# STAT 243: Model Selection with Genetic Algorithms using GA

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#### 1 Introduction

A genetic algorithm has the following steps:

- 1. Calculate fitness of chromosomes.
- 2. Select chromosomes to form a mating pool based on their fitness.
- 3. Recombine parent chromosomes from the mating pool.
- 4. Apply mutation to produce the resulting generation of chromosomes.

#### 2 Code

We took the S3 approach to object-oriented programming for our package and created functions that were as modular as possible to facilitate code creation, maintenance and testing.

For a given data set, e.g. the built-in airquality data set in R, the user can carry out model selection for an ordinary linear regression of the variable Ozone on other variables in the data set with the main function in the package as follows:

ga <- select\_model(data = airquality, yvar = "Ozone")</pre>

Finer control of other parameters in the genetic algorithm for model selection is possible by changing the other function arguments. More details can be found in the GA manual in the Appendix.

The output of the results can be viewed using the following commands:

```
summary(ga)
model(ga)
```

The result of this function is an object of GA class that contains the settings, model data, final population of chromosomes/models, model evaluation values of this population and all results of model selection using the genetic algorithm.

In the genetic algorithmic approach to model selection, a population of models, i.e. chromosomes with number of genes equal to the number of model variables under consideration, and with each gene taking a value of 1 if the model variable is included and 0 otherwise, is first initialized. This population then undergoes many iterations of reproduction. In the reproduction stage, each model/chromosome is then evaluated based on the desired model selection criterion, e.g. Akaike's Information Criterion. Chromosomes are then selected into the mating pool based on how well they perform on the model selection criterion.

Next, 2 parent chromosomes are randomly selected from the mating pool to form a child chromosome, with some probability of recombination/crossover occurring in the process. This is repeated until the desired number of child chromosomes for the next generation is reached. Finally, mutation is applied with a low probability to each gene in the population of child chromosomes. The resulting population of child chromosomes forms the next generation. The whole process is repeated for a desired number of iterations. The model/chromosome with the minimum value of the model evaluation criterion across all generations is then the best model.

The following subsections elaborate on the main subfunctions in the GA package; for more detailed documentation, please refer to the GA manual in the Appendix.

#### initialize function

We sample uniformly from the set of  $\{0, 1\}$  with replacement as many genes as is required, i.e. the product of the number of variables under consideration and the population size desired, for the initial population of chromosomes.

#### evaluate function

We compute the value of the model evaluation criterion for every model/chromosome in the population. The default model evaluation criterion is Akaike Information Criterion (AIC). The user can

also choose to use Bayesian Information Criterion (BIC) or define his/her own function.

#### select function

The default selection method is "rank", which refers to Linear Rank Selection (LRS). In LRS, chromosomes are first given ranks  $r_i$  for i = 1, ..., n, where n is the number of chromosomes in the population. The chromosome with the best (minimum) model evaluation criterion is assigned a rank of n. Chromosomes are then selected into the mating pool randomly with probability proportional to their relative rank, until the desired size of the mating pool is reached. This is done with the following algorithm:

- 1. Calculate for each chromosome its probability to be selected,  $p_i = \frac{r_i}{n}$ . Since the best chromosome is given the largest rank, it also has a highest probability of being selected.
- 2. Calculate the cumulative probability for each chromosome to be selected,  $pc_i = \sum_{j=1}^{i} p_j$ .
- 3. Generate a random number u uniformly in the range [0, 1].
- 4. Select the chromosome with index i if  $pc_i < u < pc_{i+1}$
- 5. Repeat until the desired number of chromosomes in the mating pool is select.

The alternative selection method is "tournament", which refers to Tournament Selection. The idea is simple; in Tournament Selection, we randomly select 2 chromosomes from the population. The chromosome with the better model evaluation criterion is selected into the mating pool. This process is repeated (with replacement of both chromosomes each time) until the desired number of chromosomes in the mating pool is reached.

#### recombine function

Recombination occurs with probability prob\_recombine for every set of 2 parent chromosomes; the child chromosome is simply a copy of the first parent chromosome if no recombination occurs. We implemented three methods of recombination: crossover at one point ("onepoint"), crossover at two points ("twopoint") and uniform crossover ("uniform").

For one-point crossover, a break point index b is uniformly sampled from the set of  $\{1, ..., g\}$ , where g is the number of genes on each chromosome. The resulting child chromosome then takes genes 1 to b from the first parent and genes b+1 to g from the second parent.

For two-point crossover, two break point indices  $b_1$  and  $b_2$  are uniformly sampled without replacement from the set of  $\{1, ..., g\}$ . The resulting child chromosome then takes genes 1 to  $b_1$  from the

first parent, genes  $b_1 + 1$  to  $b_2$  from the second parent, and finally genes  $b_2 + 1$  to g from the first parent.

For uniform crossover, the child chromosome has equal probability of receiving each gene from either parent.

