record the instance in the metadata
  end
end
```

2.3 Selection

The selection operator describes the process by which individuals are chosen from the current population to generate the next. Almost always, the likelihood of an individual being selected is determined by their fitness. This is because the purpose of selection is to preserve favourable qualities and encourage some homogeneity within future generations.

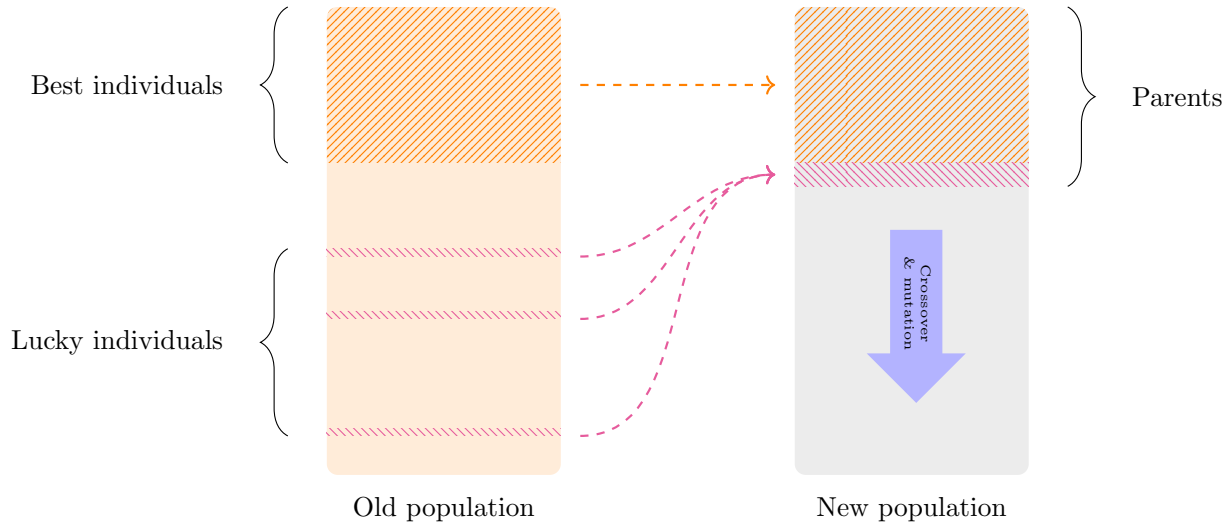


Figure 3: The selection process with the inclusion of some lucky individuals.

In EDO, a modified truncation selection method is used as can be seen in Figure 3. Standard truncation selection takes a fixed number, $n_b = \lceil bN \rceil$, of the fittest individuals in a population and makes them the “parents” of the next. The modification is an optional stage after the best individuals have been chosen. By

passing some small l to the evolutionary algorithm, a number of random individuals can be selected to be carried forward. This number is given by $n_l = \lceil lN \rceil$. It should be noted that even with this modification, no individual may be selected more than once in a single iteration but could potentially be present throughout the entire run of the algorithm.

Algorithm 4: The selection process

Data: population, population fitness, b, l
Result: A set of parent individuals
begin
 calculate n_b and n_l
 sort the population by the fitness of its individuals
 take the first n_b individuals and make them parents
 if *there are any individuals left* **then**
 take the next n_l individuals and make them parents
 end
end

It has been found that, despite its efficiency as a selection operator, truncation selection can lead an evolutionary algorithm to converge prematurely to local optima [4]. Hence, the ability to include some randomly selected individuals is included to encourage diversity throughout the run of the algorithm. This feature can be particularly useful in more complex optimisation scenarios - or for larger populations where a greater loss of diversity is seen in the selection process simply due to the nature of truncation selection [8]. As such, it should be used sparingly so as not to dominate the selection process with unwanted randomness.

2.4 Crossover

Crossover is the operation of combining two individuals in order to create at least one offspring. Often in classical evolutionary algorithms, the term “crossover” is taken literally: two bit strings are crossed at a point to produce two new bit strings. Another popular method is uniform crossover where the loci of a new individual are sampled uniformly from either parent individual. This method is adapted to support dataset manipulation here by sampling first a set of dimensions from the parents, and then inheriting entire columns.

