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Calibration and uncertainty analysis of groundwater models assisted by machine learning surrogates

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Abstract: Numerical groundwater models are widely used for environmental decision support. They are often used for predictive analysis to evaluate the consequences of management decisions. Such modelling workflow involves history matching to calibrate the model parameters and predictive analysis including quantification of prediction uncertainties. Sometimes, groundwater models are also used in a simulation-optimization framework to identify optimal values of groundwater management decision variables that meet multiple constraints. Algorithms for model inversion (calibration), non-linear uncertainty and simulation-optimization analyses typically require hundreds to millions of forward runs of the numerical groundwater models. When complex groundwater models need to be used for such analyses, long run-times and numerical instabilities limit their applicability for such computationally demanding analyses. Many studies have demonstrated the applicability of machine learning (ML) surrogate models for approximating the responses of groundwater flow and transport models (Yu et al, 2020). More recent studies have also demonstrated the applicability of ML approaches for stochastic inversion of biophysical models (MacKinlay et al, 2023). In this study we explore potential applicability of surrogate models in assisting computationally demanding inversion, optimization and uncertainty analysis.

In our first application, limited runs of a complex numerical groundwater model based on the MODFLOW code were used to train a surrogate model developed using Genetic Programming. The surrogate model was developed to approximate the functional relationship between the uncertain parameters of the model and its prediction of groundwater flow and head changes induced by extraction of groundwater for coal seam gas (CSG) development. The trained and validated surrogate model was used in a simulation-optimization framework to evaluate the trade-off between predicted maximum flow and groundwater head changes and CSG water extraction. The surrogate model trained and tested using 920 forward runs of the numerical groundwater model was used to evaluate 1.5 million combinations of model parameters to approximately evaluate the predictions using the simulation-optimization framework. The analysis showed that, within plausible range of model parameters and expected rates of CSG water extraction, CSG-induced maximum flow changes increase linearly with increases in water extraction volume and are directly proportional to the CSG-induced groundwater head drawdown.

In our second application, the applicability of trained Deep Neural Network models in reducing computational cost of calibration and uncertainty analysis of a MODFLOW model was investigated. As in the first application, training data were generated using forward runs of MODFLOW model developed to simulate groundwater levels in an aquifer. Many realisations of the uncertain model parameters were sampled including spatially varying hydraulic conductivity and specific yield to train groundwater flow responses. The DNN model trained with this data set was coupled with an optimiser to identify the posterior distribution of model parameters that provide satisfactory match to observed groundwater levels. The posterior distribution of parameter obtained from the surrogate model calibration analysis was then used as the initial parameter realisations for calibrating the numerical model using conventional techniques. The posterior distributions of parameters obtained from the numerical and surrogate models were compared, including using outputs of predictive simulations.

REFERENCES

MacKinlay, D. et al., 2023, Bayesian Spatio-temporal Model Inversion With METHO, ICML Conference, Jul-2023

Yu, X., Cui, T., Sreekanth, J., Mangeon, S., Doble, R., Xin, P., ... & Gilfedder, M., 2020. Deep learning emulators for groundwater contaminant transport modelling. *Journal of Hydrology*, *590*, 125351.

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