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

This work presents a novel approach to learning the quality and performance of an algorithm through the use of evolution. When an algorithm is developed to solve a given problem, the developer is presented with questions about the performance of their proposed method, and its relative performance against existing methods. Under the current paradigm, the standard response to this situation is to fix some datasets and a common metric amongst the proposed method and its competitors. The algorithm is then assessed based on this metric with minimal consideration for both the appropriateness or reliability of the datasets being used, and the robustness of the method in question.

This notion is not so easily observed when travelling in the opposite direction. Suppose that, instead, the benchmark was a dataset of particular interest and a preferable algorithm was to be determined. There exist a number of methods employed across disciplines to complete this task that take into account the characteristics of the data and the context of the research problem. These methods include the use of diagnostic tests. For instance, in the case of clustering, if the data displayed an indeterminate number of non-convex blobs, then one could recommend that an appropriate clustering algorithm would be DBSCAN [4]. Otherwise, for easy scalability, k-means may be chosen.

The approach presented in this work aims to flip the paradigm described here by allowing the data itself to be unfixed. This fluidity in the data is achieved by generating data for which the algorithm performs well (or better than some other) through the use of an evolutionary algorithm. The purpose of doing so is not to simply create a bank of useful datasets but rather to allow for the subsequent studying of these datasets. In doing so, the attributes and characteristics which lead to the success (or failure) of the algorithm may be described, giving a broader understanding of the algorithm on the whole.

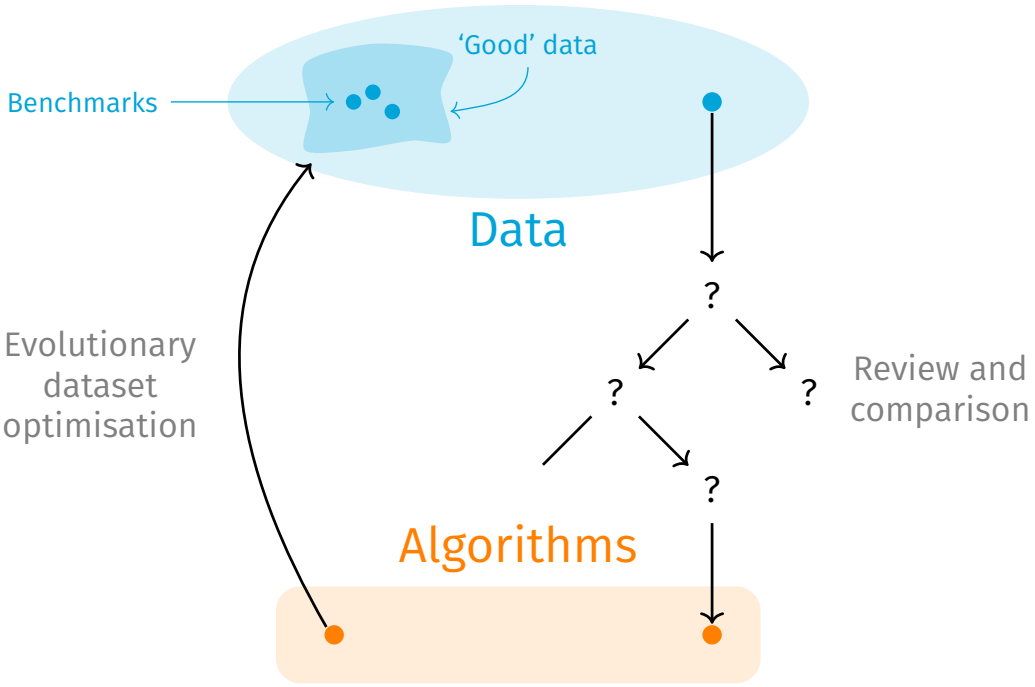

Figure 1: On the right: the path taken by data scientists currently for selecting some algorithm(s) based on their performance for a given dataset. On the left: the proposed flip to understand the space in which 'good' datasets exist.