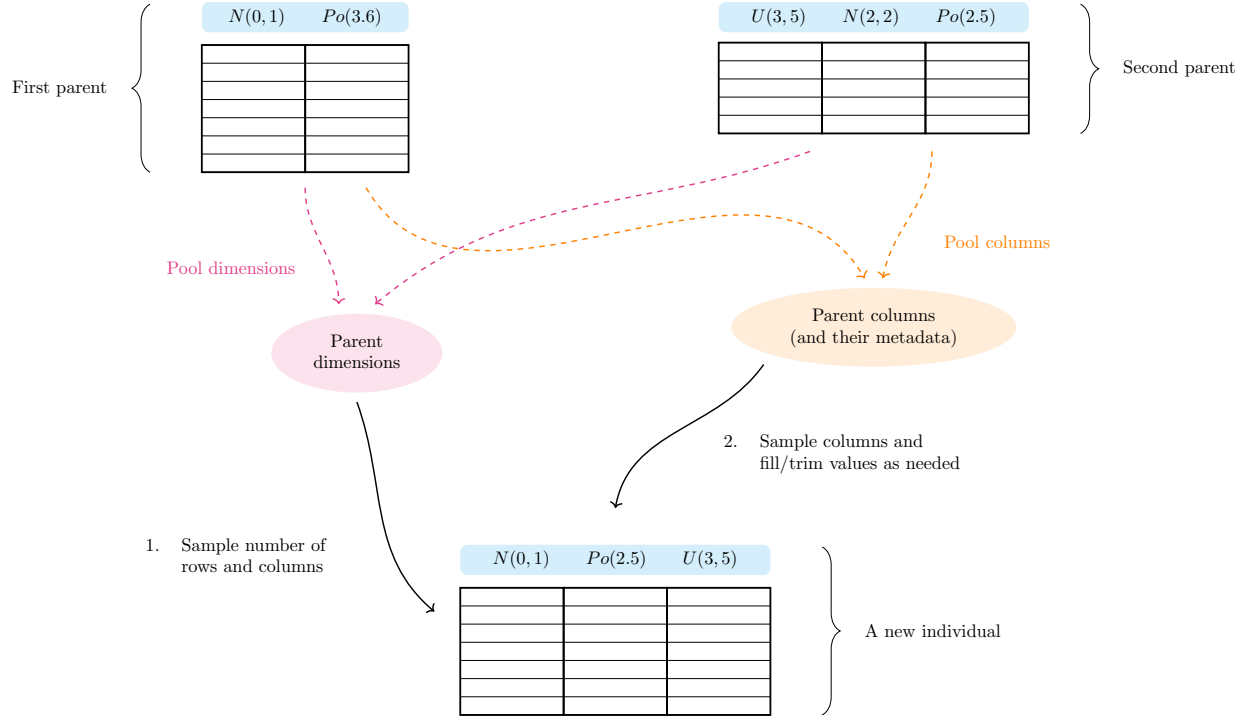


Figure 4: The crossover process.

Algorithm 5: The crossover process

Data: Two parents

Result: An offspring made from the parents ready for mutation

begin

 collate the columns and metadata from each parent in a pool

 sample each dimension from between the parents uniformly

 form an empty dataset with these dimensions

for *each column in the dataset* **do**

 sample a column (and its corresponding metadata) from the pool

if *this column is longer than required* **then**

 | randomly select entries and delete them as needed

end

if *this column is shorter than required* **then**

 | sample new values from the metadata and append them to the column as needed

end

 add this column to the dataset and record its metadata

end

end

2.5 Mutation

Mutation is used in evolutionary algorithms to encourage a broader exploration of the search space. Traditional applications with chromosome representations would mutate by run along the loci of an individual and “switching” the binary value with some constant probability. Under this framework, as has been discussed, an individual’s columns are similar to traditional loci. However, in the mutation phase multiple characteristics of an individual are susceptible to being mutated beyond the columns themselves such as the dimensions of the individual and their column metadata.

