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Assessment of model behavior and acceptable forcing data uncertainty in the context of land surface soil moisture estimation

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ABSTRACT

The sources of uncertainty in land surface models are numerous and varied, from inaccuracies in forcing data to uncertainties in model structure and parameterizations. Majority of these uncertainties are strongly tied to the overall makeup of the model, but the input forcing data set is independent with its accuracy usually defined by the monitoring or the observation system. The impact of input forcing data on model estimation accuracy has been collectively acknowledged to be significant, yet its quantification and the level of uncertainty that is acceptable in the context of the land surface model to obtain a competitive estimation remain mostly unknown. A better understanding is needed about how models respond to input forcing data and what changes in these forcing variables can be accommodated without deteriorating optimal estimation of the model. As a result, this study determines the level of forcing data uncertainty that is acceptable in the Joint UK Land Environment Simulator (JULES) to competitively estimate soil moisture in the Yanco area in south eastern Australia. The study employs hydro genomic mapping to examine the temporal evolution of model decision variables from an archive of values obtained from soil moisture data assimilation. The data assimilation (DA) was undertaken using the advanced Evolutionary Data Assimilation. Our findings show that the input forcing data have significant impact on model output, 35% in root mean square error (RMSE) for 5cm depth of soil moisture and 15% in RMSE for 15cm depth of soil moisture. This specific quantification is crucial to illustrate the significance of input forcing data spread. The acceptable uncertainty determined based on dominant pathway has been validated and shown to be reliable for all forcing variables, so as to provide optimal soil moisture. These findings are crucial for DA in order to account for uncertainties that are meaningful from the model standpoint. Moreover, our results point to a proper treatment of input forcing data in general land surface and hydrological model estimation.

1. Introduction

The estimation of soil moisture through land surface models mainly incorporates a combination of model physics, initial states, parameters, and forcing data. The majority of these components are inherent to the overall makeup of the model, defining how the model handles input forcing data. The model components are fundamental to the evaluation of land surface states in response to meteorological forcing. However, the overall uncertainty in model output is associated with uncertainties of the various model inputs and components, which interact and are strongly linked such that their respective uncertainties are difficult to separate. The input forcing data set is independent from the overall model makeup and has separate uncertainty levels for each variable as defined by their respective observation systems. While the impact of the forcing data on the accuracy of model estimation is universally recognized to be significant (Beven and Binley, 1992; De Lannoy et al., 2006; Durand and Margulis, 2008; He et al., 2011; Mantovan and Todini, 2006; Moradkhani and Hsu, 2005; Raleigh, 2013; Salamon and Feyen, 2009; Seibert, 1997; Steinschneider et al., 2012; Uhlenbrook et al., 1999; Vrugt et al., 2002; Zehe et al., 2005), its quantification remains largely unknown in most modeling procedures. That is, the majority of modeling procedures have limited knowledge about how much of a model's estimation accuracy is attributable to its forcing data uncertainty. Consequently, it is difficult to determine the level of uncertainty in forcing data that is acceptable, in the context of the model, to provide an optimal estimate of soil moisture.

The acceptable level of forcing data uncertainty, while specific to a particular model, will provide for a given model a threshold

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of uncertainty bound beyond which deterioration of the model estimation accuracy will occur. An estimate of the acceptable level of uncertainty in forcing data will separate the inaccuracies in model prediction into two categories: those that are inherent in the model, and those from the forcing data. Note that by acceptable level of uncertainty in forcing data, we are referring to the amount of uncertainty from the forcing data that is admissible/appropriate in the context of the model without deteriorating the model estimation accuracy.

An increased knowledge of forcing data uncertainty will have a crucial impact on water and climate predictions. In particular, an estimate of forcing data uncertainty will provide an important contribution, which is usually missing, to error specification in data assimilation (DA) procedures. Ensemble distributions (i.e., spread) in DA are usually generated through perturbation of input forcing data (Alemohammad et al., 2015; Clark et al., 2006; Wojcik et al., 2014), mostly with limited knowledge of the impact of forcing error on model ensemble spread. Forcing data uncertainty is also critical in climate change studies and forecasting systems (Nagler et al., 2008; Raleigh, 2013; Schär et al., 2004; Steinschneider et al., 2012; Troch et al., 2009), to provide an estimate of the changes (and uncertainties) in model output in response to variability in forcing data. An understanding of the impact of forcing data uncertainty on model prediction will therefore provide the capability to estimate the level of variability that is required in weather systems and forecasts to initiate triggers in water resource systems.

Few studies including Liu and Gupta (2007); Vrugt and Robinson (2007); Wagener et al. (2003); and He et al. (2012) have examined uncertainty in model components, and even fewer (Alemohammad et al., 2015; Maggioni et al., 2011) have actually examined uncertainty in forcing data in relation to the model output. Consequently, this study quantifies the uncertainty threshold in forcing data that can be incorporated into the Joint UK Environment Simulator (JULES) model in the context of soil moisture estimation without a significant deterioration in model estimation accuracy, for the Yanco area in southeast Australia. It also provides a methodology to estimate an acceptable threshold of forcing data uncertainty in the JULES model through three modeling approaches. These modeling approaches are model calibration, data assimilation, and multi-dimensional clustering which is used to assess values in model decision space (i.e., the interval defined by both model parameters and input forcing variables). The calibration and data assimilation procedures employ computational techniques from the state-of-the-art multi-objective evolutionary strategy. Specifically, the calibration is based on the Non-dominated Sorting Genetic Algorithm - II (NSGA-II) developed by Deb et al. (2002), whereas the DA method uses the evolutionary data assimilation (EDA) scheme demonstrated in Dumedah and Walker (2014b); Dumedah et al. (2015); and Dumedah (2015).

The three modeling approaches: calibration, data assimilation, and multi-dimensional clustering used in this study provide unique roles toward the overall goal of quantifying forcing data uncertainty in land surface modeling. Calibration, though subject to a specific time period of observation data, has an important role in determining optimized values in model decision space to generate model outputs which best match observed data. It is noted that the calibration procedure is supplementary and represents an intermediate step to the data assimilation procedure. Data assimilation has been widely credited for its ability to update model predictions through time, and to account for uncertainties in model and observation data. However, the temporal changes in model decision space resulting from data assimilation holds the potential for assessing model behavior under changing hydro-meteorological conditions. The temporal characteristic of DA is crucial in this study in order to assess the temporal evolution of the impact of forcing data uncertainty on the JULES model at different uncertainty levels across time. Consequently, this study uses data assimilation to provide an archive of updated ensemble members in model decision space through several assimilation time periods. The role of the multi-dimensional clustering is to determine commonalities in model decision space for the calibration output and the updated ensemble members.

1.1. Study area, data sets, and the land surface model

The case study demonstration is for soil moisture estimation in the Yanco area in southeast Australia. The study location is at one station (i.e., Y10) out of thirteen OzNet soil moisture monitoring stations in the Yanco area (Smith et al., 2012). The Y10 location has flat topography, along with grassland, scattered trees and loamy textured soil. The study location has extensive soil moisture and meteorological instrumentation, and has provided almost continuous time series of data for validation.

The land cover data set was obtained through the Australian National Dynamic Land Cover Dataset (DLCD) (Lymburner et al., 2011), which was generated from the 16-day Enhanced Vegetation Index composite collected at 250 m spatial resolution from the Moderate Resolution Imaging Spectroradiometer. The soil properties information including texture, bulk density, saturated hydraulic conductivity, and soil layer thicknesses for horizons A and B were obtained from the Digital Atlas of Australian Soils, through the Australian Soil Resource Information System (McKenzie et al., 2000). The meteorological forcing data including incoming short and long wave radiations, air temperature, precipitation, wind speed, pressure, and specific humidity were obtained from the meteorological record at the study location.

The soil moisture estimation model used is JULES, a tiled model of sub-grid heterogeneity for simulating water and energy fluxes between a vertical profile of variable soil layers, land surface, vegetation, and the atmosphere (Best et al., 2011). JULES allows specification of numerous soil layers and variable thickness of soil layers, together with nine land surface types including broadleaf, needleleaf, grass (temperate and tropical), shrub, urban, inland water, bare soil, and ice-covered surfaces. The JULES model requires initialization for variables including the temperatures and the moisture contents of the soil layers; temperature, density, and albedo of the snowpack if present; the temperature and intercepted rain and snow on the vegetation canopy; the temperature and depth of ponded water on the soil surface, and an empirical vegetation growth index.

