On the Design and Implementation of Genetic Algorithms for Multivariate Feature Selection

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Repository: https://github.berkeley.edu/andrew-c-ma/genetic-algo

Installation: 'R CMD INSTALL GA'

Abstract

This paper explores the creation of a genetic algorithm for feature selection in multivariate regression models followed by images and examples of its deployment. While stable methods such as step-wise regression are sure to converge to an optimal solution for feature selection problems, genetic algorithms have an advantage over regression models for models with large numbers of covariates. Step-wise regression algorithms must test every single combination of features in order to arrive at the optimal solution, while genetic algorithms may converge to a candidate solution much quicker with less computational cost, leading large increases in computational efficiency.

Introduction

Our package allows for the implementation of genetic algorithms with the goal of selecting optimal feature combinations resulting in the highest 'fitness' metric for generalized regression models.

The structure of our GA package is modular and uses vectorized calculations for efficiency and speed. While largely functional, our program does use some object oriented programming such as the ability to pass user-defined function between various supporting functions and the utilization of function outputs as objects in other helper functions. This streamlined approach can be seen in *Fig 1.* below, where each step produces an object that can be read into the next step of our algorithm.

Finally, we chose binary encoding for genes because each linear regression model either does or does not have any given feature; a bit-wise encoding scheme is both efficient and effective for feature selection problems due to its simplistic and intuitive adaptation.

Design & Development

As shown above in *Fig. 1*, we create an initial generation of genes with a desired population size and 0-1 assignment probability between 0 and 1. For each iteration, we score the fitness of the entire population - if elitism is selected, the top proportion of the population is protected from randomized selection, via the `apply_elitism()` function. The remainder of the population undergoes a parent selection process, followed by crossover and mutation. This results in the $n + 1^{th}$ generation, which undergoes a termination check - if predetermined conditions are not met, we loop through this process again to engender new generations of genes.

Population Initialization & Termination Conditions

Before the deployment of a genetic algorithm, there are several issues surrounding the initialization of the first generation. Our helper functions create generation matrix with rows representing the individual creatures and column representing the number of genes. As mentioned above, the presence of a feature is indicated by a '1' in the indexed position, and '0' for its absence. However, if one feels strongly about a particular sequence of genes, custom user inputs for population elements is also available as a parameter.

Default parameters were chosen based on convention - mutation rates were set at 0.03 and crossover at 0.9. Moreover, we are utilizing binary encoding due to our goal being the optimal selection of features. Due to

