Some results on optimal allocation in two–step sequential design

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Abstract—In nonlinear situations, optimal experimental conditions generally depend upon unknown parameters to be estimated from the data collected during the experiments. A natural approach then consists in designing the experiments sequentially, that is, alternating estimation and design phases. We consider the determination of the optimal allocation of the resource between two design steps when the design strategies at each step are fixed.
Key words—Optimal design; sequential design; approximate design.

1 Introduction

We consider a nonlinear regression model, with observations y_k given by

$$y_k = \eta(\bar{\boldsymbol{\theta}}, x_k) + \epsilon_k \,,$$

where $\bar{\boldsymbol{\theta}} \in \Theta$ is the true value of the model parameters, with $\Theta \subset \mathbb{R}^p$ a compact set, x_k denotes the experimental conditions for the k-th observation and is assumed to belong to a compact set, $\{\epsilon_k\}$ is an i.i.d. sequence of normal variables $\mathcal{N}(0, \sigma^2)$, with σ known, and $\eta(\boldsymbol{\theta}, x)$ is the model response for the value $\boldsymbol{\theta}$ of the model parameters and experimental conditions x. The response is assumed to be nonlinear in $\boldsymbol{\theta}$ and two times continuously differentiable with respect to $\boldsymbol{\theta}$.

Experimental design for parameter estimation is considered, and we wish to choose experimental conditions $\Xi_1^N = \{x_1, \ldots, x_N\}$, with $N \geq p$ fixed, that maximize a function $\Phi(\cdot)$ (usually concave) of the Fisher information matrix

$$\mathbf{M}(\boldsymbol{\theta}, \Xi_1^N) = \frac{1}{\sigma^2} \sum_{i=1}^{N} \frac{\partial \eta(\boldsymbol{\theta}, x_i)}{\partial \boldsymbol{\theta}} \frac{\partial \eta(\boldsymbol{\theta}, x_i)}{\partial \boldsymbol{\theta}^T} \,.$$

For instance,

$$\Phi(\mathbf{M}) = \log\det[\mathbf{M}] \quad \text{or} \quad \Phi(\mathbf{M}) = -\mathrm{trace}[\mathbf{M}^{-1}] \tag{1}$$

are classical choices. We consider the situation where the experiments can be performed sequentially in *two steps*. First, a design $\Xi^{(1)} = \Xi_1^n$ with n observations is chosen. The values $Y_1^n = \{y_1, \ldots, y_n\}$ of these observations are then used to design the experiment $\Xi^{(2)} = \Xi_{n+1}^N$ for the second stage, with $N - n$ observations. Note that the total number of observations and the number of design stages are fixed, and no convergence issue is thus considered.