Plan for the paper

1. Introduction

Merge the introduction from the two chapters of the thesis

2. Model Definition

2.1 Completely randomised design for the Phase 1 Experiment

2.2 Randomised block design and Balanced Incomplete block design for the Phase 1 experiment

2.3 Randomised block design with one fixed factor for the Phase 2 experiment

3. Define objective function – summarise the objective function from the thesis

3.1 The aim is to find a design with the minimal confounding of the factors between the Phase 1 and Phase 2 experiments.

3.2 To assume all the factors from the Phase 2 experiment as random. Use the projection matrix with all the random factors of the Phase 2 experiment swept for defining the information matrix and optimality criteria.

3.3 Completely randomised design for the Phase 1 Experiment

Presents the single objective function –

structural balanced for the block factor from the Phase 1 experiment

treatment allocation of Phase 1 experiment is connected

treatment average efficiency factor is maximised

3.4 Randomised block design and Balanced Incomplete block design for the Phase 1 experiment

Presents the two objective functions for this case

Keep the block factor from the Phase 1 experiment structural balanced and the treatment allocation of Phase 1 experiment connected at all time.

First objective function is to maximise the residual degrees of freedom.

Second objective function is to maximise the treatment average efficiency factor.

4. Construct the initial design for the MudPIT-iTRAQ experiments.

The Phase 2 experiment is arranged with a randomised block design with block size of 4 or 8. In addition, there is one treatment factor associated with tag effects from the Phase 2 experiment. This layout is typical in the high-throughput biotechnology experiments where multiple samples are being quantified at the same time.

4.1 Completely randomised design

4.2 Randomised block design and Balanced Incomplete block design, for example,

1 technical replicate – random assign allocating

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Run | Tag | | | |
| 114 | 115 | 116 | 117 |
| 1 | 1 | 2 | 3 | 4 |

2 technical replicates – paired allocating for the same technical replicates

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Run | Tag | | | |
| 114 | 115 | 116 | 117 |
| 1 | 1 | 2 | 3 | 4 |
| 2 | 2 | 1 | 4 | 3 |

3 technical replicates

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Run | Tag | | | |
| 114 | 115 | 116 | 117 |
| 1 | 1 | 2 | 3 | 4 |
| 2 | 3 | 1 | 2 | 4 |
| 3 | 2 | 3 | 1 | 4 |

4 technical replicates – 4-by-4 Latin square

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Run | Tag | | | |
| 114 | 115 | 116 | 117 |
| 1 | 1 | 2 | 3 | 4 |
| 2 | 2 | 1 | 4 | 3 |
| 3 | 3 | 4 | 1 | 2 |
| 4 | 4 | 3 | 2 | 1 |

5. Simulated annealing algorithm

5.1 Temperature control – determining the temperature range for the SA

modified accelerate cooling method

5.2 Swapping with respect to the technical replicates

5.3 Different stages of swapping to further reduce the search space.

6. Presents the package with examples

7 Conclusions