The JULES model parameters and forcing variables together with their descriptions and intervals are presented in Table 1. The model parameters and forcing variables were allowed to be varied within ± 10% of their original values through a relative measure. It is noteworthy that the ± 10% interval is based on the soil texture variability as obtained from McKenzie et al. (2000), and does not represent the actual variability for model parameters and forcing variables. The original values of model parameters and forcing variables were based on the soil, land cover, and meteorological forcing data such that they are physically meaningful for the study location in the context of the JULES model. The soil moisture data set used to drive the calibration and assimilation was the surface 5cm depth of in-situ soil moisture at the Y10 location.

2. Methods

The framework used to assess the acceptable forcing data uncertainty in this study comprises of a number of modeling procedures. Specifically, four procedures were used including: (i) a calibration procedure to estimate model parameters, (ii) a data assimilation procedure using both model parameters and forcing variables, (iii) a data assimilation procedure using perturbed

Table 1
Description of model parameters and forcing data variables for the JULES model.

Parameter	Description	Interval
	Model Parameters	
b	Exponent in soil hydraulic characteristics curve	± 10%
sathh	Absolute value of the soil matric suction at saturation (m)	± 10%
hsatcon	Hydraulic conductivity at saturation ($kgm^{-2}s^{-1}$)	± 10%
sm-sat	Volumetric soil moisture content at saturation (m^3 water per m^3 soil)	± 10%
sm-crit	Volumetric soil moisture content at critical point (m^3 water per m^3 soil)	± 10%
sm-wilt	Volumetric soil moisture content at wilting point (m^3 water per m^3 soil)	± 10%
hcap	Dry heat capacity ($Jm^{-3}K^{-1}$)	± 10%
hcon	Dry thermal conductivity ($Wm^{-1}K^{-1}$)	± 10%
albsoil	Soil albedo	± 10%
	Meteorological Forcing Variables	
SWR	Downward component of shortwave radiation at the surface (Wm^{-2})	± 10%
LWR	Downward component of longwave radiation at the surface (Wm^{-2})	± 10%
rain	Rainfall ($kgm^{-2}s^{-1}$)	± 10%
tempr	Atmospheric temperature (K)	± 10%
wind	Wind speed (ms^{-1})	± 10%
press	Surface Pressure (Pa)	± 10%
spHum	Atmospheric specific humidity ($kgkg^{-1}$)	± 10%
	Initial State Variables	
canopy	Amount of intercepted water that is held on each tile (kgm^{-2})	updated
tstar-t	Surface or skin temperature of each tile (K)	updated
t-soil	Temperature of each soil layer (K)	updated
sthuf	Soil wetness for each soil layer; mass of soil water expressed as a fraction of water content at saturation	updated

forcing variables with calibrated model parameters held constant, and (iv) a multi-dimensional clustering procedure to determine temporally persistent values in model decision space. The sections below describe these modeling procedures in greater detail.

2.1. Evolutionary strategy

The overall modeling method is based on the concept of evolutionary algorithm. Evolutionary algorithm is a powerful computational procedure which uses the concept of biological evolution to solve mathematical optimization problems. Essentially, the evolutionary algorithm defines a mathematical problem into a population of candidate members where the members compete for limited resources under several environmental conditions for survival and subsequent breeding of child members. By competition, the members are evaluated based on objectives such as the proximity of modeled soil moisture to in-situ data. The high performing members are chosen to reproduce for future populations whereas low performing members are discarded. A candidate member is defined by its internal properties called a genotype and its expressed behavior called a phenotype. When applied to hydrology, the genotype represents model decision variables which are made up of a vector string of values for model parameters and forcing variables, whereas the phenotype is equivalent to the model output such as soil moisture.

The genotype information for several candidate members represent a biological genome-like data, upon which several genome mappings can be undertaken. Two of those mapping methods are gene expression and genome-wide association (Dear, 1997, 2001), which were used to evaluate the model behavior. Gene expression examines how changes in individual genes (such as soil hydraulic conductivity) affect the model response (e.g. the overall soil moisture output) in phenotype space. Genome-wide association focuses on the relationships between genes in genotype space and how they interact to trigger particular expressions in phenotype space.

2.2. Calibration procedure

The role of calibration in this study is to provide an ensemble of optimized model parameter values subject to a fixed time period of soil moisture observation. The study encourages the use of ensemble members instead of a single member because of their capability to provide different pathways to matching the observation data. It is acknowledged that calibration is generally limited to a specific time period of observation data, and that improved performance of the model is not guaranteed outside the observation time period (Beven, 2001; Dumedah et al., 2012a; 2012b; Fenicia et al., 2008). It should be noted that the model parameter values obtained from model calibration were only used for the observation time period in this study.

The calibration method used is based on the NSGA-II procedure shown in Fig. 1. The NSGA-II is an advanced multi-objective evolutionary algorithm and has been applied in several sources including Bekele and Nicklow (2007); Confesor and Whittaker (2007); Dumedah et al. (2010); Khu and Madsen (2005); and Dumedah and Coulibaly (2012b). In the NSGA-II procedure, an initial population P_r of size $2n$ was generated through Latin hypercube sampling to ensure even sampling of the entire model decision space. The members in subsequent populations were generated based on the evolutionary operators including tournament selection, mutation and crossover. A tournament selection is a multi-objective optimization approach which ranks candidate members in a population by allowing two members to compete in terms of their performance on multiple evaluation objectives. This ranking procedure, usually referred to as nondominance sorting, provides a nondominance level which indicates how many members a chosen member dominates (i.e., the number of members the given member performed better than), and how many members dominate the member under consideration (i.e., the number of members which performed better than the chosen member). Mutation is an evolutionary variation operator which makes changes to a candidate member in terms of its genomic makeup. A crossover is a breeding operator which produces a child member by combining the genotype information from two parent members.

The P_r members were applied into the land surface model to generate soil moisture predictions, where they were evaluated against perturbed soil moisture observation data using root mean square error (RMSE) in Eq. (1) and bias in Eq. (2). The RMSE and bias evaluate different aspects of the model as they are independent over the calibration time period. The rationale to perturb the observation data was to match the model output against an inter-

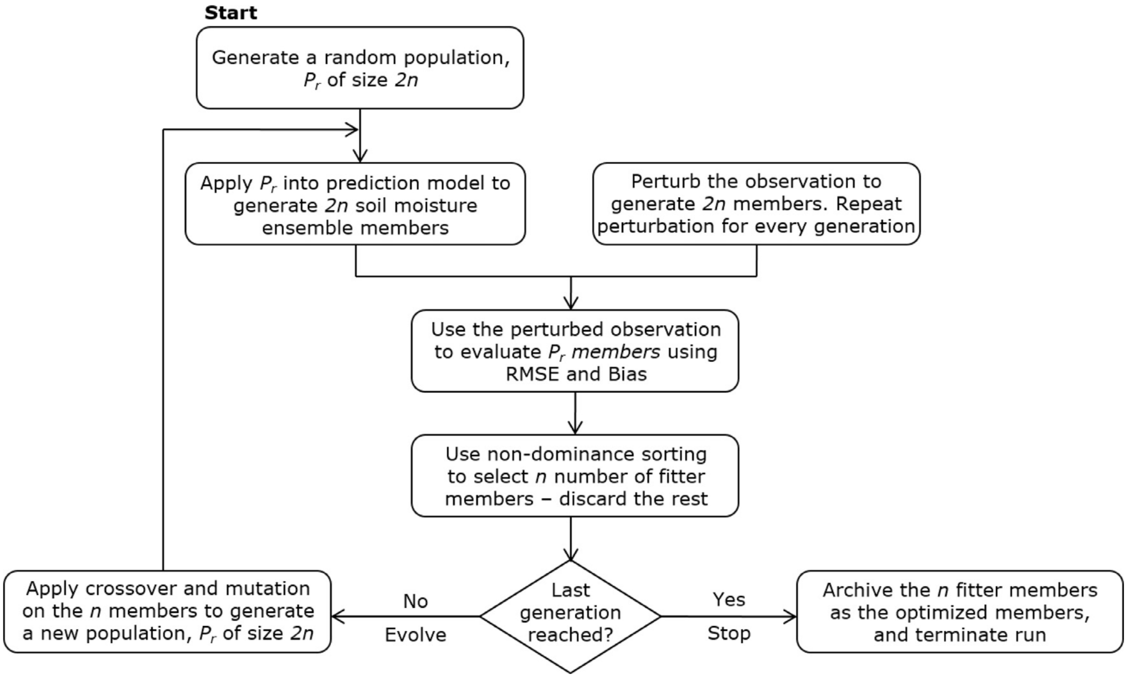


Fig. 1. Computational procedure of the calibration approach based on the NSGA-II method.

