STAT 243:
Model Selection with
Genetic Algorithms using `GA`

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1 Introduction

A genetic algorithm is an optimization technique that mimics the biological process of natural selection. The basic strategy is to take a population of candidate solutions and "evolve" them over many generations towards an optimal solution. Continuing the biology analogy, the population is typically represented as a collection of a series of bits called chromosomes. A fitness function is evaluated at each iteration to determine how well the current population of chromosomes solves the objective function. A genetic algorithm has the following steps:

1. Calculate fitness of chromosomes. Often, the fitness is the value of the objective function solving the optimization. The better the fitness, the better solution the chromosomes will provide.

2. Select chromosomes to form a mating pool based on their fitness. This process is performed stochastically, with more fit chromosomes having a higher probability of being selected.

3. Recombine parent chromosomes from the mating pool. This is the first step in producing the next generation of chromosomes in which the parents' genes are combined.

4. Apply mutation to produce the resulting generation of chromosomes. After crossover, each gene in the resulting population has a finite probability to flip its value.

5. Repeat until either a set number of generations is reached.

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(data = airquality, yvar = "Ozone")
```

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_for_mating 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, $p_i = \frac{r_i}{\sum\limits_{i=1}^{n} r_i}$. 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, $pc_i = \sum\limits_{j=1}^{i} p_j$.
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:

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

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

Automated testing of auxilliary functions was performed using R's `testthat` package. This approach has several advantages over manual testing. It provides functions that allow the user to clearly define expected inputs, outputs, and errors while testing. Additionally, re-testing simply involves running the test file again, and multiple test files can be run at once. Finally, it displays test progress visually, showing whether each tests passes, fails, or produces an error.

Each function was tested for correct inputs and outputs. The number of inputs, their class, and their dimensions was specified using the `expect_that(x, equals(y))` and `expect_that(x, is_a(y))` functions. Similarly, the number of outputs, their class, and their dimensions were specified using the same functions. Further constraints on certain inputs and outputs were tested as well. Since chromosomes are composed of bits, the elements in the population matrix must be either zero or one. This specification was tested by ensuring that the minimum of the population is 0 and the maximum is 1.

Although most functions had stochastically determined outputs and thus their exact values could not be predicted, the `mutate` function had two testable outcomes. First, if the mutation rate was set to zero, no genes were expected to mutate, so the output population should be the exact same as the input population. Secondly, if the mutation rate were one, all of the genes in the population should switch their value. Both of these scenarios were tested to ensure proper behavior in the `mutate` function.

A testing function was written for each function in the `ga` package. These files can be found in the /testing folder of the Github repository. All testing files can be run at once using the `test_dir(‘‘ /testing’’)` command in R.

After ensuring that each function takes proper inputs and returns desired outputs, each method were also tested using small data sets to see if they functions properly. In order to test the functionality of our genetic algorithm, we employed a larger, more realistic data set. We compared the models selected using our genetic algorithim with a well-known model selection method, the stepwise model selection using AIC, implemented in R in the `stepAIC` function available in the `MASS` package.

This data set was obtained from surveys about how video games affect grades. There are 15 variables in the data set – time (number of hours play), like (whether like to play), where (where to play), freq (how often), busy (play if busy), educ (playing educational), sex, age, home (computer at home), math (hate math), work (number of hours work per weeek), own (own PC), cdrom (PC has CD-rom), email (have Email) and grade. The dependent variable is grade. Completed data were obtained from 91 students during Fall 1994 at Berkeley. The data source can be found at the Stat Labs website for University of California, Berkeley.

The following results are obtained using our genetic algorithim.

