Surrogate-assisted Bayesian inversion for landscape and basin evolution models

Rohitash Chandra[1,2], Danial Azam[1], Arpit Kapoor[3], and R. Dietmar Müller[1]

[1]EarthByte Group, School of Geosciences, University of Sydney, NSW 2006, Sydney, Australia
[2]Centre for Translational Data Science, University of Sydney, NSW 2006, Sydney, Australia
[3] Department of Computer Science and Engineering, SRM Institute of Science and Technology, Tamil Nadu, India

Correspondence: Rohitash Chandra (rohitash.chandra@sydney.edu.au)

Abstract.

The complex and computationally expensive features of landscape evolution models pose a significant challenge in the inference and optimisation of unknown parameters. Bayesian inference provides a methodology for estimation and uncertainty quantification of free model parameters. In our previous work, we developed parallel tempering Bayeslands as a framework for parameter estimation and uncertainty quantification for the landscape evolution model called Badlands. Parallel tempering Bayeslands features high-performance computing with dozens of processing cores running in parallel to enhance computational efficiency. Although we use parallel computing, the procedure remains computationally challenging since thousands of samples need to be drawn and evaluated. In large-scale landscape and basin evolution problems, a single model evaluation can take from several minutes to hours, and in some instances, even days. Surrogate-assisted optimisation has been used for several computationally expensive engineering problems which motivate its use in optimisation and inference of complex geoscientific models. The use of surrogate models can speed up parallel tempering Bayeslands by developing computationally inexpensive models to mimic expensive ones. In this paper, we apply surrogate-assisted parallel tempering where that surrogate mimics a landscape evolution model including erosion, sediment transport and deposition, by estimating the likelihood function that is given by the model. We employ a neural network-based surrogate model that learns from the history of samples generated. The entire framework is developed in a parallel computing infrastructure to take advantage of parallelisation. The results show that the proposed methodology is effective in lowering the overall computational cost significantly while retaining the quality of solutions.

1 Introduction

The Bayesian methodology provides a probabilistic approach for the estimation of free parameters in complex models (Sambridge, 1999; Neal, 1996; Chandra et al., 2019b). Hence, a can view a deterministic geophysical forward model as a probabilistic model via Bayesian inference, which provides a rigorous approach to uncertainty quantification as opposed to optimisation

methods. The approach is also known as Bayesian inversion which has been used for landscape evolution (Chandra et al., 2019c, a), geological reef evolution models (Pall et al., 2018) and other geoscientific models (Sambridge, 1999, 2013; Scalzo et al., 2019). Markov Chain Monte Carlo (MCMC) sampling is typically used to implement Bayesian inference that involves the estimation and uncertainty quantification of unknown parameters (Hastings, 1970; Metropolis et al., 1953; Neal, 2012, 1996). Parallel tempering MCMC (Marinari and Parisi, 1992; Geyer and Thompson, 1995) features multiple replicas to provide a balance between exploration and exploitation which makes them suitable for irregular and multi-modal distributions (Patriksson and van der Spoel, 2008; Hukushima and Nemoto, 1996). In contrast to canonical sampling methods, we can implement parallel tempering MCMC more easily in a multi-core or parallel computing architecture (Lamport, 1986).

In our previous work, we presented parallel tempering Bayeslands for parameter estimation and uncertainty quantification for landscape evolution models (LEMs) (Chandra et al., 2019c). Parallel tempering Bayeslands features high performances parallel computing to enhance the efficiency of estimating free parameters of a Badlands model. Although we used parallel computing, the procedure was computationally challenging since thousands of samples were drawn and evaluated (Chandra et al., 2019c). In large-scale LEMs, a single model can take hours to days. Hence, it is useful to find ways to improve parallel tempering Bayeslands. Such problems are common for complex forward models of physical processes that can take several hours to days and months to evaluate a single model run. One of the ways to address this problem is using surrogate-assisted estimation.

Surrogate assistant optimisation refers to the use of statistical and machine learning models used for developing approximate simulation of the actual model (Jin, 2011). Many optimisation methods lack a rigorous approach for uncertainty quantification, leading to Bayesian inversion as an alternative, particularly for complex geophysical numerical models (Sambridge, 2013, 1999). The major advantage of a surrogate model is its computational efficiency when compared to the equivalent numerical physical forward model (Ong et al., 2003; Zhou et al., 2007). In the optimization literature, surrogate utilization is also known as response surface methodology (Montgomery and Vernon M. Bettencourt, 1977; Letsinger et al., 1996), applicable for a wide range of engineering problems (Tandjiria et al., 2000; Ong et al., 2005) such as aerodynamic wing design (Ong et al., 2003). Several approaches have been used to improve the way surrogates are utilised. (Zhou et al., 2007) combined global and local surrogate models to accelerate evolutionary optimisation. (Lim et al., 2010) presented a generalised surrogate-assisted evolutionary computation framework to unify diverse surrogate models during optimisation and taking into account uncertainty in estimation. Jin (Jin, 2011) reviewed a range of problems such as single, multi-objective, dynamic, constrained, and multi-modal optimisation problems (Díaz-Manríquez et al., 2016). In the Earth sciences, examples for surrogate assisted approaches include modeling water resources (Razavi et al., 2012; Asher et al., 2015), atmospheric general circulation models (Scher, 2018), computational oceanography (van der Merwe et al., 2007), carbon-dioxide (CO2) storage and oil recovery (Ampomah et al., 2017), and debris flow models (Navarro et al., 2018).

Given that Bayeslands is implemented using parallel computing, the challenge is in implementing surrogates across different processing cores. Recently, we developed surrogate-assisted parallel tempering has for Bayesian neural networks, which used a global-local surrogate framework to execute surrogate training in the master processing core that manages the replicas running in parallel (Chandra et al., 2018). The global surrogate refers to the main surrogate model that features training data combined

from different replicas running in parallel cores. Local surrogate model refers to the surrogate model in the given replica that incorporates knowledge from the global surrogate to make a prediction given new input data (sample or proposal). Note that the training only takes place in the global surrogate and the prediction or estimation for pseudo-likelihood only takes place in the local surrogates. The method gives promising results where prediction performance is maintained while lowering computational time using surrogates.

In this paper, we present an application of surrogate-assisted parallel tempering (Chandra et al., 2018) for Bayesian inversion of surface process models that employ parallel computing infrastructure. We use the Badlands LEM (Salles et al., 2018) as a case study to demonstrate the framework. Overall, the framework features the surrogate-model which mimics the Badlands model and estimates the likelihood function to evaluate the proposed parameters. We employ a neural network model as the surrogate that learns from the history of samples from the parallel tempering MCMC. We apply the method to several selected benchmark landscape evolution and sediment transport/deposition problems and show the quality of the estimation of the likelihood given by the surrogate when compared to the actual Badlands model.

2 Background and Related Work

2.1 Bayesian inference

Bayesian inference is typically implemented by employing MCMC sampling methods that update the probability for a hypothesis as more information becomes available. The hypothesis is given by a prior probability distribution (also known as the prior) that expresses one's belief about a quantity (or free parameter in a model) before some data is taken into account. Therefore, MCMC methods provide a probabilistic approach for estimation of free parameters in a wide range of models (Raftery and Lewis, 1996; van Ravenzwaaij et al., 2016). The likelihood function is a way to evaluate the sampled parameters for a model with given observed data. In order to evaluate the likelihood function, one would need to run the given model, which in our case is the Badlands model. The likelihood function is used with the Metropolis-criteria to either accept or reject a proposal. When accepted, the proposal becomes part of the posterior distribution, which essentially provides the estimation of the free parameter with uncertainties. The sampling process is iterative and requires thousands of samples are drawn until convergence. In our case, convergence is defined by a predefined number of samples or until the likelihood function has reached a specific value.

2.2 Badlands model and Bayeslands framework

LEMs incorporate different driving forces such as tectonics or climate variability (Whipple and Tucker, 2002; Tucker and Hancock, 2010; Salles et al., 2018; Campforts et al., 2017; Adams et al., 2017) and combine empirical data and conceptual methods into a set of mathematical equations. *Badlands* (basin and landscape dynamics) (Salles et al., 2018) is an example of such a model that can be used to reconstruct landscape evolution and associated sediment fluxes (Howard et al., 1994; Hobley et al., 2011). We use the *Badlands* LEM (Salles et al., 2018) to simulate landscape evolution and sediment transport/deposition

of selected areas, in order to provide estimation with uncertainty quantification of the unknown parameters such as *precipitation* rate and rock *erodibility* coefficient. The Badlands LEM simulates landscape dynamics which requires an initial topography exposed to climate and geological factors over time.

Bayeslands essentially provides the estimation of unknown Badlands parameters with Bayesian inference via MCMC sampling. We use the final or present-day topography at time T and expected sediment deposits at selected intervals to evaluate the quality of proposals during sampling. In this way, we constrain the set of unknown parameters given by θ using ground-truth data, $\mathbf{D}$. The prior distribution (also known as prior) refers to one's belief in the distribution of the parameter without taking into account the evidence or data. The goal of Bayeslands is to estimate θ so that the simulated topography by Badlands can resemble the ground-truth topography $\mathbf{D}$ to some degree. Bayeslands samples the posterior distribution $p(\theta|\mathbf{D})$ using principles of Bayes rule

$$p(\theta|\mathbf{D}) = \frac{p(\mathbf{D}|\theta)p(\theta)}{P(\mathbf{D})}$$

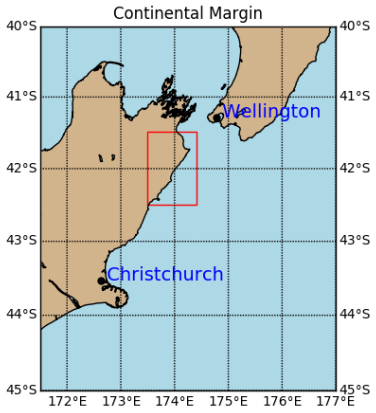
where, $p(\mathbf{D}|\theta)$ is the likelihood of the data given the parameters, $p(\theta)$ is the prior, and $p(\mathbf{D})$ is a normalizing constant and equal to $\int p(\mathbf{D}|\theta)p(\theta)d\theta$. We note that the prior ratio cancels out since we use a uniform distribution for the priors.