This proposed flip has a number of motivations, and below is a non-exhaustive list of some of the problems that are presented by the established evaluation paradigm:

1. How are these benchmark examples selected? There is no true measure of their reliability other than their frequent use. In some domains and disciplines there are well-established benchmarks so those found through literature may well be reliable, but in others less so.

2. Sometimes, when there is a lack of benchmark examples, a 'new' dataset is simulated to assess the algorithm. This begs the question as to how and why that simulation is created. Not only this, but the origins of existing benchmarks is often a matter of convenience rather than their merit.

3. In disciplines where there are established benchmarks, there may still be underlying problems around the true performance of an algorithm:

(i) As an example, work by Torralba and Efros [17] showed that image classifiers trained and evaluated on a particular dataset, or datasets, did not perform reliably when evaluated using other benchmark datasets that were determined to be similar. Thus leading to a model which lacks robustness.

(ii) The amount of learning one can gain as to the characteristics of data which lead to good (or bad) performance of an algorithm is constrained to the finite set of attributes present in the benchmark data chosen in the first place.

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 (displayed in Figure 2) allows for the efficient solving of problems that are otherwise beyond the scope of traditional search and optimisation methods. It should be clear that the study of algorithm quality falls into this category of problems.

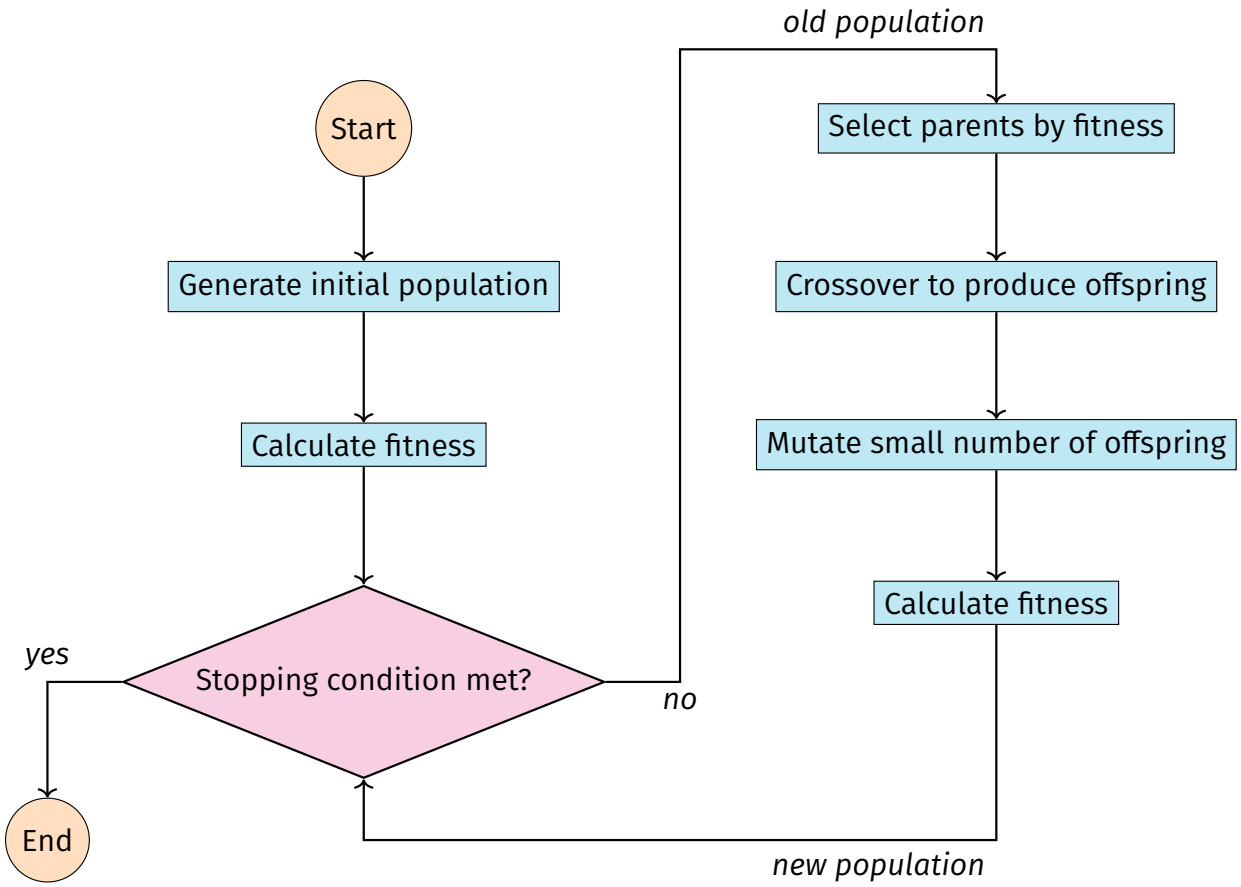

Figure 2: A general schematic for an evolutionary algorithm.

The use of EAs to generate artificial data, however, is not a new concept; these methods have been used to develop techniques for the automated testing of software with a goal of achieve maximal coverage or to support structural tests [6, 11, 14]. Such methods also have a long history in the parameter optimisation of algorithms, and recently in the automated design of convolutional neural network architecture [15, 16].