#### mutate function

We generate as many Bernoulli variables as there are genes in the population of chromosomes. For each gene, we set:

$$new\_gene \sim \begin{cases} Bernoulli(\texttt{prob\_mutate}), & \text{if current\_gene} = 0 \\ Bernoulli(1-\texttt{prob\_mutate}), & \text{if current\_gene} = 1 \end{cases}$$

This is equivalent to mutating each gene (i.e. changing a value of 1 to 0 and vice versa) with a probability of prob\_mutate, but doing it in this manner allows for vectorized operations.

# 3 Testing

## 4 Contributions

#### 4.1 Code writing

General structure: JRN Functions: JRN, YH

#### 4.2 Code testing

Function testing: EB

Overall function tests: YH

# 4.3 Documentation

Manual creation: EB

Project write-up: Introduction (EB), Code (JRN), Testing (EB, YH)

# 5 Appendix

GA-package

Genetic algorithm for model variable selection

#### Description

Final project for Statistics 243. An R package that implements a genetic algorithm for variable selection in linear and GLM problems.

#### **Details**

Package: GA-package Type: Package

Version: 1.0

Date: 2014-12-13

#### Author(s)

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#### References

G. Givens and J. Hoeting. Computational Statistics, 2nd ed. (2012).

#### See Also

https://github.com/jrnew/genetic-algo

#### Examples

```
# Select regression variables for airquality data using lm model and AIC criterion
select_model(
 data = airquality,
 yvar = "Ozone",
 xvars = NULL,
 model = "lm",
  criterion = "AIC",
 pop_size = 100L,
 method_select = "rank",
 method_recombine = "onepoint",
 prob_recombine = 0.6,
 prob_mutate = 0.01,
 num_max_iterations = 100L,
 seed = 123,
 do_parallel = FALSE
)
```

select\_model

Carry out model selection with a genetic algorithm.

#### Description

Main function for carrying out model selection with a genetic algorithm.

#### Usage

```
select_model(data, yvar, xvars = NULL, model = "lm", glm_family = NULL,
    criterion = "AIC", pop_size = 100L, method_select = "rank",
    method_recombine = "onepoint", prob_recombine = 0.6, prob_mutate = 0.01,
    num_max_iterations = 100L, seed = 123, do_parallel = FALSE)
```

#### Arguments

| data  | Data frame  |
|-------|---|
| yvar  | Character; Name of column containing response variable                      |
| xvars | Character vector; Default is all column names that are not yvar; Name(s) of |
|       | column(s) containing set of explanatory variables to select on.             |

model Character; "lm" (default) or "glm"; Linear model or generalized linear model.

glm\_family Character if model is "glm", NULL otherwise; "binomial", "gaussian" (de-

fault), "Gamma", "inverse.gaussian", "poisson", "quasi", "quasibinomial", "quasipois-

son"; A family function that gives the error distribution and link function to

be used in the model.

criterion "AIC" (default) or "BIC"; Criterion to be minimized.

pop\_size Integer; Default is 100; Number of chromosomes per generation.

method\_select

String; "rank" (linear rank selection) (default) or "tournament"; Method to

select chromosomes for inclusion in mating pool.

method\_recombine

String; "onepoint" (default), "twopoint", "uniform"; Type of crossover, at one

point, at two points or uniformly (at all possible points).

prob\_recombine

Numeric, between 0 and 1; Default is 0.6; Probability of recombination.

prob\_mutate Numeric, between 0 and 1; Default is 0.01; Probability of mutation.

num\_max\_iterations

Non-negative integer; Default is 100; Maximum number of iterations before

algorithm is stopped.

seed Non-negative integer; Default is 123; Random seed for reproducibility.

do\_parallel Logical; Default is FALSE; Do in parallel?

evaluate\_once Do evaluation once.

#### Description

Do evaluation for a chromosome by calculating model selection criterion.

#### Usage

```
evaluate_once(model_data, xvars_select, model = "lm", glm_family = NULL,
    criterion = "AIC")
```

#### Arguments

model Character; "lm" (default) or "glm"; Linear model or generalized linear model.

glm\_family Character if model is "glm", NULL otherwise; "binomial", "gaussian" (de-

fault), "Gamma", "inverse.gaussian", "poisson", "quasi", "quasibinomial", "quasipois-

son"; A family function that gives the error distribution and link function to

be used in the model.

criterion "AIC" (default) or "BIC"; AIC or BIC.

model\_data; Object of class model\_data.

xvars\_select;

Logical vector;

#### Value

Numeric; Value of criterion.

evaluate

Do evaluation.

#### Description

Do evaluation for chromosomes in population by calculating model selection criterion.

