**Simulated annealing algorithm section**

Based on the objective function defined in the previous section, I need to address the each of following issues associated with the simulated annealing algorithm,

* The modified starting design versus any random starting design.
* The accelerated cooling method versus standard cooling method.
* Pair swapping method versus one-to-one swapping method.
* Two-stages swapping method versus standard swapping method.

These four issues are explored using a two-phase experiment comprised with one specific set of design parameters:

Phase 1 experiment - 6 treatments, 3 biological replicates, 2 technical replicates,

Phase 2 experiment – 9 runs and 4 tags.

For the Phase 1 experiment, the 6 treatments are denoted by “a”, “b”, “c”, “d”, “e” and “f”. Since 3 biological replicates are used, this means 3 animals are assigned to each treatment which gives a total of 15 animals. These 15 animals are denoted by upper case letters of “A” to “R”. The theoretical ANOVA of the Phase 1 experiment can be presented as follows,

$ANOVA

DF Ani

Between Ani

Trt 5 1

Residual 12 1

$EF

Trt eff.Trt

Between Ani

Trt 3 1

Since the animals is the observational and experimental units, all the information is in the between animals stratum for this first phase experiments. In the random effects table, there are 5 degrees of freedom (DF) associated with the treatment effects; hence, there are 12 DF remains associated with the residual mean squares in the between animals stratum. In addition, all treatment information is in the between animals stratum as shown in the fixed effects table.

1. Comparing the modified starting design to a random starting design.

The modified starting design for assigning the animals to the runs and tags is to group a pair of animals of the identical technical replicates and allocating them in a sector of 2 runs and 2 tags. For this experiment, since the total number of runs needed is 9; hence, the last pair of animals is assigned to the last run. The pair of animas can be Animals “A” and “B”, Animals “C” and “D” to Animals “Q” and “R”. The allocation of the animals to runs and tags can be shown as follows,

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Run | Tag | | | |
| 114 | 115 | 116 | 117 |
| 1 | A | B | C | D |
| 2 | B | A | D | C |
| 3 | E | F | G | H |
| 4 | F | E | H | G |
| 5 | I | J | K | L |
| 6 | J | I | L | K |
| 7 | M | N | O | P |
| 8 | N | M | P | O |
| 9 | Q | Q | R | R |

The bold box in this animal allocation represents the pair of the animals. Note that the animal is confounded with both runs and tags. More specifically, the animal is confounded with a tag contrast of 114, 115 versus 116, 117. For the relationship between runs and animals, the runs can be separated into 5 groups according to the pairs of animals that are assigned. This means 4 DF associated with the animals are confounded with the runs, or we can also say that 4DF associated with the animals should be in the between runs stratum.

The treatment allocation to runs and tags is based on the assignments of treatments to animals of the Phase 1 experiments. The treatment design is shown as follows,

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Run | Tag | | | |
| 114 | 115 | 116 | 117 |
| 1 | a | b | c | d |
| 2 | b | a | d | c |
| 3 | e | f | a | b |
| 4 | f | e | b | a |
| 5 | c | d | e | f |
| 6 | d | c | f | e |
| 7 | a | b | c | d |
| 8 | b | a | d | c |
| 9 | e | e | f | f |

The bold box in this treatment allocation represents each pair of treatments from the pair of the animals. The treatment is also confounded with both runs and tags. The treatment is also confounded with the confounded with a tag contrast of 114, 115 versus 116, 117.

The initial temperature is set at 100, this means the initial search for the optimal designs allows the values from the objective function to be worse than 100.

The simulated annealing algorithm was implemented using the optima function in R program for one million iterations. There is another parameter called tmax, which is the number of iteration at each temperature, this is set at 1000. This search takes just over nine minutes to complete.

After applying the simulated annealing using the modified starting design to start the search, this is shown that simulated annealing could not improve the designs since the result from the objective function was already at very high value of 97.62.

Using a random starting design, the simulated annealing algorithm does improve the design based on the objective function from 51.56 to 76.272. Note this value is still lower than using than objective function from the modified starting design.

1. Comparing the accelerated cooling method described by John and Whitaker (1993) to standard cooling method.

John and Whitaker (1993) mentioned that the convergence of the standard simulated annealing algorithm can be very slow and the solution may be far from optimal. This issue can be resolve from modifying the cooling schedule.

The cooling schedule of the current standard simulated annealing base on the optim function in R is

where temp is the initial temperature, t is the current iteration step and tmax is the number of iteration at each temperature. The operator “\” denotes the integer division, i.e. division removing the remainders. With initial temperature of 100 and tmax equals to 1000, after one million iterations the temperature has reduced to 7.239. This final temperature may still be too high to find the optimal design.

The modified revision of the cooling schedule separates the one million iterations into 10 levels of one hundred thousand iterations. At the first level, the initial temperature and tmax are still 100 and 1000, respectively; but the number of iterations is reduced to one hundred thousand iterations. Then, at the next level, the initial temperature is reduced by an half giving 50. The solution from the simulated annealing of the previous level is used as the starting design to start the search. The tmax and the number of iteration are remained the same of 100 and one hundred thousand. This process repeats again with initial temperature reduced by a half giving 25, 12.5 and till the tenth level of the simulated annealing algorithm is performed. The initial temperature of the tenth level is reduced to 0.1953125 and the final one hundred thousand iterations, the temperature is reduced to 0.01697941. Note that total number of the iteration is still one million, therefore the time required to complete this simulated annealing algorithm remain the same.