3 Methodology

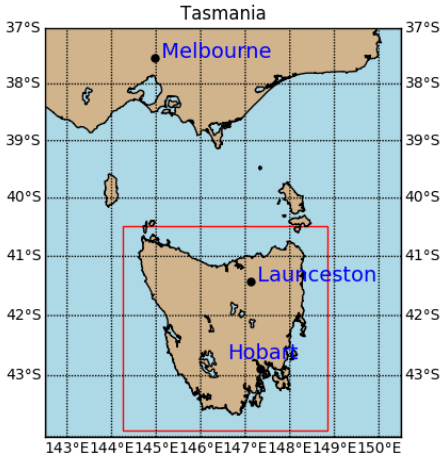
3.1 Benchmark landscape evolution problems

We select two benchmark landscape problems from parallel tempering Bayeslands (Chandra et al., 2019c) that were adapted from earlier work (Chandra et al., 2019a). These include *Continental Margin (CM)* and *Synthetic-Mountain* LEMs which are chosen due to their computational time for a single model. Both of these problems use less than ten seconds to run a single model on a single central processing unit (CPU). These problems are well suited for a parameter evaluation for the proposed surrogate-assisted Bayesian inversion framework. In order to demonstrate an application which is computationally expensive, we introduce another problem, which features the landscape evolution of Tasmania, Australia, for a million years that features the region shown in Figure 1. The Synthetic-Mountain landscape evolution is a synthetic problem while the Continental-Margin problem is a real-world problem based on the topography of a region along the eastern margin of the South Island of New Zealand as shown in Figure 1. We then use Badlands to evolve the initial landscape with parameter settings given in Table 1 and Table 2 and create the respective problems synthetic ground-truth topography.

The initial and synthetic ground-truth topographies along with erosion/deposition for these problems appear in Figure 2 and 3, respectively. Note that the figure shows that the Synthetic-Mountain is flat in the beginning, then given a constant uplift rate along with weathering with constant precipitation rate creates the mountain topography. We use present-day topography as the initial topography in the Continental-Margin and Tasmania problems, whereas, a synthetic flat region for Synthetic-Mountain initial topography. The problems involve an erosion-deposition model history that is used to generate synthetic ground-truth data for the final model state that we then attempt to recover. Hence, the likelihood function given in the following subsection takes both the landscape topography and erosion-deposition ground-truth into account. The Continental-Margin and Tasmania



(a) Continental-Margin



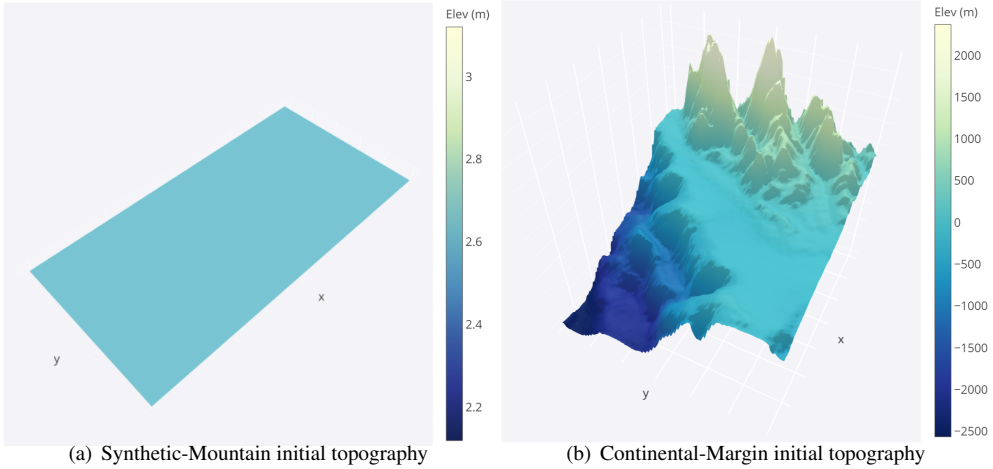
(b) Tasmania

Figure 1. Location of (a) Continental-Margin problem shown taken from South Island of New Zealand (llcrnrlon =173.5 ° East, llcrnrlat=-42.5° South, urcrnrlon=174.5° East, urcrnrlat=-41.5° South). (b) Tasmania, Australia (llcrnrlon =144.5 ° East,llcrnrlat=-43.5° South, urcrnrlon=148.5° East,urcrnrlat=-40.5° South). Note the following abbreviations: llcrnrlon refers to longitude of lower left hand corner, llcrnrlat refers to latitude of lower left hand corner. urcrnrlon refers to longitude of upper right hand corner and urcrnrlat refers to latitude of upper right hand corner of the desired map domain (degrees).

cases feature six free parameters (Table 2) whereas the Synthetic-Mountain features 5 free parameters. Note that the marine diffusion coefficients are absent for the Synthetic-Mountain problem since the region does not cover or overlap with coastal and marine areas. The main reason behind choosing the two benchmark problems is due to their nature, i.e. the Synthetic-Mountain problem features uplift rate, which is not present in the Continental-Margin problem. The Continental-Margin problem features other parameters such as the marine coefficients. The Tasmania problem features a much bigger region; hence, it takes more computational time for running a single model. The common feature in all three problems is that they model both the elevation and erosion/deposition topography. Furthermore, we draw the priors from a uniform distribution with a lower and upper limit given in Table 3.

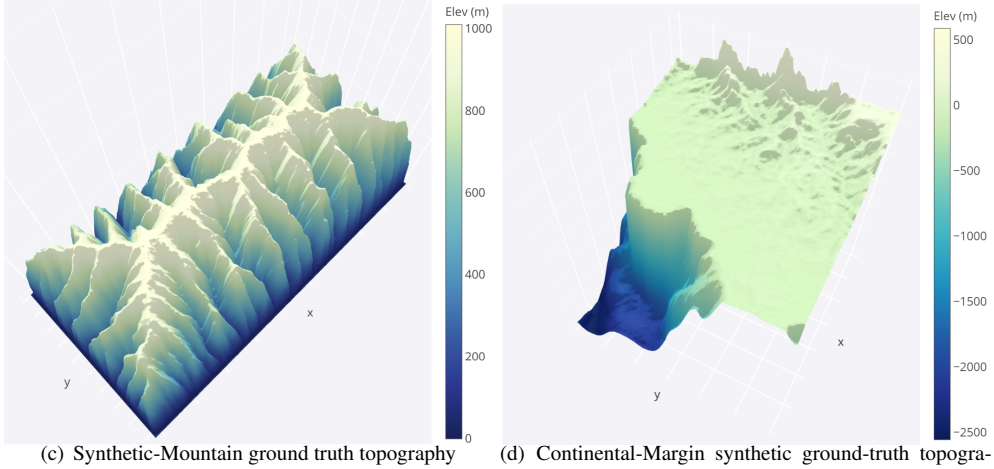
Topography	Evo.(years)	Length [km, pts]	Width [km, pts]	Res. factor	Run-time (s)
Continental-Margin	1 000 000	[136.0, 136]	[123.0, 123]	1	7.5
Synthetic-Mountain	1 000 000	[80,202]	[40,102]	1	10
Tasmania	1 000 000	[510,523]	[537,554]	1	71.3

Table 1. In the given landscape evolution problems, the run-time represents approximately the duration for one model to run on a single central processing unit (CPU).



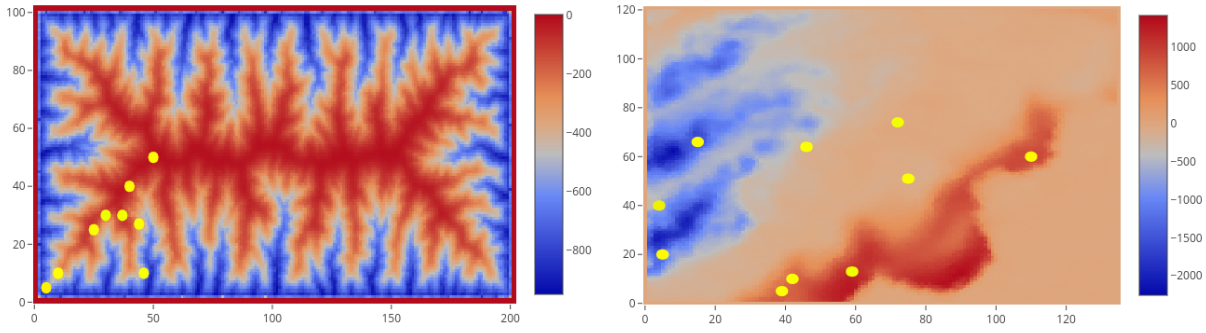
(a) Synthetic-Mountain initial topography

(b) Continental-Margin initial topography



(c) Synthetic-Mountain ground truth topography

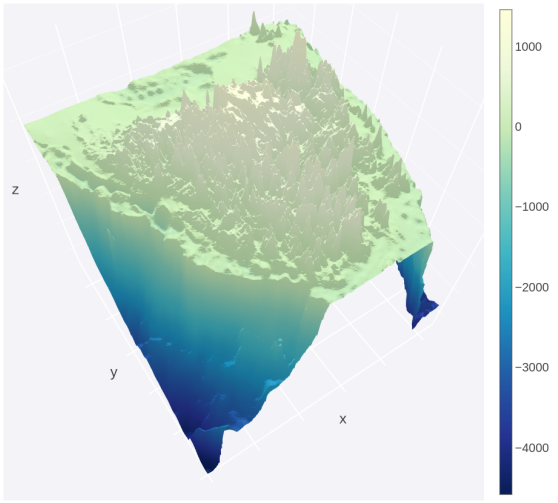
(d) Continental-Margin synthetic ground-truth topography



