



## Research paper

# Bayeslands: A Bayesian inference approach for parameter uncertainty quantification in Badlands

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## ABSTRACT

Bayesian inference provides a rigorous methodology for estimation and uncertainty quantification of unknown parameters in geophysical forward models. Badlands is a landscape evolution model that simulates topography development at various space and time scales. Badlands consists of a number of geophysical parameters that needs estimation with appropriate uncertainty quantification; given the observed present-day ground truth such as surface topography and the stratigraphy of sediment deposition through time. The inference of the unknown parameters is challenging due to the scarcity of data, sensitivity of the parameter setting, and complexity of the model. In this paper, we take a Bayesian approach to provide inference using Markov chain Monte Carlo sampling (MCMC). We present *Bayeslands*; a Bayesian framework for Badlands that fuses information obtained from complex forward models with observational data and prior knowledge. As a proof-of-concept, we consider a synthetic and real-world topography with two parameters for Bayeslands; namely, precipitation and erodibility. We demonstrate the challenge in sampling irregular and multi-modal posterior distributions using a likelihood surface that has a range of sub-optimal modes. The results of the experiments show that Bayeslands yields a promising distribution of the selected Badlands parameters.

## 1. Introduction

A new generation of Earth evolution models has recently emerged with the capability to link models for dynamic and isostatic topography through time (Flament et al., 2013) with landscape evolution models (Braun and Sambridge, 1997; Coulthard, 2001; Whipple and Tucker, 2002; Tucker and Hancock, 2010; Salles and Duclaux, 2015; Campforts et al., 2017; Adams et al., 2017; Pazzaglia, 2003; Chen et al., 2014). This provides a model for landscape evolution in response to surface uplift and subsidence over a large range of spatial scales, and track sediments from source to sink (Salles, 2016; Salles et al., 2017). Geophysical forward models depend on uncertain initial and boundary conditions (Scott and Zhang, 1990); such as global sea level, spatial and temporal variations in precipitation, and rock erodibility (Godard et al., 2006; Rejman et al., 1998). These models are calibrated against ground truth data which include the present-day topography and river geometries, total sediment thickness, sediment stratigraphy (constraining the time-dependence of sedimentation) and sedimentation rates, the time-dependent rock exhumation history from thermochronology data, geologically mapped paleocoastlines and geological data that constraints sediment provenance.

Bayesian inference provides a framework for combining information from various sources to estimate and quantify uncertainty of an unknown parameter in a rigorous manner (Chair and Varshney, 1988). The diverse source of information includes expert knowledge, ground-truth data, and knowledge from physical processes embedded in geophysical models (Notarnicola and Posa, 2001; Moon and So, 1995). Markov Chain Monte Carlo sampling methods (MCMC) implement Bayesian inference to sample from a posterior probability distribution (Hastings, 1970; Metropolis et al., 1953). In the past few decades, Bayesian methods became popular in geophysics (Malinverno, 2002; Mosegaard and Tarantola, 1995; Sambridge, 1999), where the emphasis has shifted from optimization methods (Sen and Stoffa, 2013) to inference, due to the need for rigorous uncertainty quantification given sparse and incomplete data (Gallagher et al., 2009). The application of Bayesian inference via MCMC methods in Earth science has been demonstrated in a number of papers, such as characterizing geochronological data that describe the age of rocks and fossils (Jasra et al., 2006), modelling the effect of climate changes in land surface hydrology (Raje and Krishnan, 2012), calibrating hydrologic models (Thyer

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et al., 2015), flood frequency analysis (Gaál et al., 2010), inferring sea-level and sediment supply from the stratigraphic record (Charvin et al., 2009), and inferring groundwater contamination sources (Wang and Jin, 2013). However, in the context of landscape evolution models, to our knowledge there is no work that employs MCMC methods to fuse information given by complex forward models with observational data.

Landscape evolution models (LEMs) are characterized by parameters that interact in a complicated fashion and feature a high dimensional parameter space given time dependent parameters that represent climate factors for thousands to millions of years (Salles, 2016). Basin and landscape dynamics (Badlands) is an unusual example of a landscape evolution model for not only simulating topography development through time, but also tracking sediments from source to sink, with the capability to create synthetic basin stratigraphies (Salles, 2016; Salles et al., 2017). We focus on using the Badlands software here because, despite the general abundance of landscape modelling software, there is no other mature open-source software that allows the simultaneous modelling of erosion, sediment transport and sedimentation. Badlands models feature a number of unknown parameters which need to be estimated given incomplete and sparse observational datasets which remains a major challenge in the field. The challenge is in estimating the unknown parameters given model complexity, lack of gradient information to construct efficient proposals, and computationally expensive models. The posterior distribution of the parameters in these models can feature multiple modes and discontinuities which create further challenges. These have hindered the uptake of Bayesian inference methods for landscape evolution models (Salles, 2016; Salles et al., 2017).

This paper presents Bayeslands, a framework for inference and uncertainty quantification in the Badlands model for basin and landscape evolution. We evaluate the performance of Bayeslands in terms of prediction accuracy of the final elevation and sediment erosion/deposition over time. Moreover, we present a visualization of the likelihood surfaces of the respective problem for a better understanding of the posterior distribution.

## 2. Background and related work

### 2.1. Bayesian inference

Bayesian inference regarding a quantity of interest  $\theta$ , is made via the posterior distribution denoted by  $p(\theta|\mathbf{D})$ , where  $\mathbf{D}$  denotes the data. This posterior probability is proportional to the product of the likelihood  $p(\mathbf{D}|\theta)$  and the prior  $p(\theta)$ , i.e.  $p(\theta|\mathbf{D}) \propto p(\mathbf{D}|\theta)p(\theta)$ . The prior distribution  $p(\theta)$ , reflects existing knowledge or belief about  $\theta$  gathered from previous research and expert opinion. This prior is then updated via the likelihood  $p(\text{data}|\theta)$ , as data are acquired. The likelihood  $p(\mathbf{D}|\theta)$  defines how likely the given value of  $\theta$  is given some data. The posterior probability quantifies the probability that  $\theta$  takes on a particular value (if  $\theta$  is a discrete) or a range of values (if  $\theta$  is continuous). The posterior distribution,  $p(\theta|\mathbf{D})$ , is rarely available in closed form; hence, sampling based methods such as MCMC are used for approximation.

MCMC methods use the Metropolis–Hastings algorithm to obtain draws of  $\theta$  from some proposal distribution. The draws of  $\theta$  are then accepted with a probability which ensures that the Markov chain satisfies the detailed balance condition (Tierney et al., 1998). If the proposed values are not accepted, then the chain stays at its current value. Under certain conditions, the draws of  $\theta$  will converge to draws from the stationary distribution  $p(\theta|D)$ .

The proposals distributions can include random-walk proposals (Haario et al., 1999), full conditional proposals known as Gibbs sampling (Casella and George, 1992), and proposals which use gradients (Neal, 2011), such as the No U-Turn (NUTS) sampler of Hamiltonian MCMC (Hoffman and Gelman, 2014; Girolami and Calderhead, 2011). The performance of these methods and their variants have been well studied in the literature; see Robert and Casella (2010) for a review.

Open-source Bayesian statistical packages have made the implementation of MCMC methods easier to facilitate researchers without a background in Bayesian statistics (Fonnesbeck et al., 2015; Drummond et al., 2012).

### 2.2. Basin and landscape dynamics with Badlands model

Over the last decades, many numerical models have been proposed to simulate how Earth's landscape has evolved over geological time scales in response to different driving forces such as tectonics and climatic variability (Whipple and Tucker, 2002; Tucker and Hancock, 2010; Salles and Duclaux, 2015; Campforts et al., 2017; Adams et al., 2017). These models combine empirical data and conceptual methods into a set of mathematical equations that can be used to reconstruct landscape evolution and associated sediment fluxes (Howard et al., 1994; Hobley et al., 2011). They are currently used in a variety of research fields including hydrology (Raje and Krishnan, 2012), modelling sea level fluctuations, erosion, and sediment supply to basins and margins (Charvin et al., 2009), and to study the interplay between landscape degradation, vegetation and gully erosion (Bastola et al., 2018; Gallen, 2018).

The Badlands model simulates regional to continental sediment deposition and associated sedimentary basin architecture (Howard et al., 1994; Salles et al., 2017; Salles, 2016). In its most simple formulation, the landscape surface elevation changes in response to the interaction of three types of processes, (i) tectonic plate movement, (ii) diffusive processes and the associated smoothing effects, and (iii) water flow and the associated erosion. The change in elevation  $z$  with respect to time  $t$  is given by

$$\frac{\partial z}{\partial t} = -\nabla \cdot q_s + u \quad (1)$$

where,  $u$  in  $\text{m yr}^{-1}$  is a source term that represents tectonic uplift. The total downhill sediment flux  $q_s$  is defined by

$$q_s = q_r + q_d \quad (2)$$

$q_s$  is the volumetric sediment flux per unit width ( $\text{m}^2 \text{ yr}^{-1}$ ).  $q_r$  represents transport by fluvial system and  $q_d$  hillslope processes both in  $\text{m}^2 \text{ yr}^{-1}$ .

