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Sampling efficiency in Monte Carlo based uncertainty propagation strategies: Application in seawater intrusion simulations

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ABSTRACT

The implementation of Monte Carlo simulations (MCSs) for the propagation of uncertainty in real-world seawater intrusion (SWI) numerical models often becomes computationally prohibitive due to the large number of deterministic solves needed to achieve an acceptable level of accuracy. Previous studies have mostly relied on parallelization and grid computing to decrease the computational time of MCSs. However, another approach which has received less attention in the literature is to decrease the number of deterministic simulations by using more efficient sampling strategies. Sampling efficiency is a measure of the optimality of a sampling strategy. A more efficient sampling strategy requires fewer simulations and less computational time to reach a certain level of accuracy. The efficiency of a sampling strategy is highly related to its space-filling characteristics.

This paper illustrates that the use of optimized Latin hypercube sampling (OLHS) strategies instead of the widely employed simple random sampling (SRS) and Latin hypercube sampling (LHS) strategies, can significantly improve sampling efficiency and hence decrease the simulation time of MCSs. Nine OLHS strategies are evaluated including: improved Latin hypercube sampling (IHS); optimum Latin hypercube (OLH) sampling; genetic optimum Latin hypercube (GOLH) sampling; three sampling strategies based on the enhanced stochastic evolutionary (ESE) algorithm namely φ_p-ESE which employs the φ_p space-filling criterion, CLD-ESE which utilizes the centered L_2-discrepancy (CLD) space-filling criterion, and SLD-ESE which uses the star L_2-discrepancy (SLD) space-filling criterion; and three sampling strategies based on the simulated annealing (SA) algorithm namely φ_p-SA which employs the φ_p criterion, CLD-SA which uses the CLD criterion, and SLD-SA which utilizes the SLD criterion. The study applies SRS, LHS and the nine OLHS strategies to MCSs of two synthetic test cases of SWI. The two test cases are the Henry problem and a two-dimensional radial representation of SWI in a circular island. The comparison demonstrates that the CLD-ESE strategy is the most efficient among the evaluated strategies. This paper also demonstrates how the space-filling characteristics of different OLHS designs change with variations in the input arguments of their optimization algorithms.

1. Introduction

Numerical models have found widespread applications in system understanding and future predictions of seawater intrusion (SWI) into coastal aquifers [1,2]. However in some instances SWI simulations are carried out without any historical data available for model calibration, or more commonly without any information on the boundary conditions that might prevail in the simulation of future time intervals (refer to [1] for an example related to the recharge boundary conditions). In both cases, model predictions are entirely reliant on the assumptions made by the modeler regarding model structure and inputs [3]. The unreliability or uncertainty in model structure and inputs propagates through the model and results in uncertainty of the output quantities of interest (QoI). Quantifying this uncertainty is known as uncertainty propagation (UP) analysis [4]. The same problem also arises in the presence of historical data for model calibration. In this case, model inputs are affected by uncertainty due to a number of factors such as the concept of equifinality in model calibration [5] and the existence of stochastic, measurement, representativity and parameter uncertainties. Equifinality arises from the fact that in the process of model calibration, many complex SWI models lack "optimum" parameter sets and instead have many distinct sets of input parameter values within a model structure that are consistent with