val of the observation data (i.e., observation with error distribution) instead of a fixed value.

$$RMSE = \sqrt{\frac{\sum_{t=1}^{n}(y_{s,t} - y_{o,t})^2}{n}} \tag{1}$$

where: $y_{s,t}$ is the simulated output for time t, $y_{o,t}$ is the perturbed observation value for time t, and n is the calibration time period.

$$Bias = \frac{\sum_{t=1}^{n}(y_{s,t} - y_{o,t})}{n} \tag{2}$$

Using values from the evaluation objectives (RMSE and bias), non-dominated sorting (based on tournament selection) was performed on the members in P_r after which n high performing members were selected through tournament selection. The remaining less performing members were discarded. The n high performing members were used to reproduce a new population P_r of size $2n$ through variation operators including crossover and mutation. This cycle of creating a new population of members, their evaluation, sorting and selection represents a complete evolutionary cycle called a generation. The population P_r was evolved over several generations whereas the members in P_r undergo variation at each stage of evolution to generate the final Pareto-optimal set. The Pareto-optimal set comprising of several model scenarios were retained as the optimal calibrated values for the model.

2.3. Overall data assimilation procedure

The DA approach used in this study is the EDA method, shown in Fig. 2. The EDA procedure unifies temporal updating from traditional DA with the multi-objective evolutionary strategy, to concurrently explore the internal dynamics of a prediction model in an adaptive and temporal manner. The EDA is unique in its approach because its updated members have model outputs and values in model decision space, where this inherent link preserves water and energy balance in model outputs. Several investigations have been undertaken with the EDA including soil moisture (Dumedah and Walker, 2014b), brightness temperature (Dumedah et al., 2011), streamflow (Dumedah and Coulibaly, 2012a), and its comparison to the ensemble Kalman filter and particle filter (Dumedah and Coulibaly, 2013).

The multi-objective evolutionary strategy used in the EDA in this study is the NSGA-II. It is notable that the EDA approach is flexible to accommodate other evolutionary algorithms such as Strength Pareto Evolutionary Algorithm (Zitzler et al., 2004; 2001; Zitzler and Thiele, 1999), Pareto Archived Evolution Strategy (Knowles and Corne, 2000), or Pareto Envelope based Selection II (Corne et al., 2001). The EDA procedure incorporates the NSGA-II procedure described at the calibration stage, except that some changes were included to account for temporal updating of the model, observation and model uncertainties, and sequential update of population members. The NSGA-II's role in the EDA procedure is limited to evolution of population members over several generations, their evaluation using multiple objectives, selection of high performing members to reproduce new members, and variation of members using evolutionary operators.

The EDA begins the initial assimilation time step with the creation of an initial population, P_r as in the NSGA-II procedure. The members in P_r were evaluated using absolute difference in Eq. (3) and cost function in Eq. (4) to account for model and observation uncertainties. The high performing members were selected based on the estimated values of absolute difference and the cost function. The selected members were then used to create new members, after which the evolutionary cycle was repeated over several generations. After the last generation, the high performing members which remain competitive across all the generations were chosen as the updated ensemble members for the current assimilation time step. The updated members were then used to make a forecast for the next assimilation time step and to estimate the model background error. The assimilation time step was incremented to a new time step, with the current updated members used as the seed population. The evolutionary cycle including evaluation, selection and variation were repeated for the new population to determine the updated ensemble for the new assimilation time step. The evolutionary procedure, the update and the forecasting steps were repeated to generate the updated ensem-

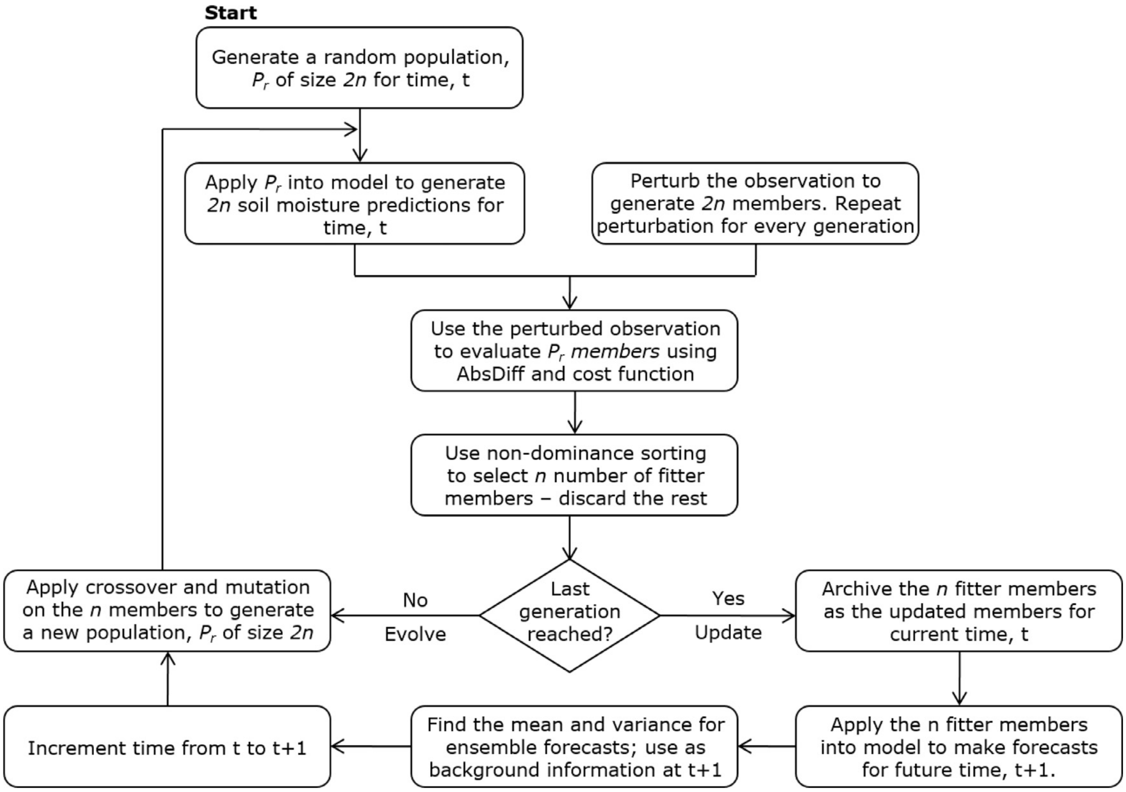


Fig. 2. Computational procedure of the EDA method (adapted from Dumedah (2012)).

ble for each assimilation time step. It is noteworthy that the updated members for each assimilation time step were selected from among several populations of members that have been evaluated over numerous generations.

$$AbsDiff = |y_{s,i} - y_{o,i}| \tag{3}$$

$$J = \sum_{i=1}^{k} J(y_i) = \sum_{i=1}^{k} \left\{ \frac{\left(y_{s,i} - y_{b,i}\right)^2}{\sigma_b{}^2} + \frac{(y_{s,i} - y_{o,i})^2}{\sigma_o{}^2} \right\} \tag{4}$$

$y_{s,\ i}$ = the analysis (i.e., the searched) value for ith data point which minimizes $J(y_i)$.

$y_{b,\ i}$ = background value for ith data point.

$y_{o,\ i}$ = perturbed observed value for ith data point.

σ_b^2= variance for background soil moisture error.

σ_o^2 = variance for observed soil moisture error.

k = number of data points (k is set to 1 for sequential data assimilation).

2.3.1. Data assimilation using both model parameters and forcing variables

Data assimilation has been widely recognized in the literature (Dumedah, 2015; Evensen, 2003; Houtekamer and Mitchell, 2005; Reichle, 2008; Weerts et al., 2010), for its ability to account for uncertainties in model and observation, along with its forecasting and temporal updating capabilities. Nonetheless, an underestimated property of DA is its temporal changes in model decision space for initial states, parameters, and forcing variables to produce the updated output. An assessment of this temporal evolution in model decision space has been shown to provide valuable information about model behavior (Dumedah, 2015; Dumedah and Walker, 2014a). This section therefore draws upon the hydrologic genome mapping in Dumedah (2015) to assess model behavior in relation to model parameters and forcing variables.