#### 2.2.1. Fluvial system

Badlands uses a triangular irregular network (TIN) to solve the geomorphic equations presented in Braun and Sambridge (1997). The continuity equation is defined using a finite volume approach and relies on the method described in Tucker et al. (2001). To solve channel incision and landscape evolution, the algorithm follows the  $O(n)$ -efficient ordering method from Braun and Willett (2013). This is based on a single-flow-direction (SFD) approximation assuming that water goes down the path of the steepest slope (O'Callaghan and Mark, 1984).

Several formulations of river incision have been proposed to account for long term evolution of fluvial system (Tucker and Hancock, 2010; Chen et al., 2014). These formulations describe different erosional behaviours. They include detachment-limited incision, which is governed by bed resistance to erosion, and transport-limited incision, which is governed by the capacity of the flow to transport sediment available on a river bed. Mathematical representation of the erosion process is often assumed to follow a stream power law (Hobley et al., 2017). These relatively simple approaches have two main advantages. First, they have been shown to approximate the first order kinematics of landscape evolution across geologically relevant timescales ( $>10^4$  years). Second, neither the details of long term catchment hydrology nor the complexity of sediment mobilization dynamics are required. However, other formulations are sometimes necessary when addressing specific aspects of landscape evolution.

In this paper, our main objective centres around the estimation with uncertainty quantification of the parameters in Badlands. We use the

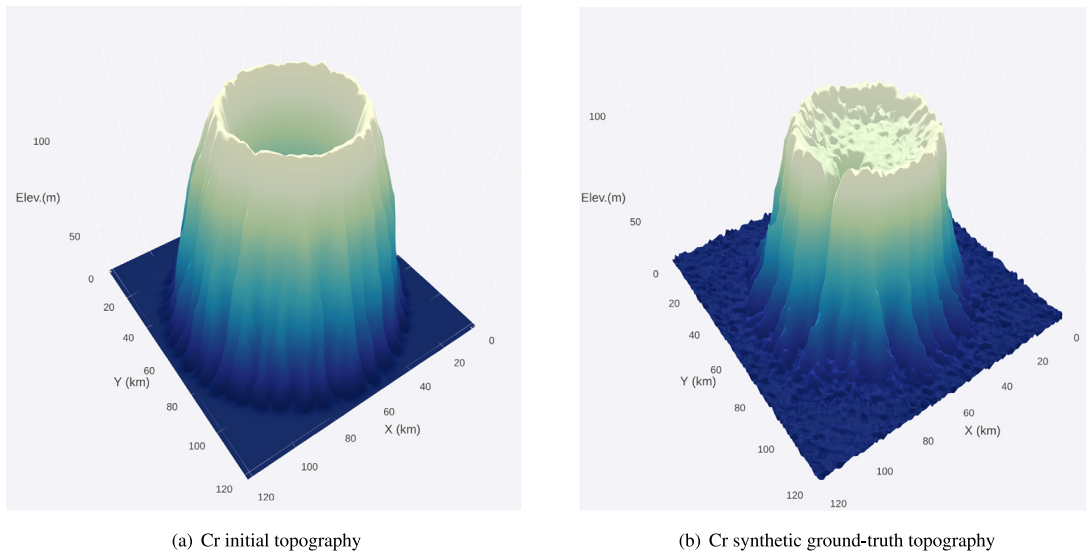


Fig. 1. Cr: Initial (panel a) and eroded ground-truth topography (panel b) after 50,000 years.

Table 1

Values used for generation of synthetic ground-truth topographies (Cr and CM). The simulated time that is represented by Badlands is given in years while the run-time for executing a single Badlands model is given in seconds (s).

Topography	Time ( $t$ yrs)	$\rho$ (m/yr)	$\epsilon$	Run-time (s)
Cr	50,000	1.5	$5.e-5$	0.8
CM	1000,000	1.5	$5.e-6$	1.1

default fluvial incision law available in *Badlands* which is based on the detachment-limited stream power law. The erosion rate  $\dot{e}$  depends on drainage area  $A$  ( $m^2$ ), net precipitation  $P$  (m/yr) and local slope  $S$  which takes the form

$$\dot{e} = \epsilon (P \cdot A)^m S^n \quad (3)$$

where,  $\epsilon$  is a dimensional coefficient describing the erodibility of channel bed as a function of rock strength, bed roughness and climate,  $m$  and  $n$  are dimensionless positive constants. The default formulation assumes  $m = 0.5$  and  $n = 1$ . Using this incision law, sediment deposition occurs solely in topographically closed depression and marine locations.

### 2.2.2. Hillslope processes

Along hillslopes, we state that the flux of sediment is proportional to the gradient of topography and a linear diffusion law commonly referred to as soil creep is used (Tucker and Hancock, 2010; Salles and Duclaux, 2015). This is formulated as a diffusion equation

$$\frac{\partial z}{\partial t} = \kappa \nabla^2 z \quad (4)$$

in which,  $\kappa$  is the diffusion coefficient and can be defined with different values for the marine and land environments. It encapsulates, in a simple formulation, a variety of processes operating over short ranges on the superficial veneer of soils and sediments.  $\kappa$  varies as a function of substrate, lithology, soil depth, climate and biological activity.

## 3. Materials and methods

### 3.1. Creation of synthetic data

In order to evaluate the performance of Bayeslands, we consider two synthetic topographies that include the development of river systems, mountain ranges and sediment transport from source to sink. We refer to them as Crater (Cr) and Continental-Margin (CM) and provide further details as follows:

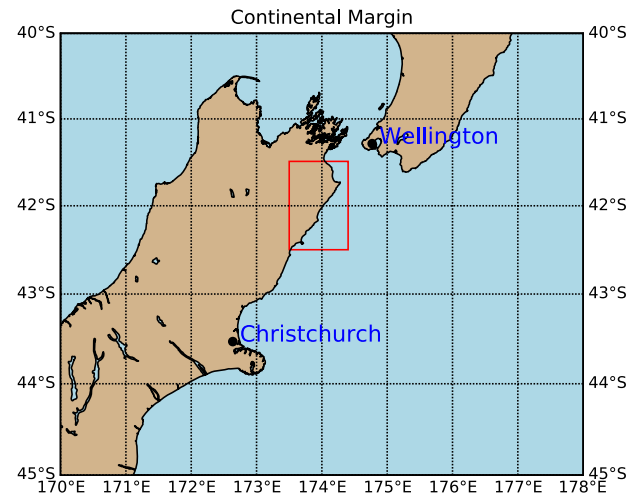
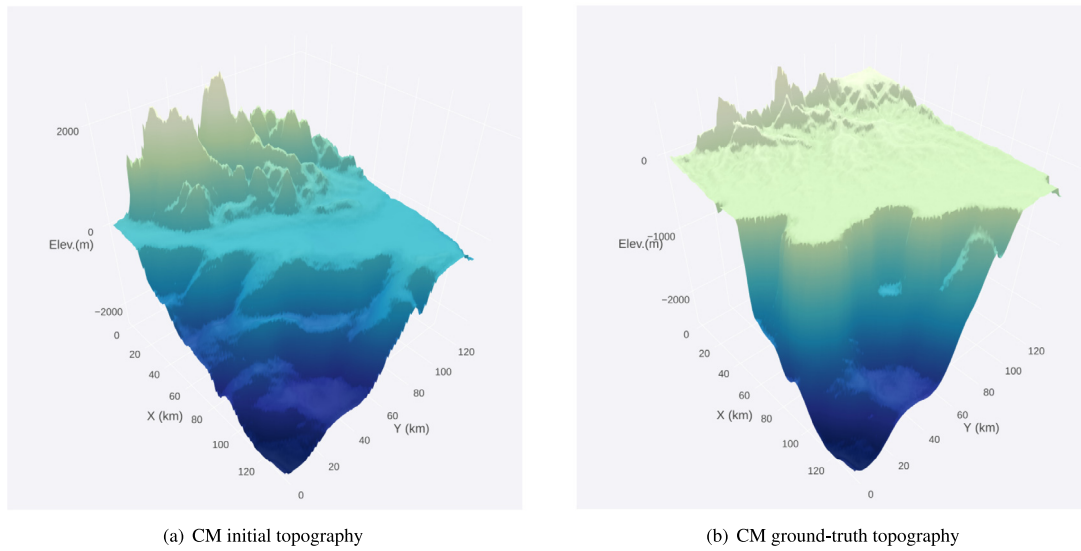
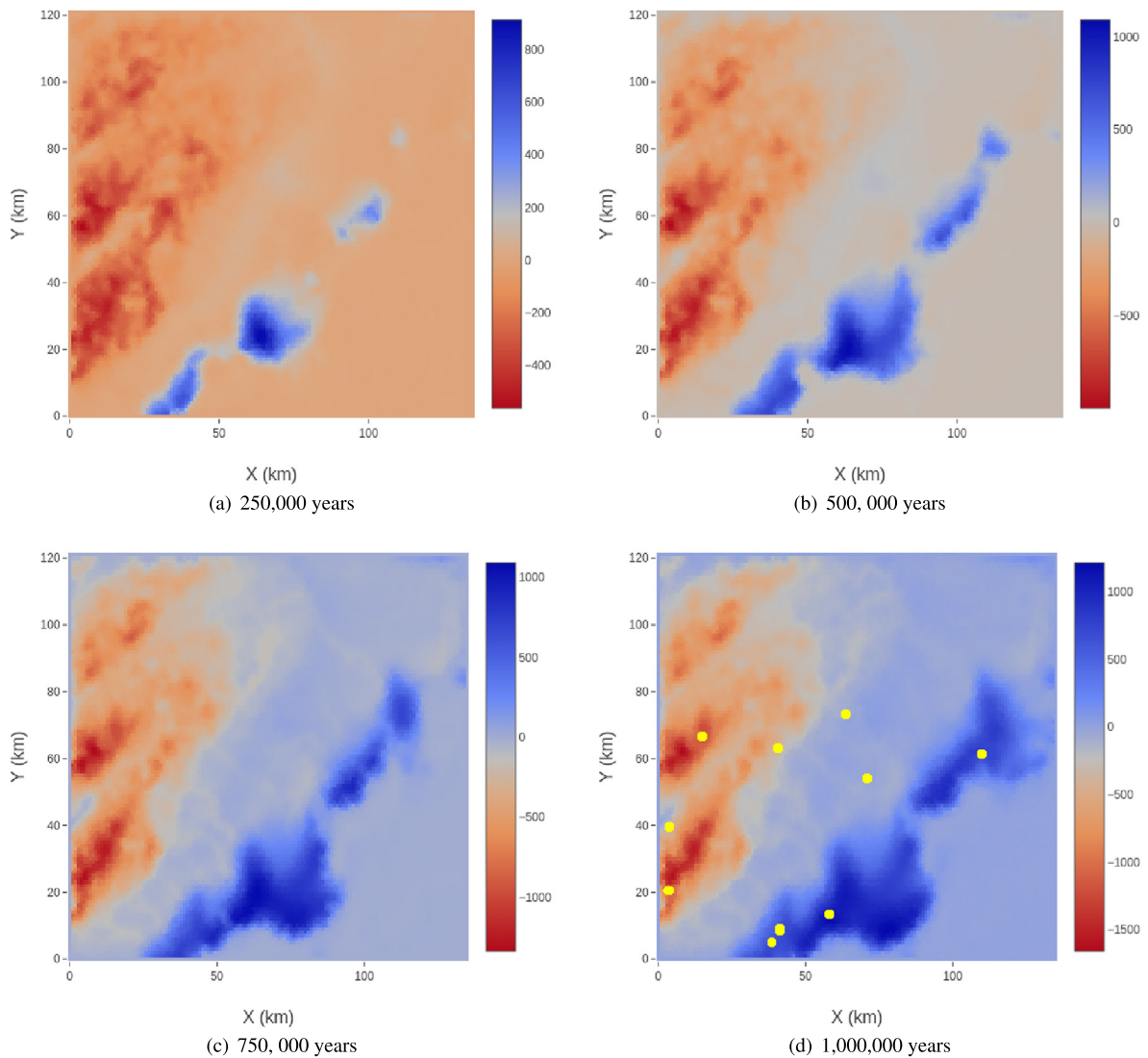


