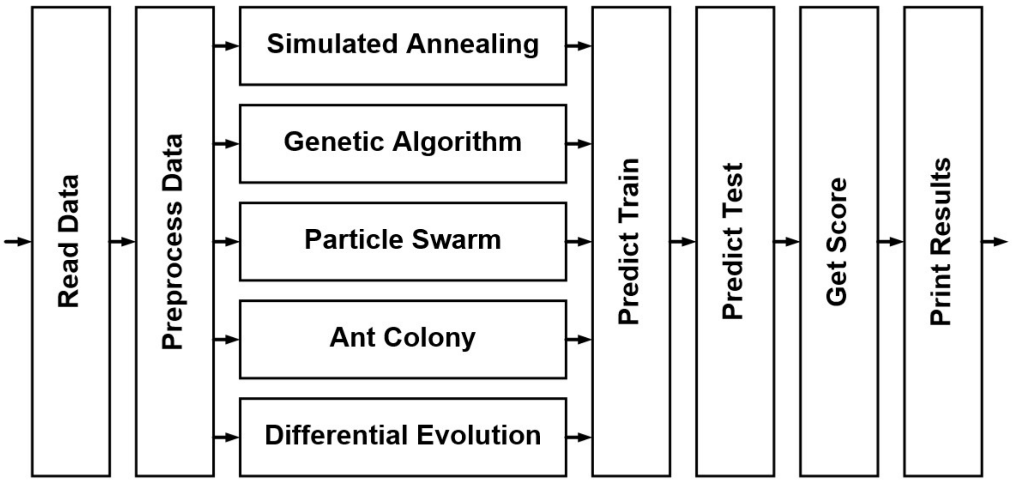
Bio-marker selection problem for logistic regression model utilizing Meta-heuristic Algorithms

Overview

The flow chart of this project is as follows



- Read Data: directly read the data from the excel file
- Preprocess Data
  (1) Add cross terms $x_i x_j$ (We ignore the triple terms $x_i x_j x_k$ since it requires large memory)
  (2) The above data is set as the solution space. The goal is to find 30 selection from it.
- Simulated Annealing (SA)
  (1) Initialize temperature
  (2) Randomly select a solution
  (3) Calculate neighbor solution (We randomly pick a bio-marker for the first 30 selection)
  (4) If the neighbor sol. has better cost, update the sol. Otherwise, update the sol. with a probability based on the difference of the cost and the current temperature.
  (5) Reduce temperature
  (6) Return to (3) and run until iteration terminates
- Genetic Algorithm (GA)
  (1) Generate random parent genes
  (2) Calculate fitness of all parent genes and leave the best few with better fitness
  (3) Apply single point crossover within the remain parent genes to generate children genes (The remain parents and the childern will have the same amount as the original parent)
  (4) Apply mutation on the children genes (randomly select one bio-marker and replace by a random bio-marker)
  (5) Return to (2) and run until iteration terminates
- Particle Swarm (PS) : Swarm intelligent based
  (1) Generate random particles
  (2) Calculate fitness of each particles
  (3) Update the particle based on the local best, global best or random perturbation
  (4) Return to (2) and run until iteration terminates
- Ant Colony (AC)
  (1) Randomly generate large amount of solutions as solution space (Our graph is contruct by single layer with number of sample nodes)
  (2) Randomly generate ants, each represent a solution (The number of ants is much smaller than the number of solution)
  (3) Calculate fitness of each ants
  (4) Decay pheromone of each solution
  (5) Increase pheromone of the best fitness ant
  (6) Return to (2) and run until iteration terminates
- Differential Evolution (DE)
  (1) Generate random parent particles

(2) Randomly select three parent particles and generate a children particles
(3) Run (2) until amount of children particles is the same as parent particles
(4) Replace a parent particle by a children particle if it has worse fitness
(5) Return to (2) and run until iteration terminates

- Predict Train: predict training data by logistic regression based on the selected index
- Predict Test: predict test data set based on the previous logistic regression model

Simulation Setting

Algor.	Num. of particle	Num. of iterations
SA	1	1000
GA	10	100
PS	10	100
AC	10	100
DE	10	100

