Separable Formulations of Optimum Experimental Design Problems

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Abstract: In this talk, we consider multi-experiment nonlinear optimum experimental design problems. These lead to optimal control problems which are non-standard in the sense that the objective function is not of Mayer or Lagrange type. They can be solved numerically by general purpose NLP solvers by discretizing the controls and regarding the states as dependent variables. However, this often leads to poor convergence properties. We present reformulations of the problem that transform it into a standard optimal control problem. It is then possible to attack this problem via the direct approach with state-of-the-art methods such as multiple shooting. This allows us to make use of the greater robustness and superior convergence properties of the multiple shooting approach. The reformulation gives rise to a highly structured NLP due to the multiple shooting discretization as well as due to the peculiarities of the optimum experimental design problem. We highlight some of these structures in the constraints, the objective function, and the Hessian matrix of the Lagrangian, and present ways to exploit them leading to efficient SQP methods tailored to optimum experimental design problems. Numerical results are presented comparing the new multiple shooting capable formulations to an existing implementation.

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