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Nomenclature

n	sample size
x	uncertain input variable(s)
$S(x)$	output quantity of interest
$f_X(x)$	probability density function describing the uncertainty of x
$E()$	expected value
$x_1, x_2, \ldots, x_n$	n sample of x
$\bar{S}_n(x)$	Monte Carlo estimate of $E(S(x))$
u	nonempty subset of the coordinate indices
C^u	u dimensional unit cube
$\Omega = \{1, \ldots, \theta\}$	set of coordinate indices
Y	set of n points $\{y_1, \ldots, y_n\}$
J_y	s dimensional interval uniquely defined by Y
J_{y_u}	projection of J_y on C^u
$Vol(J_{y_u})$	volume of a subset J_{y_u}
$N(Y_u, J_u)$	number of points of Y_u falling in J_{y_u}
CLD	centered L_2-discrepancy
$d_i^1, d_i^2, \ldots, d_i^u$	n samples within u
d_i	set of n samples within u
p	characterizes the L_p norm
φ_p	a family of distance based criteria
dup	valid candidate points in the improved Latin hypercube sampling strategy
N_R	number of rows in a matrix
N_C	number of columns in a matrix
eps	the optimal stopping criterion in the optimum Latin hypercube sampling strategy
$maxSweeps$	the maximum number of times the columnwise–pairwise algorithm is applied to all the columns in the optimum Latin hypercube sampling strategy
pop	the number of designs in the initial population of the genetic algorithm
gen	the number of generations over which the genetic algorithm is applied
$pMut$	the probability that a mutation occurs in a column of the offspring in the genetic algorithm
J_{ESE}	new designs generated in the inner loop of the enhanced stochastic evolutionary optimization algorithm
T_h	acceptance threshold in the enhanced stochastic evolutionary optimization algorithm
$inner\_it_{ESE}$	number of iterations of the inner loop in the enhanced stochastic evolutionary optimization algorithm
$outer\_it_{ESE}$	number of iterations of the outer loop in the enhanced stochastic evolutionary optimization algorithm
L_{new}	new sample design in each step of the simulated annealing algorithm
L_{old}	sample design in the previous step of the simulated annealing algorithm
SC	an space-filling criterion
T	temperature in the simulated annealing algorithm
T_0	the initial temperature in the simulated annealing algorithm
α	cooling factor in the simulated annealing algorithm
it_{SA}	number of iterations in the simulated annealing algorithm
H1, H2, …, H5	reference nodes of the Henry problem
$P_{H1}, P_{H2}, \ldots, P_{H5}$	pressures in the reference nodes of the Henry problem
$C_{H1}, C_{H2}, \ldots, C_{H5}$	concentrations in the reference nodes of the Henry problem
I1, I2, …, I5	reference nodes of the two-dimensional radial island problem
$C_{I1}, C_{I2}, \ldots, C_{I5}$	concentrations in the reference nodes of the two-dimensional radial island problem
k	permeability of the aquifer in the Henry problem
Q	total constant fresh-water inflow on the inland boundary in the Henry problem
μ	mean of the n-run analysis
μ_i	mean of the ith repetition of Monte Carlo simulations
σ	standard deviation of the n-run analysis
σ_i	standard deviation of the ith repetition of Monte Carlo simulations
μ_{ref}	means of the reference solutions
σ_{ref}	standard deviations of the reference solutions
κ	excess kurtosis of the n-run analysis
n_r	number of repetitions in the analysis
PI	percent improvement

the data available for calibration [3]. Stochastic uncertainty occurs due to randomness as an objective fact of the phenomenon, most notably in defining SWI boundary conditions [6]. Measurement uncertainty is caused by the intrinsic noise of measurement apparatus [7]. Representativity uncertainty arises from the difference between the spatial and temporal sampling footprint of measurements and the defined spatial and temporal representation of reality within the framework of the SWI numerical model [8,9]. Parameter uncertainty is the epistemic uncertainty resulting from the lack of knowledge about input parameters which cannot be directly observed and are often empirically determined [10]. Parameter uncertainty is particularly important in the estimation of input parameters such as longitudinal and transverse dispersivities and large-scale hydraulic conductivities.

UP analysis allows the modeler to estimate the effects of quantified input uncertainties (described by fuzzy or probability distributions) on the model output QoI, and there by replace deterministic solutions with a range of solutions accommodated with their respective probabilities [3,4,6]. The probabilistic representation of output QoI can then be used to estimate prediction intervals, probabilities for the failure of specific management plans or the exceedance of critical thresholds in SWI risk assessments. It should be noted that UP analysis does not replace history matching or model calibration. However model calibration (especially in the form of stochastic inverse modeling) can provide valuable information for probabilistic characterisation of model inputs which can then be fed into the UP analysis procedure [3].

Monte Carlo simulations (MCSs) are the most common approaches for propagating uncertainty in mathematical and computational models, most notably because they are: (1) transparent and simple to implement, (2) non-intrusive and able to employ existing codes, (3) capable of solving a large class of uncertainty propagation problems, (4) easy to parallelize because they fall into the category of embarrassingly parallel algorithms, (5) robust for discontinuities, (6) suitable for many probability distribution types (e.g. normal, gamma, beta, Poisson, Weibul, etc.), (7) appropriate for large number of uncertainties, (8) shown to converge, although slowly, without stringent regularity conditions and at the same rate independent of the dimension of random variables, (9) they also invoke fewer assumptions and require less user-inputs than other propagation tools such as polynomial chaos expansions [11], and (10) their accuracy can be fixed in advance according to the level of risk associated with a decision [4,12–16]. As a result, Monte Carlo based UP is progressively finding applications in many