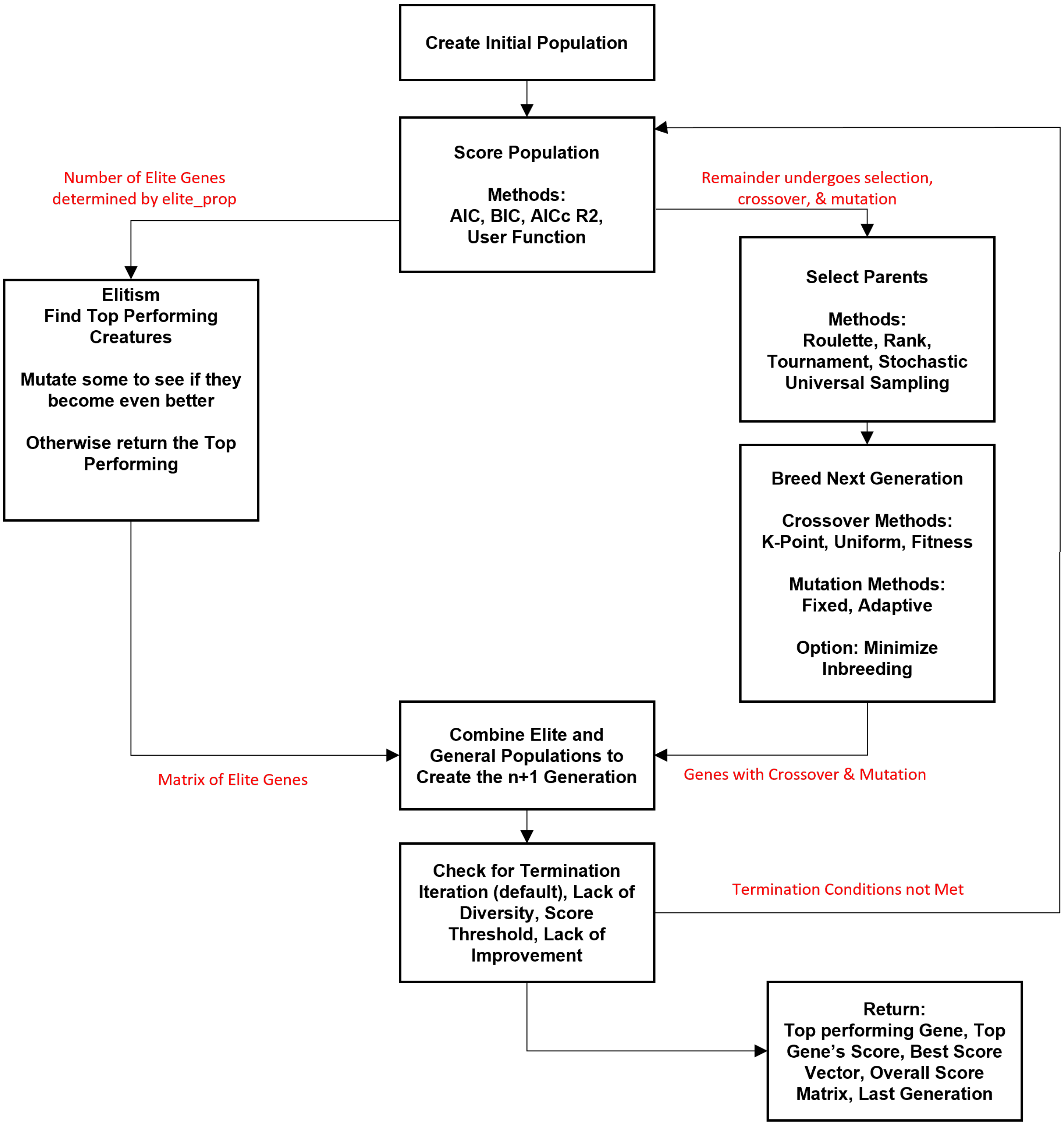


Figure 1: Flowchart of Genetic Algorithm

the heavy dependence on context, parameter initialization for GA's must be carefully considered, alongside factors such as population size, termination conditions,etc.

Finally, there are three termination conditions, which we are checking at the end of each generation after the first. The conditions are:

- Max number of generations reached
- Variance of our fitness scores is less than a constant close to 0 - this implies a lack of diversity within our population or arrival at an estimate that is close to the true solution
- Convergence to the true fitness value, shown through no consistent improvement of fitness scores through the generations

The Creation of a New Generation

Next, we will explain the functionality of our scoring, crossover, and mutation functions, which are applied to each generation of genes. As seen in *Fig 1.*, there is a divergence of data after the scoring step, where $\textit{crossover percentage} = 1 - \textit{elitism percentage}$. Genes that fall under our elitism criteria undergo mutation, but are guaranteed a place in the $n + 1^{th}$ generation.

