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Research papers

Emulator-enabled approximate Bayesian computation (ABC) and uncertainty analysis for computationally expensive groundwater models

Tao Cui[a,*], Luk Peeters[b], Dan Pagendam[c], Trevor Pickett[a], Huidong Jin[d], Russell S. Crosbie[b], Matthias Raiber[a], David W. Rassam[a], Mat Gilfedder[a]

[a] CSIRO Land and Water, GPO Box 2583, Brisbane, QLD 4001, Australia
[b] CSIRO Land and Water, PMB 2, Glen Osmond, SA 5064, Australia
[c] CSIRO Data61, GPO Box 2583, Brisbane, QLD 4001, Australia
[d] CSIRO Data61, GPO Box 1700, Canberra, ACT 2601, Australia

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ABSTRACT

Bayesian inference provides a mathematically elegant and robust approach to constrain numerical model predictions with system knowledge and observations. Technical challenges, such as evaluating a large number of models with long runtimes, have restricted the application of Bayesian inference to groundwater modeling. To overcome such technical challenges, we use Gaussian process emulators to replace a transient regional groundwater MODFLOW model for computing objective functions during model constraining. The regional model is designed to assess the potential impact of a proposed coal seam gas (CSG) development on groundwater levels in the Richmond River catchment, Clarence-Moreton Basin, Australia. The emulators were trained using 4000 snapshots derived from the MODFLOW model and subsequently used to replace the MODFLOW model in an Approximate Bayesian Computation (ABC) scheme. ABC was deemed the more appropriate choice as it relaxes the need to derive an explicit likelihood function that the formal Bayesian analysis requires. The study demonstrated the flexibility of the Gaussian process emulators, which can accurately reproduce the original model behavior at a fraction of the computational cost (from hours to seconds). The gain in computational efficiency using the proposed approach allows the global calibration and uncertainty algorithms to become more feasible for computationally demanding groundwater models. Based on the ABC analysis, the probability for the simulated CSG development causing a water table change of more than 0.2 m was less than 5%. In addition to a probabilistic estimate of the prediction, an added value of emulator-assisted ABC inference is providing information on the extent to which observations can constrain parameters and predictions, as well as the flexibility to include various quantitative and qualitative parameter constraining information.

1. Introduction

Doherty (2011) states that "… a model cannot promise the right answer. However, if properly constructed, a model can promise that the right answer lies within the uncertainty limits which are its responsibility to construct". This statement is a reflection of the need to shift the focus of groundwater modeling from seeking a single optimal prediction to a prediction distribution that encompasses the range of predictions that are consistent with observations. Uncertainty analysis can be considered as the process to achieve such a distribution to support evidence-based decision making. Predictive uncertainty can be quantified through (i) forward propagation of input uncertainty or (ii) an inverse assessment of parameters where historical measurements are available to constrain the model (Beven, 2007; Refsgaard et al., 2007). Most practical groundwater modeling applications belong to the latter type, aiming to inform decision-making for water resource management. The inverse assessment of uncertainty requires sampling the prior distribution of parameters to yield posterior parameter distributions conditioned on observations.

A multitude of methods for assessing the predictive uncertainty using various sampling strategies have been reported in the literature, such as pure Monte Carlo (MC) sampling, stratified sampling, importance sampling, projection-based sampling, or combinations of them (Beven, 2008). Among those, the null space Monte Carlo (NSMC) (Herckenrath et al., 2015; James et al., 2009; Sepúlveda and Doherty, 2015) is probably the most widely used method in groundwater

* Corresponding author.
E-mail address: Tao.Cui@csiro.au (T. Cui).

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modelling, especially for computationally expensive groundwater models either due to large spatial and temporal scales or coupled multiple processes. Although the projection-based NSMC can significantly reduce computational cost and allow a non-linear uncertainty analysis for computationally intensive groundwater models, the posterior-distribution is always surrounding a pre-calibrated parameter set using a gradient-based sampling algorithm. The method is sensitive to initial parameter assignment and prone to local minima when the model is not linear (or not approximately linear), although the bias may be minimized to some extent by multiple starting-points NSMC (Keating et al., 2010; Tavakoli et al., 2013). Meanwhile, with the continuous rise in computing power and improvement of data measurements, Bayesian analysis based on holistic sampling algorithms has become increasingly popular for posterior parameter inference in other fields (Sadegh and Vrugt, 2014; Vrugt and Sadegh, 2013). However, two key issues have hindered the application of Bayesian inference in groundwater modelling, although other factors exist (Pappenberger and Beven, 2006), such as a steep learning curve, and a lack of well-documented and robust tools with a user-friendly interface.

The first factor is the heavy computational burden for most practical groundwater models. Despite the advances in algorithmic sampling efficiencies (Maier et al., 2014; J. A. Vrugt et al., 2009), the number of model runs required to accurately approximate the posterior distributions are counted in tens to hundreds of thousands for highly parameterized groundwater models (Keating et al., 2010). Constraining wide and uninformative prior parameter distributions for a complex regional groundwater model through Bayesian inference using a holistic search algorithm requires an often prohibitively large number of model runs. Model emulation has a great potential to overcome this particular issue. The principle of model emulation is to use computationally-efficient algorithms to replace computationally-demanding models. Emulators are also known as surrogate models, meta-models, reduced models, proxy models, lower fidelity models, and response surfaces (Razavi et al., 2012). Numerous model emulation techniques have been explored in various disciplines, and they can be broadly categorized into three classes; data-driven methods, projection-based methods, and multi-fidelity methods (Asher et al., 2015; Robinson et al., 2008).

