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Optimal design criteria - prediction vs. parameter estimation

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G-optimality is a popular design criterion for optimal prediction, it tries to minimize the kriging variance over the whole design region. A G-optimal design minimizes the maximum variance of all predicted values. If we use kriging methods for prediction it is self-evident to use the kriging variance as a measure of uncertainty for the estimates. Though the computation of the kriging variance and even more the computation of the empirical kriging variance is computationally very costly and finding the maximum kriging variance in high-dimensional regions can be time demanding such that we cannot really find the G-optimal design with nowadays available computer equipment in practice. We cannot always avoid this problem by using space-filling designs because small designs that minimize the empirical kriging variance are often non-space-filling.

D-optimality is the design criterion related to parameter estimation. A D-optimal design maximizes the determinant of the information matrix of the estimates. D-optimality in terms of trend parameter estimation and D-optimality in terms of covariance parameter estimation yield basically different designs. The Pareto frontier of these two competing determinant criteria corresponds with designs that perform well under both criteria.

Under certain conditions searching the G-optimal design on the above Pareto frontier yields almost as good results as searching the G-optimal design in the whole design region. In doing so the maximum of the empirical kriging variance has to be computed only a few times though.

The method is demonstrated by means of a computer simulation experiment based on data provided by the Belgian institute *Management Unit of the North Sea Mathematical Models* (MUMM) that describe the evolution of inorganic and organic carbon and nutrients, phytoplankton, bacteria and zooplankton in the Southern Bight of the North Sea.