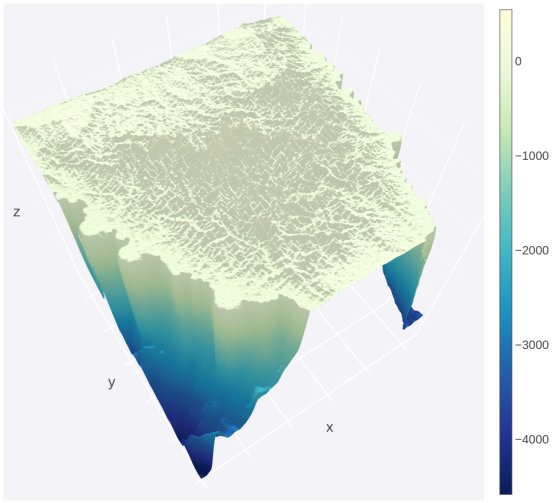
(e) Synthetic-Mountain erosion-deposition map

(f) Continental-Margin erosion-deposition map

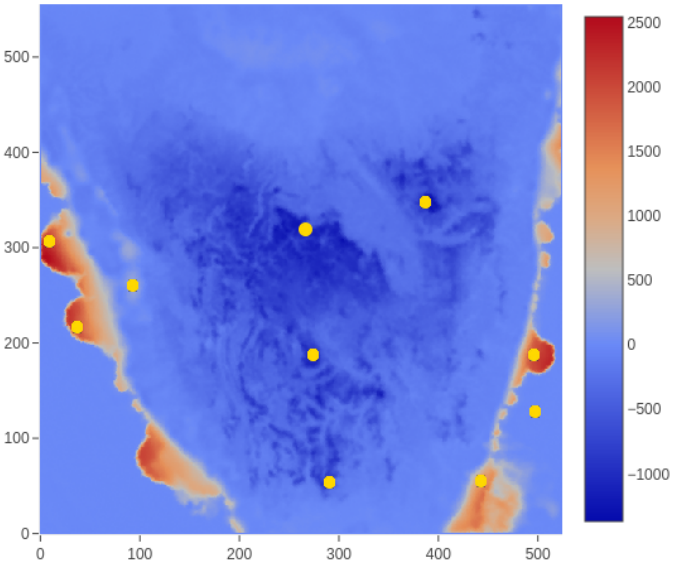
Figure 2. Synthetic-Mountain: Initial and eroded ground-truth topography after a million years of evolution. Continental Margin (CM) : Initial and eroded ground-truth topography and sediment after one million years. The erosion-deposition that forms sediment deposition after one million years is also shown. Note that x-axis represents the latitude, y-axis represents the longitude and that aligns with Figure 1 for the CM problem. The elevation in meters is given by the z-axis which is further shown as a colour-bar. The Synthetic-Mountain problem does not align with actual landscape.



(a) Tasmania initial topography



(b) Tasmania final topography



(c) Tasmania erosion-deposition map

Figure 3. Tasmania: initial and eroded ground-truth topography along with erosion-deposition that shows sediment deposition after one million years evolution. Note that x-axis represents the latitude, y-axis represents the longitude and that aligns with Figure 1 for the Tasmania problem. The elevation in meters is given by the z-axis which is further shown as a colour-bar.

Topography	Rainfall (m/a)	Erod.	n-value	m-value	c-marine	c-surface	Uplift (mm/a)
Continental-Margin	1.5	5.0-e06	1.0	0.5	0.5	0.8	-
Synthetic-Mountain	1.5	5.0-e06	1.0	0.5	-	-	1.0
Tasmania	1.5	5.0-e06	1.0	0.5	0.5	0.8	-

Table 2. True values of parameters

Topography	Rainfall (m/a)	Erod.	n-value	m-value	c-marine	c-surface	uplift
CM-ext.	[0,3.0]	[3.0-e06, 7.0-e06]	[0, 2.0]	[0, 2.0]	[0.3, 0.7]	[0.6, 1.0]	-
Synthetic-Mountain	[0,3.0]	[3.0-e06, 7.0-e06]	[0, 2.0]	[0, 2.0]	-	-	[0.1, 1.7]
Tasmania	[0,3.0]	[3.0-e06, 7.0-e06]	[0, 2.0]	[0, 2.0]	[0.3, 0.7]	[0.6, 1.0]	-

Table 3. Prior distribution range of model parameters

Topography	Pt. 1	Pt. 2	Pt. 3	Pt. 4	Pt. 5	Pt. 6	Pt. 7	Pt. 8	Pt. 9	Pt. 10
Continental Margin	(4,40)	(6,20)	(14,66)	(39,8)	(40,5)	(42,10)	(59,13)	(68,40)	(72,44)	(75,51)
Synthetic-Mountain	(5,5)	(10,10)	(20,20)	(30,30)	(40,40)	(50,50)	(25,25)	(37,30)	(44,27)	(46,10)
Tasmania	(260,320)	(400,350)	(270,180)	(290,50)	(500,120)	(500,195)	(44,200)	(5,315)	(450,50)	(95,260)

Table 4. Erosion-deposition (sediment) coordinates used in likelihood evaluation

3.2 Bayeslands likelihood function

The Bayeslands likelihood function captures the quality of topography simulation along with the quality of successive erosion-deposition, which denotes the sediment thickness evolution through time. More specifically, the likelihood function evaluates the quality of the proposals by taking into account the difference between the final simulated Badlands topography and the ground-truth topography. The likelihood function also considers the difference between the simulated and ground-truth sediment thickness at selected time intervals, which has been adapted from previous work (Chandra et al., 2019c) and given as follows.

The initial topography is denoted by $\boldsymbol{D}_0$ with $\boldsymbol{D}_0 = (D_{0,s_1} \ldots, D_{0,s_n})$, where s_i corresponds to site s_i, with the coordinates given by the latitude u_i and longitude v_i.

We assume an inverse gamma (IG) prior $\tau^2 \sim IG(\nu/2, 2/\nu)$. We integrate it so that the likelihood for the topography at time $t = T$ is

$$L_l(\boldsymbol{\theta}) \propto \prod_{i=1}^{n} \left(1 + \frac{(D_{s_i,T} - f_{s_i,T}(\boldsymbol{\theta}))^2}{\nu}\right)^{-\frac{\nu+1}{2}} \tag{1}$$

where, the subscript l, in $L_l(\boldsymbol{\theta})$ denotes that it is the landscape likelihood to distinguish it from a sediment likelihood.

We note that Badlands produces successive time-dependent topographies; however, only the final topography $\mathbf{D}_T$ is used for the calculation of the elevation likelihood because usually little ground-truth information is available for the detailed evolution of surface topography. In contrast, sediments preserve the stratigraphic record of the time-dependence of sedimentation and can be used to ground-truth the time-dependent evolution of surface process models that include sediment transport and deposition. Given that the sediment erosion/deposition values at time t, $\mathbf{z}_t$, are simulated by the Badlands model, given $\boldsymbol{\theta}$ plus some Gaussian noise

$$z_{s_j,t} = g_{s_j,t}(\boldsymbol{\theta}) + \eta_{s_j,t} \text{ with } \eta_{s_j t} \sim (0, \chi^2) \tag{2}$$

Similar to the likelihood function for the topography, the sediment likelihood $L_s(\boldsymbol{\theta})$, after integrating out χ^2 is

$$L_s(\boldsymbol{\theta}) \propto \prod_{t=1}^{T} \prod_{j=1}^{J} \left(1 + \frac{(z_{s_j,t} - g_{s_j,t}(\boldsymbol{\theta}))^2}{\nu}\right)^{-\frac{\nu+1}{2}} \tag{3}$$

We then have a combined likelihood taking both elevation and sediment/deposition into account

$$L(\boldsymbol{\theta}) = L_s(\boldsymbol{\theta}) \times L_l(\boldsymbol{\theta}). \tag{4}$$

We note that given that the sediment erosion/deposition is temporal, we could have a hierarchical Bayesian model (Chib and Carlin, 1999; Wikle et al., 1998) with two stages for MCMC sampling, that evaluates the respective likelihoods, which could be future work.

Alg. 1 Surrogate-assisted Bayeslands

Data: Ground-truth topography dataset

Result: Posterior distribution of unknown parameters θ (precipitation and erodibility

i. Initialize M replicas, $\theta_1, \theta_2, \ldots, \theta_M$ with corresponding temperature values $T_1, T_2, \ldots, T_M$
ii. Set all replicas in ensemble as $alive$; $alive = M$
iii. Define the surrogate interval (ψ), and maximum number of samples for each replica (R_{max}).

(Note: The highlighted region of the algorithm shows different processing cores. We highlighted the manager process in blue and ensemble of replica processes running in parallel in pink.)

while $(alive \neq 0$ **do**
    Stage 0: Prepare manager process to execute each replica in parallel cores
    for *each replica* r *in* M **do**
        while $(i < R_{max})$ **do**
            Stage 1.0: Metropolis Transition
            for *each* s *in* ψ **do**
                1.1 Random-walk, $\theta_s^* = \theta_s + \epsilon$
                1.2 L_{local} calculate:
                Draw κ
                if $\kappa < S_{prob}$ *and* $s > \psi$ **then**
                    Estimate L_{local} from local surrogate's prediction, $L_{surrogate}$
                    1.3 Copy global surrogate knowledge to local surrogate
                    1.4 Predict $L_{surrogate}$ value with the proposed θ_i^*.
                    1.5 L_{past} = mean(L_{s-1}, L_{s-1}, L_{s-2})
                    1.6 Assign L_{local} = (0.5 * $L_{surrogate}$) + 0.5 * L_{past}
                    1.7 Save L_s = L_{local}
                else
                    L_{local} = true-likelihood, given by Likelihood function in Equation (**??**))
                end
                1.8 Draw α from uniform distribution
                if $\alpha \leq L_{local}(\theta_s \rightarrow \theta_s^*)$ **then**
                    Update replica state, $\theta_s \leftarrow \theta_s^*$
                end
                1.9 Increment i
            end
            Stage 2.0: Replica Transition:
            2.1 Draw β from a Uniform distribution [0,1]
            if $\beta \leq P(\theta_i \leftrightarrow \theta_{s+1})$ **then**
                2.2 Signal() manager process 2.3 Exchange neighboring Replica, $\theta_i \leftrightarrow \theta_{s+1}$
            end
            Stage 3.0: Check when to end the process
            if $i == R_{max} - 1$ **then**
                3.1 Signal() manager process
                3.2 decrement number of replica processes $alive$
            end
        end
        Stage 4.0: Signal() manager process
        4.1 Set Θ which features history of proposals Φ (θ) and response λ (L_{local})

        Stage 5.0: Global Surrogate Training

        for *each replica* **do**
            5.1 Get Θ which features history of proposals Φ (θ) and response λ (L_{local})
            5.2 Append proposal list to X
            5.3 Append likelihood list to Y
        end
        5.4 Train global surrogate model with input X and output Y
        5.5 Save global surrogate model parameters
    end
end
Stage 6: Combine predictions and posterior from respective replicas in the ensemble.