For genes that undergo normal parent selection, there are a multitude of available methods available to users:

1. Roulette - selects parents randomly proportionally to their fitness; this process favors parents with the highest fitness
2. Rank - selects parents proportional to their rank, similar to Roulette but proportions are not assigned randomly
3. Tournament - selects n candidates at random and the fittest from filtered pool becomes a parent
4. Stochastic Universal Sampling - works like roulette but a user specified number of parents are selected at a fixed interval afterwards

After the parents are chosen, there exist a multitude of crossover parameters which may also be chosen by the user. For simplicity's sake, 'uniform' seems to be safest with a default of two parents creating offspring. However, other recognized crossover methods include fitness & k-point; Uniform Crossover selects each individual gene of the next offspring one at a time assigning it from a parent randomly at a proportion equal to the number of parents. Fitness generates each individual gene randomly from a parent proportionally to the fitness of each parent. K-Point crossover breaks the gene at k points, and randomly assigns each point to one of the parents, the offspring being the combination of those segments. k = 1 is a 1-point crossover. See *Fig 3.*

Lastly, mutation is applied at either a fixed or adaptive rate. Fixed mutation mutates each gene allele of every gene in the population at a fixed rate, while adaptive mutation allows for changes in the mutation rate based on the diversity of the population. Parameters associated with mutation include maximum mutation rate, a minimum mutation rate and an inflection point to generate a logistic function of the populations diversity.

One area associated with mutation worth investigating would be the **minimization of inbreeding**; this involves comparisons of parents before breeding to ensure that there are sufficient differences between the sequence of genes. Parent-pairs with high levels of similarity are penalized, and this leads to an increase in diversity.

Testing & Examples

This section contains multiple examples of applications with our package. The first two are examples pulled from select()'s help function (`?select`). The third example involves a large dataset from generate_data() and the deployment of adaptive mutation in combination with inbreeding-minimization

