# GreedyExperimentalDesign: Finding Experimental Designs using Greedy Search with Random Restarts

## Adam Kapelner

Queens College, City University of New York Department of Mathematics

#### Abstract

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## 1. Introduction

Assume a randomized controlled two-arm experiment with n subjects and treatment (T) and control (C) denoted by the n-binary vector  $\mathbf{1}_T$  where entries of 1 in location i indicates subject i was administered T and entries of 0 indicates C. Define the number of treatments  $n_T := \sum_{i=1}^n \mathbf{1}_{T,i}$  and the number of controls  $n_C := n - n_T$ . For each subject, p covariates  $\mathbf{X} := [\mathbf{x}_1, \dots, \mathbf{x}_p]$  are measured. Define  $\bar{\mathbf{X}}_T$  as the p-vector of sample averages for each of the covariates in subjects where  $\mathbf{1}_T = 1$  (the treatments) and  $\bar{\mathbf{X}}_C$  as the p-vector of sample averages for each of the covariates in subjects where  $\mathbf{1}_T = 0$  (the controls). The investigator will eventually measure one response for each subject collected in the n-vector  $\mathbf{y}$ , but this is not our current interest. We assume that each of the p covariates is standardized.

There are many functions of  $\mathbf{1}_T$  and X that will yield higher efficiency when testing null hypotheses about effects of the treatment. Below are a few:<sup>1</sup>

- 1.  $n_T/n$  which measures the balance of treatment allocations. 0.5 is the optimal value.
- 2.  $\sum_{j=1}^{p} |\bar{X}_{T,j} \bar{X}_{C,j}|$  which is a measure of balance between the covariate distributions. Covariate distribution permitting, zero is the optimal value.
- 3.  $\frac{n_T n_C}{n} \left( \bar{\boldsymbol{X}}_T \bar{\boldsymbol{X}}_C \right)^{\top} \boldsymbol{S}_{\boldsymbol{X}}^{-1} \left( \bar{\boldsymbol{X}}_T \bar{\boldsymbol{X}}_C \right)$  is a Mahalanobis-like distance metric. Covariate distribution permitting, zero is the optimal value.

For many of our proposals below we will fix  $n_T/n$  to be 0.5 and then minimize one of the other two objective functions.

There are also metrics which measure the similarity between the two joint densities  $f_T$  and  $f_C$  which we may want to explore later.

# 2. Greedy Switches Algorithm

Draw one vector from the space of  $\binom{n}{n/2}$  possible balanced  $\mathbf{1}_T$  vectors. Create a list of the indices of size n/2 corresponding to where  $\mathbf{1}_T = 1$  (call it  $I_T$ ). Create a list of the indices of size n/2 corresponding to where  $\mathbf{1}_T = 0$  (call it  $I_C$ ). For every pair in  $I_T \times I_C$ , switch the 0 and 1 within  $\mathbf{1}_T$  and record the resulting value of the objective function. For all possible  $n^2/4$  possible switches (of which all preserve  $n_T/n = 0.5$ ), find the switch which yielded the minimum value of the objective function. Make that switch inside  $\mathbf{1}_T$ . Continue in this fashion until you can no longer improve the objective value.

### Replication

The stable version of **GreedyExperimentalDesign** will be soon on CRAN and the development version is located at <a href="https://github.com/kapelner/GreedyExperimentalDesign">https://github.com/kapelner/GreedyExperimentalDesign</a>. The package code is under the GPL3 and LGPL licenses. Results, tables, and figures found in this paper can be replicated via the scripts located in the GreedyExperimentalDesign/vignettes folder within the git repository.

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### Affiliation:

Adam Kapelner Department of Mathematics Queens College, City University of New York 64-19 Kissena Blvd Room 325 Flushing, NY, 11367

E-mail: kapelner@qc.cuny.edu URL: http://kapelner.com