The EDA procedure was used to perform assimilation into the JULES model through perturbation of both model parameters and forcing variables. The contribution of EDA in this section is to provide genome-like data for model parameters and forcing variables across all assimilation time periods, and subsequent gene expression and genome-wide evaluation. The EDA procedure with variable model parameters and forcing data across assimilation time steps was used to provide a large archive of updated values in model decision space. These updated values in model decision space were evaluated using the multi-dimensional clustering method described in Section 2.4 (also employed in Dumedah (2015)) to determine unique mappings in the genotype space for both model parameters and forcing variables.

2.3.2. Data assimilation using forcing variables only

The EDA procedure in this section was designed to provide forcing data uncertainty evolution through time, while the model parameters were held constant at the optimal ensemble values obtained from the calibration procedure. The rationale for this approach is to minimize the influence of model parameters while generating the genome-like data for forcing variables only. The EDA with changing values of only forcing variables across several assimilation time steps provide a large archive of updated values in model decision space. Similarly, the ensemble archive was evaluated using the multi-dimensional clustering method described in Section 2.4 in order to determine the unique mappings in the genotype space for forcing variables only.

2.4. Assessment of values in model decision space

The updated ensemble members obtained from the EDA procedure have model outputs in terms of soil moisture and values in model decision space. This section focuses on the assessment of the updated values in model decision space (i.e., genotype space).

It is noted that all subsequent descriptions are in reference to the genotype space. The updated values in model decision space are equivalent to a biological genome-like data which can be used to develop a hydrologic genomic map (Dumedah, 2015). As a genome-like data, different knowledge discovery methods can be used to examine unique properties such as gene expression for micro-array analysis, feature selection for unique role of features, genome-wide associations for interaction between genes, or sequence analysis for gene signal analysis (Dear, 2001).

One kind of hydrologic genomic map is the dominant pathway; dominant because it determines temporally stable/persistent locations across several time periods, and pathway because it connects unique locations for different model components. By location in reference to genome-like data, a specific subset in the model decision space is implied. The temporally stable locations signify a commonality in values that persist for a model decision variable when evaluated across several assimilation time periods. Given that these locations are in genotype space, they represent unique sub-regions of individual genes which persist or survived across multiple time periods. It is worth noting that the pathway characteristic encompasses genome-wide association as it explores the interaction between model decision variables. The temporal persistence property exemplifies gene expression as it provides the capability to evaluate temporally stable genes and their impact or expression on soil moisture (in phenotype space).

The dominant pathway was determined by performing a multi-dimensional hierarchical clustering on the archive of updated members in model decision space. Clustering is an exploratory approach that is well suited for this kind of analysis, because it requires limited assumptions about the distribution of the data set. The clustering performed on updated members ensured the determination of temporally stable locations, while the multi-dimensional aspect of the clustering performed ensured that interactions between model decision variables were preserved.

To measure the distribution of updated members, each model decision variable was normalized and a Euclidean metric was used to estimate the distance between the normalized vectors. Several numbers of cluster groupings were explored through the knee method (Thorndike, 1953), to determine the appropriate number of clusters which best identified the distinct groups in the data set. After determining the suitable number of clusters, the cluster group with the largest ensemble membership was chosen to represent the dominant pathway.

3. Setup of model, calibration and data assimilation runs

The model was setup in a way that both calibration and assimilation procedures were undertaken for the JULES model over a three year time period from 2012 to 2015. The same modeling periods for calibration and assimilation ensured that values can be compared in model decision space. The NSGA-II procedure was used to calibrate the JULES model leading to an ensemble estimate of values for both model parameters and forcing variables which produce soil moisture output from JULES to best match the observation in-situ soil moisture. The initial population in the NSGA-II was generated from Latin hypercube sampling by using the intervals for model parameters and forcing variables in Table 1. The observation in-situ soil moisture was perturbed to within ± 0.03 m^3/m^3 of their original values, based on outcomes from Smith et al. (2012). Based on the standard NSGA-II procedure (Deb et al., 2002), a crossover probability of 0.8 and a mutation probability of $\frac{1}{n}$ (where n is the number of variables) were used. In the calibration, a population of 40 members was evolved through 250 generations, leading to an optimized ensemble of 20 members. Given the number of generations used, the population size was deemed suitable as it is more than two times the number of variables under consideration.

Two independent assimilation procedures were undertaken, both run across the same time period as in the calibration procedure. The first assimilation, denoted full DA, applied the EDA method in concert with the procedure outlined in Section 2.3.1 to generate an updated archive of model parameters and forcing variables through assimilation of in-situ soil moisture observation into the JULES model. The second assimilation, denoted forcing DA, used the EDA method in concert with the procedure presented in Section 2.3.2 to generate an updated archive of forcing variables only, through assimilation of in-situ soil moisture observation into the JULES model. In the forcing DA procedure, the model parameters were held constant at the optimized ensemble model parameters values obtained at the calibration stage.

The soil moisture observation error in both EDA procedures was set to ± 0.03 m^3/m^3, whereas the model error was derived from the ensemble members which evolve between and at each assimilation time step, with the background error estimated from the seed population between assimilation time steps. The initial population in the full DA was created through Latin hypercube sampling by using the intervals for model parameters and forcing variables in Table 1. Similarly, the initial population in the forcing DA approach used the same procedure except that only forcing variables were used to generate the initial population. The probabilities for crossover and mutation in both EDA procedures were set using the same procedure as in the calibration stage. In both EDA procedures, a population of 40 members was evolved over 10 generations, to produce an updated ensemble of 20 members for each assimilation time step. The updated ensembles were archived for subsequent evaluation using multi-dimensional clustering procedure.

4. Results and discussion

4.1. Evaluation in phenotype space - soil moisture output

The resulting outcomes of the model runs include the updated soil moisture in phenotype space and an archive of values for model decision variables in genotype space. The key focus of this study is examination of the results in genotype space, however a provisional evaluation of the estimated soil moisture against in-situ data is an important initial step. The updated soil moisture from the full DA and forcing DA are evaluated by their comparison against in-situ soil moisture at 5 cm soil depth, in Fig. 3.

The evaluation is based on two numerical measures: root mean square error (RMSE) and coefficient of determination (R), together with a graphical one-to-one plot. The RMSE measures the overall closeness of the soil moisture estimate to the observed in-situ data, and R accounts for the overall temporal association between the estimation and observation. The graphical one-to-one plot provides a visual departure of the soil moisture estimate from observed values, with perfectly matched values lying on the diagonal line. Overall, the forcing DA output closely matches the in-situ soil moisture and has better accuracy values than the full DA output based on the evaluation measures. Specifically, the forcing DA method improved the accuracy of the full DA output by 35% in terms of RMSE and about 7% for R.

Additionally, the root-zone soil moisture estimates from both full and forcing DA methods are compared against root-zone in-situ data at soil depths of 15 cm and 45 cm in Fig. 4. The soil moisture estimation accuracy generally decreased with increasing soil depth, such that, the highest estimation accuracy was obtained at the surface 5 cm soil depth with the lowest accuracy at the deeper 45 cm soil depth. The soil moisture estimation accuracy at the 15 cm soil depth is almost similar to those obtained for the surface 5 cm soil depth. Similarly, the forcing DA output at the 15 cm soil