The unconstrained learning style of methods such as neural networks aligns with that proposed in this work. By allowing the EA to explore and learn about the search space in an organic way, a more unprejudiced level of insight can be established that is free from any particular framework or agenda.

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-values fitness function, f, which acts on a single dataset to give a single fitness score.
- A population size, $N \in \mathbb{N}$.
- A maximum number of iterations, $M \in \mathbb{N}$.
- A selection parameter to detail the proportion of the fittest individuals to carry forward, $b \in [0, 1]$.
- A mutation probability, $p_m \in [0, 1]$.
- Limits on the number of rows a dataset can have:

$$R \in \left\{(r_{\min}, r_{\max}) \in \mathbb{N}^2 \mid r_{\min} \leq r_{\max}\right\}$$

- Limits on the number of columns a dataset can have:

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

  for each $j = 1, \ldots, |\mathcal{P}|$. That is, C defines the minimum and maximum number of columns a dataset may have from each distribution 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 $\mathcal{P}$, $w = \left(w_1, \ldots, w_{|\mathcal{P}|}\right)$.
- A second selection parameter, $l \in [0, 1]$, to allow for a small proportion of "lucky" individuals to be carried forward.
- 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 [10, 13]. 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.

Algorithm 1: The evolutionary dataset optimisation algorithm

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

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 per-

Algorithm 2: Creating a new population

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

spective. Lower level 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:

- Stopping when no improvement in the best fitness is found within some K consecutive iterations [8].
- Utilising global behaviours in fitness to indicate a stopping point [9].
- Constant decreasing in mutation probability by varied amounts across the available attributes [7].

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.