3.3 Surrogate-assisted Bayeslands

The surrogate model learns from the relationship between the set of input parameters and the response given by the true (Badlands) model. In our case, the input is the set of proposals by the respective replica samplers in the parallel tempering algorithm. The likelihood estimation by the surrogate model is called the pseudo-likelihood.

In a parallel computing environment, we need to take into account the cost of inter-process communication, which must be limited to avoid computational overhead. As given in our past implementation (Chandra et al., 2019c), the *swap interval* refers to the number of iterations after which each replica pauses and can undergo a replica transition. After the swap proposal is accepted or rejected, the replicas are resumed, and they continue iterating while undergoing Metropolis transition in between the swap intervals. We incorporate the surrogate-assisted estimation into the multi-core parallel tempering algorithm. Our previous work (Chandra et al., 2018) used a *surrogate interval* that determines the frequency of training by collecting the history of past samples with their likelihood from the respective replicas.

Taking into account that the true model is represented as $y = f(x)$, the surrogate model provides an approximation in the form $\hat{y} = \hat{f}(x)$, such that $y = \hat{y} + e$ where e represents the difference or error. The task of the surrogate model is to provide an estimate for the pseudo-likelihood by training from the history of proposals which is given by the set of input $\mathbf{x_{r,s}}$ and likelihood y_s where s represents the sample and r represents the replica. Hence, we create the training dataset Φ for the surrogate by fusion of $\mathbf{x_{r,s}}$ across all the replica for a given surrogate interval ψ, which can be formulated as follows

$$\begin{aligned} \Phi &= (\mathbf{x_{1,s}}, \ldots, \mathbf{x_{1,s+\psi}}, \ldots, \mathbf{x_{M,s}}, \ldots, \mathbf{x_{M,s+\psi}}) \\ \lambda &= (y_{1,s}, \ldots, y_{1,s+\psi}, \ldots, y_{M,s}, \ldots, y_{M,s+\psi}) \end{aligned} \tag{5}$$

where, $\mathbf{x_{r,s}}$ represents the set of parameters proposed at sample s, $y_{r,s} = \log\left(p(\mathbf{y}|\mathbf{x_{r,s}})\right)$ is the likelihood which is dependent on data and the Badlands LEM, M is the total number of replicas. Θ denotes the training surrogate dataset which features input Φ and response λ at the end of every surrogate interval denoted by $s + \psi$. Therefore, the pseudo likelihood $\hat{y}$ is given by $\hat{y} = \hat{f}(\Theta)$, where $\hat{f}$ is the surrogate model. The likelihood in training data is altered, with respect of the temperature, since it has been changed by taking L_{local}/T_r for given replica r. We undo this change by multiplying the likelihood by the respective temperature, which is a data processing step for the surrogate model.

We present surrogate-assisted Bayeslands in Algorithm 1 that features parallel processing of the ensemble of replicas. The highlighted region in colour pink of the Algorithm 1 shows different processing cores running in parallel, shown in Figure 4 where the manager process is highlighted. Due to multiple parallel processing replicas, it is not straightforward to implement when to terminate sampling. Hence, the termination condition waits for all the replica processes to end where the number of active or *alive replica process* are monitored in the master process. Hence, we begin by setting the number of alive replicas in the ensemble ($alive = M$). The replicas that sample θ_n are assigned values using a uniform distribution $[-\alpha, \alpha]$; where α defines the range of the respective parameters. We then assign the user-defined parameters which include the number of replica

samples R_{max}, swap-interval R_{swap}, surrogate interval, ψ, and surrogate probability S_{prob} which determines the frequency of employing the surrogate model for estimating the pseudo-likelihood.

xxx

The samples that cover the first surrogate interval makes up the initial surrogate training data Θ, which features all the replicas. We then train the surrogate to estimate the pseudo-likelihood when required according to the surrogate probability. Figure 4 shows how the manager processing unit controls the respective replicas, which samples for the given surrogate interval. Then, the algorithm calculates the replica transition probability for the possibility of swapping the neighbouring replicas. The information flows from replica process to manager process using *signal()* via inter-process communication given by the replica process as shown in Stage 2.2, 3.1 and 4.0 of Algorithm 1, and further shown in Figure 4.

To enable better estimation for the pseudo-likelihood, we retrain the surrogate model for remaining surrogate interval blocks until the maximum time (R_{max}). The surrogate model is trained only in the manager process. Then the algorithm passes the surrogate model copy with the trained parameters to the ensemble of replica processes for estimating the pseudo-likelihood. The samples associated with the true-likelihood only becomes part of the surrogate training dataset. In Stage 1.4 of Algorithm 1, the pseudo-likelihood ($L_{surrogate}$) provides an estimation with given proposal θ_s^*. Stage 1.5 calculates the likelihood moving average of past three likelihood values, L_{past} = mean($L_{s-1}, L_{s-1}, L_{s-2}$). In Stage 1.6, we combine the moving average likelihood with the pseudo-likelihood to give a prediction that considers the present replica proposal and taking into account the past, L_{local} = (0.5 * $L_{surrogate}$) + 0.5 * L_{past}. The surrogate training can consume a significant portion of time which is dependent on the size of the problem in terms of the number of parameters and also the surrogate model used, along with the training algorithm. We evaluate the trade-off between quality of estimation by pseudo-likelihood and overall cost of computation for the true likelihood function for different types of problems.

We validate the quality of estimation from the surrogate model by the root mean squared error (RMSE) which considers the difference between the true likelihood and the pseudo-likelihood. This can be seen as a regression problem with multi-input (parameters) and a single output (likelihood). Hence, the RMSE is given by

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$$

where y_i and $\hat{y}_i$ are the true likelihood and the pseudo-likelihood values, respectively, N is the number of cases the surrogate is used during sampling.

We further note that the framework uses parallel tempering MCMC in the first stage of sampling and then transforms into the second stage where the temperature ladder is changed such that $T_i = 1$, for all replicas, $i = 1, 2, ..., N$. This strategy enables exploration is the first stage and exploitation in the second stage. We combine the respective replica accepted proposals once the termination condition is met and show their mean and standard deviation in the results.

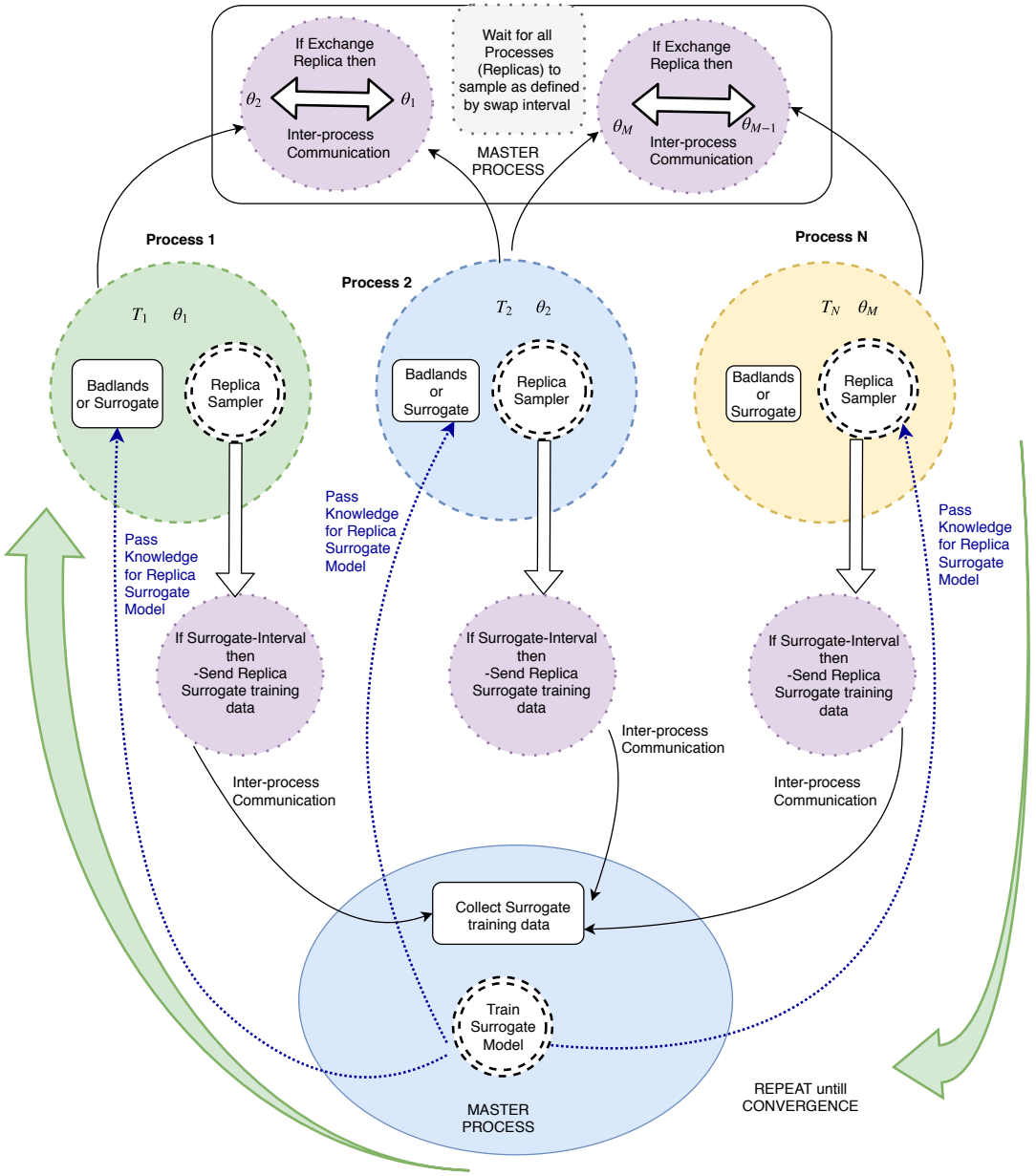


Figure 4. Surrogate-assisted Bayeslands using the parallel tempering framework. We carry out the training in the master process, which features the global surrogate model. The replica processes provide the surrogate training dataset to the master process using inter-process communication. We employ a neural network model for the surrogate model. After training, we transfer the knowledge (neural network weights) to each of the replicas to enable estimation of pseudo-likelihood. Refer to Algorithm 1 for further details.