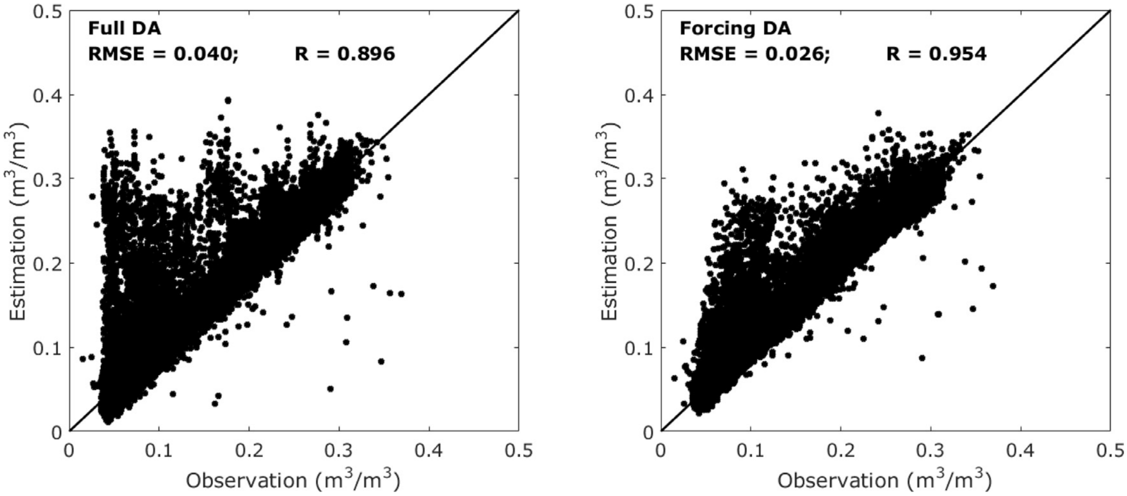
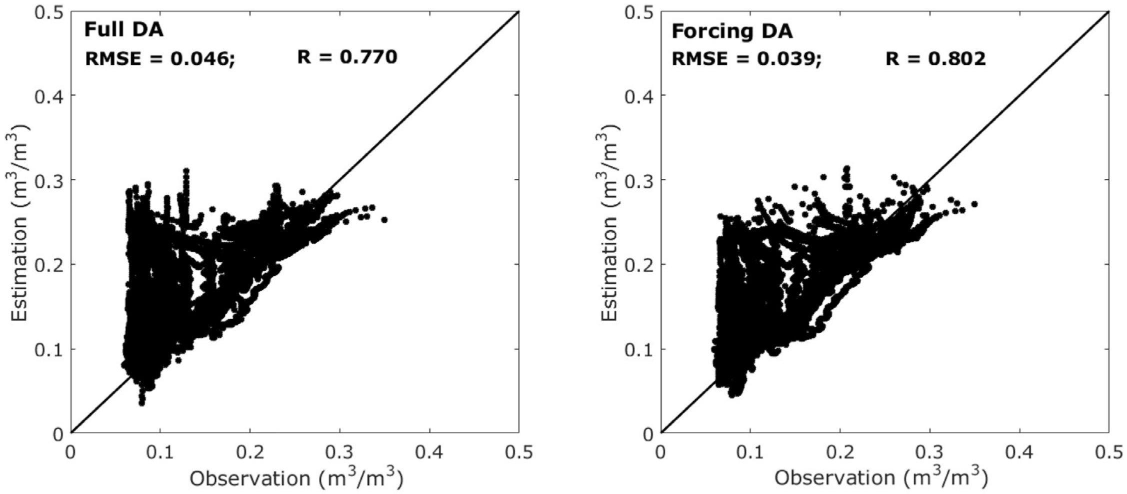
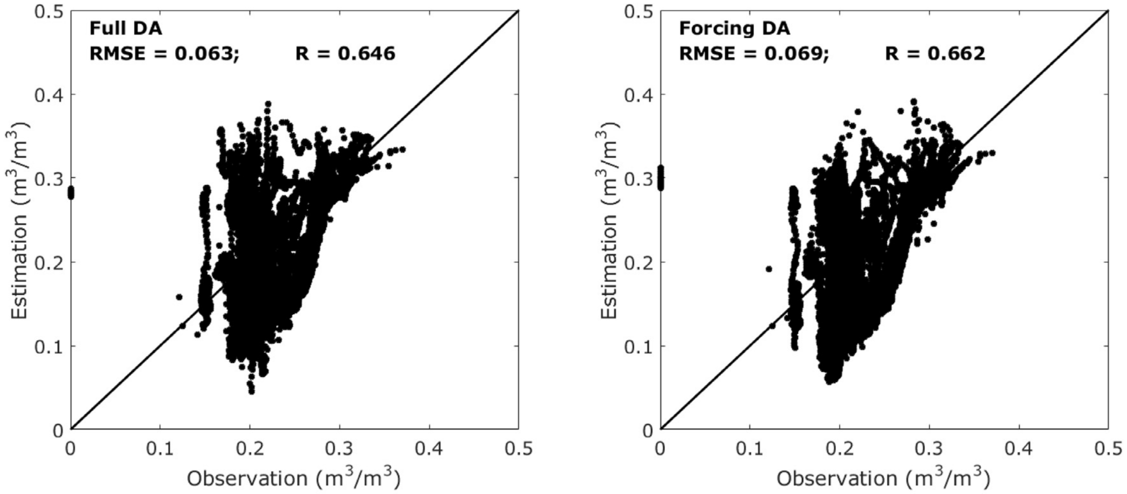


Fig. 3. Evaluation of updated near surface soil moisture (based on RMSE in m^3/m^s and coefficient of determination) of the full DA and forcing DA against in-situ soil moisture at 5 cm soil depth.



(a) Soil depth: $15cm$



(b) Soil depth: $45cm$

Fig. 4. Evaluation of root-zone soil moisture (based on RMSE in m^3/m^s and coefficient of determination) of the full DA and forcing DA against in-situ soil moisture at 15 cm and 45 cm soil depths.

depth performed better than the full DA output based on the evaluation measures. At the 15 cm soil depth, the forcing DA method improved the estimation accuracy of the full DA method by 15% in terms of RMSE and about 4% for R. However, there is little discernible difference in the evaluation values between the full and forcing DA outputs for the 45 cm soil depth. The impact of the differences between the two assimilation approaches is limited to the 5 cm and 15 cm outputs, with negligible impact at the deeper 45 cm soil depth. That is, the forcing DA has a positive impact on the soil moisture estimation accuracy at the upper soil layers, and no observable impact at the deeper 45 cm soil depth.

4.2. Evaluation in genotype space - model decision variables

Two types of evaluation were undertaken to assess the model outputs in genotype space. The two types of evaluation include gene expression with a focus on one model decision variable at a time, and genome-wide association with a focus on interactions between all model decision variables. These evaluations are presented in greater detail in the sections below.

4.2.1. Gene expression - dominant cluster

Ideally, the goal of gene expression is to determine how different values of an individual model decision variable trigger a response or an expression in phenotype space, soil moisture estimate in this case. However, in this assimilation procedure, the optimal estimate of soil moisture has been determined to best account for uncertainties in both soil moisture observation and model estimation. That is, the soil moisture estimate in phenotype space is definitive based on the operating uncertainties. To achieve this definitive estimate of soil moisture, changes were made in genotype space for individual model decision variables. As a result, the gene expression in this case is focused on assessing the changes that were made by each model decision variable across several time periods, in order to obtain competitive soil moisture estimation. In other words, the objective is on temporal evolution of individual model decision variables and subsequent determination of a subset of the genotype space that is deemed to be temporally stable.

The procedure employed to assess gene expression examined individual genes (that is, each model decision variable) and their response across time, which were used to generate the competitive soil moisture estimates in phenotype space. That is, this section focuses on the assessment of independent response from each model decision variable with no influence from other model decision variables. To do this, the analysis procedure outlined in Section 2.4 was employed on each model decision variable, to determine the dominant cluster together with its coverage of the decision space. For each variable, the dominant cluster represents a subset of the model decision space where values were persistently chosen (i.e. temporally stable) to produce competitive soil moisture across several time periods. The corresponding coverage of the dominant cluster indicates the weight or level of dominance in model decision space in terms of frequency of occurrence. The coverage is expressed as percentage, with 0% indicating no weight and 100% indicating the maximum weight.

