

On evaluating the gradient of the optimum experimental design objective function

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In the talk we discuss an enhancement of the software VPLAN that allows the evaluation of the objective function's gradient in the reverse mode of algorithmic differentiation (AD).

The theory of AD to evaluate gradients is rather well-understood. This is reflected in the numerous ready-to-use software packages. However, the objective function of optimum experimental design is not of the typical form. It requires the evaluation of derivatives of the state trajectory of some DAE, followed by numerical linear algebra computations.

To evaluate the derivatives of the state trajectory we use the differential algebraic equation (DAE) integrator DAESOL-II. It supports internal numerical differentiation in the forward and reverse mode of AD. Derivatives in the forward mode are evaluated in univariate Taylor polynomial arithmetic. The model functions of the DAEs are given as Fortran files for speed reasons. Their derivatives are generated by the tool Tapenade. Therefore one is confronted with the problem to provide a mapping between sets of coefficients of univariate Taylor polynomials, derivative tensors and the output of Tapenade. We discuss how this mapping can be accomplished.

Additionally, we discuss how the derivatives of the numerical linear algebra can be evaluated in a numerically stable manner and discuss challenges that have to be addressed in the future. At last we show a runtime comparison between the forward and reverse mode.