Objective function

In this problem, the number of training samples is n_s, the number of features in each data is n_f and the number of prediction classes is n_y. Then the training input data is represented by $\mathbf{X} \in R^{n_s \times n_f}$ and the training output is $\mathbf{y} \in R^{n_s \times 1}$.
The objective function of this problem is
$\arg\min_{\mathcal{I} \in \mathcal{A}} \frac{\sum 1(\mathbf{y}, \hat{\mathbf{y}})}{n_s}$, representing the prediction accuracy, where $\hat{\mathbf{y}}$ is generate from the logistic regression model $LR(\mathbf{X}_{:,\mathcal{I}}, \mathbf{y})$ and the $1(.)$ function is defined as

$$1(x_1, x_2) = \begin{cases} 1, \text{ when } x_1 = x_2 \\ 0, \text{ otherwise} \end{cases}.$$

Performance Results

The trainging performance:

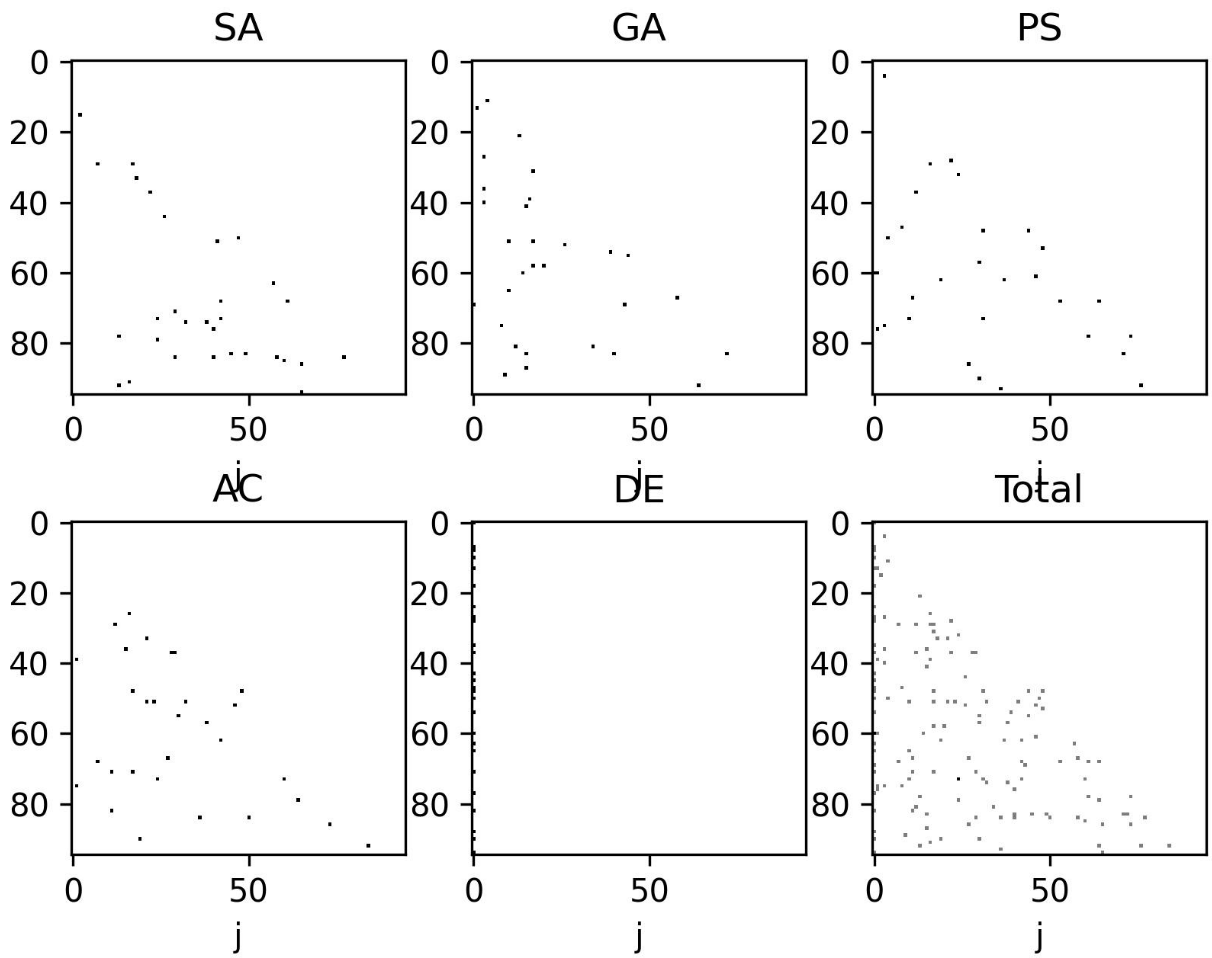
Algor.	Class 1	Class 2	Class 3	Class 4	Class 5	Mean Acc.
SA	0.964842	0.954932	0.876357	0.959179	1	0.951062
GA	0.967437	0.958943	0.907504	0.961538	1	0.959084
PS	0.958943	0.957291	0.884379	0.958707	1	0.951864
AC	0.963426	0.957055	0.878952	0.958707	1	0.951628
DE	0.962718	0.956583	0.86621	0.956583	1	0.948419