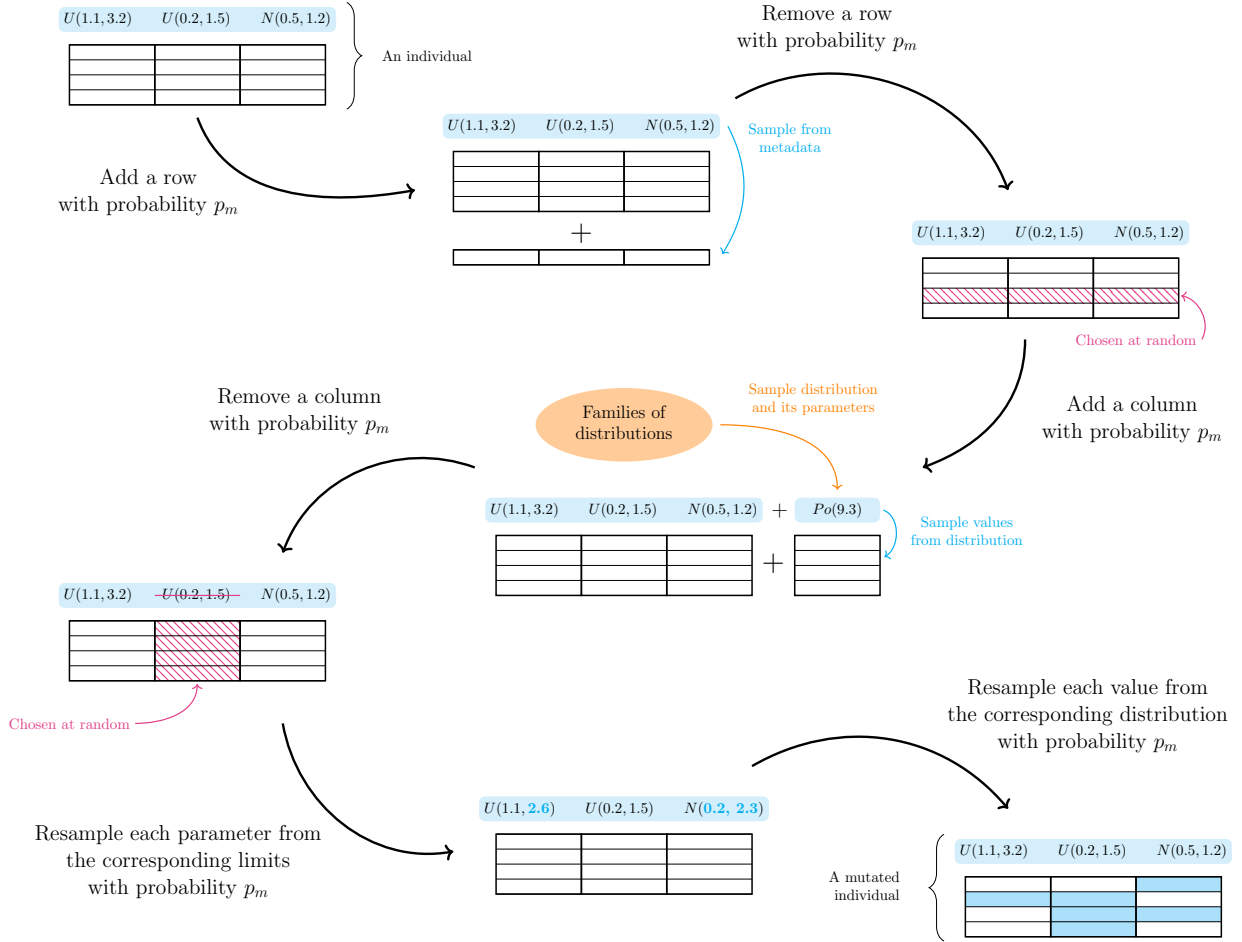


Figure 5: The mutation process.

The mutation process, seen in Figure 5 and defined in Algorithm 6, is deliberately fine so that all aspects of an individual can be changed in a meaningful yet fluid way. Each of the potential mutations occur with the same probability, p_m , but the way in which columns are maintained assure that (assuming

appropriate choices for f and \mathcal{P}) many mutations in the metadata and the dataset itself will only result in some incremental change in the individual's genetics and fitness overall - at least relatively so to, say, a completely new individual.

2.6 Shrinking

The potential benefits of adapting the search space of an EA has been well-discussed in the domain of complex optimisation problems. During the development of EDO, two methods were considered to do this. Each of these methods relied on a law relating a successive generation's search space with its predecessor. It should be noted that in both cases the methods were adapted to conform with the choice to represent individuals as they are rather than as bit strings.