Fig. 2. Map showing the region (highlighted in red) for the Continental-Margin problem selected from the South Island of New Zealand. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

- Cr: We simulate the geomorphological evolution over 50,000 years of a synthetic crater-type digital elevation model created by Badlands. The size of the crater is  $0.24 \times 0.24$  kilometer (km) squared. The topography is evaluated at a grid of  $123 \times 123$  points (pixels). The resolution factor which defines the distance between two adjacent points in the grid. In this case, the resolution factor is 0.02 km/point. Fig. 1 shows the initial and the final topography after 50,000 years of evolution by Badlands. The final topography is used as the ground-truth topography.
- CM: Using Badlands, we simulate the geomorphological evolution over 1000,000 years using a digital elevation model from present day South Island in New Zealand as shown in Fig. 2. This region is represented by  $91 \times 81$  points that covers 136 by 123 km squared; hence, the resolution factor is 1.5 km/point. Fig. 3 shows the initial and the final or ground-truth topography by Badlands. Note that the CM topography is typically a 1 arc-minute global relief model of Earth's surface that integrates land topography and ocean bathymetry. Fig. 4 presents the sediment erosion/deposition for selected time-frames with selected locations used by the Bayeslands framework.



**Fig. 3.** CM: Initial and eroded ground-truth topography after 1000,000 years.



**Fig. 4.** Sediment erosion/deposition for Continental-Margin topography for 4 selected time-frames, panels (a) - (d). Note that the erosion is negative while deposition is positive which is shown by the legend in metres. The yellow points mark the selected locations of the sediment data.



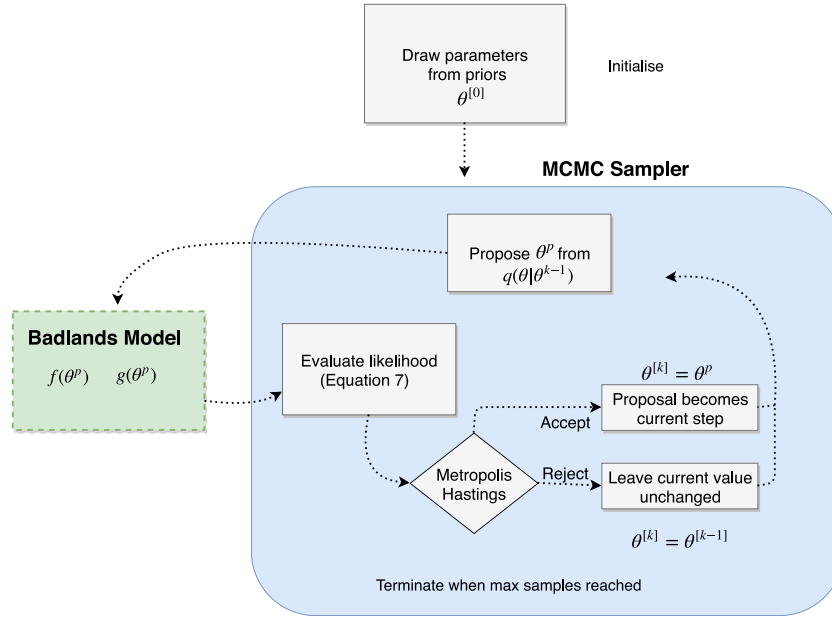


Fig. 5. Bayeslands framework employing MCMC random-walk sampler and Badlands model. Further details are given in Algorithm 1.

Table 1 shows the set of parameters that were used to create the ground-truth topography described above. We assume the final topographies are observed in the present; by which we imply that the Cr topography began evolution 50,000 years ago while the CM topography began evolution 1000,000 years ago. Hence, the ground-truth or observed topography data ( $Y^{obs}$ ) refers to the topography of present age, where  $t = T$ . The goal of Bayeslands is to sample and obtain a posterior distribution of the free parameters that governs Badlands. The posterior distribution is used to make inference about the free parameters which includes prediction and uncertainty quantification.

### 3.2. Bayeslands model and priors

#### 3.2.1. Model for topography

In order to implement the model, we take a probabilistic approach and assume that the observed elevation at time  $t$ , longitude  $i$  and latitude  $j$ , is generated from a signal plus noise model

$$y_{t,i,j} = g_{t,i,j}(\theta) + e_{t,i,j} \quad (5)$$

where,  $y_{t,i,j}$  is the elevation,  $g(\theta)$  is the signal that depends on the unknown parameters  $\theta$ , and  $e_{t,i,j} \sim \mathcal{N}(0, \tau^2)$  is the noise. In this model,  $\theta$  is equal to precipitation ( $\rho$ ) and erodibility ( $\epsilon$ ). The notation  $N(\mu, \sigma^2)$  refers to the normal distribution with mean ( $\mu$ ) and variance ( $\sigma^2$ ). The noise in Eq. (5) reflects the fact that the elevation, at any point in time, will be affected by factors other than those in the Badlands model.

Let  $\mathbf{Y}_T = (\mathbf{Y}_{T,1}, \dots, \mathbf{Y}_{T,n})$ ; where,  $\mathbf{Y}_{T,j} = (y_{T,1,j}, \dots, y_{T,n,j})'$  is the matrix of observed elevations across an  $n \times n$  grid of latitude and longitude at time  $t$ . We place an inverse gamma,  $IG(\nu/2, 2/\nu)$  prior on  $\tau^2$  and integrate it out of the likelihood, denoted by  $L_{Y_T}(\theta)$ , to give

$$L_{Y_T}(\theta) \propto \prod_{j=1}^n \prod_{i=1}^n \left( 1 + \frac{(y_{T,i,j} - g_{T,i,j}(\theta))^2}{\nu} \right)^{-\frac{\nu+1}{2}} \quad (6)$$

We note that the mean function  $g(\theta)$  has no closed form representation in  $\theta$ . Therefore, we cannot write down the likelihood as an explicit function of  $\theta$ . However, given there exists a deterministic relationship between  $\theta$  and  $g(\theta)$ , then  $P(\mathbf{Y}_t | \theta, \tau^2) = P(\mathbf{Y}_t | g(\theta), \tau^2)$ . We place uniform priors on precipitation and erodibility, and the limits of the uniform distributions are given in Table 2

Table 2

Prior range with minimum and maximum values for precipitation ( $\rho$ ) and erodibility ( $\epsilon$ ).

Topography	$\rho$ [min., max.]	$\epsilon$ [min., max.]
Cr	[0.0–3.0]	[3.e–5, 7.e–5]
CM	[0.0–3.0]	[3.e–6, 7.e–6]

#### 3.2.2. Model for sediment erosion/deposition

Due to the issue of multi-modality in complex models, there can be a number of possible values of  $\rho$  and  $\epsilon$  which gives rise to the same topography. To constrain the number of possible values, we use information featured in the sediment erosion/deposition history.