3.4 Surrogate model

To choose a particular surrogate model, we need to consider the computational resources for training the model during the sampling process. Our literature review showed that Gaussian process models, neural networks, and radial basis functions (Broomhead and Lowe, 1988) are popular choices for surrogate models. We note that Badlands LEM features about a dozen of free parameters in the simplest case of implementation, this increases when taking into account spatial and temporal dependencies. For instance, the precipitation rate for a million years can be represented by a single parameter or by 10 different parameters that capture every 100,000 years for 10 different regions. This can account for 1,000 parameters instead of 1. Considering hundreds or thousands of unknown Badlands LEM parameters, the surrogate model needs to be efficiently trained without taking lots of computational resources. The flexibility of the model to have incremental training is also needed and hence, we rule out Gaussian process models since they have limitations in training given that the size of the dataset increases (Rasmussen, 2004). Therefore, we use neural networks as the choice of the surrogate model and the training data and neural network model can be formulated as follows.

The surrogate model use training data denote by Φ and λ defined in Equation (5), where Φ is the input and λ is the desired output of the model. The prediction of the model is denoted by $\hat{\lambda}$. We use a feedforward neural network as the surrogate model. Given input $\mathbf{x_t}$, $f(\mathbf{x}_t)$ is computed by the feedforward neural network with one hidden layer defined by the function

$$f(\mathbf{x}_t) = g\left(\delta_o + \sum_{h=1}^{H} v_j g\left(\delta_h + \sum_{d=1}^{I} w_{dh}\mathbf{x_t}\right)\right) \tag{6}$$

where δ_o and δ_h are the bias weights for the output o and hidden h layer, respectively. v_j is the weight which maps the hidden layer h to the output layer. w_{dh} is the weight which maps $\mathbf{x_t}$ to the hidden layer h and $g(.)$ is the activation function for the hidden and output layer units. We use ReLU (rectified linear unitary function) as the activation function. The learning or optimisation task then is to iteratively update the weights and biases to minimise the cross-entropy loss $J(\mathbf{W}, \mathbf{b})$. This can be done using gradient update of weights using Adam (adaptive moment estimation) learning algorithm (Kingma and Ba, 2014) and stochastic gradient descent (Bottou, 1991, 2010). We experimentally evaluate them for training feedforward network for the surrogate model in the next section.

3.5 Design of Experiments

We provide an experimental study of the proposed surrogate-assisted parallel tempering (SAPT-Bayeslands) framework for selected LEMs. We compare the results with our parallel tempering Bayeslands framework (PT-Bayeslands) presented in an earlier study (Chandra et al., 2019c). The first part of the experiment features the accuracy of the surrogates in comparison with the actual model, while the second part features the integration of SAPT for the Badlands model. We used *Keras* neural networks library (Chollet et al., 2015) for implementation of the surrogate. We provide the open-source software package that implements Algorithm 1 along with benchmark problems and experimental results [1].

[1] Surrogate-assisted parallel tempering Bayeslands: https://github.com/badlands-model/surrogate-pt-Bayeslands

We first investigate the effects of different surrogate training procedures and parameter evaluation for SAPT-Bayeslands using smaller problems. Afterwards, we apply the methodology to our selected landscape evolution problems. More specifically, we design the experiments as follows.

- We generate a dataset for training and testing the surrogate for the Synthetic-Mountain and Continental-Margin landscape evolution problems. We use the neural network model for the surrogate and evaluate different training techniques.
- We evaluate if the transfer of knowledge from previous surrogate interval is better than no transfer of knowledge for Synthetic-Mountain and Continental-Margin problems. Note this is done only with the data generated from the previous step.
- We integrate the surrogate model into parallel tempering (SAPT-Bayeslands) and evaluate the effectiveness of the surrogate in terms of prediction of likelihood and overall time reduced is evaluated. Due to the computational requirements, we only consider Synthetic-Mountain and Continental-Margin problems.
- SAPT-Bayeslands is applied to the Tasmania landscape evolution problem and compared with PT-Bayeslands.

In SAPT-Bayeslands and PT-Bayeslands, we employ a random-walk proposal distribution implemented by perturbing the chain in the respective replica with a small amount of Gaussian noise with a parameter specific step-size or standard deviation. The step-size β_i for parameter i is chosen to be a combination of a fixed step size $\phi = 0.02$, common to all parameters, multiplied by the range of possible values for parameter i so that $\beta_i = (a_i - b_i) * \phi$, where, a_i and b_i represent the maximum and minimum limits of the priors for parameter and are given in Table 2.

Similarly, we use a geometric temperature ladder with a maximum temperature of $T_{max} = 10$ for determining the temperature level for each of the replicas. In trial experiments, the selection of these parameters depended on the performance in terms of the number of accepted samples and prediction accuracy of elevation and sediment/deposition. We used replica-exchange or swap interval value, $R_{swap} = 10$ samples that determine when to check whether to swap with the neighbouring replica. In previous work (Chandra et al., 2019c), we observed that increasing the number of replicas up to a certain point does not necessarily mean that we get better performance in terms of the computational time or prediction accuracy. In this work, we limit the number of replicas as $R_{num} = 10$ for all experiments along with fixed maximum samples of 10 000 samples. We use a 15% burn-in which discards the portion of initial samples. This is a standard practice required for convergence which shows that the sampling discards the invariant and only considers the joint posterior distribution. We evaluate the performance quality of the SAPT-Bayeslands and PT-Bayeslands framework in terms of total simulation time, and root-mean-squared-error (RMSE) of the predicted elevation and erosion-deposition in the topography.

4 Results

4.1 Surrogate accuracy

To implement the surrogate model, we need to evaluate the training algorithm such as Adam and stochastic gradient descent (SGD). Furthermore, we also evaluate specific parameters such as the size of the surrogate interval (batch-ratio), the neural network topology for the surrogate and the effectiveness of either training from scratch or to utilise previous knowledge for surrogate training (transfer and train). We create a training dataset from the cases where the true likelihood was used, which compromises the history of the set of parameters proposed with the corresponding likelihood. This is done for standalone evaluation of the surrogate model, which further ensures that the experiments are reproducible since different experimental runs create different dataset depending on the exploration during sampling. Hence, we create a benchmark data set from the history of samples proposed with their likelihood [2]. We then evaluate the neural network model designated for the surrogate using two major training algorithms which featured the Adam optimiser and stochastic gradient descent. The parameters that define the neural network surrogate model used for the experiments are given in Table 5. Note that the train size in Table 5 refers to the maximum size of the data set. The training is done in batches where the batch ratio determines the training data set size, as shown in Table 6.

Table 5. Neural network architecture for the different problems

Dataset	Input	Output	Hidden layers [H1, H2, H3]	Train size	Test size
Continental-Margin	6	1	[64,35,24]	8073	879
Synthetic-Mountain	5	1	[65,35,25]	8073	879

Table 6 presents the results for the experiments that took account of the training data collected during sampling for two benchmark problems (Continental-Margin and Synthetic-Mountain). Note that, we report the mean value of the mean-squared-error (MSE) for the given batch ratio from ten experiments. The batch ratio is taken, in relation to the maximum number of samples across the chains (R_{max}/R_{num}). We normalise the likelihood values (outcomes) in the dataset between [0,1]. Although in most cases, the accuracy of the neural network is slightly better when training from scratch with combined data; however, there is a considerable trade-off with the time required to train the network. The results show that the transfer and train methodology, in general, requires much lower computational time when compared to training from scratch by combined data. Moreover, in comparison to SGD and Adam training algorithms, we observe that SGD achieves slightly better accuracy than Adam for Continental-Margin problem. However, Adam, having an adaptive learning rate, outperforms SGD in terms of the time required to train the network. Thus, we can summarise that transfer and train method is better since it saves significant computation time with a minor trade-off with accuracy.

[2]

Table 6. Evaluation of surrogate training accuracy

Dataset	Batch-ratio	Transfer and train				Train from scratch			
		SGD		Adam		SGD		Adam	
		MSE	Time(s)	MSE	Time(s)	MSE	Time(s)	MSE	Time(s)
Continental-Margin	0.1	0.0198	19.40	0.0209	31.23	0.0199	88.17	0.0206	122.41
	0.2	0.0197	26.95	0.0211	56.84	0.0197	67.74	0.0199	100.49
	0.3	0.0199	25.53	0.0212	61.41	0.0197	70.71	0.0205	268.16
	0.4	0.0195	70.42	0.0193	48.28	0.0194	46.07	0.0188	140.90
Synthetic-Mountain	0.1	0.0161	40.38	0.0097	54.45	0.0161	282.0	0.0081	347.94
	0.2	0.0134	52.87	0.007	70.65	0.0139	185.025	0.007	857.38
	0.3	0.0129	65.105	0.0088	73.035	0.0123	179.36	0.0088	543.019
	0.4	0.0164	50.14	0.0048	87.67	0.0066	149.26	0.0038	653.85

4.2 Surrogate-assisted Bayeslands

In the experiments, we investigated the effects of the surrogate probability (s-prob) and surrogate interval (batch-ratio) on the accuracy and time duration of the experiments. We report the accuracy of the prediction by the mean square error (RMSE) of the predicted topography with the real synthetic topography. Note that we report the mean and standard deviation (mean and std) of accepted samples over the sampling time after removing the burn-out period. We report the computational time in seconds.

