Ensemble Methods for Geothermal Model Calibration

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# ABSTRACT

A typical geothermal model requires significant computational resources to simulate and can contain hundreds of unknown parameters. The process of estimating these parameters, often referred to as model calibration, is a difficult task; traditional methods such as Markov chain Monte Carlo generally require running a prohibitively large number of simulations to obtain accurate results. Ensemble methods form an alternative class of algorithms for approximating the solution to the calibration pro­­­­blem and have the potential to provide accurate results using considerably fewer simulations. Ensemble methods have been used successfully to calibrate large, complex models in areas including petroleum engineering, oceanography, and weather forecasting. There are, however, few examples of applications of these methods to geothermal reservoir modelling. In addition, the wide variety of ensemble methods that have been developed mean there is a need for numerical studies that examine their respective benefits and drawbacks when applied to specific problems. To support the effective use of ensemble methods for geothermal reservoir model calibration, we review several widely used ensemble methods and demonstrate their performance on a synthetic reservoir model.

# 1. Introduction

Reservoir modelling is an important tool in the sustainable management of geothermal resources. The effectiveness of a reservoir model depends on the degree to which it reflects reality. A key component of developing an effective model is the calibration process, which involves identifying model parameters that provide an acceptable match to field data. In the context of reservoir modelling, the parameters of interest typically include the subsurface permeability structure and the strength and magnitude of the hot mass upflow at the base of the model, while the data typically include downhole temperature and pressure measurements.

The complexity of the typical geothermal system and the sparse, noisy nature of

The calibration problem is an ill-posed inverse problem

An alternative to the optimisation-based approach is to pose the model calibration problem as one of statistical inference. In particular, the Bayesian framework (Aster, Kaipio) allows for the natural incorporation of various sources of uncertainty into the calibration process. A key difference between the Bayesian approach and classical methods is that the solution to the calibration problem is not a single set of parameters; instead, it is an entire probability distribution, referred to as the posterior, which characterises the uncertainty in the parameters in the parameters that remains after accounting for the data. This

Allows for natural incorporation of risk and uncertainty

The complexity of the typical reservoir model means that the posterior is seldom available in closed form; instead, it is generally characterized using samples, using methods including Markov chain Monte Carlo (MCMC) and sequential Monte Carlo (SMC). These methods are exact, in the sense that the resulting samples are distributed according to the true posterior. However, in the geothermal context, these algorithms generally require a prohibitive number of simulations to obtain accurate results without the use of a surrogate model (Maclaren, Cui).

The challenges associated with the use of exact sampling methods for problems with complex models and large state or parameter spaces have motivated the development of methods that provide an approximate characterisation of the posterior using significantly fewer model runs. A feature common to many of these methods is that, under a Gaussian prior distribution and a linear model, the samples they generate are distributed according to the posterior. Under a nonlinear model, however, this does not hold in general. There is therefore a need to have an understanding of how well these algorithms do…?

Among the most widely-used methods for approximately characterising the posterior are linearisation of the forward model about the point in parameter space with the greatest posterior density (the maximum-a-posteriori estimate) (Omagbon), and randomised maximum likelihood (RML) (Kitandis, Oliver), in which one repeatedly solves a stochastic optimisation problem to obtain sets of parameters distributed in regions of high posterior density.

An alternative class of algorithms for approximate Bayesian inference are ensemble methods, in which a small ensemble (group of parameter sets) is combined with data, in an iterative manner, such that the distribution of the ensemble approximates the posterior. The first ensemble-based algorithm was the ensemble Kalman filter (Evensen), which was developed for the purpose of state estimation of dynamical systems, and has been used extensively in many areas of geophysics, including weather forecasting and oceanography. A great deal of subsequent research, however, has focused on the development of ensemble methods for approximating the solutions of inverse problems within the Bayesian framework. Such methods are often referred to as iterative ensemble smoothers (IES), or as forms of ensemble Kalman inversion (EKI). An advantage of ensemble methods over methods such as randomised maximum likelihood is that they do not require the computation of derivatives, which can be expensive; instead, these are approximated using the ensemble.

Though ensemble methods have begun to see some use within the geothermal community (), there exist few studies that investigate the

In this work, we present

# 2. Calibration in a Bayesian Framework

We consider problems in which the unknown parameters, , and the observations, , are related through

where denotes the forward model, and is a vector of additive measurement errors. The process of applying the forward model to find using a particular instance of is referred to as solving the forward problem. The inverse, or calibration problem, by contrast, is the process of estimating given a set of observations .

The Bayesian approach to solving the calibration problem requires us to first form a prior distribution; that is, a mathematical representation of expert knowledge on the likely values of the parameters prior to data being observed. Data, once collected, is then combined with the prior to form the posterior distribution using Bayes’ theorem, which we express here as

In the above, denotes the prior, denotes the likelihood, which expresses the probability of the data given a particular instance of the parameters, and denotes the posterior, or the conditional density of the parameters given the observations.

If we assume that the prior is Gaussian, with mean and covariance , and that the distribution of the errors is Gaussian, with mean and covariance , it can be shown (see, e.g., Tarantola 2005) that the posterior takes the form

where , , and denotes the Euclidean norm. When the forward model is linear, the posterior is also Gaussian; however, the

# 3. Ensemble Methods

We describe two ensemble methods that have been used extensively in the geosciences: the ensemble smoother with multiple data assimilation (ES-MDA) and ensemble randomised maximum likelihood (EnRML).