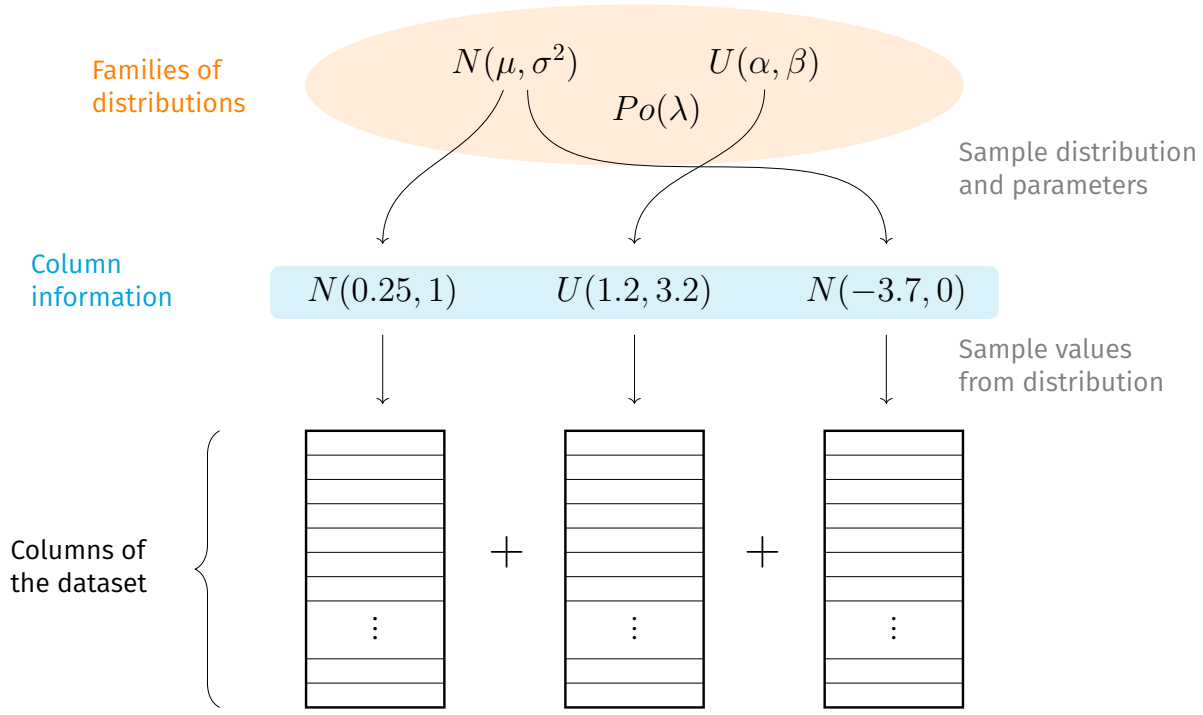

Figure 3: An example of how an individual is first created.

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 3, 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

Input: $R, C, \mathcal{P}, w$
Output: 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.

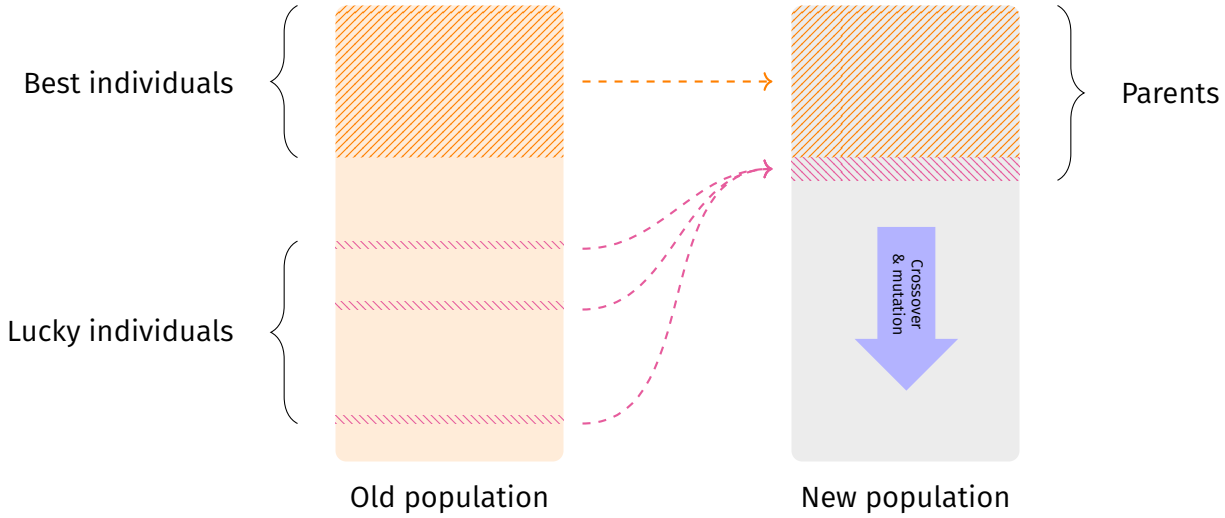

Figure 4: The selection process with the inclusion of some lucky individuals.