The validation performance:

Algor.	Class 1	Class 2	Class 3	Class 4	Class 5	Mean Acc.
SA	0.966316	0.938947	0.848421	0.962105	1	0.943158
GA	0.970526	0.932632	0.858947	0.978947	1	0.948211
PS	0.981053	0.941053	0.858947	0.974737	1	0.951158
AC	0.974737	0.932632	0.837895	0.964211	1	0.941895
DE	0.983158	0.938947	0.833684	0.968421	1	0.944842

Bio-marker Selection Results

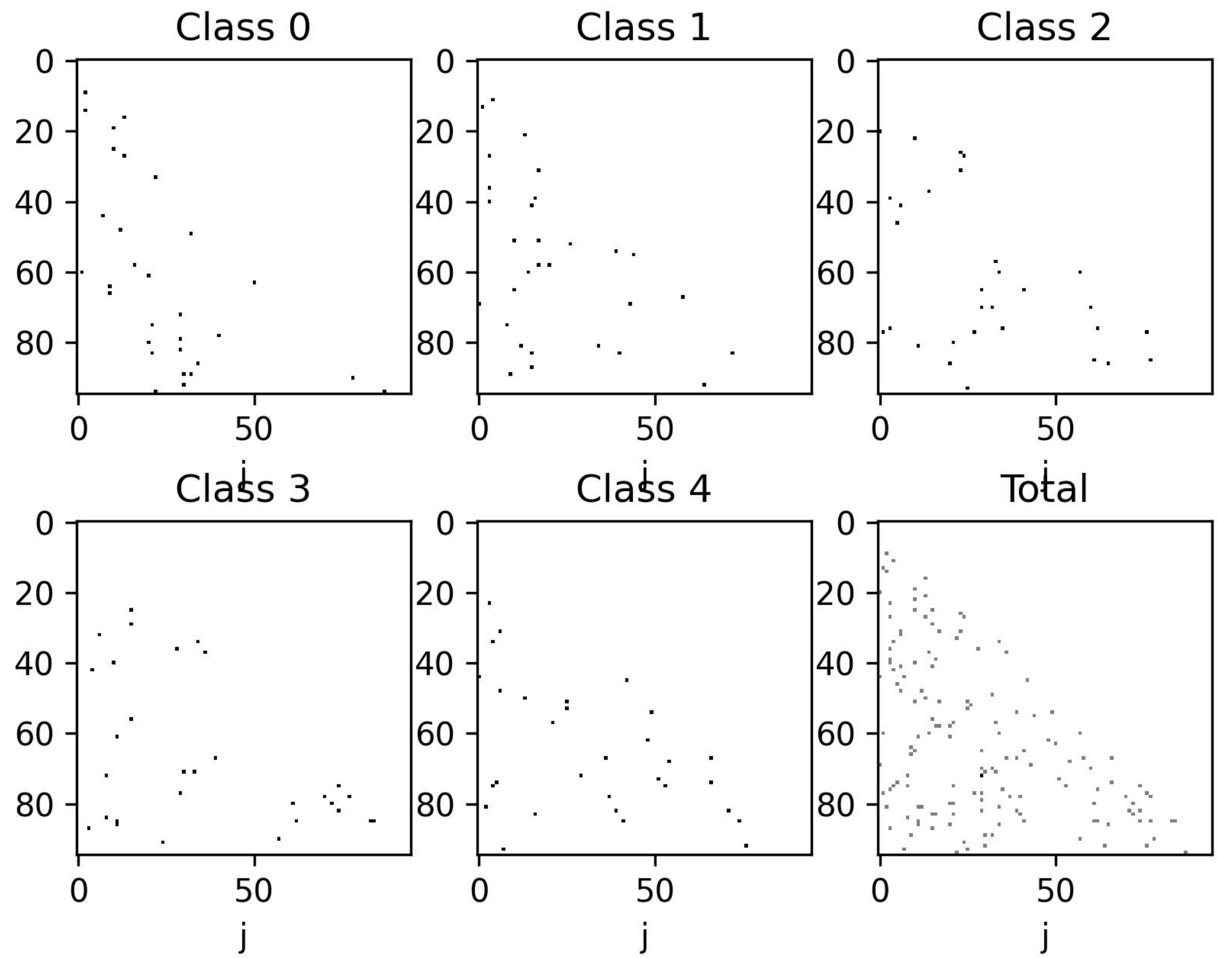
The follow figure shows the selection of each algorithm for class 2



