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Are covariances meaningless in criteria for optimal designs for prediction?

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Classical optimality criteria for the allocation problem of experimental designs usually focus on the minimization of the variance of estimators.

Optimal designs for parameter estimation somehow minimize the variance of the parameter estimates. Some criteria just use the variances (A-optimality, E-optimality) whereas other criteria also implicitly consider the covariances of the parameter estimates (D-optimality, C-optimality).

Traditional criteria for optimal designs for prediction minimize the variances of the predicted values, e.g. G-optimal designs minimize the maximum variance of predictions or I-optimal designs minimize the average prediction variance over the design space. None of these criteria consider the covariances of the predictions. If we want to control the variation of all (i.e. more than just one of) the predictions we should think of measures for the overall variation of a multivariate data set:

The so-called *total variation* of a random vector is simply the trace of the population variance-covariance matrix. This is minimized with V-optimal designs.

The problem with total variation is that it does not take into account correlations among the predictions. This is done by an alternative measure of overall variance, the so-called *generalized variance* introduced by Wilks 1932. The larger the generalized variance the more dispersed are the data.

The generalized variance is defined as the determinant of the covariance matrix and minimizing this determinant might serve as optimality criterion as well as other related criteria based on the condition number of the covariance matrix.

The different optimality criteria are compared by means of a computer simulation experiment producing spatio-temporal data.

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