```r
data <- read.table("../data/video.txt", header = TRUE, quote = "\"")
ga <- select(data,
                   yvar = "grade",
                   pop_size = nrow(data)*2,
                   num_max_iterations = 50,
                   model = "glm",
                   glm_family = "gaussian")
```

```
res <- summary(ga)


## Model 1 :
##  grade ~ where + freq + busy + sex + home + math
##  AIC = 157.6
##  --------------------------------------------------
## Model 2 :
##  grade ~ freq + educ + sex + home + math
##  AIC = 158.2
##  --------------------------------------------------
## Model 3 :
##  grade ~ freq + busy + sex + home + math
##  AIC = 158.3
##  --------------------------------------------------
## Model 4 :
##  grade ~ where + freq + busy + sex + home + math + own
##  AIC = 158.4
##  --------------------------------------------------
## Model 5 :
##  grade ~ where + freq + busy + sex + home + math + email
##  AIC = 158.6
##  --------------------------------------------------
```

The following results are obtained using the `stepAIC` function.

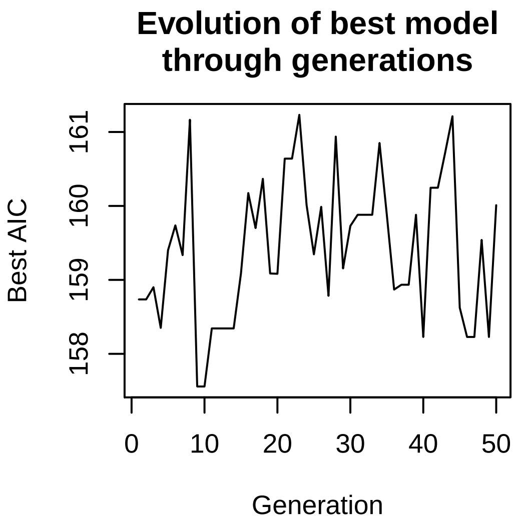
```
library(MASS)
mod <- glm(grade ~ ., data = data)
res_step <- stepAIC(mod)