As stated previously, we only have ground-truth data of the landscape topography in the present day denoted by  $T$ . The likelihood given by Eq. (6) evaluates the Badlands parameters  $\theta$  to ground-truth topography  $y_{T,i,j}$ . The estimates for surface topography at previous timescales are often unavailable. However, sedimentary basins contain a record of erosion and deposition which is available as total sediment thickness of as a stratigraphic sequence; i.e. sediment thickness through space and time, for  $t < T$ . Therefore, the information from sedimentary deposits can be incorporated into the likelihood. Let  $z_{t,j}$  be the thickness of the sediment at time  $t$ , at location  $j$ . We assume that the deposition also depends upon  $\theta$ , via a signal plus noise model, whereby

$$z_{t,j} = f_{t,j}(\theta) + \eta_{t,j}$$

where,  $f(\theta)$  is the signal that represents sediment thickness given by the Badlands model, for a given value of  $\theta$  and  $\eta \sim \mathcal{N}(0, \sigma^2)$  is the noise. Analogous to the topography data, we integrate out  $\sigma^2$  and the likelihood function  $L_Z(\theta)$  for the sediment data given by

$$L_Z(\theta) \propto \prod_{i=1}^{n_t} \prod_{j=1}^m \left( 1 + \frac{(z_{t,j} - f_{t,j}(\theta))^2}{\nu} \right)^{-\frac{\nu+1}{2}} \quad (7)$$

where,  $n_t$  is the number of times that the sediment thickness is recorded and  $m$  is the number of points at which the sediment is measured.

### 3.3. Bayeslands framework

We take a Bayesian approach and estimate the topography via Badlands using the posterior mean of the selected parameters,  $E(y_{T,i,j}^* | \mathbf{Z}_t, \mathbf{Y}_T)$ . The posterior mean is equal to

$$E(y_{T,i,j}^* | \mathbf{Z}_t, \mathbf{Y}_T) = \int E(y_{T,i,j}^* | \mathbf{Y}_T, \theta) p(\theta | \mathbf{Z}_t, \mathbf{Y}_T) d\theta$$

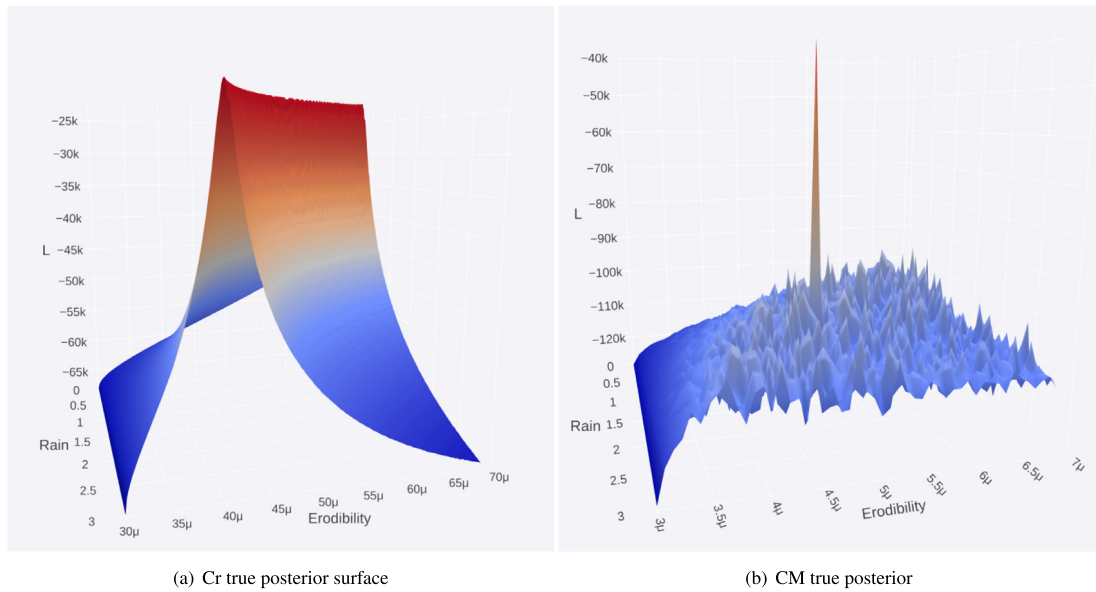


Fig. 6. True posterior (log-likelihood) surfaces for Cr and Continental-Margin topography as a function of precipitation  $\rho$  and epsilon  $\epsilon$  obtained by a grid-search.

and an estimate of it is

$$\hat{E}(y_{T,i,j}^* | \mathbf{Z}, \mathbf{Y}_T) = \frac{1}{M} \sum_{j=1}^M E(y_{T,i,j}^* | Z_i, Y_T, \theta^{[j]}) \quad (8)$$

where,  $\theta^{[j]} \sim p(\theta | \mathbf{Y})$  is obtained via MCMC in Bayeslands as shown in Algorithm 1. That is we draw each element of  $\theta$  from a proposal distribution,  $q(\theta | \theta^c)$ , conditional on the current value of  $\theta$ , denoted by  $\theta^c$ . The proposed value of  $\theta^p$  is accepted with probability

$$\alpha = \min \left\{ 1, \frac{L_{Y_T}(\theta^p) L_Z(\theta^p)}{L_{Y_T}(\theta^c) L_Z(\theta^c)} \right\} \quad (9)$$

which ensures the convergence of the chain to its stationary distribution,  $p(\theta | \mathbf{Y}, \mathbf{Z})$ . Note that as  $q(\cdot)$  is symmetric and  $p(\theta)$  is the product of independent uniform priors,  $\alpha$  reduces to the likelihood ratio. The inference regarding the selected parameters are given via the joint posterior  $p(\theta | \mathbf{Y}, \mathbf{Z})$ .

Fig. 5 gives an overview of the Bayeslands framework that employs the MCMC sampler for the Badlands model. Algorithm 1 begins by initializing values of precipitation and erodibility by drawing from the respective prior distribution for the selected parameters given in Table 2. The algorithm then proceeds by proposing new values of the parameter (Step 1) from the normal distribution as the proposal distribution, with mean  $\theta^{[i-1]}$  and the step-size ( $\phi_p$  and  $\phi_e$ ). Conditional on these proposed values, Badlands is executed for the maximum time (e.g. Cr = 50,000 years) which produces outputs that include the successive sediment erosion/deposition and topographies (Step 2). The choice of a random-walk proposal distribution was due to the unavailability of gradients for the selected parameters in the Badlands model. The likelihood given by Eq. (7) is then evaluated by considering the final topography and the successive erosion deposition values at selected locations (e.g. Fig. 4). Once the likelihood is computed, the Metropolis–Hasting criterion is used for determining whether to accept or reject the proposal (Step 3). If the proposal is accepted, the chain moves to this proposed value. If rejected, the chain stays at the current value (Step 4). The process is repeated until the convergence criterion is met, which in this case is the maximum number of samples defined by the user. Note that the software package in Python along with data is given online.<sup>1</sup>

#### Algorithm 1 Bayeslands framework

Initialize  $\theta = \theta^{[0]}$  by drawing  $\theta^{[0]}$  from the prior  $\theta^{[0]} \sim p(\theta)$

For  $i = 1 : \text{Samples}$

- 1: Propose a value  $\theta^{[p]} | \theta^{[i-1]} \sim q(\theta^{[i-1]})$ , where  $q(\cdot)$  is the proposal distribution.
- 2: Given  $\theta^{[p]}$ , execute *Badlands* and compute  $g_{T,max,i,j}(\theta^{[p]})$ , and  $f_{t,i,j}(\theta^{[p]})$
- 3: Calculate the acceptance probability  $\alpha$ , as given by Eq (9).
- 4: Generate  $u \sim U(0, 1)$  and set  $\theta^{[i]} = \theta^{[p]}$  if  $\alpha < u$ . Otherwise, set  $\theta^{[i]} = \theta^{[i-1]}$ .

#### 3.4. Experimental setting and evaluation

In order to evaluate the performance of Bayeslands on the problems (CM and Cr) presented previously, we consider the following issues and metrics:

1. Visualization of the true posterior surface evaluated across the grid;
2. Bayeslands MCMC sampling and posterior distributions;
3. Prediction of the topography and sediment erosion/deposition.