#### Usage

```
evaluate(pop, model_data, model = "lm", glm_family = NULL,
    criterion = "AIC", do_parallel = FALSE)
```

#### Arguments

pop Matrix of population of chromosomes.

model\_data Object of class model\_data.

model Character; "lm" (default) or "glm"; Linear model or generalized linear model.

glm\_family Character if model is "glm", NULL otherwise; "binomial", "gaussian" (de-

fault), "Gamma", "inverse.gaussian", "poisson", "quasi", "quasibinomial", "quasipois-

son"; A family function that gives the error distribution and link function to

be used in the model.

criterion "AIC" (default) or "BIC"; Criterion to be minimized.

do\_parallel Logical; Default FALSE; Do in parallel?

#### Value

Numeric vector; Evaluation values for all chromosomes in the current generation.

initialize

Initialize first generation of chromosomes.

#### Description

Initialize first generation of chromosomes completely randomly.

#### Usage

initialize(pop\_size, num\_vars)

#### Arguments

pop\_size Non-negative integer; Number of chromosomes in population.

num\_vars Non-negative integer; Number of variables in model under consideration/ num-

ber of genes in each chromosome.

#### Value

A matrix of size pop\_size x num\_vars with 1's and 0's.

Mutate genes in the population.

mutate

#### Description

Mutate each gene in the population at a pre-defined rate.

#### Usage

```
mutate(pop, prob_mutate = 0.01)
```

#### Arguments

pop Matrix; Population of chromosomes.

prob\_mutate Numeric, between 0 and 1; Default is 0.01; Probability of mutation.

#### Value

Matrix of population of chromosomes that have undergone mutation.

plot.ga

Plots results from the genetic algorithm.

#### Description

Plots the best model evaluation criterion in each generation against the generation iteration.

#### Usage

```
## S3 method for class 'ga'
plot(ga, num_view = 3)
```

#### Arguments

ga Object of class ga.

num\_view Number of top models to display.

#### Value

Prints summary of top models and associated value of model selection criterion.

process\_data

Process data for input into genetic algorithm.

#### Description

Process data for input into genetic algorithm.

#### Usage

```
process_data(data, yvar, xvars = NULL)
```

#### Arguments

data Data frame

yvar Character; Name of column containing response variable.

xvars Character vector; Default is all column names that are not yvar; Name(s) of

column(s) containing set of explanatory variables to select on.

#### Value

A list object named model\_data containing:

data Data frame; Processed data with only relevant columns.

yvar Character; Name of column containing response variable.

xvars Character vector; Name(s) of column(s) containing set of explanatory variables to select on.

num\_vars Integer; Length of xvars.

recombine\_once

Recombine once.

#### Description

Carry out crossover of two parent chromosomes to produce one child chromosome.

#### Usage

```
recombine_once(parent1, parent2, method = "onepoint")
```

#### Arguments

| parent1 | Integer vector of 1st parent chromosome containing 1's and 0's.                |
|---------|--|
| parent2 | Integer vector of 2nd parent chromosome containing 1's and 0's.                |
| method  | String; "onepoint" (default), "twopoint", "uniform"; Type of crossover, at one |

point, at two points or uniformly (at all possible points).

#### Value

Integer vector of child chromosome containing 1's and 0's.

recombine Recombine.

#### Description

Carry out crossover of parent chromosomes in a mating pool.

#### Usage

```
recombine(pop_mating, pop_size, method = "onepoint", prob_recombine = 0.6,
   do_parallel = FALSE)
```

#### Arguments

pop\_mating Matrix of population of chromosomes that form the mating pool.

pop\_size Integer; Number of chromosomes in a generation.

method String; "onepoint" (default), "twopoint", "uniform"; Type of crossover, at one

point, at two points or uniformly (at all possible points).

prob\_recombine

Numeric, between 0 and 1; Default is 0.6; Probability of recombination.

do\_parallel Logical; Default FALSE; Do in parallel?

#### Value

Matrix of population of chromosomes resulting from recombination.

reproduce Wrapper function for reproduction stage.

### Description

Wrapper function for reproduction stage.

#### Usage

```
reproduce(ga, iteration, do_parallel = FALSE)
```

#### Arguments

ga Object of class ga. iteration Iteration number.

#### Value

Updated ga list object.

select

 $Select\ chromosomes\ for\ recombination.$ 

#### Description

Select chromosomes for recombination based on fitness.

#### Usage

```
select(pop, evaluation, method = "rank", do_parallel = FALSE)
```

#### Arguments

pop Matrix; Population of chromosomes.

evaluation Numeric vector; Evaluation values of all chromosomes in population.

method String; "rank" (linear rank selection) (default) or "tournament"; Method to

select chromosomes for inclusion in mating pool.

do\_parallel Logical; Default FALSE; Do in parallel?

#### Value

Matrix of population of chromosomes that form the mating pool.

summary.ga

Display summary of results from the genetic algorithm.

#### Description

Outputs the top models selected from the genetic algorithm.

# Usage

```
## S3 method for class 'ga'
summary(ga, num_view = 5)
```

# Arguments

ga Object of class ga.

num\_view Number of top models to display.

# Value

Prints summary of top models and associated value of model selection criterion.