## Start:  AIC=167.2
## grade ~ time + like + where + freq + busy + educ + sex + age +
##     home + math + work + own + cdrom + email
##
##         Df Deviance AIC
## - age    1     23.6 165
## - where  1     23.6 166
## - time   1     23.6 166
## - like   1     23.7 166
## - educ   1     23.8 166
## - cdrom  1     23.8 166
## - work   1     23.9 166
## - email  1     23.9 167
## - busy   1     23.9 167
## <none>         23.6 167
## - math   1     24.2 168
## - own    1     24.2 168
## - freq   1     24.6 169
## - home   1     25.8 174
## - sex    1     27.4 179
##
## Step:  AIC=165.3
## grade ~ time + like + where + freq + busy + educ + sex + home +
##     math + work + own + cdrom + email
##
##         Df Deviance AIC
## - where  1     23.7 164
## - time   1     23.7 164
## - like   1     23.8 164
## - educ   1     23.8 164
## - cdrom  1     23.8 164
## - work   1     23.9 165
## - busy   1     24.0 165
## - email  1     24.0 165
## <none>         23.6 165
## - math   1     24.2 166
## - own    1     24.3 166
## - freq   1     24.6 167
## - home   1     25.9 172
## - sex    1     27.5 178
##
## Step:  AIC=163.7
## grade ~ time + like + freq + busy + educ + sex + home + math +
##     work + own + cdrom + email
##
##         Df Deviance AIC
## - like   1     23.9 162
## - cdrom  1     23.9 162
## - busy   1     24.0 163
## - time   1     24.0 163
## - work   1     24.0 163
## - educ   1     24.1 164
## - math   1     24.2 164
## <none>         23.7 164
## - email  1     24.2 164
## - own    1     24.4 165
## - freq   1     24.8 166
## - home   1     26.1 170
## - sex    1     27.9 177
##
## Step:  AIC=162.4
## grade ~ time + freq + busy + educ + sex + home + math + work +
##     own + cdrom + email
##
##         Df Deviance AIC
## - cdrom  1     24.1 161
## - time   1     24.2 162
## - work   1     24.2 162
## - busy   1     24.2 162
## - math   1     24.3 162
## - email  1     24.4 162
## - educ   1     24.4 162
## <none>          23.9 162
## - own    1     24.6 163
## - freq   1     25.0 164
## - home   1     26.2 169
## - sex    1     27.9 175
##
## Step:  AIC=161.2
## grade ~ time + freq + busy + educ + sex + home + math + work +
##     own + email
##
##         Df Deviance AIC
## - time   1     24.4 160
## - work   1     24.4 160
## - busy   1     24.5 161
## - math   1     24.5 161
## - educ   1     24.6 161
## <none>          24.1 161
## - email  1     24.6 161
## - own    1     24.7 162
## - freq   1     25.1 163
## - home   1     26.6 168
## - sex    1     28.6 175
##
## Step:  AIC=160.3
## grade ~ freq + busy + educ + sex + home + math + work + own +
##     email
##
##         Df Deviance AIC
## - work   1     24.7 160
## - busy   1     24.8 160
## - email  1     24.8 160
## - educ   1     24.9 160
## - math   1     24.9 160
## <none>         24.4 160
## - own    1     25.0 161
## - freq   1     25.6 163
## - home   1     27.1 168
## - sex    1     28.7 173
##
## Step:  AIC=159.6
## grade ~ freq + busy + educ + sex + home + math + own + email
##
##         Df Deviance AIC
## - email  1     25.1 159
## - busy   1     25.2 159
## - own    1     25.2 159
## - educ   1     25.2 159
## <none>         24.7 160
## - math   1     25.8 162
## - freq   1     25.9 162
## - home   1     27.3 167
## - sex    1     28.8 171
##
## Step:  AIC=159.2
## grade ~ freq + busy + educ + sex + home + math + own
##
##        Df Deviance AIC
## - own   1     25.5 159
## - educ  1     25.6 159
## - busy  1     25.6 159
## <none>        25.1 159
## - math  1     26.2 161
## - freq  1     26.3 161
## - home  1     27.8 166
## - sex   1     29.2 171
##
## Step:  AIC=158.6
## grade ~ freq + busy + educ + sex + home + math
##
##        Df Deviance AIC
## - busy  1     26.0 158
## - educ  1     26.0 158
## <none>        25.5 159
## - math  1     26.6 160
## - freq  1     26.7 161
## - home  1     27.8 164
## - sex   1     29.4 169
##
## Step:  AIC=158.2
## grade ~ freq + educ + sex + home + math
##
##        Df Deviance AIC
## <none>        26.0 158
## - freq  1     26.7 159
## - math  1     26.8 159
## - educ  1     27.4 161
## - home  1     28.4 164
## - sex   1     29.8 168
```

The best model found using genetic algorithim was: y ∼ where + freq + busy + sex + home + math, with an AIC of 157.56. This result is better than that of 158.23 that we obtained using the `stepAIC` function.

Finally, we plotted the best AIC for each generation to see how the best AIC has changed over generations.

```
par(cex = 0.8)
plot(ga)
```



From the plot, we can see that the best model was found at generation 9.

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)

Eddie Buehler, Yang Hu, JR New

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
)

# With a user-defined model evaluation criterion function
rsquared <- function(lm) {
  mod <- summary(lm)
  return(-mod\$r.squared)
}
ga <- select_model(data = airquality,
                   yvar = "Ozone",
                   model = "lm",
                   criterion = "rsquared",
                   criterion_function = rsquared)
```

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” (default), ”Gamma”, ”inverse.gaussian”, ”poisson”, ”quasi”, ”quasibinomial”, ”quasipoisson”; 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” (default), ”Gamma”, ”inverse.gaussian”, ”poisson”, ”quasi”, ”quasibinomial”, ”quasipoisson”; 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" (default), "Gamma", "inverse.gaussian", "poisson", "quasi", "quasibinomial", "quasipoisson"; 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/ number of genes in each chromosome.

Value

A matrix of size pop_size x num_vars with 1's and 0's.

`mutate` *Mutate genes in the population.*

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 algorithim.*

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 algorithim.*

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.