## 3.1 Ensemble Smoother with Multiple Data Assimilation

In the linear-Gaussian case,

We first sample an initial ensemble, , from the prior. At each subsequent iteration , we first compute the matrices of scaled differences, and , from the previous ensemble, which are defined as

In the above, and denote the mean of the ensemble parameters and predictions from the previous iteration, respectively.

We then compute the ensemble estimates of the covariance of the modelled observations, , and the cross-covariance between the parameters and modelled observations, , using

We then update ensemble member, , where , using

where ).

In the linear-Gaussian case, the samples generated used ES-MDA are distributed according to the true posterior if the inflation factors satisfy

This can be observed through a factorisation of the likelihood (Stordal xx).

This is, in general, still adhered to even when the model is nonlinear.

## 3.2 Ensemble Randomised Maximum Likelihood

An alternative group of ensemble methods (Chen and Oliver, White) share characteristics of the optimisation-based framework of RML. Unlike RML, however, these methods perform the optimisation on all ensemble members simultaneously, and, at each step of the optimisation, use an “average” gradient, estimated using the ensemble itself, when updating each ensemble member. Here, we describe the method of Chen and Oliver (2013), which is an ensemble approximation of the Levenberg-Marquardt algorithm (see, e.g., Nocedal and Wright).

At iteration , each ensemble member is updated using

where . In the above, denotes the ensemble estimate of the sensitivity matrix, which is given by

where denotes the pseudoinverse of . The sensitivity matrix encodes the number of the

convergence

adjusting lambda

## 3.3 Additional Considerations

Though the standard forms of ES-MDA and EnRML have been applied successfully to many inverse problems within the geosciences, they can encounter issues as a result of sampling errors that arise when a small ensemble is used.

Spurious correlations

It is well-known that, at each iteration, the updated ensemble lies within the span of the initial ensemble.

If a small ensemble is used and the dimensionality of the parameter space is large (that is, ), there may exist regions of parameter space with high posterior density that cannot be reached by the ensemble.

Much of the work on

(Zhang…)

There is a need, however,

# 4. Synthetic Reservoir Model

To test each ensemble method, we use a two-dimensional slice model, discretised on a grid, with dimensions of . We consider the problem of estimating the (isotropic) permeability within each block of the model grid, as well as the magnitude of the upflow at the base of the model. All other parameters are assumed to be known.

The rock in the reservoir is assumed to have a porosity of , a density of , a thermal conductivity of , and a specific heat of . The top boundary of the model is set to a constant pressure of and a temperature of ; this represents an atmospheric boundary condition. We impose a constant heat flux of through the bottom boundary, with the exception of the cell at the centre of the boundary, which is associated with an unknown mass flux of fluid with an enthalpy of . The side boundaries are closed.

4.1 Prior Parametrization

In their standard form, the update

For instance, we may wish to model the reservoir as being composed of a small number of rock formations with common physical characteristics, or to enforce bounds on range of acceptable permeabilities or the strength of the mass upflow at the base of the model.

Accounting for discontinuities in the model parameters or adhering to

This amounts to decomposing the forward model as , where is a nonlinear function mapping each ensemble member to the set of geological parameters it represents, and is the reservoir simulator.

### 4.1.1 Permeability Parametrization

Something about log-permeabilities

We partition the model domain into three distinct subdomains; a shallow high-permeability region (), a low-permeability clay cap (), and a deep high-permeability region (). We assume that the top of the clay cap is located (one gridblock) beneath the surface across the model domain. We treat the position of the bottom of the clay cap, however, as unknown. The permeability at an arbitrary location, , is therefore given by

where , and are functions that describe the (log)-permeability in regions , and , and and are functions that describe the top and bottom surfaces of the clay cap. We set , which reflects a prior assumption that the position of the top of the clay cap is known. However, we treat the bottom of the clay cap as unknown, giving a Gaussian process prior with a mean, , of , and a covariance function of

where we use a standard deviation of and a characteristic length-scale of .

We use the level set method to model the (log-)permeability field, , in each region. The level set method is commonly used in subsurface modelling to generate distinct zones with common geophysical characteristics (Muir 2020, Nicholson 2020, Tso 2021), the boundaries of which are defined using the contours of a continuous underlying function, which we refer to as the level set function.

In each region, we take the underlying level set function to be a Gaussian random field with the anisotropic covariance function given by

where is a diagonal matrix that encodes the characteristic length-scales of the correlations in each direction,

### 4.1.2 Mass Upflow Parametrization

We assume that the magnitude of the mass upflow at the base of the model is uniformly distributed on the interval , where and are equal to and respectively.

We apply the mapping , where denotes the cumulative density function of the unit normal distribution.

## 4.4 Observations

TODO

## 4.5 Simulation

We use the Waiwera simulator (Croucher et al, 2020) to run the model. Incon stuff…

# 5. Results

# 6. conclusion

Bayesian stuff with MCMC (possibly beyond the realm of the computational resources we currently have available)

Hyperparameters

3d inversion

Incorporating initial conditions into the inversion.

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