Role and Applications of Higher order Derivatives in Optimal Design of Experiments

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Abstract: Typically, the optimal experimental design (OED) objective function Φ is a function that depends on the covariance matrix $C \in \mathbb{R}^{N_p \times N_p}$ of the parameters $p \in \mathbb{R}^{N_p}$. The covariance matrix C is itself a complicated expression in $J = (J_1, J_2)$, where $J_1 \in \mathbb{R}^{N_M \times N_p}$ is the sensitivity of the measurement model functions and $J_2 \in \mathbb{R}^{N_C \times N_p}$ the sensitivity of the constraint functions w.r.t. the parameters p. In particular, the following NLP has to be solved:

$$\min_{q \in \mathbb{R}^{N_q}} \Phi(C(J(q))),$$

where

$$C = \begin{pmatrix} I & 0 \end{pmatrix} \begin{pmatrix} J_1^T J_1 & J_2^T \\ J_2 & 0 \end{pmatrix}^{-1} \begin{pmatrix} J_1^T J_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} J_1^T J_1 & J_2^T \\ J_2 & 0 \end{pmatrix}^{-T} \begin{pmatrix} I \\ 0 \end{pmatrix}.$$

Recently, there has been growing interest in new robust formulations of the OED problem. The robust objective functions $\tilde{\Phi}$ are often functions of the original objective function and its derivatives. I.e.:

$$\tilde{\Phi} \equiv \tilde{\Phi}(\Phi, \nabla\Phi, \nabla^2\Phi, \dots).$$

We discuss several formulations and their uses/limits. We show how the theory Algorithmic Differentation can be applied to obtain the required higher order derivatives of Φ.

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