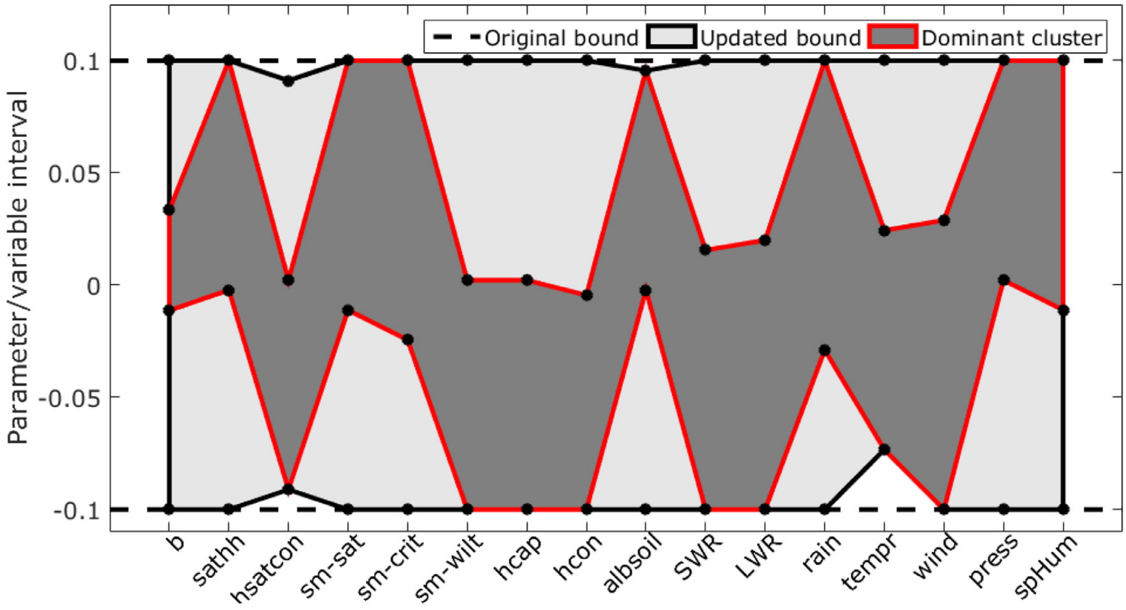
The dominant cluster and its corresponding coverage were determined from an archive of values for each model decision variable obtained from both the full DA and forcing DA outputs. For the full DA output, the dominant cluster and its coverage for each model decision variable are presented in Fig. 5. The dominant cluster is equivalent to a subset of the model decision space, with its coverage representing the level of temporal persistence or stability. In the context of genomic mapping, the dominance cluster represents a unique feature in model decision space which has survived several changes in hydro-meteorological conditions. It is noted that, in the dominant cluster plot, the lines connecting the model decision variables are imaginary and do not signify an interaction between the variables. The number of clusters used in the clustering of individual model decision variables range from two to six, meaning that the dominant cluster is determined from among several clusters ranging from two to six. This range of clustering is important to better understand the significance of the coverage of each dominant cluster.

From the full DA output, it was found that the range between the minimum and maximum values of the dominant cluster in relation to the model ensemble range is about 50% across all model decision variables. That is, the dominance clustering procedure have reduced the entire model decision space by half. The significance of this reduction is measured by the overall coverage, which was determined to be about 60% across all model decision variables. This demonstrates that the overall dominant cluster representing a subset of the genotype space are temporally stable for 60% of the time to provide competitive soil moisture estimates.

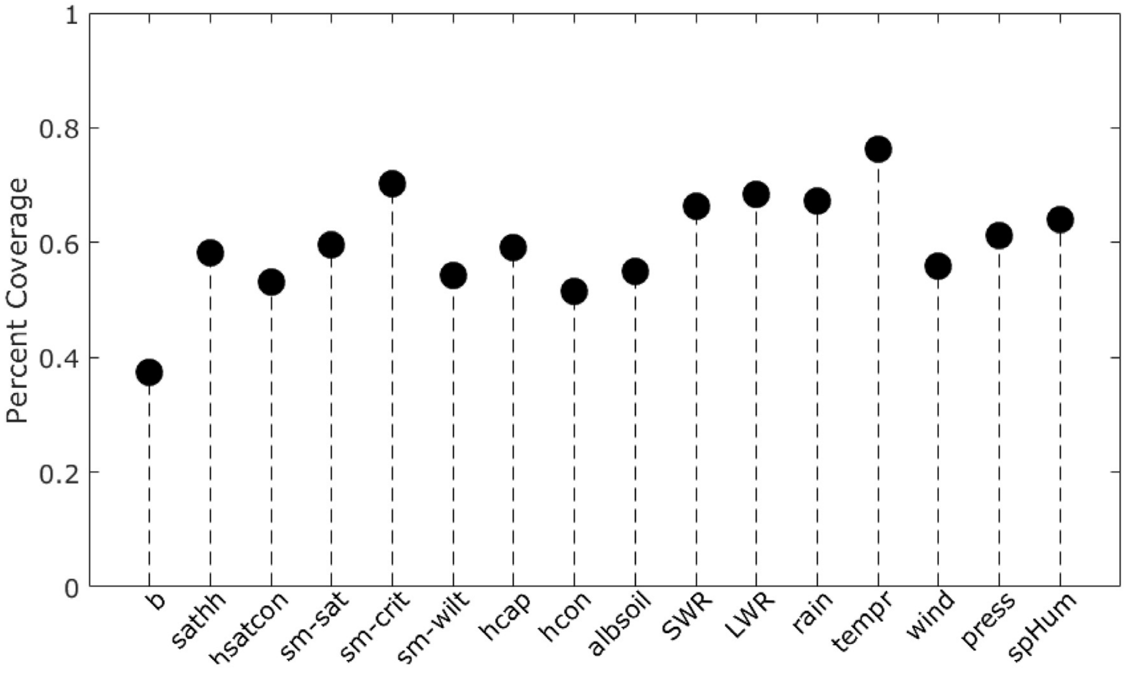
For the forcing DA output, the dominant cluster and its coverage for each model decision variable are presented in Fig. 6. It is noted that only forcing model decision variables are considered here since model parameter decision variables were predetermined and assigned to ensemble values obtained from calibration procedure outlined in Section 2.2. From the forcing DA output, it is found that the range between the minimum and maximum values of the dominant cluster in relation to the model ensemble range is about 45% across all model decision variables. That is, the dominance clustering procedure reduced the entire model decision space by 55%. The significance of this reduction is measured by the overall coverage, which is determined to be about 60% across all forcing model variables. This demonstrates that the overall dominant cluster representing a subset of the genotype space for forcing variables are temporally stable for 60% of the time to provide optimal soil moisture estimation.

In the context of gene expression, the resulting dominant clusters for the individual input forcing variables represent the acceptable uncertainty bound needed in the JULES model to provide optimal estimates of soil moisture. It is notable that this acceptable uncertainty bound is in the context of individual forcing variables; the interaction between variables is accounted for under genome-wide evaluation. This estimate of acceptable uncertainty bounds, based on gene expression, need validation to verify their robustness and reliability to other hydro-meteorological situations. Using the dominant clusters from both full and forcing DA outcomes, the acceptable level of uncertainty for the input forcing variables are validated by finding the overlapping decision space between the two sets of dominant clusters.

The validation of the acceptable uncertainty bound is presented in Fig. 7, showing the overlapping decision space for input forcing variables. The degree of overlap between the two sets of dominant clusters indicates the level of validity for the individual variables, with 100% overlap meaning the highest validity and 0% indicating the lowest validity. A variable with an invalid uncertainty bound means that no consistent subset of the model decision space has been found and that random subsets are equally capable of having the most influence on the output soil moisture. Shortwave and longwave radiations have 100% validity, with the lowest overlap area obtained in air pressure with 4% validity. Among all seven input forcing variables, only air pressure and specific humidity were deemed invalid based on their overlapping area in decision space. The remaining five forcing variables have an overlapping area of about 85% and were satisfactorily deemed valid. Overall, the validation results show that the acceptable uncertainty bound estimated for the five forcing variables are considered reliable for the JULES model in this study area.