In this figure, the i, j represents the two-way bio-marker $x_i x_j$ while i, i represents the ony-way bio-marker x_i

We find that the bio-marker selection are totally different.

The follow figure shows the selection of each algorithm for class GA



Similarly, the selected bio-markers are mostly different.

We define $T_{i,j}$ as the two way ratio $D_i D_j$ if $i = j$; otherwise, $T_{i,j}$ is define as the one-way ratio D_i (Notice that the index start from 0)
Also, D_i is define as $\frac{F_k}{R_l}$ where $k = i \bmod 19$ and $l = \lfloor \frac{i}{5} \rfloor$
The 30 bio-marker selection for each algorithm and each class is shown as follows:

SA

- Class 0
  $T_{91,9}, T_{92,59}, T_{53,67}, T_{86,27}, T_{72,75}, T_{67,14}, T_{91,25}, T_{89,68}, T_{85,31}, T_{4,77}, T_{40,45}, T_{52,18}, T_{7,62}, T_{31,84}, T_{90,11}, T_{88,11}, T_{62,28}, T_{33,74}, T_{72,88}, T_{78,9}, T_{49,15},$
- Class 1
  $T_{20,5}, T_{57,61}, T_{16,67}, T_{45,40}, T_{24,27}, T_{79,59}, T_{84,67}, T_{16,9}, T_{44,27}, T_{64,87}, T_{42,65}, T_{62,28}, T_{62,2}, T_{64,53}, T_{64,88}, T_{61,74}, T_{64,93}, T_{16,44}, T_{16,93}, T_{72,86}, T_{70,5},$
- Class 2
  $T_{60,1}, T_{4,3}, T_{70,9}, T_{21,6}, T_{63,41}, T_{0,76}, T_{63,67}, T_{72,69}, T_{71,15}, T_{39,58}, T_{65,72}, T_{66,23}, T_{10,56}, T_{12,56}, T_{86,0}, T_{6,3}, T_{81,12}, T_{42,18}, T_{11,76}, T_{62,23}, T_{43,23}, T_{30,8}$
- Class 3
  $T_{30,53}, T_{16,25}, T_{91,77}, T_{68,72}, T_{74,73}, T_{64,34}, T_{91,19}, T_{29,30}, T_{38,53}, T_{5,26}, T_{71,91}, T_{87,33}, T_{37,71}, T_{64,39}, T_{26,29}, T_{66,18}, T_{51,53}, T_{40,75}, T_{61,91}, T_{59,2}, T_{31,8}$
- Class 4
  $T_{32,79}, T_{83,15}, T_{62,69}, T_{41,33}, T_{27,75}, T_{30,6}, T_{79,3}, T_{60,58}, T_{33,21}, T_{54,61}, T_{47,17}, T_{7,93}, T_{65,33}, T_{29,30}, T_{89,4}, T_{9,76}, T_{5,18}, T_{57,7}, T_{55,30}, T_{84,12}, T_{43,60}, T_{6}$