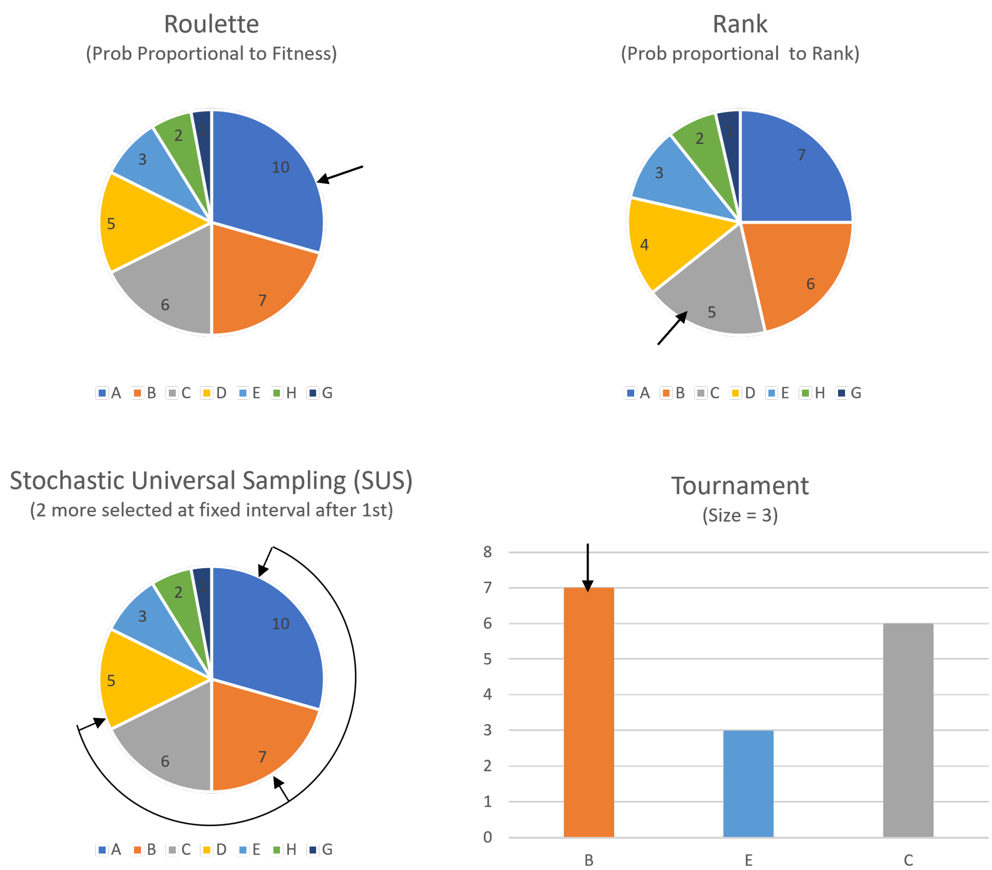


Figure 2: Select Parent Methods

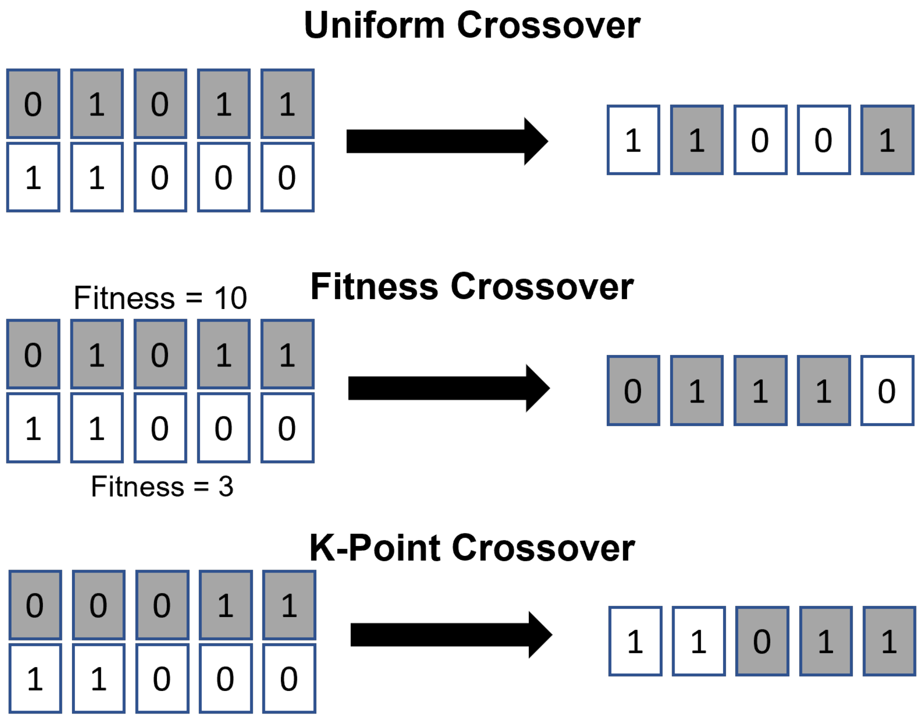


Figure 3: Mutation Types

techniques. For conciseness, we load the functions using `source('reportDemo.R')` and the code can be reviewed in our Github.

We did a lot of initial research into different methods for genetic algorithm; at a cursory level, any genetic algorithm design has to balance speed of convergence and computational complexity. The code for this final example can be found in 'Final_Demo.R', so we simply state the results without proof below:

- **Method 1: Fast-Convergence** - two parents, 1-point crossover, high elitism, high mutation
- **Method 2: Multi-Parent** - four parents, lower elitism, lower mutation, uniform crossover
- **Method 3: Adaptive** - two parents lower elitism, adaptive mutation, minimize inbreeding.

For this experiment, note that our sample dataset is designed such that regression coefficients are sure to be in decreasing order and between the values of [1,50]. See ?generate_data(). We run each method five times taking the average system.time() and also scoring the SSE using the formula below:

$SSE = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$

From the results, it is clear that maintaining diversity had better results (minimizing SSE). However we also see that elitism appears to be computationally wasteful and increases computational time while not providing significant decreases in model metrics or SSE.Finally, let's explore the differing rates of convergence with respect to parent selection methods:

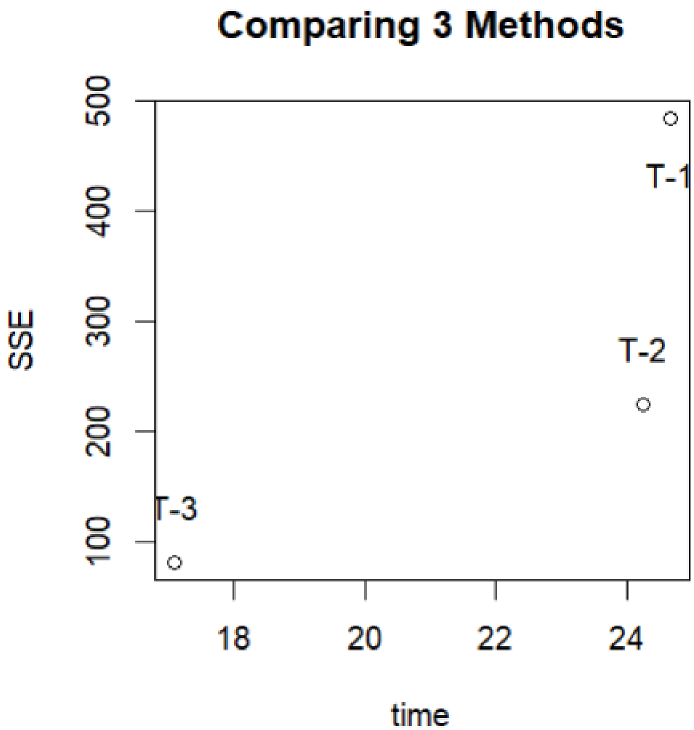


Figure 4: Comparison of Methods

	time	SSE
1	24.664	484
2	24.254	225
3	17.088	81

Figure 5: SSE and Time

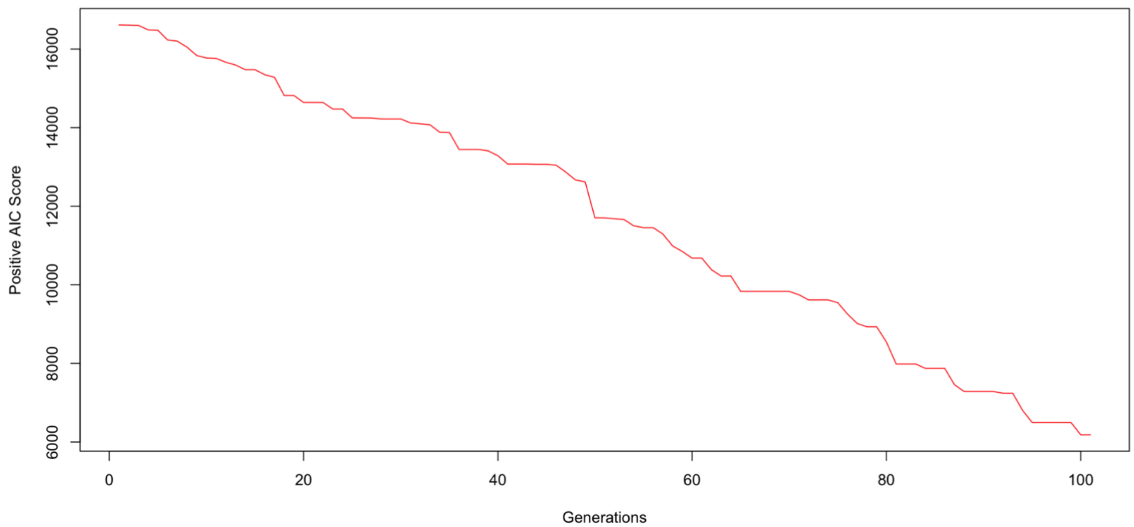
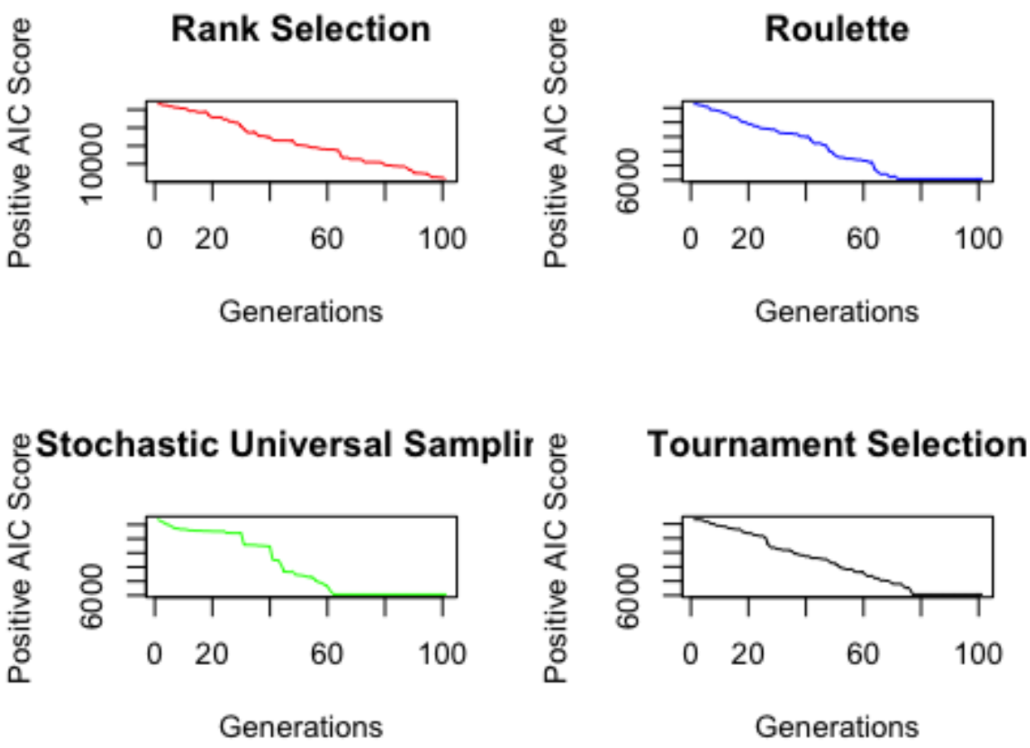