(a) Dominance cluster for full data assimilation

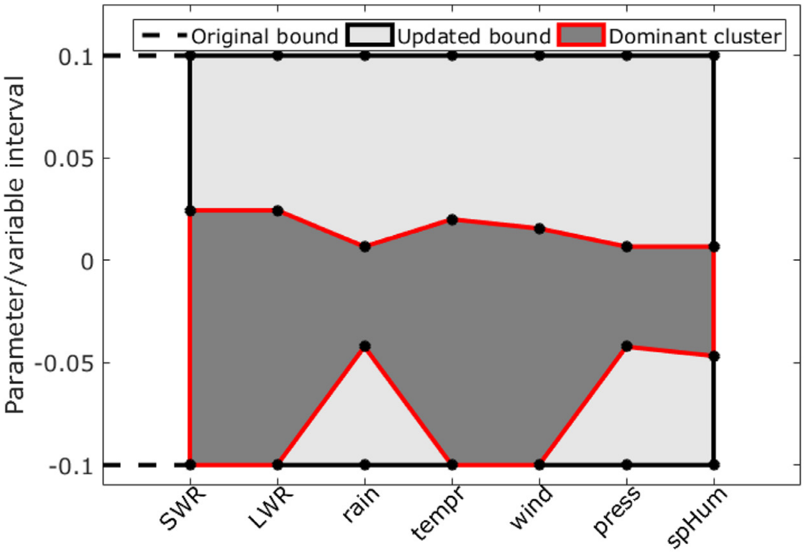


(b) Coverage of dominance cluster for full data assimilation

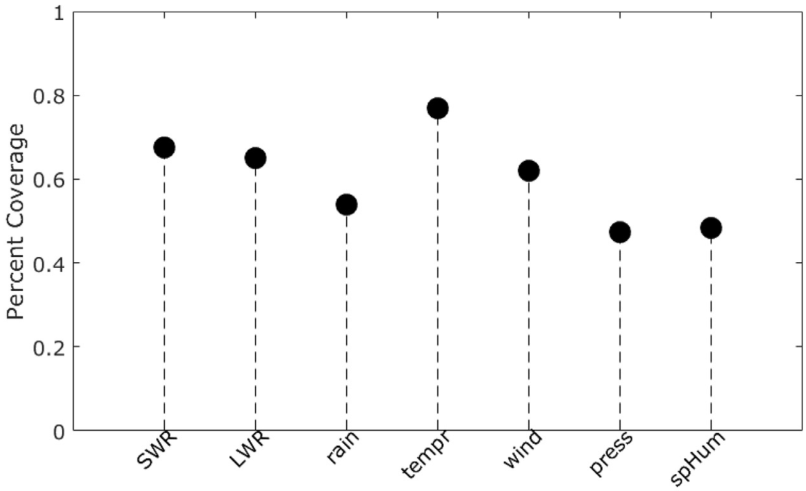
Fig. 5. Dominant cluster and its corresponding coverage for individual model decision variables obtained from full DA output.

4.2.2. Genome-wide association - dominant pathway

By definition, genome-wide association examines the interactions and relationships between model decision variables and their collective response in phenotype space. A similar approach is employed here with some modifications. To determine optimal soil moisture in phenotype space across several time periods, changes were made in genotype space by evaluating several pathways in model decision space. Given the operating uncertainties in observation and model estimation, the optimal soil moisture is mostly definitive and was achieved by finding distinct pathways in model decision space. As a result, the objective here was to find those model decision pathways that are persistent across several time periods. The genome-wide evaluation focuses on the interactions between model decision variables, their temporal evolution, and determination of temporally stable pathways in genotype space. The genome-wide association was examined by using the procedure in Section 2.4 to determine the dominant pathway for model decision variables. The dominant pathway is the persistent pathway frequently chosen in model decision space to produce competitive soil moisture across several time periods.



(a) Dominant cluster for forcing data assimilation



(b) Coverage of dominant cluster for forcing data assimilation

Fig. 6. Dominant cluster and its corresponding coverage for individual model decision variables obtained from forcing DA output.

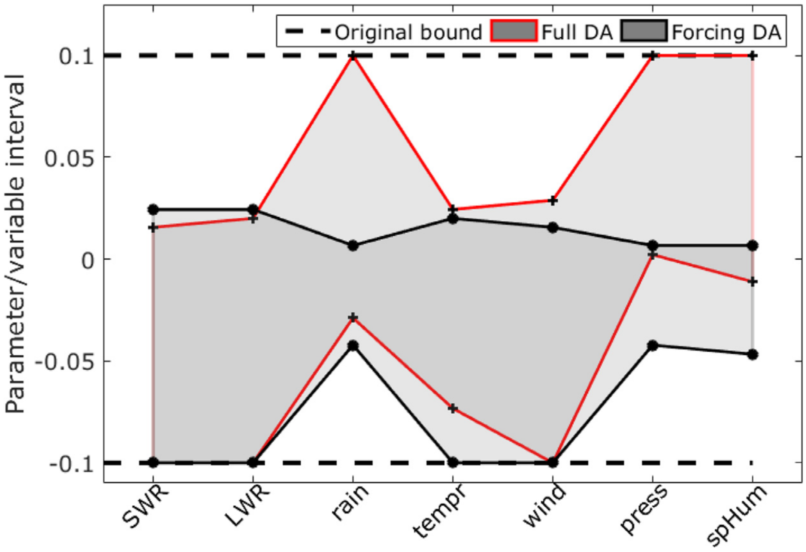
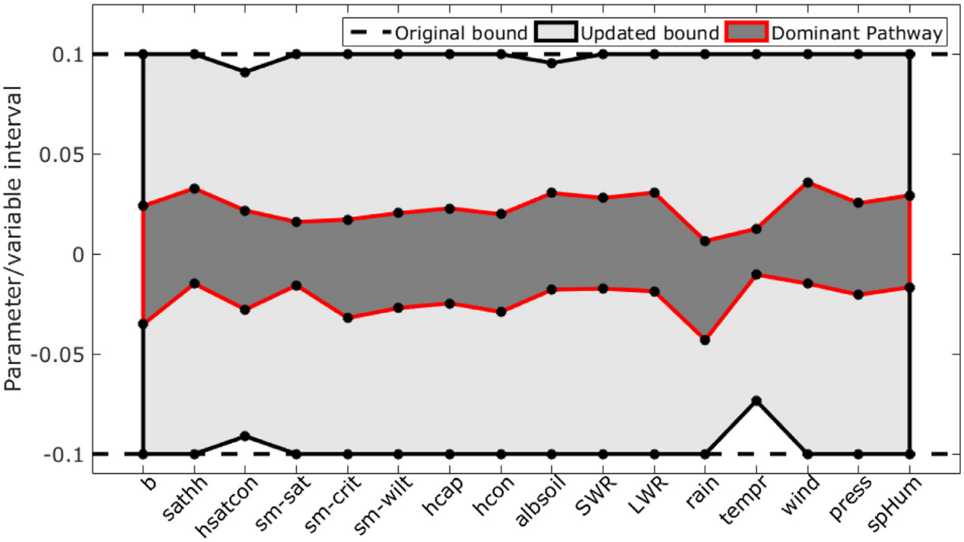
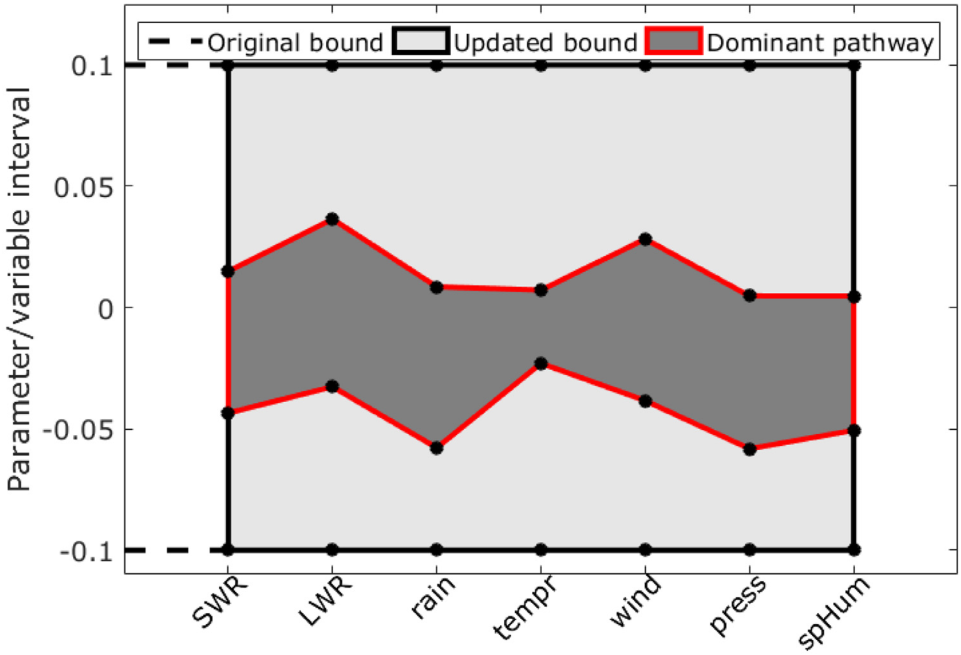


Fig. 7. Validation of acceptable uncertainty bound based on gene expression showing the overlapping decision space for input forcing variables.



(a) Dominant pathway for full data assimilation



(b) Dominant pathway for forcing data assimilation

Fig. 8. Dominant pathway model decision variables obtained independently for full DA and forcing DA outputs.

The dominant pathways obtained independently for the full DA and forcing DA outputs are presented in Fig. 8. In the full DA output, the range between the minimum and maximum values of the dominant pathway in relation to the model ensemble is about 22%. That is, the dominant pathway reduced the entire model decision space by 78%. The corresponding coverage of the dominant pathway was determined to be 30%, based on an optimal number of seven cluster groups. From the forcing DA output, it was found that the range between the minimum and maximum values of the dominant pathway in relation to the model ensemble range was about 30%, representing a 70% reduction of the entire model decision space. The significance of this reduction was measured by the overall coverage, which was determined to be about 30%, based on an optimal number of 8 cluster groups.