GA

- Class 0
  $T_{91,9}, T_{92,59}, T_{53,67}, T_{86,27}, T_{72,75}, T_{67,14}, T_{91,25}, T_{89,68}, T_{85,31}, T_{4,77}, T_{40,45}, T_{52,18}, T_{7,62}, T_{31,84}, T_{90,11}, T_{88,11}, T_{62,28}, T_{33,74}, T_{72,88}, T_{78,9}, T_{49,15},$
- Class 1
  $T_{20,5}, T_{57,61}, T_{16,67}, T_{45,40}, T_{24,27}, T_{79,59}, T_{84,67}, T_{16,9}, T_{44,27}, T_{64,87}, T_{42,65}, T_{62,28}, T_{62,2}, T_{64,53}, T_{64,88}, T_{61,74}, T_{64,93}, T_{16,44}, T_{16,93}, T_{72,86}, T_{70,5},$

- Class 2
  $T_{60,1}, T_{4,3}, T_{70,9}, T_{21,6}, T_{63,41}, T_{0,76}, T_{63,67}, T_{72,69}, T_{71,15}, T_{39,58}, T_{65,72}, T_{66,23}, T_{10,56}, T_{12,56}, T_{86,0}, T_{6,3}, T_{81,12}, T_{42,18}, T_{11,76}, T_{62,23}, T_{43,23}, T_{30,8}$
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  $T_{30,53}, T_{16,25}, T_{91,77}, T_{68,72}, T_{74,73}, T_{64,34}, T_{91,19}, T_{29,30}, T_{38,53}, T_{5,26}, T_{71,91}, T_{87,33}, T_{37,71}, T_{64,39}, T_{26,29}, T_{66,18}, T_{51,53}, T_{40,75}, T_{61,91}, T_{59,2}, T_{31,8}$
- Class 4
  $T_{32,79}, T_{83,15}, T_{62,69}, T_{41,33}, T_{27,75}, T_{30,6}, T_{79,3}, T_{60,58}, T_{33,21}, T_{54,61}, T_{47,17}, T_{7,93}, T_{65,33}, T_{29,30}, T_{89,4}, T_{9,76}, T_{5,18}, T_{57,7}, T_{55,30}, T_{84,12}, T_{43,60}, T_{6}$

PS

- Class 0
  $T_{91,9}, T_{92,59}, T_{53,67}, T_{86,27}, T_{72,75}, T_{67,14}, T_{91,25}, T_{89,68}, T_{85,31}, T_{4,77}, T_{40,45}, T_{52,18}, T_{7,62}, T_{31,84}, T_{90,11}, T_{88,11}, T_{62,28}, T_{33,74}, T_{72,88}, T_{78,9}, T_{49,15},$
- Class 1
  $T_{20,5}, T_{57,61}, T_{16,67}, T_{45,40}, T_{24,27}, T_{79,59}, T_{84,67}, T_{16,9}, T_{44,27}, T_{64,87}, T_{42,65}, T_{62,28}, T_{62,2}, T_{64,53}, T_{64,88}, T_{61,74}, T_{64,93}, T_{16,44}, T_{16,93}, T_{72,86}, T_{70,5},$
- Class 2
  $T_{60,1}, T_{4,3}, T_{70,9}, T_{21,6}, T_{63,41}, T_{0,76}, T_{63,67}, T_{72,69}, T_{71,15}, T_{39,58}, T_{65,72}, T_{66,23}, T_{10,56}, T_{12,56}, T_{86,0}, T_{6,3}, T_{81,12}, T_{42,18}, T_{11,76}, T_{62,23}, T_{43,23}, T_{30,8}$
- Class 3
  $T_{30,53}, T_{16,25}, T_{91,77}, T_{68,72}, T_{74,73}, T_{64,34}, T_{91,19}, T_{29,30}, T_{38,53}, T_{5,26}, T_{71,91}, T_{87,33}, T_{37,71}, T_{64,39}, T_{26,29}, T_{66,18}, T_{51,53}, T_{40,75}, T_{61,91}, T_{59,2}, T_{31,8}$
- Class 4
  $T_{32,79}, T_{83,15}, T_{62,69}, T_{41,33}, T_{27,75}, T_{30,6}, T_{79,3}, T_{60,58}, T_{33,21}, T_{54,61}, T_{47,17}, T_{7,93}, T_{65,33}, T_{29,30}, T_{89,4}, T_{9,76}, T_{5,18}, T_{57,7}, T_{55,30}, T_{84,12}, T_{43,60}, T_{6}$