Table 7 and 8 shows the performance of the respective methods (PT-Bayeslands and SAPT-Bayeslands) with respective parameter settings for the Continental-Margin and Synthetic-Mountain problems. In SAPT-Bayeslands, we observe that there not a significant difference in the accuracy of elevation or erosion/deposition given different values of surrogate probability. Howsoever, there is a significant difference in terms of the computational time. Greater surrogate probability gives more usage of surrogates through which we save computational time. Furthermore, we notice that there is not a significant difference in the accuracy of prediction or computational time given different values of the batch-ratio. Figure 5 and 6 provides a visualization in the elevation prediction accuracy when compared to actual ground-truth between the two methods. We also give the prediction accuracy of erosion/deposition for 10 chosen points taken at selected locations shown in Table 4. Although both methods provide erosion-deposition prediction for 4 successive time intervals, we only show the final time interval due to lack of space for the respective problems. We notice that although the prediction accuracy is lower by SAPT-Bayeslands, the visualisation shows that the mean prediction of the topography is close to ground-truth, which is well covered by the credible interval. Figure 8 and Figure 9 show the true likelihood and prediction by the surrogate for the Continental-Margin and Synthetic-Mountain problems, respectively. We notice that at certain intervals given in Figure 8, given by different replica, there is inconsistency in the predictions. Moreover, Figure 9 shows that the log-likelihood is very chaotic, and hence there is difficulty in providing robust prediction at certain points in the time given by samples for the respective replica.

Table 7. Surrogate evaluation for Continental-Margin problem

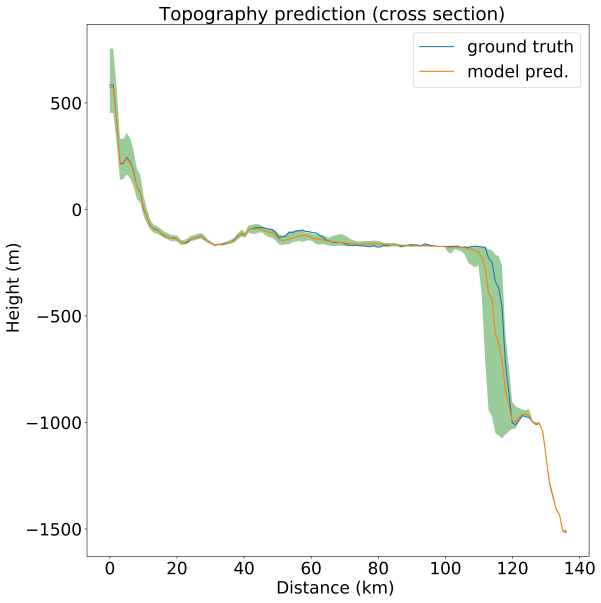
				[Elevation]		[Erosion-Deposition]			
Data-set	method	s-prob	batch-ratio	mean	std	mean	std	time (min)	time saved (%)
Continental-Margin	PT-Bayeslands	N/A	N/A	60.05	10.45	49.23	14.65	84.50	N/A
	SAPT-Bayeslands	0.25	0.10	119.37	31.48	106.13	32.54	78.36	7.27 %
	SAPT-Bayeslands	0.25	0.15	138.41	22.14	124.30	29.24	74.98	11.27 %
	SAPT-Bayeslands	0.25	0.20	123.09	37.00	112.45	35.45	76.77	9.15 %
	SAPT-Bayeslands	0.50	0.10	137.86	29.42	123.89	27.87	49.89	40.96 %
	SAPT-Bayeslands	0.50	0.15	131.14	37.31	117.59	34.58	54.27	35.78 %
	SAPT-Bayeslands	0.50	0.20	130.74	36.59	120.30	30.34	56.46	33.18 %
	SAPT-Bayeslands	0.75	0.10	126.16	29.50	116.11	26.23	34.17	65.48 %
	SAPT-Bayeslands	0.75	0.15	127.60	32.73	115.08	34.48	34.32	59.38 %
	SAPT-Bayeslands	0.75	0.20	125.18	33.70	114.73	37.86	36.98	56.24 %

Table 8. Surrogate evaluation results for Synthetic-Mountain. Mean Squared Error (MSE) values and Time elapsed for various surrogate intervals and probabilities

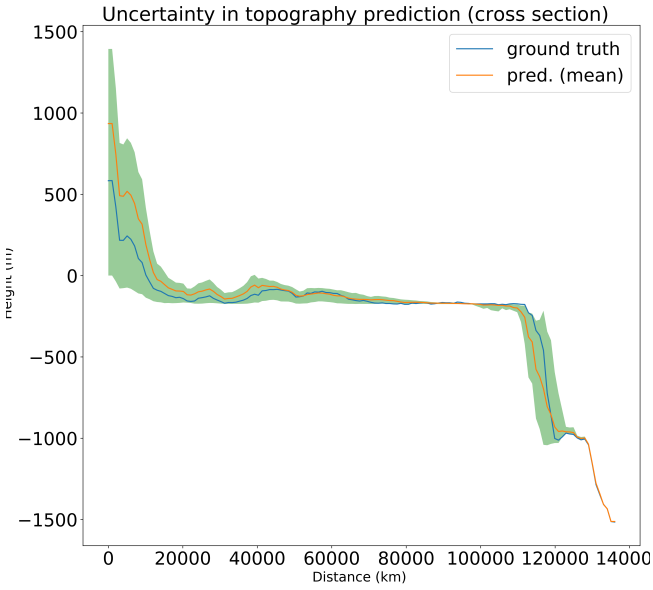
				Elevation		Erosion-Deposition			
Data-set	method	s-prob	batch-ratio	mean	std	mean	std	time (min)	time saved (%)
Synthetic-Mountain	PT-Bayeslands	N/A	N/A	4.87	1.68	1.41	0.34	128.20	N/A
	SAPT-Bayeslands	0.25	0.10	17.51	32.05	5.09	12.32	100.77	21.40 %
	SAPT-Bayeslands	0.25	0.15	22.50	28.90	7.97	12.16	101.98	20.45 %
	SAPT-Bayeslands	0.25	0.20	11.66	26.65	3.11	10.38	110.57	13.75 %
	SAPT-Bayeslands	0.50	0.10	18.79	35.75	5.51	14.11	71.35	44.34 %
	SAPT-Bayeslands	0.50	0.15	23.67	30.34	8.59	12.83	75.21	41.33 %
	SAPT-Bayeslands	0.50	0.20	12.77	28.95	3.61	11.42	80.33	37.34 %
	SAPT-Bayeslands	0.75	0.10	26.99	42.75	8.69	17.06	44.72	65.12 %
	SAPT-Bayeslands	0.75	0.15	24.18	30.31	8.75	12.66	49.64	61.28 %
	SAPT-Bayeslands	0.75	0.20	11.49	25.63	2.89	9.33	54.91	57.17 %

Table 9 gives the results for Tasmania, which is a bigger and computationally expensive problem. We select a suitable combination of the set of parameters evaluated in the previous experiments (s-prob = 0.5 and batch-ratio is 0.15). We used a maximum of 10 000 samples with 10 replicas. We notice that the performance of SAPT-Bayeslands is similar to PT-Bayeslands as shown in Figure 7, and we save 41.27 percent of computational time.

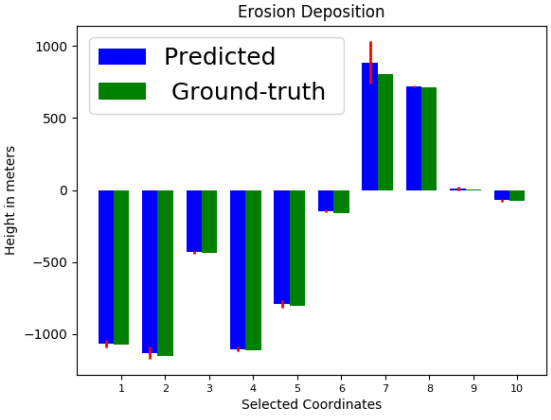
We observe that the surrogate probability is directly related to the computational performance; this is obvious since computational time depends on how often we use the surrogate. Our concern is about the prediction performance, especially while



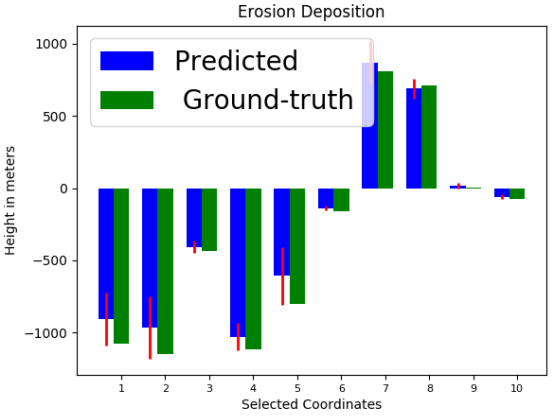
(a) Continental Margin (PT-Bayeslands)



(b) Continental Margin (SAPT-Bayeslands)

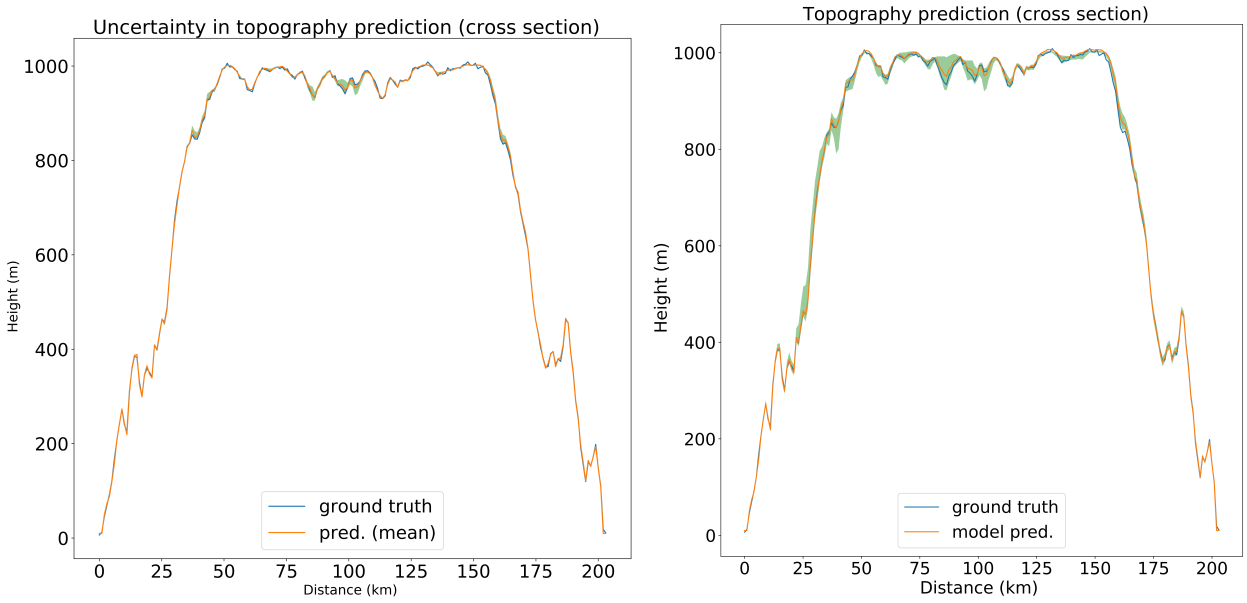


(c) Continental Margin (PT-Bayeslands)



