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Predicting groundwater heads in alluvial aquifers: Benchmarking different model classes and machine-learning techniques with BMA/S

Thomas Wöhling^{1,2} and Oliver Crespo Delgadillo¹

¹TUD Dresden University of Technology, Chair of Hydrology, Dresden, Germany (thomas.woehling@tu-dresden.de) ²Lincoln Agritech, Lincoln, New Zealand

Groundwater heads are commonly used to monitor storage of aquifers and as decision variables for groundwater management. Alluvial gravel aquifers are often characterized by high transmissivities and a corresponding strong seasonal and inter-annual variability of storage. The sustainable management of such aquifers is challenging, particularly for already tightly allocated aquifers and in increasingly extreme and potentially drier climates, and might require the restriction of groundwater abstraction for periods of time. Stakeholders require lead-in time to prepare for potential restrictions of their consented takes.

Groundwater models have been used in the past to support groundwater decision making and to provide the corresponding predictions of groundwater levels for operational forecasting and management. In this study, we benchmark and compare different model classes to perform this task: (i) a spatially explicit 3D groundwater flow model (MODFLOW), (ii) a conceptual, bucket-type Eigenmodel, (iii) a transfer-function model (TFN), and (iv) three machine learning (ML) techniques, namely, Multi-Layer Perceptron models (MLP), Long Short-Term Memory models (LSTM), and Random Forrest (RF) models. The model classes differ widely in their complexity, input requirements, calibration effort, and run-times. The different model classes are tested on four groundwater head time series taken from the Wairau Aquifer in New Zealand (Wöhling et al., 2020). Posterior parameter ensembles of MODFLOW (Wöhling et al., 2018) and the EIGENMODEL (Wöhling & Burbery, 2020) were combined with TFN and ML variants with different input features to form a (prior) multi-model ensemble. Models classes are ranked with posterior model weights derived from Bayesian model selection (BMS) and averaging (BMA) techniques.

Our results demonstrate that no "model that fits all" exists in our model set. The more physicsbased MODFLOW model is not necessarily providing the most accurate predictions, but can provide physical meaning and interpretation for the entire model region and outputs at locations where no data is available. ML techniques have generally much lower input requirements and short run-times. They show to be competitive candidates for groundwater head predictions where observations are available, even for system states that lie outside the calibration data range.

Because the performance of model types is site-specific, we advocate the use of multi-model

ensemble forecasting wherever feasible. The benefit is illustrated by our case study, with BMA uncertainty bounds providing a better coverage of the data and the BMA mean performing well for all tested sites. Redundant ensemble members (with BMA weights of zero) are easily filtered out to obtain efficient ensembles for operational forecasting.

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