The first was developed to be a two-part process based on a linear law with two parameters: a shrink factor, $s \in (0, 1)$, and the maximum number of iterations $M \in \mathbb{N}$ [2]. The adapted method would be as follows. For all iterations, $t \geq sM$, no shrinking would take place. However, for all previous iterations, the suggested method would take the parents found during selection and act on each component of the search space. That is, for each iteration, $t < sM$, every component would have its lower and upper limits, denoted by l_t and u_t respectively, adjusted so that they are centred about the mean parent value, μ , and be such that:

$$u_{t+1} - l_{t+1} = (u_t - l_t) \left(1 - \frac{t}{sM}\right)$$

More specifically, the adjusted limits would be calculated as follows:

$$\begin{aligned} l_{t+1} &= \max \left\{ l_t, \mu - \frac{1}{2}(u_t - l_t) \left(1 - \frac{t}{sM}\right) \right\} \\ u_{t+1} &= \min \left\{ u_t, \mu + \frac{1}{2}(u_t - l_t) \left(1 - \frac{t}{sM}\right) \right\} \end{aligned}$$

The second method was for use in a genetic algorithm which mapped weighted bit strings to some pre-defined interval with lower and upper bounds [1]. The proposed method would rely on a power law with a single parameter: some shrink factor, $s \in [0, 1]$. Again, at each iteration, the parents would be taken and every component's limits would be adjusted so that they were centred about the mean parent value, μ , such that:

$$u_{t+1} - l_{t+1} = (u_t - l_t)s^t$$

The process by which the values of l_{t+1} and u_{t+1} would be found are equivalent to the above but with a

Algorithm 6: The mutation process

Data: An individual, p_m , R , C , \mathcal{P} , w

Result: A mutated individual

begin

 sample a random number $r \in [0, 1]$

if $r < p_m$ *and adding a row would not violate R* **then**

 sample a value from each distribution in the metadata

 append these values as a row to the end of the dataset

end

 sample a new $r \in [0, 1]$

if $r < p_m$ *and removing a row would not violate R* **then**

 remove a row at random from the dataset

end

 sample a new $r \in [0, 1]$

if $r < p_m$ *and adding a new column would not violate C* **then**

 create a new column using \mathcal{P} and w

 append this column to the end of the dataset

end

 sample a new $r \in [0, 1]$

if $r < p_m$ *and removing a column would not violate C* **then**

 remove a column (and its associated metadata) at random from the dataset

end

for *each distribution in the metadata* **do**

for *each parameter of the distribution* **do**

 sample a random number $r \in [0, 1]$

if $r < p_m$ **then**

 sample a new value from within the distribution parameter limits

 update the parameter value with this new value

end

end

end

for *each entry in the dataset* **do**

 sample a random number $r \in [0, 1]$

if $r < p_m$ **then**

 sample a new value from the associated column distribution

 update the entry with this new value

end

end

end

different shift term:

$$l_{t+1} = \max \left\{ l_t, \mu - \frac{1}{2}(u_t - l_t)s^t \right\} \quad (1)$$

$$u_{t+1} = \max \left\{ u_t, \mu + \frac{1}{2}(u_t - l_t)s^t \right\} \quad (2)$$

From these brief definitions alone, these methods appear to be largely indistinguishable. However, following a wider discussion around how EDO would work for the general user, it was decided that the first method be rejected in favour of the second. It was found that the second method having fewer parameters was a particularly redeeming feature; this removed any hidden or otherwise unwanted interactions between a parameter dedicated to the shrink process, s , and the maximum number of iterations, M , which is often used as a fallback stopping criterion in complex problem domains.

Algorithm 7: Shrinking the mutation space

Data: parents, current iteration, \mathcal{P}, M, s
Result: A new mutation space focussed around the parents
begin
 for *each distribution in \mathcal{P}* **do**
 for *each parameter of the distribution* **do**
 get the current values for parameter over all parent columns
 find the mean of the current values
 find the new lower (1) and upper (2) bounds around the mean
 set the parameter limits
 end
 end
end

3 Numerical examples

- The x^2 example from the docs is a nice easy one to illustrate things
- Something stochastic
- Make use of the moving parts (linear focus of the mutation space, dwindling mutation probability, stopping conditions)
- If not the k -modes initialisation example, then another clustering one. Maybe k -means versus DBSCAN to show DBSCAN works better on non-convex clusters.

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