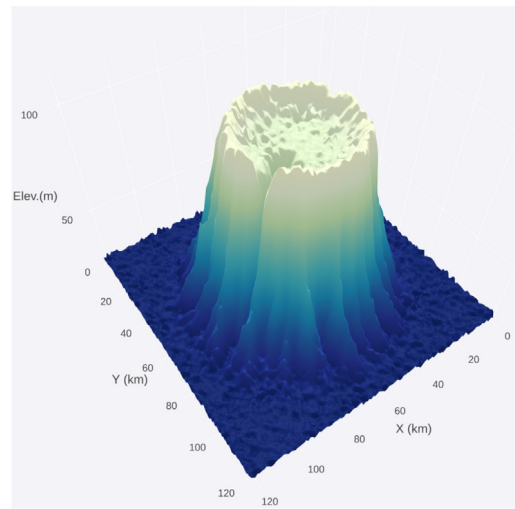
We present the metrics for evaluating Bayeslands using the Badlands outputs (predicted topography and sediment erosion/deposition). We highlight that although a series of topographies are generated by Badlands, only the final topography is used for evaluation, while selected sediment erosion/deposition is used. The root mean squared-error (RMSE) is used as the metrics for evaluation where the final topography elevation (elev) and sediment erosion/deposition (sed) respectively are given by

$$\text{RMSE}_{\text{elev}} = \sqrt{\frac{1}{n \times m} \sum_{i=1}^n \sum_{j=1}^m (g(\hat{\theta}_{T,i,j}) - g_{T,i,j}(\theta))^2}$$

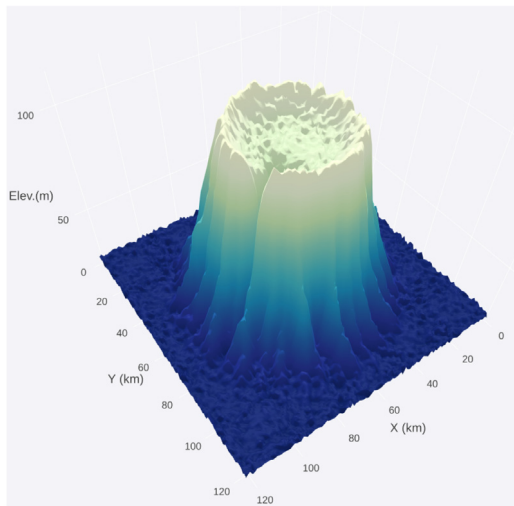
$$\text{RMSE}_{\text{sed}} = \sqrt{\frac{1}{n_t \times v} \sum_{t=1}^{n_t} \sum_{j=1}^m (f(\hat{\theta}_{t,i,j}) - f(\theta_{t,i,j}))^2}$$

where,  $\hat{\theta}$  is an estimated value of  $\theta$ , chosen according to some criteria and  $\theta$  is the true value on which the ground truth topographies and sediment thickness were based.  $f(\cdot)$  and  $g(\cdot)$  represent the outputs of the Badlands model, as defined earlier while  $m$  and  $n$  represent the size of the selected topography.  $v$  is the total number of selected points from sediment erosion/deposition as shown in Fig. 4 over the selected time frame,  $n_t$ .

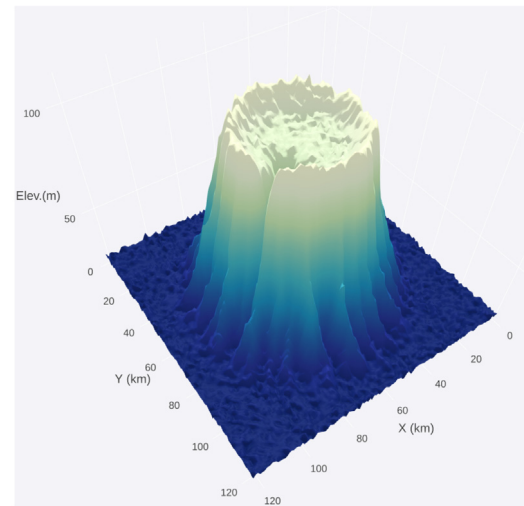
<sup>1</sup> Bayeslands: <https://github.com/intelligentEarth/Bayeslands>.



(a) Cr (true value from Table 3)



(b) Cr topography (Combination 1 from Table 3)



(c) Cr topography (Combination 5 from Table 3)

**Fig. 7.** Cr: Selected cases showing that there is not much difference between the different combinations (unique modes) of the parameters when compared to the true-values.

We use the information about uniform priors for the respective parameters from Table 2. We construct proposal distributions using a covariance matrix, which is assumed to be diagonal with entries equal to the square of step-size ( $\phi$ ). We performed several trial experiments to evaluate an optimal  $\phi$ , and use  $\phi_p = 0.03$ , for precipitation for both cases (Cr and CM). In the case for erodibility, CM uses  $\phi = 4.e - 8$ , while Cr uses  $\phi_e = 4.e - 7$ . We evaluate Bayeslands for selected number of samples with a 10% burn-in period. Note that burn-in is considered as the initial sampling period before the draws in the chain are assumed to be from the invariant distribution, which in this case is the joint posterior. The different number of samples are used to check the convergence properties of the MCMC.

The overall computation time taken for Bayeslands for each experiment is also reported. We use an Intel Core i7-8700 Processor (Hexa-core, 3.2 Giga-Hertz) for all the experiments. Note that parallel computing was not used in the implementation of Bayeslands.

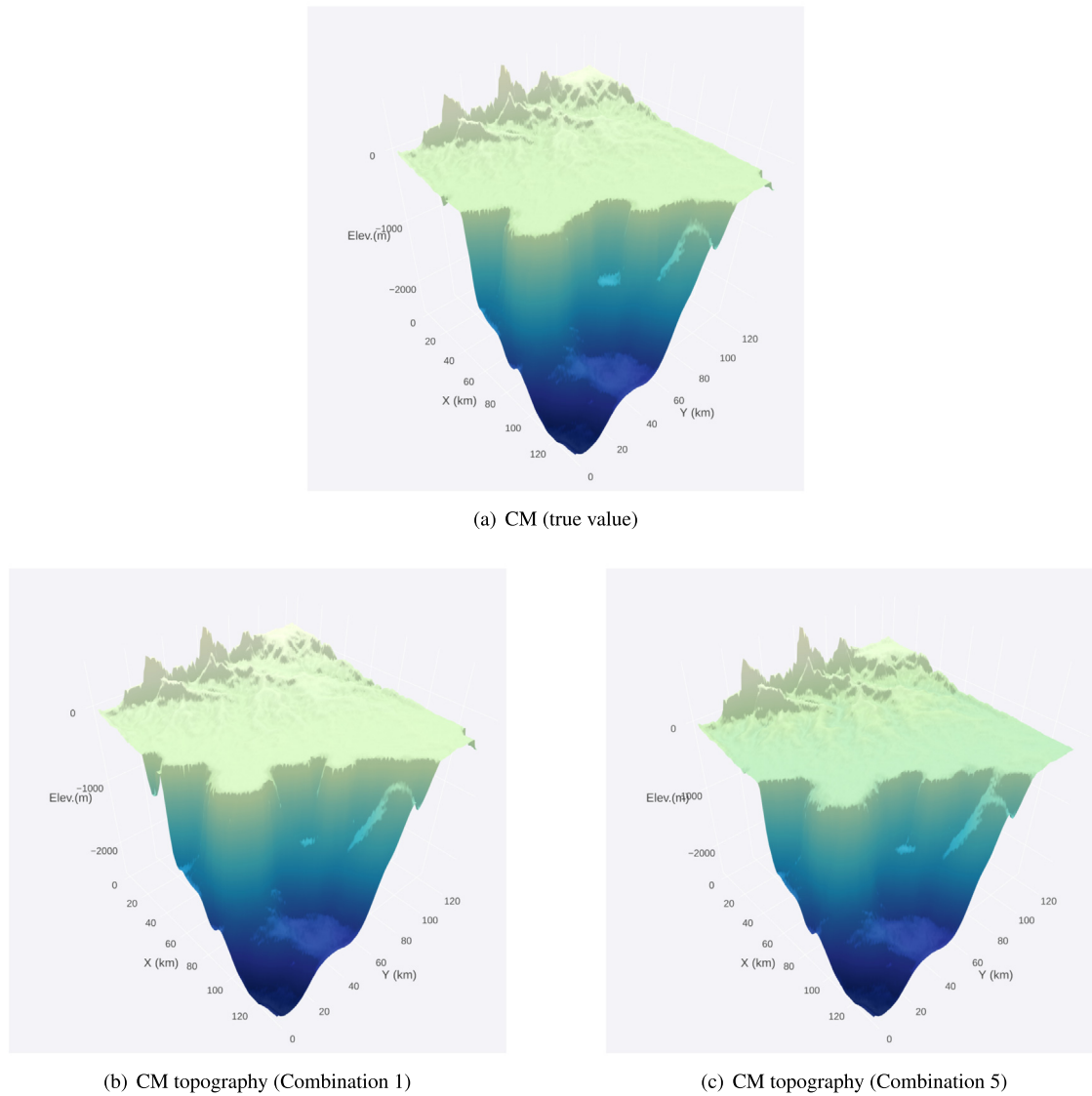
## 4. Results

### 4.1. Visualization of the true posterior surface

To illustrate the difficulty of making inference in geophysical inversion problems, we produce the posterior surface (up to a proportionality

constant), evaluated across a grid of values for  $\rho$  and  $\epsilon$ . We note that it is only computationally and visually possible to produce these plots for very low dimensional problems, and yet these surfaces demonstrate the challenges of MCMC sampling. Fig. 6 panel (a) presents the posterior surface for the Cr topography and shows that this surface is more sensitive to erodibility than precipitation. It also shows that there is no unique mode for precipitation and erodibility. Several combinations of precipitation and erodibility give the same posterior value, indicated by the ridge. Fig. 6 panel (b) presents the posterior surface for CM which is in sharp contrast to the posterior surface for the Cr. Although it shows the existence of a unique global maximum, there are a number of local maxima, which makes the exploration of the surface very challenging.

Table 3 presents the top 10 combinations of the parameters with minimal RMSE values. Note that the first combination (true-value) shows the actual values that were used to generate the ground-truth topography, hence the corresponding RMSE values are 0. Figs. 7 and 8 give a visualization of the ground truth topography. Panel (a) corresponds to the topography giving the lowest RMSE, while panel (b) corresponds to the topography with the 5th lowest RMSE. It can be seen that there is not much difference between the sub-optimal and optimal values, particularly for the CM problem in Fig. 8.