The emulator is typically a black-box or statistical model that is trained on a set of model inputs and their corresponding outputs. A well-trained emulator can yield relatively accurate and precise predictions for new inputs such as parameter values and forcing variables that were not part of the original training set. Emulators have gained popularity for performing tasks such as model calibration, sensitivity analysis and uncertainty analysis, where a model must be run a large number of times. Some popular choices in the literature have included Gaussian processes (GPs) (Kennedy and O'Hagan, 2001; Liu and West, 2009; O'Hagan, 2006; Sacks et al., 1989), Neural Networks (Kourakos and Mantoglou, 2009; Yan and Minsker, 2006), Random Forests (Hooten et al., 2011; Leeds et al., 2014) and Generalized Additive Models (GAMs) (Stanfill et al., 2015; Storlie et al., 2009; Strong et al., 2014). Table 1 summarizes the recent applications of model emulation in applied groundwater modeling. Although these previous studies significantly advanced our understanding of groundwater model emulation, to the authors' knowledge, GP emulators have not been previously applied to regional groundwater models that are used to provide environmental impact assessment of deep resource development in a sedimentary basin. These models needs to include both the shallow unconsolidated aquifers where most receptors are located and the deep porous rock formations where resource development occurs (Raiber et al., 2015); such models are complex and highly non-linear (Cui et al., 2018a; Sreekanth et al., 2018).

Gaussian process emulators (O'Hagan, 2006) are mathematically very close to Kriging interpolation (Kleijnen, 2009); they are robust and well-establish tools for accurate representation of complex response surfaces derived from numerical models. They were chosen in this study as they: (1) can provide a probabilistic estimate of the uncertainty in the emulated prediction (Rasmussen and Williams, 2006), (2) are straightforward and quick to generate, (3) can be easily tailored to individual predictions, and (4) allow flexible parameterization (Bastos and O'Hagan, 2009). Razavi et al. (2012) and Asher et al. (2015) have provided a thorough review on the application of surrogate models in water resources along with a comprehensive comparison among different types of emulators.

The second critical issue that limits the application of Bayesian inference is the difficulty to define an explicit likelihood function for complex and non-linear groundwater models. Although different likelihood functions can be derived based on some assumptions, such as that the error residuals are normally distributed with a variance related to the observation uncertainty, this observation uncertainty is however often very difficult to establish and the assumptions are often not realistic (Hill and Tiedeman, 2007). The Approximate Bayesian Computation (ABC) framework (Nott et al., 2012; Vrugt and Sadegh, 2013) relaxes the need for computing an explicit likelihood function by using summary statistics or multiple objective functions. ABC has its roots in the rejection sampling in which only those parameter combinations that meet specific defined acceptance criteria are accepted. This is in contrast with formal Bayesian analysis where parameter combinations are accepted based on a likelihood function. ABC is also superior in diagnostic model calibration by defining multiple summary statistics that capture different aspects of the modelled system (Vrugt and Sadegh, 2013). ABC has been recently applied in hydrology by Nott et al. (2012) and Vrugt and Sadegh (2013), however and to the authors' knowledge, it has not been applied in groundwater modelling yet.

Another critical challenge that the classical groundwater model calibration faces is the design of the objection function. Different weight factors are usually applied to different types of numerical observations to ensure that every type of observation does influence the model calibration, however, the determining the weights is not straightforward and is usually subjective (Doherty, 2015). Qualitative

Table 1
Summary of recent applications of model emulation in applied groundwater modeling.

Paper	Emulation technique	Numerical model	Discretization	Study area	Purpose
Laloy et al. (2013)	Polynomial chaos expansion (PCE)	Steady-state groundwater flow	113 km^2, 14 layers	Nete Basin, Belgium	Posterior inference of a highly parameterized groundwater flow model
Wu et al. (2014)	Polynomial chaos expansion (PCE)	Coupled SW-GW model	9106 km^2, 5 layers	Zhangeye Basin, China	Monte Carlo uncertainty analysis
Wu et al. (2015)	Support vector machines (SVM)	Coupled SW-GW model	9106 km^2, 5 layers	Zhangeye Basin, China	Optimize SW/GW ratio in irrigation
Xu et al. (2017)	Support vector regression (SVR)	3D transient groundwater model	844 km^2, 3 layers	Spokane Valley-Rathdrum Prairie, United States	Investigate the impact of structure error on calibration and prediction
Rajabi and Ketabchi (2017)	Gaussian process emulator (GP)	3D transport model	90.5 km^2, 2 layers,	Kish Island, Iran	Optimization of coastal groundwater management
Cui et al. 2018a,b (this paper)	Gaussian process emulator (GP)	3D transient groundwater model	8230 km^2, 6 layers,	Clarence-Moreton Basin, Australia	Improve computational efficiency for global model calibration and uncertainty analysis