In EDO, a modified truncation selection method is used as can be seen in Figure 4. 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

Input: population, population fitness, b, l
Output: 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 [5]. 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 [12]. 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.

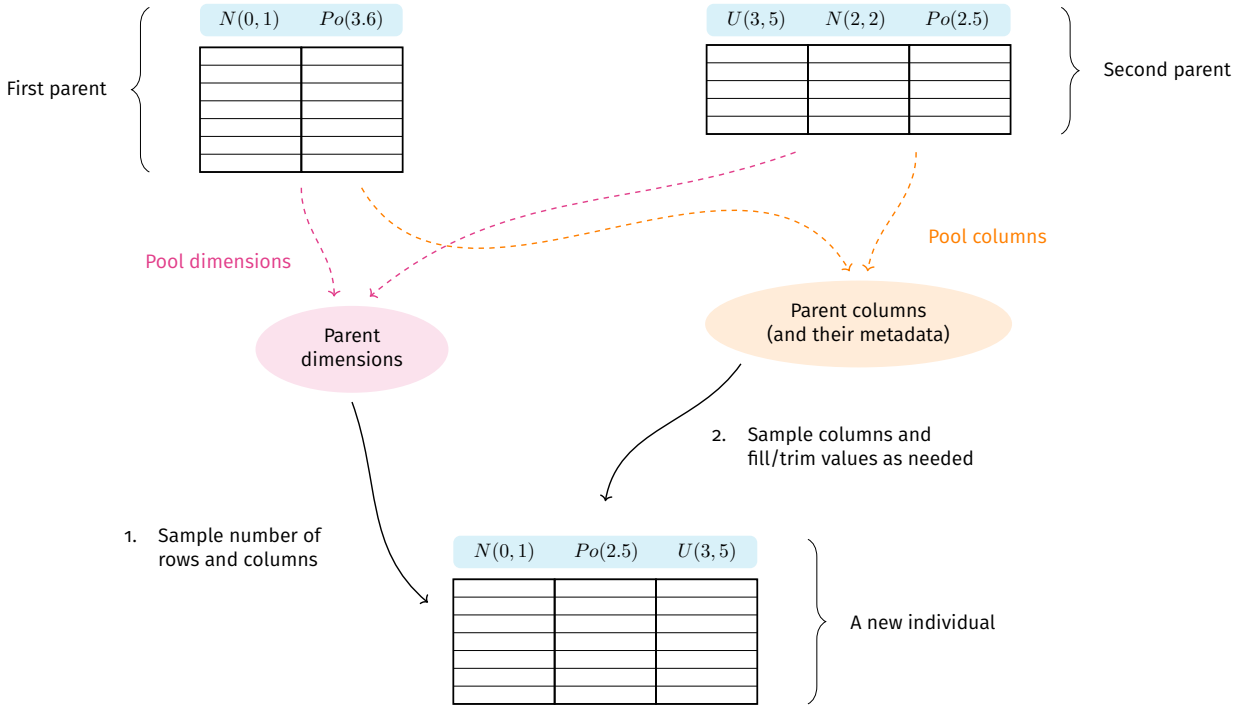

Figure 5: The crossover process.