AC

- Class 0
  $T_{91,9}, T_{92,59}, T_{53,67}, T_{86,27}, T_{72,75}, T_{67,14}, T_{91,25}, T_{89,68}, T_{85,31}, T_{4,77}, T_{40,45}, T_{52,18}, T_{7,62}, T_{31,84}, T_{90,11}, T_{88,11}, T_{62,28}, T_{33,74}, T_{72,88}, T_{78,9}, T_{49,15},$
- Class 1
  $T_{20,5}, T_{57,61}, T_{16,67}, T_{45,40}, T_{24,27}, T_{79,59}, T_{84,67}, T_{16,9}, T_{44,27}, T_{64,87}, T_{42,65}, T_{62,28}, T_{62,2}, T_{64,53}, T_{64,88}, T_{61,74}, T_{64,93}, T_{16,44}, T_{16,93}, T_{72,86}, T_{70,5},$
- Class 2
  $T_{60,1}, T_{4,3}, T_{70,9}, T_{21,6}, T_{63,41}, T_{0,76}, T_{63,67}, T_{72,69}, T_{71,15}, T_{39,58}, T_{65,72}, T_{66,23}, T_{10,56}, T_{12,56}, T_{86,0}, T_{6,3}, T_{81,12}, T_{42,18}, T_{11,76}, T_{62,23}, T_{43,23}, T_{30,8}$
- Class 3
  $T_{30,53}, T_{16,25}, T_{91,77}, T_{68,72}, T_{74,73}, T_{64,34}, T_{91,19}, T_{29,30}, T_{38,53}, T_{5,26}, T_{71,91}, T_{87,33}, T_{37,71}, T_{64,39}, T_{26,29}, T_{66,18}, T_{51,53}, T_{40,75}, T_{61,91}, T_{59,2}, T_{31,8}$
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DE

- Class 0
  $T_{91,9}, T_{92,59}, T_{53,67}, T_{86,27}, T_{72,75}, T_{67,14}, T_{91,25}, T_{89,68}, T_{85,31}, T_{4,77}, T_{40,45}, T_{52,18}, T_{7,62}, T_{31,84}, T_{90,11}, T_{88,11}, T_{62,28}, T_{33,74}, T_{72,88}, T_{78,9}, T_{49,15},$
- Class 1
  $T_{20,5}, T_{57,61}, T_{16,67}, T_{45,40}, T_{24,27}, T_{79,59}, T_{84,67}, T_{16,9}, T_{44,27}, T_{64,87}, T_{42,65}, T_{62,28}, T_{62,2}, T_{64,53}, T_{64,88}, T_{61,74}, T_{64,93}, T_{16,44}, T_{16,93}, T_{72,86}, T_{70,5},$
- Class 2
  $T_{60,1}, T_{4,3}, T_{70,9}, T_{21,6}, T_{63,41}, T_{0,76}, T_{63,67}, T_{72,69}, T_{71,15}, T_{39,58}, T_{65,72}, T_{66,23}, T_{10,56}, T_{12,56}, T_{86,0}, T_{6,3}, T_{81,12}, T_{42,18}, T_{11,76}, T_{62,23}, T_{43,23}, T_{30,8}$
- Class 3
  $T_{30,53}, T_{16,25}, T_{91,77}, T_{68,72}, T_{74,73}, T_{64,34}, T_{91,19}, T_{29,30}, T_{38,53}, T_{5,26}, T_{71,91}, T_{87,33}, T_{37,71}, T_{64,39}, T_{26,29}, T_{66,18}, T_{51,53}, T_{40,75}, T_{61,91}, T_{59,2}, T_{31,8}$
- Class 4
  $T_{32,79}, T_{83,15}, T_{62,69}, T_{41,33}, T_{27,75}, T_{30,6}, T_{79,3}, T_{60,58}, T_{33,21}, T_{54,61}, T_{47,17}, T_{7,93}, T_{65,33}, T_{29,30}, T_{89,4}, T_{9,76}, T_{5,18}, T_{57,7}, T_{55,30}, T_{84,12}, T_{43,60}, T_{6}$

Statistical Test

We apply the ANOVA test between each pair of algorithms, the α value is taken as 0.05. Also, we run each algorithm for 4 times for the statistical test.