**Fig. 8.** CM: Selected cases showing that there is not much difference between the different combinations (sub-optimal modes) of the parameters when compared to the true-values.

#### 4.2. Inference using Bayeslands

Table 4 gives details on the number of iterations (samples) in the MCMC sampling scheme, the corresponding time taken, and the prediction performance as measured by  $RMSE_{elev}$  and  $RMSE_{sed}$  and their total,  $RMSE_{total}$ . We find that  $RMSE_{total}$  decreased (improved) with the increase in sample size from 10,000 to 50,000 for the Cr topography. This improvement is in both  $RMSE_{elev}$  and  $RMSE_{sed}$ , suggesting that the MCMC scheme for this landscape had not converged within the first 10,000 samples. A similar trend is seen in the CM topography.

Fig. 9, panel(a) shows the trace plot of accepted proposals in MCMC sampling for precipitation  $\rho$ , while panel (b) is a histogram estimate of the posterior distribution for the Cr topography. Note that the vertical line in red in the respective figures shows the true value and the major goal of the experiments was to check if Bayeslands framework can recover the true value. In the case of the Cr topography, we find that the MCMC sampling estimate of the posterior distribution is reasonable. It has one of the modes near the true values of precipitation and erodibility the MCMC chain appears to mix well, although with a high degree of auto-correlation. We note that the MCMC sampling recovered few different modes as reported by the trace plot of the posterior distribution. In contrast, the CM topography (Fig. 10) MCMC

sampling procedure shows that the chains have difficulty in escaping local modes, hence they are stuck (shown in the trace-plot) for longer time periods when compared to the Cr topography trace-plots. As evident by the trace plots, there little mixing. The histogram estimates of precipitation and erodibility are not peaked around the true values for these parameters. Instead they are multimodal with modal values corresponding to local maxima, given by the coloured dashed vertical lines. The difference in these results are not surprising, when one considers that the CM topography's likelihood surface is very complex when compared with that of the Cr, resulting in the need for longer sampling time and better or adaptive MCMC proposal schemes from better traversal.

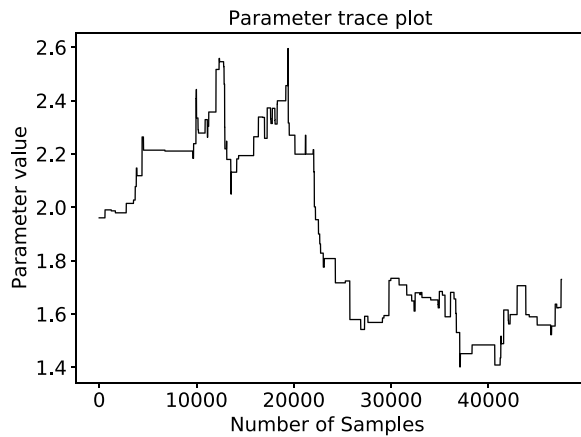
Despite the difficulty in recovering the true parameter values, the prediction for the landscape topographies are astonishingly accurate. This is evident from the predicted topography; Figs. 11 and 12 which are visually similar to the ground truth, Figs. 1 and 3. Moreover, the cross-sections shown in Figs. 13 and 14 show good accuracy with 95% credible interval which highlight the accuracy of the prediction. Fig. 15 shows the predicted evolution of the sediment thickness for both topographies. Interestingly, the CM predictions appear to be more accurate than those of the Cr landscape. However, this may be due to the different scales. We note that the sediment thickness of the Cr



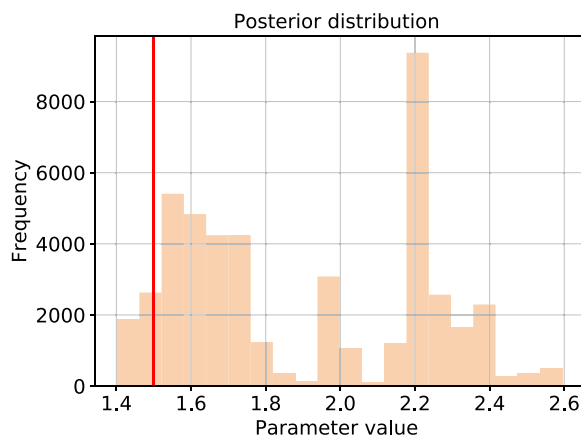
**Table 3**

Columns 3–4 are combinations of parameters of precipitation  $\rho$  and erodibility  $\epsilon$  that give near optimal performance; in terms of  $RMSE_{total}$  for Cr and CM.

Combination	Topography	Precipitation	Erodibility	$RMSE_{elev}$	$RMSE_{sed}$	$RMSE_{total}$
True-value	Cr	1.50	5.00e-5	0.00	0.00	0.00
1		1.14	5.72e-5	1.05	0.26	1.31
2		2.94	3.56e-5	1.05	0.26	1.32
3		2.40	3.96e-5	1.04	0.27	1.32
4		2.58	3.80e-5	1.05	0.26	1.32
5		1.98	4.36e-5	1.04	0.27	1.32
6		0.78	6.92e-5	1.06	0.26	1.32
7		2.28	4.04e-5	1.05	0.27	1.32
8		1.08	5.88e-5	1.06	0.26	1.32
9		1.02	6.04e-5	1.05	0.27	1.32
10		0.90	6.44e-5	1.07	0.26	1.32
True-value	CM	1.50	5.00e-6	0.00	0.00	0.00
1		2.64	3.96e-6	69.85	27.63	97.48
2		2.70	4.20e-6	69.71	28.55	98.26
3		1.38	4.68e-6	69.84	33.44	103.20
4		2.10	4.28e-6	68.59	42.70	111.35
5		2.58	3.40e-6	73.42	42.97	116.43
6		2.34	4.04e-6	102.2	15.30	117.51
7		2.94	3.88e-6	79.58	40.55	120.10
8		2.76	3.64e-6	104.61	15.64	120.35
9		1.20	5.56e-6	69.45	51.14	120.51
10		0.78	6.76e-6	105.72	27.98	123.77



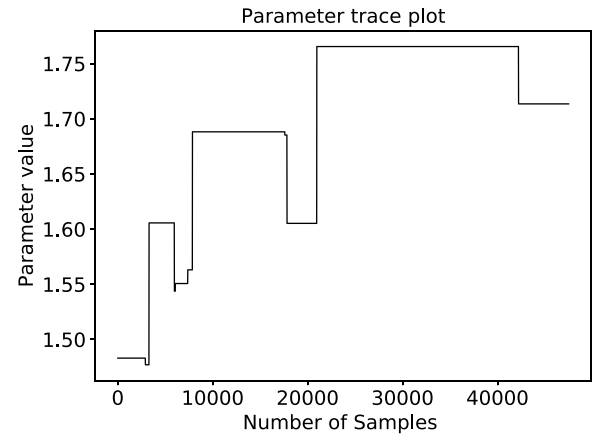
(a) Trace-plot of accepted samples



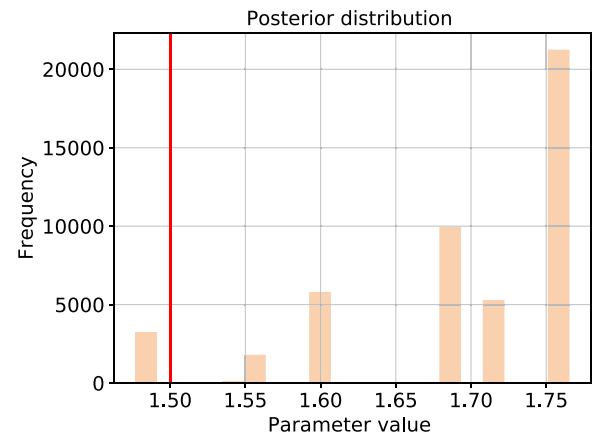
(b) Posterior distribution

**Fig. 9.** Cr: Panel (a) is a trace plot of the Cr precipitation ( $\rho$ ) posterior for 50,000 samples, while panel (b) is a histogram estimate of the posterior distribution. The vertical red line shows true value.

topography is two orders of magnitude less than that of CM which makes differences appear larger.



(a) Trace-plot of accepted samples



(b) Posterior distribution

**Fig. 10.** Panel (a) is a trace plot of the CM precipitation ( $\rho$ ) posterior for 50,000 samples, while panel (b) is a histogram estimate of the posterior distribution. The vertical red line shows true value.

**Table 4**

Results for Bayeslands MCMC sampling.

Topography	Samples	Accepted %	Time (hours)	$RMSE_{elev}$	$RMSE_{sed}$	$RMSE_{total}$
Cr	10,000	2.35	2.26	3.69	4.56	8.25
	25,000	0.28	5.43	3.10	4.34	7.44
	50,000	0.22	8.68	1.26	0.95	2.21
CM	10,000	0.47	4.20	133.90	83.28	217.20
	25,000	0.05	10.66	131.5	62.64	194.10
	50,000	0.04	19.29	94.26	29.69	123.90

## 5. Discussion

In this paper, we presented a logically consistent Bayesian framework to estimate and quantify uncertainty for selected parameters that govern LEMs. This was achieved by embedding a LEM (Badlands) within a probabilistic model. Although we used Badlands, we stress that the approach is general; it can accommodate any LEM and other geophysical forward models where the outputs are a deterministic function of the inputs, for instance Underworld models to explore the geothermal potential of the crust (Quenette et al., 2015).