This approach to simulated annealing produce good solution by reducing the temperature quickly across the levels, but it also carries out the standard simulated annealing at each temperature level. The cooling schedule is known as *accelerated cooling* and the modified simulated annealing is also known as *nested simulated annealing*.

The nested simulated annealing starts a random walk across a surface with a high temperature to diversify the search. The accelerated cooling allows the search to intensify as it becomes a more local search. Therefore, gradually the random walks become more confined following the contours of the surface, with more restriction on accepting the worse designs.

Using the experiment, the accelerated cooling method again made no improvement on the modified starting design as the result form the objective function stays at 97.62. However, it does improve the result from the objective function with a random starting design with the result from the objective function of 78.647 after one million iterations. This is also shown to be better than the standard simulated annealing algorithm which obtains the design with objective function of 76.271.

1. Comparing the pair swapping method to the one-to-one swapping method.

With the modified starting design, both standard simulated annealing and nested simulated annealing could not improve the design.

The swapping method will need to modify to find the optimal design quickly and efficiently. The current swapping method is to swap any random pair of observations throughout the design. Note the modified starting design of the experiments with 2 technical replicates is to group a pair of animals and treatments and assigned them to a sector comprising 2 runs and 2 tags. Hence, the new swapping method is to swap any two random pairs of animals and treatments of the identical technical replicates.

With the pair swapping method, the optimal design, with the results of 98.189 from the objective function, has found fewer than ten thousand iterations. The nested simulated annealing was not required, because the optimal design was found within the first level of one hundred thousand iterations even with the initial temperature of 100.

1. Comparing the two-stages swapping method to the standard swapping method.

Williams and John (1996) described a two-stage swapping method for finding the optimal row-column design via simulated annealing. For this experiment, the runs and tags are considered as the rows and columns, respectively. In the first stage, the swapping only take place within runs, that means when the swapping of two observations, it has to be in the same run. The second stage is swapping within tags, which means when the two observations are swapped, these two observations have to be in the same tags. This method is attempted to reduce the search space of the simulated annealing algorithm; hence, it has ability to find a better designs more quickly.

The accelerated cooling and pair swapping methods were combined with the two-stage swapping method. Using same the accelerated cooling as described, it is achieved by separating the one million iterations into 10 levels of one hundred thousand iterations. To incorporate the two-stage swapping method, each level of one hundred thousand iterations are further separated for each of two stages; hence, each stage consists of fifty thousand iterations.

For this experiment, the pair swapping with two-stages swapping method on the modified starting design shown to be slower than the using pair swapping method alone. This is because this experiment with modified design is very easy to find the optimal design. The pair swapping method was able to find an optimal design required fewer than ten thousand iterations. As for the two-stage swapping, the optimal design could not be found within the first stage, but it only required another ten thousand iterations in the second stage to find the optimal design. Hence, the optimal designs can still be generated within sixty thousand iterations. Same using the pair swapping alone, the nested simulated annealing was not required, because the optimal design was found within the first level of one hundred thousand iterations even with the initial temperature of 100.

This may raise an question that the two-stage swapping method may not be useful, because it has no evidence on improving the design during the search. Thus, the accelerated cooling with two-stage swapping method was compared to the standard swapping method on the random starting design. After one million iterations, the design with result from the objection function of 84.97 was found which is the better design compare to using standard simulated annealing (76.27) and accelerated cooling method (78.64). Therefore, it shows that two-stage swapping method can generate a more optimal design than the standard swapping method based on the results from the objective function.

In conclusion, based on these results, I believe that using the modified starting design with accelerate cooling, pair swapping and two-stage swapping will allow user to find the optimal design more quickly and efficiently. The table of summary for comparing different method in simulated annealing is shown as follows.

Summary of table for comparing different method in simulated annealing

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Methods | Modified Starting design | Accelerated cooling method | Pair swapping | Two-stage swapping | Objective function | | Iteration |
| Before | After |
| SA |  |  |  |  | 51.555453 | 76.271591 | 1e6 |
| SA on modified starting design | ˅ |  |  |  | 97.617991 | 97.617991 | 1e6 |
| Accelerated cooling method |  | ˅ |  |  | 51.555453 | 78.647182 | 1e6 |
| Accelerated cooling method on modified design | ˅ | ˅ |  |  | 97.617991 | 97.617991 | 1e6  ((10)1e5) |
| Pair swapping method with accelerated cooling method on modified starting design | ˅ | - | ˅ |  | 97.617991 | 98.189248 | 1e4 |
| Two-stages swapping method with Pair swapping method with accelerated cooling method on modified starting design | ˅ | - | ˅ | ˅ | 97.617991 | 98.189248 | 6e4 |
| Two-stages swapping method |  |  |  | ˅ | 51.555453 | 71.125898 | 1e6 (5e5) |
| Two-stages swapping method with accelerated cooling method |  | ˅ |  | ˅ | 51.555453 | 84.970056 | 1e6  ((10)1e5  (5e4)) |