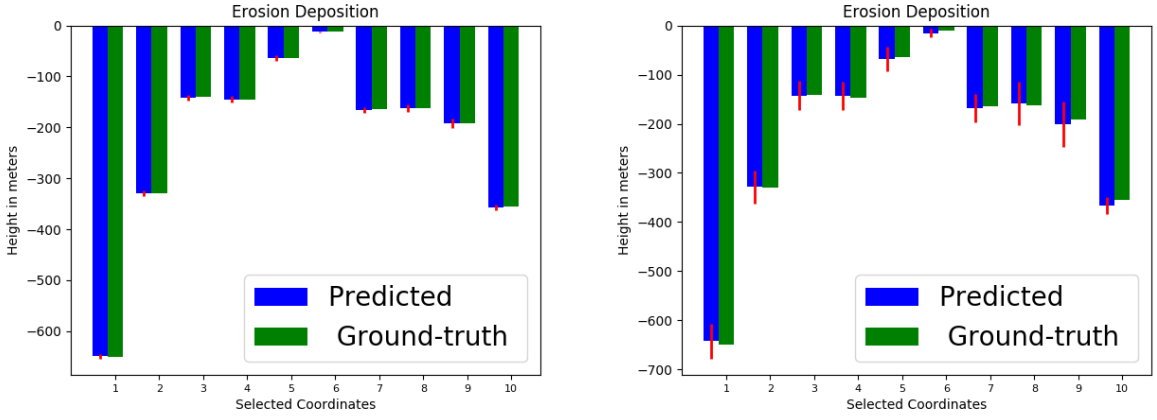
(d) Continental Margin (SAPT-Bayeslands)

Figure 5. Cross section of prediction for Continental-Margin problem. The prediction of erosion-deposition for 10 chosen points (Figure 2, Panel f) in the topography is also given.



(a) Synthetic-Mountain (PT-Bayeslands)

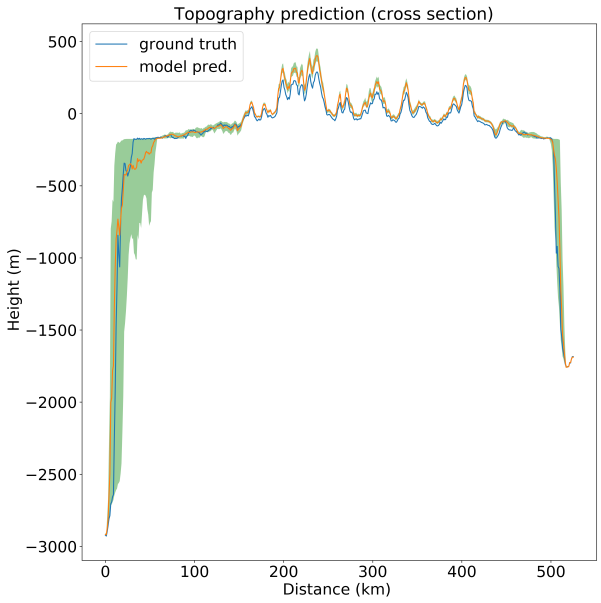
(b) Synthetic-Mountain (SAPT-Bayeslands)



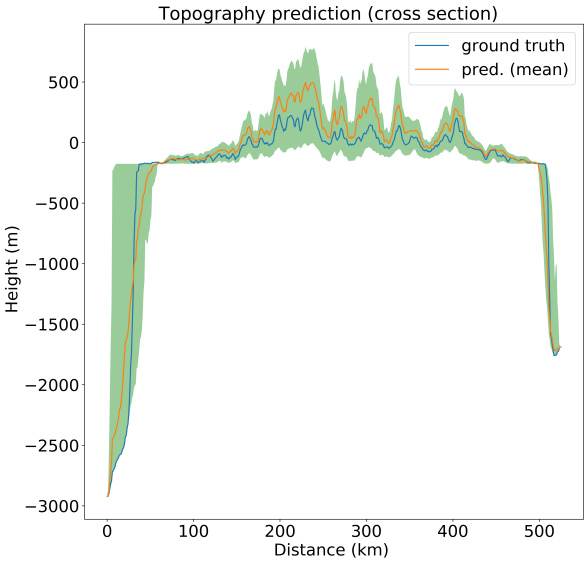
(c) Synthetic-Mountain (PT-Bayeslands)

(d) Synthetic-Mountain (SAPT-Bayeslands)

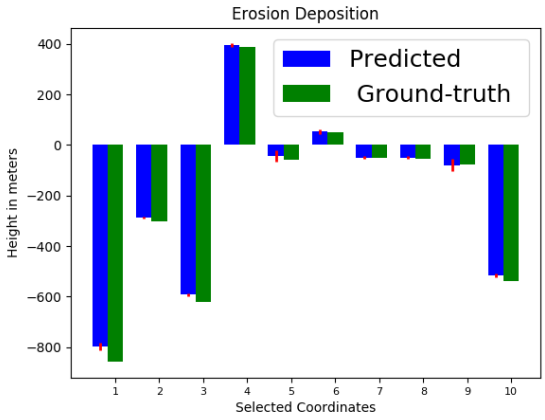
Figure 6. Cross section of prediction for Synthetic-Mountain problem. The prediction of erosion-deposition for 10 chosen points (Figure 2, Panel e) in the topography is also given.



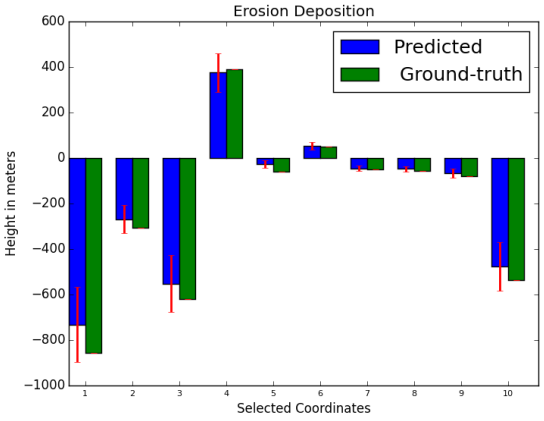
(a) Tasmania (PT-Bayeslands)



(b) Tasmania (SAPT-Bayeslands)



(c) Tasmania (PT-Bayeslands)



(d) Tasmania (SAPT-Bayeslands)

Figure 7. Cross section of prediction for Tasmania problem along with the prediction of erosion-deposition for 10 chosen points (Figure 3, Panel c) .

Table 9. Surrogate evaluation for Continental-Margin problem

				[Elevation]		[Erosion-Deposition]			
Data-set	method	s-prob	batch-ratio	mean	std	mean	std	time (min)	time saved (%)
Tasmania	PT-Bayeslands	N/A	N/A	197.27	23.42	3.9	0.5	4724.47	N/A
	SAPT-Bayeslands	0.50	0.20	235.79	32.06	3.91	0.1	2774.53	41.27 %

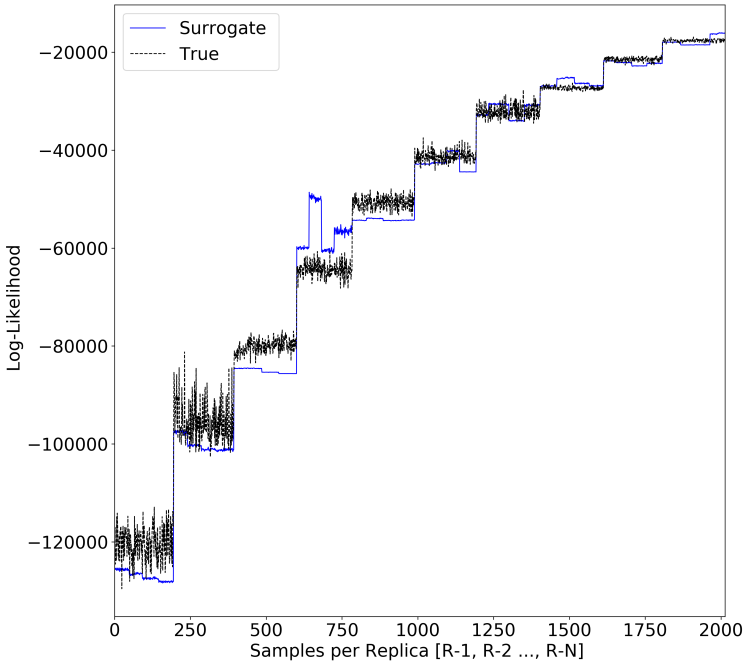


Figure 8. Surrogate likelihood vs true likelihood estimation for Continental-Margin topography