The dominant pathway obtained from the forcing DA output is the acceptable forcing data uncertainty, representing the minimum inaccuracy within which to obtain competitive soil moisture estimation without a significant deterioration in accuracy from the JULES model. This acceptable uncertainty bound was validated by comparison against the dominant pathway obtained from the full DA output. The validation of the acceptable uncertainty bound is presented in Fig. 9, showing the overlapping decision space for input forcing variables. Rainfall and air temperature have 100% validity (i.e., full overlap area), with the lowest overlap area obtained in specific humidity with 56% validity. All the forcing variables have an overlapping area of about 82% and were satisfactorily deemed valid. Overall, the validation results show that the acceptable uncertainty bound estimated for all forcing variables are reliable for the JULES model in this study area.

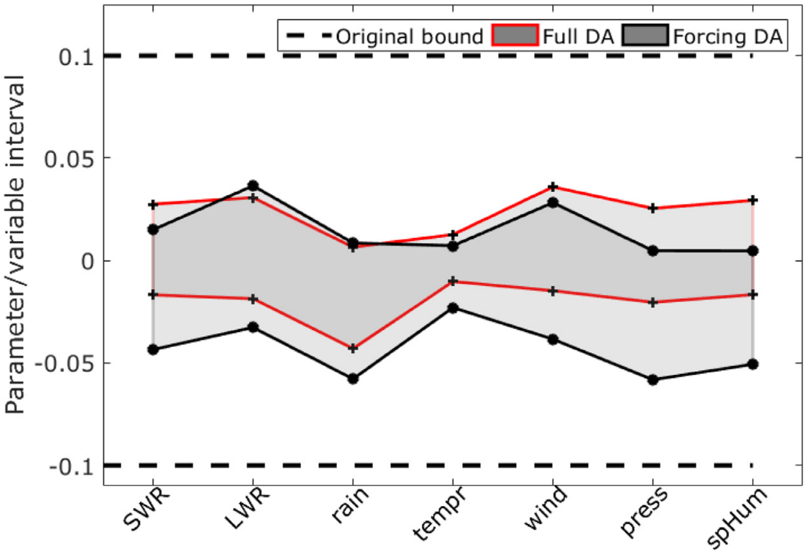


Fig. 9. Validation of acceptable uncertainty bound based on genome-wide association showing the overlapping decision space for input forcing variables.

5. Implication of findings and conclusion

This study has quantified the acceptable uncertainty needed in the JULES model to provide optimal soil moisture without a significant deterioration in the model estimation accuracy. To achieve this, two assimilation approaches were undertaken: full DA which used both model parameters and forcing variables, and forcing DA which used only forcing variables in the assimilation procedure with the model parameter values obtained through calibration. Both full DA and forcing DA were used to assimilate soil moisture into the JULES model. When model outputs from full DA and forcing DA were evaluated against surface and root-zone in-situ soil moisture, the forcing DA output was found to be superior at the surface but had similar accuracy as those from the full DA output at the root-zone. That is, the advantages of the forcing DA output were limited to the surface soil moisture at 5 cm and 15 cm soil depths. It is noteworthy that the high performance of the forcing DA does not suggest that changing of model parameter values is unnecessary. Rather, it reinforces the impact of having an adequate model parameter space, which was predetermined through the model calibration procedure.

The acceptable uncertainty was determined through a hydro genomic mapping, with the objective to find persistent commonalities in model decision space across several time periods. The evaluation focused on individual model decision variables to determine the dominant cluster, and the interaction between model decision variables to determine the dominant pathway. From the model viewpoint, the interaction between the model decision variables is the major influence on soil moisture estimation. That is, the dominant pathway is more meaningful to the model in replicating the soil moisture output. Nevertheless, the dominant cluster for each variable is crucial to better understand the subset of the model decision space which bears the most influence on the output soil moisture. As a result, the acceptable uncertainty bound was determined using both dominant cluster and dominant pathway procedures, with the later being more consequential in terms of the model and the output soil moisture.

The acceptable uncertainty determined from the forcing DA output were validated with outputs from the full DA. Based on results from the dominant cluster, five out of seven forcing variables were valid with only two variables not valid; air pressure and specific humidity. The condition of validity was based on the persistence of a subset of the model decision space across several time periods. A variable with an invalid uncertainty bound means that the representation of the variable in the model is not consistent in the context of the area and time period of study. In the dominant pathway, the findings from the validation showed that all the forcing variables are reliable and are considered temporally stable to provide optimal soil moisture estimate.

These findings have important implications on soil moisture assimilation and general environmental estimation from land surface and hydrological models. The findings show that the input forcing data have significant impact on model output, 35% in RMSE for 5 cm depth of soil moisture and 15% in RMSE for 15 cm depth of soil moisture. While the impact of input forcing data on model output has been widely recognized, this specific quantification is most crucial to illustrate its exact significance. In terms of assimilation procedures, the exact bound of acceptable uncertainty demonstrate the limits in model decision space beyond which ensemble members should be generated to be considered unique. That is, ensemble members which are generated within the limits of acceptable uncertainty cannot be considered differentiable based on this knowledge of inaccuracies in model decision space. This is crucial in DA in order to account for uncertainties that are meaningful from the model standpoint.

The acceptable uncertainty has practical significance in all types of environmental modeling. Knowledge of the acceptable uncertainty gives confidence about the reliability of the model in terms of its performance under different hydro-meteorological conditions and time periods. Because no output from a model is free from error, the knowledge of acceptable uncertainty will lead to a better interpretation of model outcomes. Notably in environmental forecasting it is crucial to know the level of changes in individual forcing variables that can trigger a rapid response/change in the model prediction. For operational prediction, the derived acceptable uncertainty for a specific model can be applied to model predictions in the future. That is, the acceptable uncertainty will help model users and forecasters to account for known model behavior and to better interpret their model outputs. Being a consequence of model behavior, the acceptable uncertainty points to specific parts of the model that need verification to ensure that their intended behavior are satisfactory under different modeling conditions. As a result, the acceptable uncertainty will provide invaluable information to model developers in their effort to fine-tune the inaccurate parts of the model.

It is also important to emphasize the novelty in our modeling paradigm. To study the model behavior, this approach took the land surface model as a whole with no assumption of its erroneous parts. The resulting genomic-like data were examined to de-construct the model decision space through gene expression and genome-wide association. As a result, the modeling approach accommodates different model configurations including the conceptual physical structure or the conceptual process structure, deterministic, stochastic, and empirical model structures. This procedure of de-construction of the model decision space is suitable for model inter-comparison studies and for the examination of alternative modeling procedures, for example, the evaluation of water infiltration rate by either Richards' equation (Richards, 1931) or Green-Ampt method (Green and Ampt, 1911) in different watersheds.

It is important to highlight the implication of the modeling approach used in this study and the findings. The study examined the behavior of the JULES model under soil moisture estimation scenario by analyzing genomic-like data using gene expression and genome-wide association methods. The genomic-like data were generated through the EDA approach, which can be undertaken for any land surface or hydrological model. As a result, the entire modeling approach can be adapted to any land surface and hydrological models for any given study area. However, the findings obtained in this study are specific to the JULES model, the study area, and the time period of study. The behavior of the JULES model in relation to its inputs and outputs found in this study will need to be examined in other study areas in order to generalize these findings. Nevertheless, this study points to a definitive approach to assess model behavior by evaluating different parts of the model, their individual expression, their interaction, and subsequent contribution to the model output.

Moreover, the findings illustrate the potential of the hydro genomic mapping, with this study demonstrating two of its derivatives; dominant cluster and dominant pathway, employed to determine the acceptable uncertainty for input forcing variables. The hydro genomic mapping has been undertaken through gene expression and genome-wide association analysis, which together provide new insight into the behavior of the JULES model. The demonstrated approach provides a definitive framework to assess the specific impact from different model components in general land surface and hydrological model estimation. The hydro genomic approach focus on mappings in model decision space from which a better understanding of the model, and its inputs and outputs can be made. Consequently, there is a need to find other derivatives of the hydro genomic mapping in order to construct a more thorough understanding of the land surface model, and its inputs and outputs.

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