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Geoscientific Model Development Discussions

Interactive comment on "Optimization of experimental designs and model parameters exemplified by sedimentation in salt marshes" *by* J. Reimer et al.

J. Reimer et al.

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We first thank the reviewer for his very insightful comments, which helped us a lot to clarify and improve this paper.

Minor comments:

p 6442ff: Say "estimation of model parameters" instead of "optimization ..."

-> changed (except at the title of the paper and the title of chapter 2)

p 6442f: Choice of the estimator: the estimator should be derived from the statistical properties/distribution of the measurement errors, e.g. a maximum likelihood estimator

-> incorporated

p 6442: Set of feasible model parameters, described by bounds: what is the use of an estimate if the bounds (which have been specified by the modeler) are active?

-> The bounds can be determined by physical meanings. For example, a concentration can not be negative thus it can be meaningful even if it is on a boundary.

-> For the presented optimal experimental design theory, it is reasonable to assume that the unknown exact parameter vector $\hat{p}$ is not at the bounds. (See assumption A5.) However, this does not mean that estimated parameters p_n are not allowed to be at the bounds.

p 6443: Can psi be assumed to be injective?

-> This is in practice certainly rarely the case. A less restrictive assumption would be the convexity.

-> changed

p 6443: Use of SQP for PE is not really a good idea, for large residuals it may converge to statistically unstable solutions, see Bock et al. 2013 better use Gauss-Newton For exp. design SQP is ok.

-> So far, we have gained good experience with SQP for PE. Can you please explain why large residual minimizers are no good estimators? Please look in the supplement for an example of a large residual minimizers which is a good estimator.

p 6443 l 24: "normally distributed"

-> changed

p 6443f: What are the regularity assumptions? E.g. for the inverse of Mn(p) it is: nabla_p fËĘT has full (column) rank.

-> regularity assumptions incorporated

p 6445 l 23-13: The operation "set to infinity" is not differentiable, which is needed for application of SQP.

-> Matlab's SQP algorithm can recover from infinity. If an infinite function value is reached during the optimization, the algorithm attempts to take a smaller step. Thus, if the optimization is started with a regular design, singular designs do not make any trouble.

-> explanation incorporated

p 6446: Experimental design: what about optimizing the x_i?

-> This formulation is useful if additional experimental designs should be chosen from a finite number of experimental designs. Otherwise, the optimization problem can be reformulated so that the additional optimal design variables have to be optimized directly.

-> explanation incorporated

p 6447 l 2: "occur nonlinearly"

-> changed

p 6447 l 24: typo: can be solved

-> changed

p 6449 l 19: For derivative based optimization of the exp design problem, e.g.. by SQP, a mixed derivative is required to compute the gradient of the objective.

-> That's right. However, the user needs to provide only the derivatives with respect to the model. All other derivatives are computed automatically and are not listed here for this reason.

p 6450 l 21: "initial guess" instead of "initial estimation"

-> changed

p 6457 l 26: "normally distributed"

-> changed

p 6458 l 11ff: If you also use the high water levels of the tidal inundation as experimental design variable, you need derivatives wrt. this quantity for the SQP optimization. How do you compute them? (In contrast, derivatives wrt. the w_i only need nabla f.)

-> The experimental design variables are not directly optimized. Instead, the corresponding weights are optimized. That is, derivatives with respect to the weightings are needed. These are automatically calculated. Derivatives with respect to the experimental design variables are not needed.

p 6459f: The phrase "maximal accuracy" is misleading. Of course the accuracy can always be improved further by performing additional measurements.

-> "maximal accuracy" replaced by "best achieved accuracy"

p 6459f: Which gamma did you choose in the robust approach? How big is the standard part of the objective compared to the robustification part?

-> The 95%-quantil of the chi-squared-distribution was used for gamma.

-> quantil incorporated

-> The standard part is around one thousandth of the robustification part. Which means that the robustification part dominates in the robust approach.

p 6459ff: Conceptionally, the relaxed solution should be better than the discrete one, because the feasible set is larger, Unless you compare local relaxed to global discrete minima which is not a fair comparison.

-> Here, the formulation was misleading. The solution of the discrete problem was compared with the solution of the continuous (relaxed) problem projected onto an integer solution.

-> In the article, the terms "exact" and "approximate" solution of the discrete problem are used now.

p 6459 l 12: typo: worst -> worse

-> changed

p 6459 l 15: "occur nonlinearly"

-> changed

p 6459 l 22f and p 6460 l 16f: This is because here the different (constant) standard deviations only mean a different scaling of the objective of the exp. design opt. problem. Only if the stqandard deviations are non-constant within the experiments, the weighting by 1/sigma becomes relevant.

-> explanation incorporated

p 6460 l 24: replace greater by bigger, e.g.

-> changed

p 6460 l 27f: This explanation sounds weird. See remark above. The behavior should depend on the actual nonlinearity of the problem.

-> On the one hand, the nonlinearity is included, by optimizing the worst case quality within a confidence region. On the other hand, the worst case quality is approximated by the solution of the linearized problem. It may be that this additional approximation offsets the gain by considering the nonlinearity.

p 6462 l 14ff: This kind of results also occurs for linear models. This may indicate why the robust approach is not needed.

-> The model is nonlinear in the parameters and the robust approach yields different results than the standard approach. The robustification part is many times larger than the standard part.

p 6472: Fig. 2: 1.input should be the "RHS of the differential equation".

-> changed

Please also note the supplement to this comment:
http://www.geosci-model-dev-discuss.net/7/C2360/2014/gmdd-7-C2360-2014-supplement.zip

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