Algorithm 5: The crossover process

```
Input: Two parents
Output: 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.

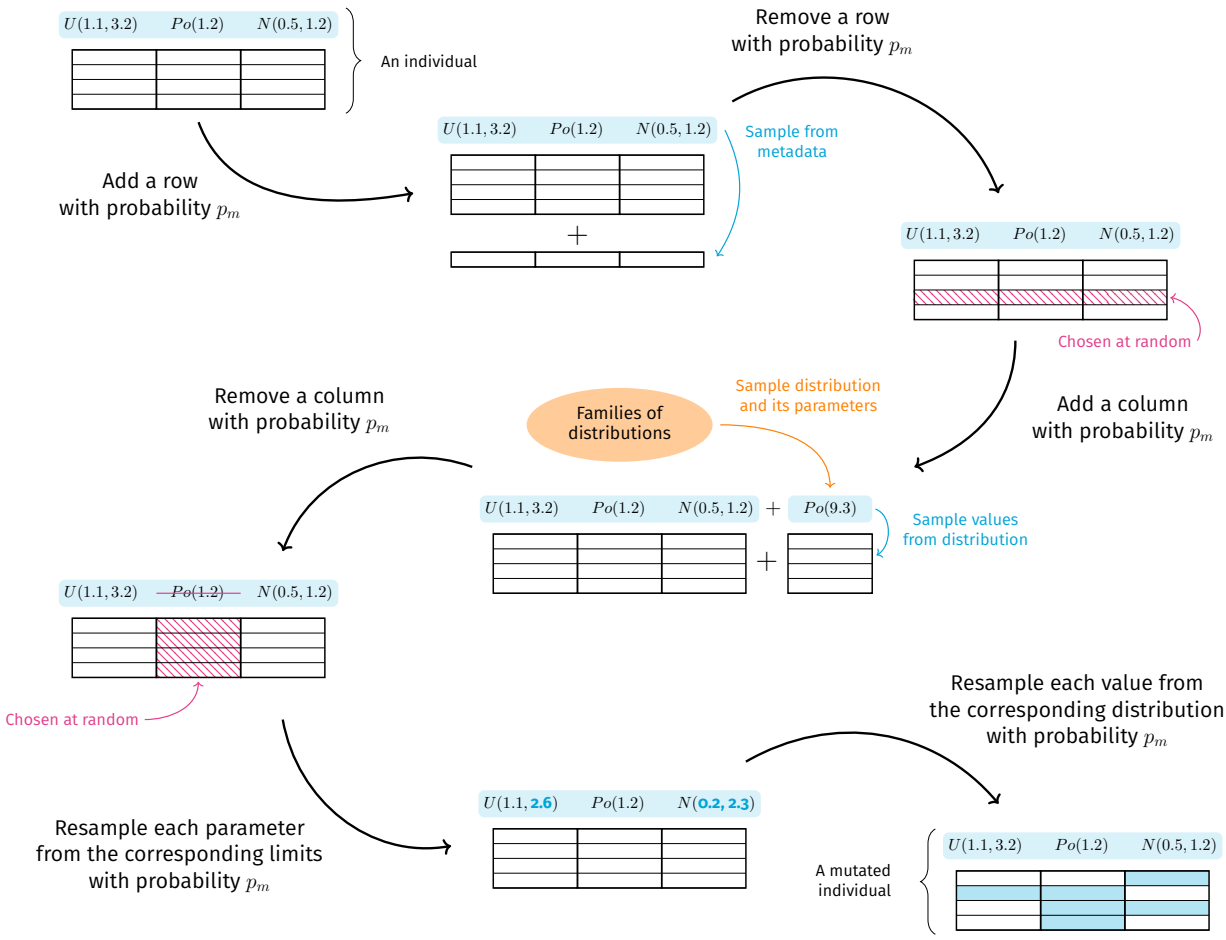

Figure 6: The mutation process.

The mutation process, seen in Figure 6 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

Algorithm 6: The mutation process

Input: An individual, p_m, R, C, $\mathcal{P}$, w
Output: 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

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:

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

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 different shift term:

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

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

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

Input: parents, current iteration, $\mathcal{P}, M, s$
Output: 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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