We made inference for only 2 free parameters (precipitation and erodibility) and assumed that they were constant over space and time. Even with this simplification, Fig. 6 shows that the posterior (likelihood) surfaces are non-standard and difficult to estimate. Multi-modality (Charvin et al., 2009) in the posterior distribution is a major concern. Multi-modality implies that multiple combinations of the

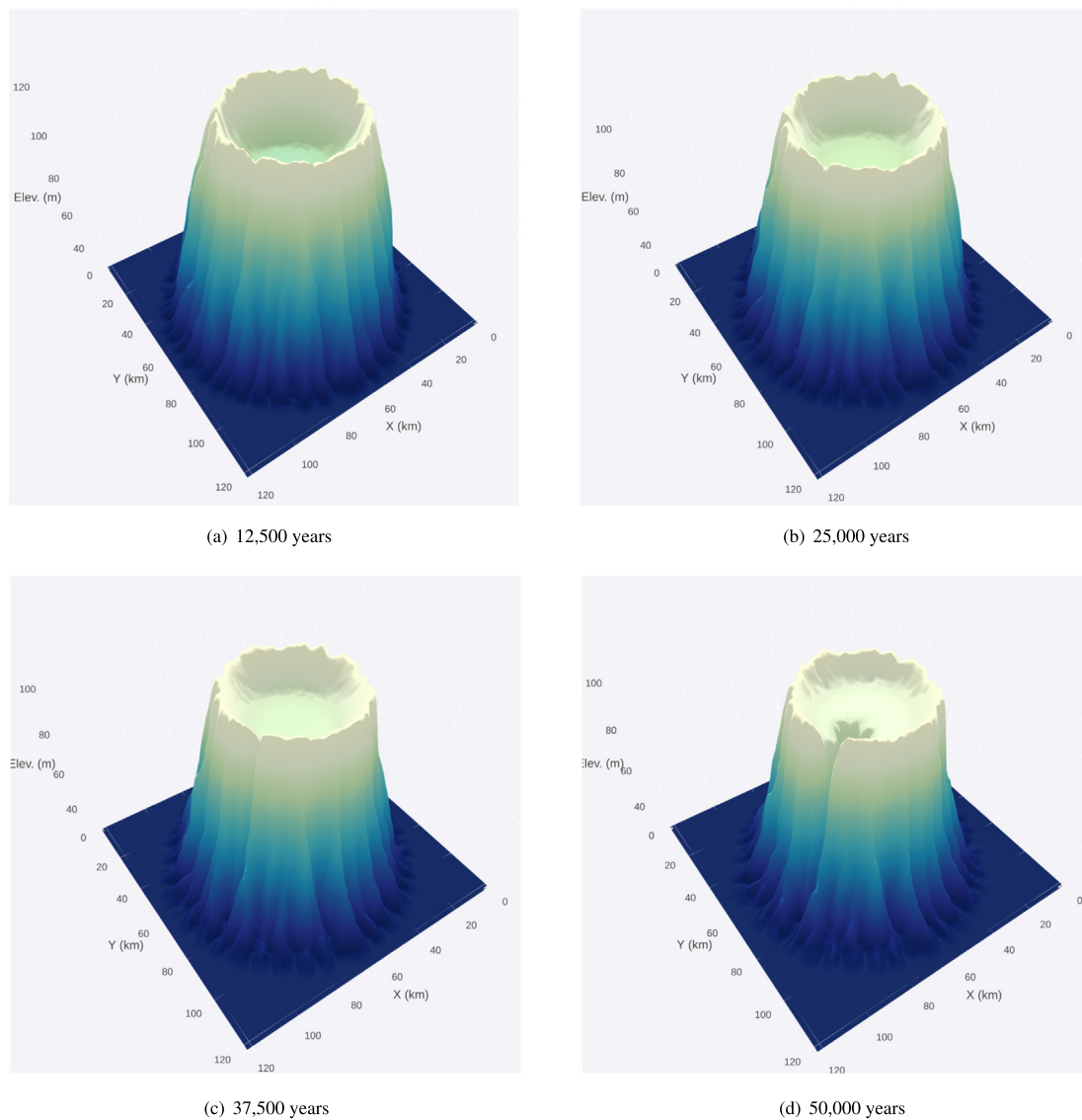


Fig. 11. Cr: Predicted topographies at selected intervals for 50,000 years.

given parameters (precipitation and erodibility) can plausibly predict or simulate the same topography, which closely resembles the synthetic or ground-truth topography (Cross and Lessenger, 1999) (e.g. Fig. 8 and Table 3). In addition to the issue of multi-modality, the posterior may be discontinuous, by which we mean the derivative does not exist which further makes MCMC sampling difficult.

Which aspects of the problem give rise to these unusual posterior surfaces? Are these surfaces a product of the data or due to complexity of the Badlands model? It is important to reflect upon the characteristics or assumptions made in geophysical models, characteristics of the topography data for a given time and location. It is worthwhile to investigate if the posterior distribution gives meaningful information about the appropriateness of the Badlands model to different topographies.

Clearly, limiting precipitation and erodibility to be constant for the entire spatial and temporal extent of a given model may not be appropriate. While this may not make much difference for small geographical regions and short time intervals; for larger areas, different regions of the topography would have different distributions of precipitation at different points of time. Moreover, the parameter values are also same throughout the entire topography evolution. This does not fully simulate geological time scales and fully capture the effects of changing climate through time. In order to implement this, the precipitation

would become a vector of parameters that define different regions expressed by grids in the map. This would increase the number of parameters and further add complexity to the model which would make the inference more difficult. Furthermore, the synthetic problems should consider larger areas that contain a variety of landscape features. This would increase the computational complexity of the model and require multi-core implementations of MCMC via high performance computing. Parallel tempering (Earl and Deem, 2005), which is an advanced MCMC method suited for multi-core implementation that better captures multi-modality, would be a natural choice to improve the performance of the sampler (Sambridge, 1999, 2013; Chandra et al., 2000).

The Bayeslands framework will form the foundation for more complex models of landscape and basin evolution. In the future, we envision to include many additional parameters in Bayeslands, including the uncertain initial model topography, global sea level fluctuations, tectonic and dynamic topography evolution, spatially varying lithospheric flexural rigidity, spatio-temporal variations in mountain uplift rates and in precipitation. Ultimately, we will be able to consider the uncertain effects of climate change and changing vegetation cover on spatio-temporal denudation rates and improve assessments on how re-vegetation may slow down the continuing erosion of degraded landscapes (Bastola et al., 2018).

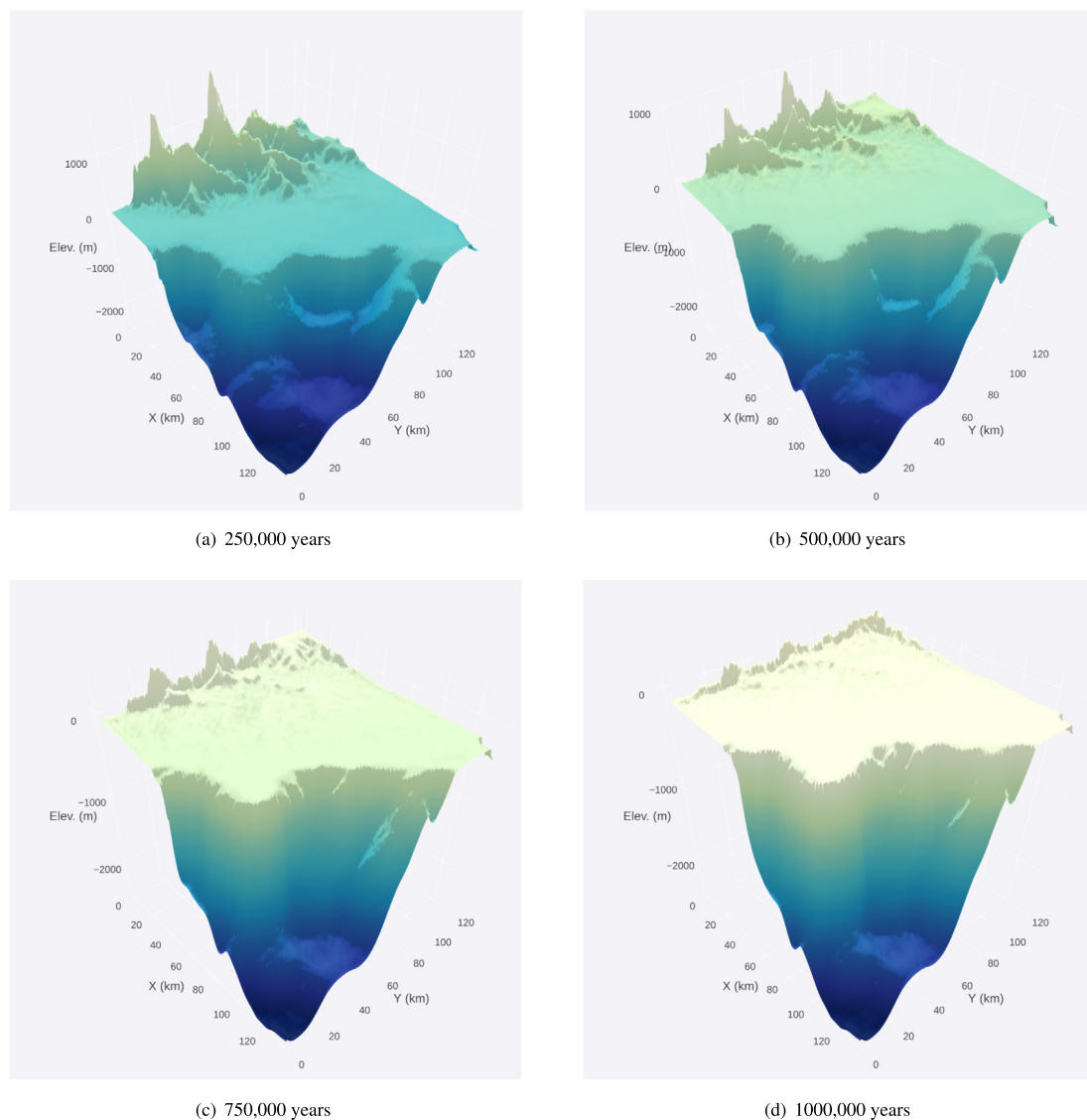


Fig. 12. CM topography evolution over time at selected intervals for 1000,000 years.

