

Computationally efficient hypothesis testing using an iterative ensemble smoother and reproducible workflows

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Many of the environmental challenges we face as a society require the use of numerical models to evaluate potential undesirable conditions using limited data and imperfect representation of natural and human systems. Iterative ensemble smoother (IES) methods are a computationally efficient and robust approach to evaluate the uncertainty of numerical models and the worth of adding additional observation sources. IES methods also provide a way to test hypotheses about modelling assumptions and conditions in problems often too complex for traditional statistical methods.

This work presents an approach to test hypotheses on undesirable outcomes in complex decision support models by taking advantage of the efficient and parallel capabilities of IES methods. The model used to illustrate the approach represents a groundwater system with around 200 observation points and more than 70,000 parameters to describe hydraulic properties and boundary conditions. The version-controlled workflow used to implement the uncertainty analysis and hypothesis testing meticulously documents each step of the analysis and takes advantage of open-source libraries to manipulate model files, implement the ensemble methods, and efficiently evaluate the fate of a contaminant of concern. After a careful evaluation of conflicts between prior parameters and observations, the prior parameter ensemble is updated by IES to improve the match between simulations and observations. Historical observations were augmented with a spatial metric representing the condition where the hypothesis could be accepted.

Results of the analysis illustrate the trade-off between fitting observations and the hypothetical undesirable outcome as well as the impact on parameter value plausibility. The computational performance and flexibility of this approach provides a robust, efficient, and reproducible decision-support modelling tool for solving mining and environmental challenges.