- The test of the 1st class

group1	group2	meandiff	p-adj	lower	upper	reject
AC	DE	-0.0009	0.8405	-0.0038	0.0019	False
AC	GA	0.0041	0.0039	0.0012	0.0069	True
AC	PS	-0.0032	0.0249	-0.006	-0.0003	True
AC	SA	0.0021	0.1971	-0.0007	0.005	False

group1	group2	meandiff	p-adj	lower	upper	reject
DE	GA	0.005	0.0006	0.0022	0.0079	True
DE	PS	-0.0022	0.16	-0.0051	0.0006	False
DE	SA	0.0031	0.0318	0.0002	0.0059	True
GA	PS	-0.0073	0.0	-0.0101	-0.0044	True
GA	SA	-0.0019	0.2652	-0.0048	0.0009	False
PS	SA	0.0053	0.0003	0.0025	0.0082	True

- The test of the 1st class

group1	group2	meandiff	p-adj	lower	upper	reject
AC	DE	-0.0002	0.9996	-0.003	0.0026	False
AC	GA	0.0032	0.0226	0.0004	0.006	True
AC	PS	-0.0012	0.6581	-0.004	0.0016	False
AC	SA	0.0002	0.9996	-0.0026	0.003	False
DE	GA	0.0034	0.0155	0.0006	0.0062	True
DE	PS	-0.0011	0.7681	-0.0039	0.0017	False
DE	SA	0.0004	0.9946	-0.0025	0.0032	False
GA	PS	-0.0044	0.0016	-0.0072	-0.0016	True
GA	SA	-0.003	0.0328	-0.0058	-0.0002	True
PS	SA	0.0014	0.5433	-0.0014	0.0042	False

- The test of the 2st class

group1	group2 m	eandiff	p-adj	lower	upper	reject
AC	DE	-0.0173	0.0	-0.0245	-0.01	True
AC	GA	0.025	0.0	0.0177	0.0322	True
AC	PS	0.0057	0.1593	-0.0015	0.013	False
AC	SA	0.0004	0.9998	-0.0068	0.0077	False
DE	GA	0.0422	0.0	0.035	0.0495	True
DE	PS	0.023	0.0	0.0157	0.0303	True
DE	SA	0.0177	0.0	0.0104	0.025	True
GA	PS	-0.0192	0.0	-0.0265	-0.012	True
GA	SA	-0.0245	0.0	-0.0318	-0.0173	True
PS	SA	-0.0053	0.2116	-0.0126	0.0019	False

- The test of the 3st class

group1	group2	meandiff	p-adj	lower	upper	reject
AC	DE	-0.0022	0.2283	-0.0054	0.0009	False
AC	GA	0.0028	0.0858	-0.0003	0.006	False
AC	PS	-0.0009	0.8805	-0.0041	0.0022	False

group1	group2	meandiff	p-adj	lower	upper	reject
AC	SA	0.0001	1.0	-0.003	0.0032	False
DE	GA	0.0051	0.0013	0.0019	0.0082	True
DE	PS	0.0013	0.7068	-0.0018	0.0044	False
DE	SA	0.0024	0.19	-0.0008	0.0055	False
GA	PS	-0.0038	0.0149	-0.0069	-0.0006	True
GA	SA	-0.0027	0.1055	-0.0058	0.0004	False
PS	SA	0.0011	0.8297	-0.0021	0.0042	False