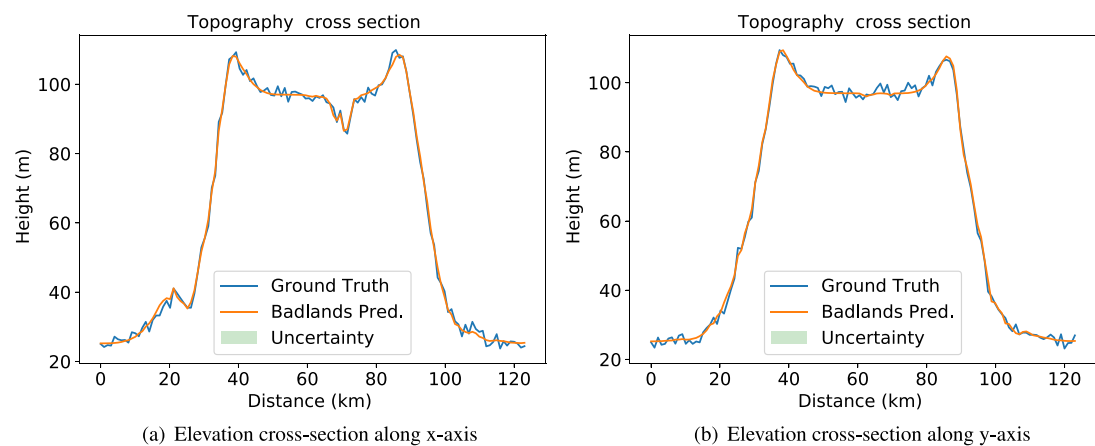
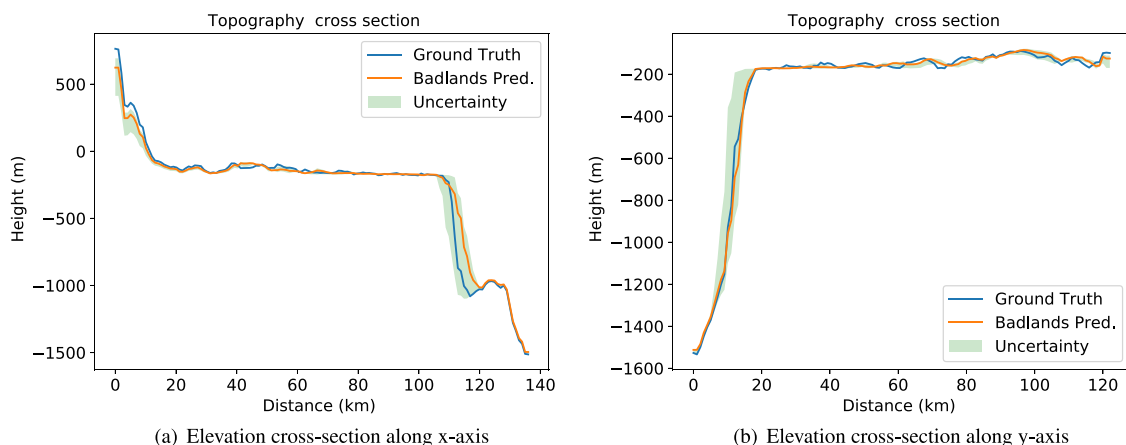
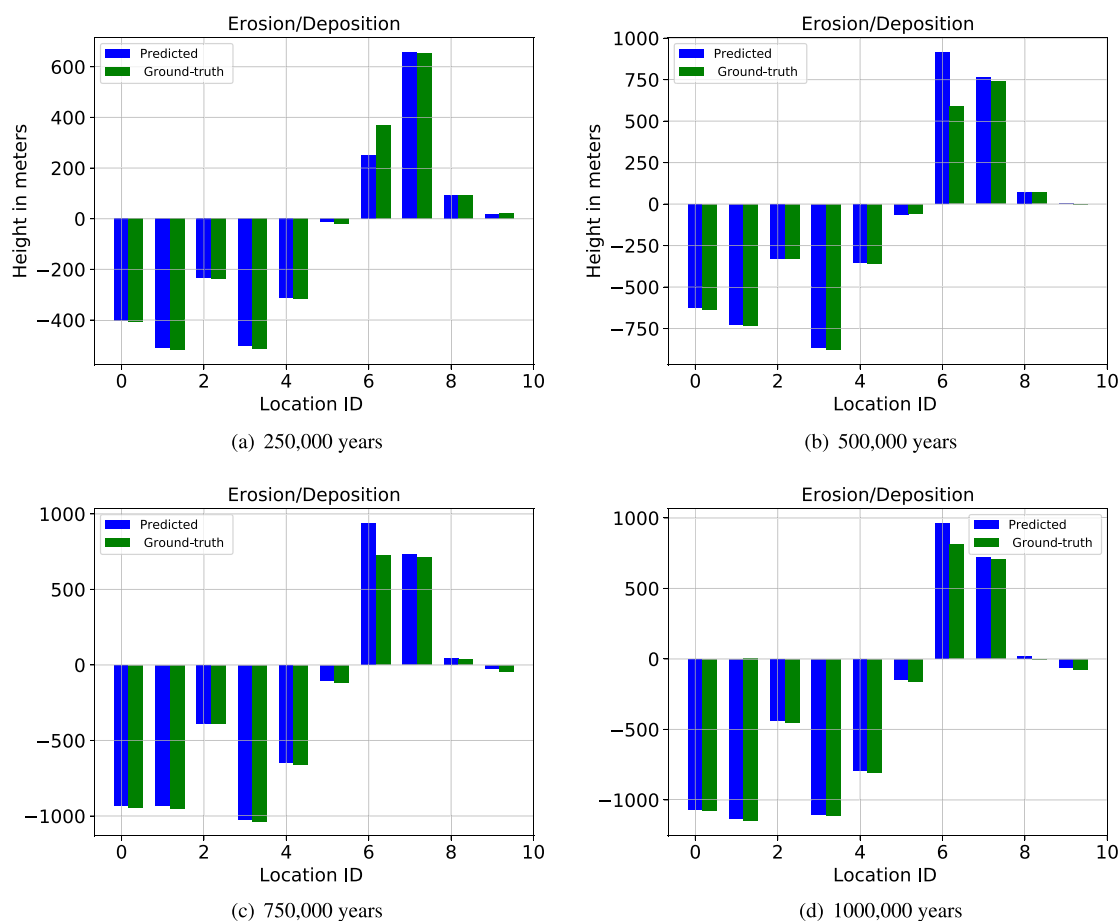


Fig. 13. Cr: Elevation cross-section taken at mid-point along  $x$ -axis and  $y$ -axis. The green shaded area corresponds to 95% credible intervals.



**Fig. 14.** CM model: Panel (a), elevation cross-section from West to East at a latitude of  $42^\circ$ . Panel (b), elevation cross-section from North to South at a longitude of  $174^\circ$ . The green shaded area shows 95% credible interval. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



**Fig. 15.** CM: Sediment erosion/deposition for selected time-frames and locations for 1,000,000 years. The selected locations (ID) are shown in Fig. 4.

## 6. Conclusions and future work

Bayeslands provides a framework for incorporating uncertainty quantification for simulated elevation and sediments in Badlands through MCMC sampling in landscape evolution models. Although promising, there are major challenges in scaling to higher dimensions for real-world applications. As the dimension increases, there can be further challenges with issues of multi-modality and exploration in such posterior distributions. The exploration of these challenging posterior distributions will require the development of new proposal

distributions for use in MCMC schemes, which reflect local geometry and/or gradient information from the Badlands model.

The Bayeslands framework can be computationally challenging since Badlands takes minutes to hours for large scale or continental problems. Hence, new computationally efficient methods, such as replacing the Badlands model with surrogate models for a proportion of the MCMC iterates needs to be developed. Speeding up computation of Bayeslands via parallel tempering in multi-core architecture is another avenue to be explored in the future.



## Supplementary material

Open source software in Python along with data is given online:  
<https://github.com/intelligentEarth/Bayeslands>.

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## CRediT authorship contribution statement

**Sally Cripps:** Methodology, Writing, Supervision.

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