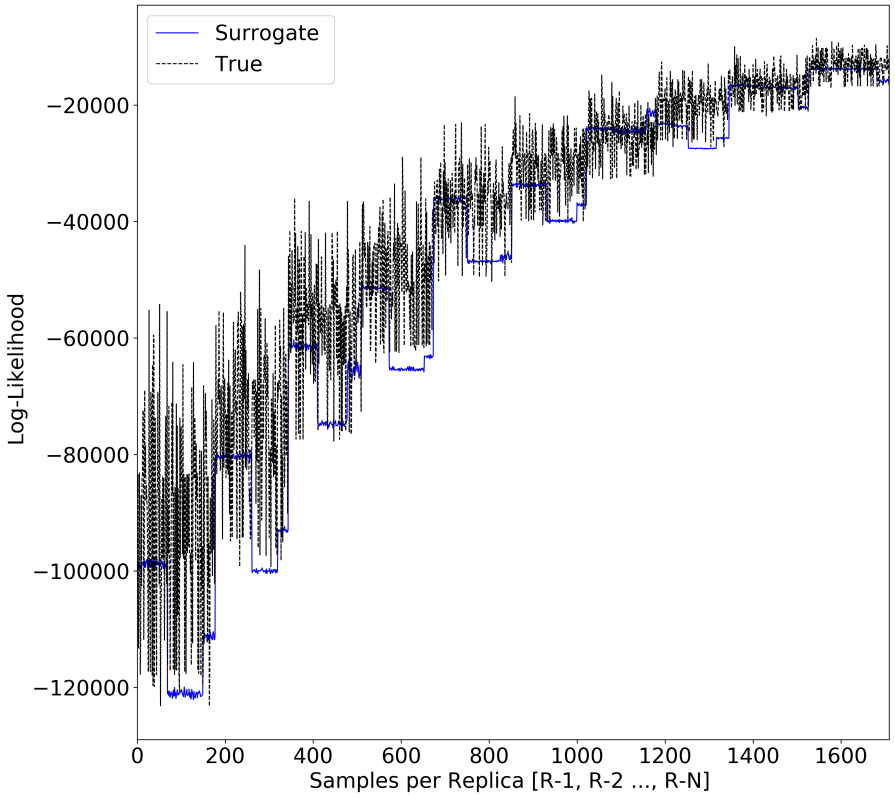


Figure 9. Surrogate likelihood vs true likelihood estimation for Synthetic-Mountain topography

increasing the use of the surrogate as it could lower the accuracy, which can result in a poor estimation of the parameters. According to the results, the accuracy is well retained we give a higher probability to the use of surrogates.In general, the proposed method achieves a lower prediction accuracy when compared to PT-Bayeslands. However, given the cross-section visualisation, we find that the accuracy given in prediction by the surrogate-based framework is not so poor. Moreover, the application to a more computationally intensive problem (Tasmania) shows that a significant reduction in computational time is achieved. We demonstrated the method using small models that run in seconds or minutes, Computational costs of continental-scale Badlands models is extensive (5-kilometre resolution for Australian continent for 149 million years is about 72 hours) and hence, in the case when thousands of samples are required, the use of surrogates can be beneficial. However, we note that improved efficiency of the surrogate-assisted Bayeslands comes at the cost of lower accuracy, and there is a trade-off between accuracy and computational time.

The results in terms of prediction accuracy given by the proposed method can be further improved in future work with the way we train the surrogates. Rather than a global surrogate model, we could use the local surrogate model on its own, where the training only takes place in the local surrogates by relying on the history of the likelihood and hence taking a univariate time series prediction approach using neural networks. Our primary contribution is in terms of the parallel computing based open-source software and the proposed underlying framework for incorporating surrogates, taking into account complex issues such as inter-process communication. This opens the road to try different types of surrogate models while using the underlying framework and open-source software.

The initial evaluation for the setup surrogate model shows that it is best to use a transfer learning approach where the knowledge from the past surrogate interval is utilised and refined with new surrogate data. This consumes much less time than accumulating data and training the surrogate from scratch at every surrogate interval. We note that in the case when we use the surrogate model for pseudo-likelihood, there is no prediction given by the surrogate model. The prediction (elevation topography and erosion-deposition) during sampling are gathered only from the true Badlands model evaluation rather than the surrogate. In this way, one could argue that the surrogate model is not mimicking the true model; however, we are guiding the sampling algorithm towards forming better proposals without evaluation of the true model. A direction forward is in incorporating other forms of surrogates, such as running low-resolution Badlands model as the surrogate, which would be computationally faster in evaluating the proposals.

Furthermore, computationally efficient implementations of landscape evolution models that only feature landscape evolution (Braun and Willett, 2013) could be used as the surrogate, while we could use Badlands model that features both landscape evolution and erosion/deposition as the true model. We could also use computationally efficient implementations of landscape evolution models that consider parallel processing (Hassan et al., 2018) in the Bayeslands framework. In this case, the challenge would be in allocating specialised processing cores for Badlands and others for parallel tempering MCMC.

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We adapted the surrogate framework from (Chandra et al., 2018) with a significant difference of featuring gradient-based proposals. Gradient-based learning or parameter estimation has been very popular in machine learning due to availability of gradient information. Due to the complexity in geological or geophysical numerical forward models, it is challenging to obtain gradients which have been the case of Badlands, landscape evolution model. We use random-walk proposals which is a canonical sampling approach with several limitations. Hence, we need to incorporate advanced meta-heuristic techniques to form non-gradient based proposals for efficient search. Our study is limited to a relatively small seat of free parameters, and a significant challenge would be to develop surrogate models with an increased set of parameters.

5 Conclusions

We presented a novel application of surrogate-assisted parallel tempering that features parallel computing for landscape evolution models using Badlands. Initially, we experimented with two different approaches for training the surrogate model, where we found that transfer learning-based approach is beneficial and could help reduce the computational time of the surrogate.

Using this approach, we present the experiments that featured evaluating certain key parameters of the surrogate-based framework. In general, we observe that the proposed framework lowers the computational time significantly while maintaining the required quality in parameter estimation and uncertainty quantification.

In future work, we envision to apply the proposed framework to more complex applications such as the evolution of continental-scale landscapes and basins over millions of years. We could use the approach for other forward models such as those that feature geological reef development or lithospheric deformation. Furthermore, the posterior distribution of our parameters require multi-modal sampling methods; hence, a combination of meta-heuristics for proposals with surrogate assisted parallel tempering could improve exploration features and also help in lowering the computational costs.

Code availability. https://github.com/intelligentEarth/surrogate-pt-Bayeslands

1 Parallel tempering MCMC

As noted earlier, parallel tempering MCMC features massive parallelism with enhanced exploration capabilities. It features several replicas with slight variations in the acceptance criteria through relaxation of the likelihood with a temperature ladder that affects the acceptance criterion. The replicas associated with higher temperature levels have more chance in accepting weaker proposals (solutions) which could help in escaping a local minimum. Given an ensemble of N replicas defined by the temperature ladder, the state of the ensemble is specified by $X = x_1, x_2, ..., x_N$, where x_i is the replica at temperature level T_i. A Markov chain is constructed to sample proposals x_i which are evaluated by the likelihood $L(x_i)$ at each replica temperature level T_i. At every iteration, the Markov chain can feature two types of transitions that include the *Metropolis transition* and the *replica transition*.

In the *Metropolis transition* phase, each replica is sampled independently to perform local *Monte Carlo* moves defined by the temperature ladder which is implemented by a change in the energy function $E(x_i)$, for each temperature level T_i. The configuration x_i^* is sampled from a proposal distribution $q_i(.|x_i)$ and the *Metropolis-Hastings* ratio at temperature level T_i is given as

$$L_{local}(x_i \rightarrow x_i^*) = exp(-\frac{1}{T_i}(E(x_i^*) - E(x_i))) \tag{1}$$

where, L represents the likelihood at the $local$ replica and the new state is accepted with probability $min(1, L_{local}(x_i \rightarrow x_i^*))$. Since the detailed balance condition holds for each MCMC replica, therefore, it holds for the ensemble system (Calderhead, 2014).

The *replica transition* phase considers the exchange of current state between two neighbouring replicas based on the Metropolis-Hasting acceptance criteria. Hence, given a probability α, pairs of replica defined by two neighbouring temperature levels, i and $i+1$ are exchanged.

$$x_i \leftrightarrow x_{i+1} \tag{2}$$

The exchange of neighbouring replicas provide an efficient balance between local and global exploration (Sambridge, 2013). The temperature ladder and replica-exchange have been of the focus of investigation in the past (Calvo, 2005; Liu et al., 2005; Bittner et al., 2008; Patriksson and van der Spoel, 2008) and there is a consensus that they need to be tailored for different types of problems given by their likelihood landscape. In this paper, the selection of temperature spacing between the replicas is carried out using a Geometric spacing methodology (Vousden et al., 2015), given as follows

$$T_i = T_{max}^{(i-1)/(M-1)} \tag{3}$$

where $i = 1, \ldots, M$ and T_{max} is maximum temperature which is user defined and dependent on the problem.

2 Training the neural network surrogate model

We note that stochastic gradient descent maintains a single learning rate for all weight updates and typically the learning rate does not change during the training. Adam (adaptive moment estimation) learning algorithm Kingma and Ba (2014) differs from classical stochastic gradient descent, as the learning rate is maintained for each network weight and separately adapted as learning unfolds. Adam computes individual adaptive learning rates for different parameters from estimates of first and second moments of the gradients. Adam features the strengths of *root mean square propagation* (RMSProp) Tieleman and Hinton (2012), and *adaptive gradient algorithm* (AdaGrad) Duchi et al. (2011). Adam has shown better results when compared to stochastic gradient descent, RMSprop and AdaGrad. Hence, we consider Adam as the designated algorithm for the neural network-based surrogate model.

The learning procedure through weight update for iteration number t can be formulated as:

$$\begin{aligned}
\Theta_{t-1} &= [\mathbf{W_{t-1}}, \mathbf{b_{t-1}}] \\
g_t &= \nabla_\Theta J_t(\Theta_{t-1}) \\
m_t &= \beta_1.m_{t-1} + (1-\beta_1).g_t \\
v_t &= \beta_2.v_{t-1} + (1-\beta_2).g_t^2 \\
\hat{m}_t &= m_t/(1-\beta_1^t) \\
\hat{v}_t &= v_t/(1-\beta_2^t) \\
\Theta_t &= \Theta_{t-1} - \alpha.\hat{m}_t/(\sqrt{\hat{v}_t} + \epsilon)
\end{aligned} \tag{4}$$

where m_t, v_t are the respective first and second moment vectors for iteration t; β_1, β_2 are constants $\in [0, 1]$, α is the learning rate, and ϵ is a close to zero constant.

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