Figure 6: Example of Convergence to true solution with population size of 50 & 'Rank' method



From the results of our experiments, we are confident that our genetic algorithm converges to an optimal solution for feature selection problems with at least a linear rate. It seems that SUS converges to an optimal solution the fastest through large increases in the fitness levels - this is similar to the conclusions drawn from stochastic gradient descent, where large jumps in the direction of greatest descent results in decreased convergence times. On the other hand, rank is a sure and steady method which seems to also converge at a linear rate. Note that of premature convergence have been avoided with the use of crossover and forced variance(diversity) within members of each generation - this greatly assist our algorithm in escaping traps of local minima!

Challenges & Future Possibilities

In this section, we will discuss challenges faced during the implementation of GA's followed by possible research directions for those who wish to dig deeper. With respect to our specific algorithm, we believe that there may be options for the implementation of parallelization - for example, the distribution of fitness scoring to multiple workers presents itself as an embarrassingly-parallel problem.

Furthermore, there are numerous challenges inherently commonly associated with genetic algorithms; many of these are influenced by our chosen parameters. Extensive research done by researchers at the University of Taluk[4] suggests that parameters must be proportional to the population size and number of generations, where unique setups such as 90% mutation / 10% crossover are optimal for models with low population numbers and large numbers of iterations, while 1% mutation / 99% crossover converge quicker for setups with large populations and finite iterations. The consequences of these parameter settings include premature convergence, local minima, and max iterations.

Many of the issues discussed above have no known definitive solutions; as of today, researchers are implementing GA's with adaptive crossover and mutation rates. One can also imagine the combination of GA's with Monte-Carlo simulation methods, where GA's are run in parallel with different parameters to arrive at converging and similar solutions; this would require deeper research into possible implementations of nested parallelization and efficient storage of data & results of simulated GA's for comparison.

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