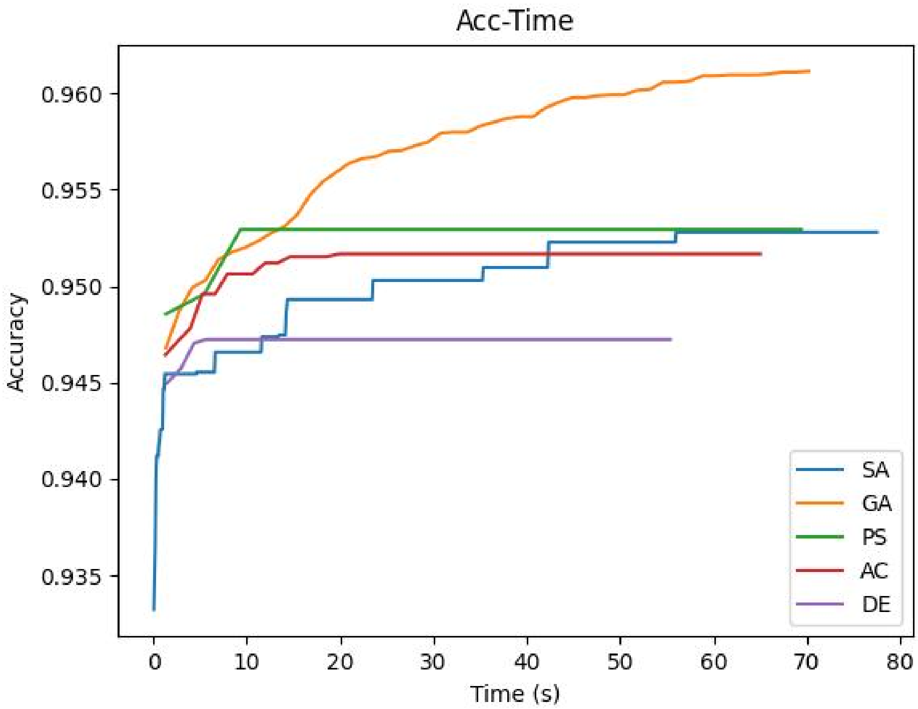
- The test of the 4st class

group1	group2	meandiff	p-adj	lower	upper	reject
AC	DE	0.0	nan	0.0	0.0	False
AC	GA	0.0	nan	0.0	0.0	False
AC	PS	0.0	nan	0.0	0.0	False
AC	SA	0.0	nan	0.0	0.0	False
DE	GA	0.0	nan	0.0	0.0	False
DE	PS	0.0	nan	0.0	0.0	False
DE	SA	0.0	nan	0.0	0.0	False
GA	PS	0.0	nan	0.0	0.0	False
GA	SA	0.0	nan	0.0	0.0	False
PS	SA	0.0	nan	0.0	0.0	False

Since all algorithm has 1 accuracy in this prediction, the ANOVA test shows no difference between all of them.

Statistical Progress Diagram Analysis

The mean accuracy of the training data to the runtime is shown as follows:



We can observe that:
(1) AC and PS can find good solution in less then 10 second, but the solution would not be improved too much after that.
(2) SA can find better solution as the iteration process runs; however, the improvement is much slower then GA.
(3) GA has improvement on the solution as the iteration process goes, and the algorithm gets the best performance after 10 seconds. This methods outperforms other methods.
In conclusion, we think that the algorithm performance comparison for this problem can be summarized as:
GA > PS > AC > SA > DE

File Description

- model/: stores final 30 selection during running 'train.py'
- select/: stores figures for bio-marker selection
- time/: store time and accuracy info. during running 'train.py' & the acc-time figure after running 'plot_time.py'
- utils/:
  - eval.py: score evaltion functions
  - optimization.py: all optimization algorithms
  - preprocess.py: read data and set solution space
- plot_selection.py: plot the bio-marker selection and save
- plot_time.py: plot the acc-time curve
- stat_test.py: perform statiscal test
- test.py: Predict the output and store to 'Test2_Answer.xlsx'
- train.py: Run optmization algorithm on the train set to select the best indices for each classes
- valid.py: Predict the output of 'Test1.xlsx' for validating the training result.

How to Run?

- To run the training and validation
  (1) Run 'train.py'
  (2) Run 'valid.py'
  (3) Run 'plot_selection.py' & 'plot_time.py' for analysis
  (4) Run 'test.py' to generate the answer
- To run the statistic test related code
  (1) Run 'python train.py --seed 1~2', to get total 4 samples

(2) Run 'stat_test.py' for statistical test on diffrerent algorithm