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Assessment of land surface model uncertainty: A crucial step towards the identification of model weaknesses

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SUMMARY

Assessment of uncertainty in land surface models is complex, mainly because of the numerous sources of error from model parameters, initial states, input forcing data, and the model structure. These sources of uncertainty interact together to impact the simulated output generated from the land surface model. To account for these uncertainties, the goal in diagnostic model evaluation has been to determine the erroneous/inadequate components of the model structure that need improvement. However, the specification of inaccurate model components is not straightforward, requiring crucial steps to determine the uncertainty contributions from individual error sources. Also, the interaction between the uncertainty sources makes it difficult to assess the impact of the individual error sources on the simulated output. The approach undertaken in this study was to quantify the specific uncertainties linked with model parameters, states, input forcing variables, and spatial variations in landscape properties, such that the remaining model uncertainty is equivalent to the inadequacy/inaccuracy associated with the model structure. This study employed the Evolutionary Data Assimilation, together with multi-dimensional clustering, to quantify these individual uncertainties for the Community Atmosphere Biosphere Land Exchange (CABLE) model, in terms of soil moisture estimation for the Yanco area in south-east Australia. The findings showed that the updated soil moisture was more accurate than both the open loop and calibrated estimates. The minimum uncertainty for model components was found to reduce the original and updated bounds by 68% and 62% respectively. The estimated model pathway has accurately reproduced the updated estimates with less than 0.02 m^3/m^3 error, and was found to be more accurate than both the calibrated and the updated estimates when evaluated against in-situ soil moisture.

1. Introduction

Numerous sources of uncertainty in land surface models have ratified data assimilation (DA) as a promising procedure to account for inaccuracies (or errors) linked to the model output and the observation data. Primarily, DA methods have been employed to improve model predictions by correcting model state trajectories (Dumedah and Coulibaly, 2013, 2012b; Thirel et al., 2010; Xie and Zhang, 2010), but very few studies (Vrugt and Sadegh, 2013; Dumedah and Walker, 2013) have actually employed DA to learn about the land surface model physics with the aim to identify weaknesses in the model structure. The need to learn about the land surface model with the capacity to assess and quantify its uncertainties has been widely recognized (Vrugt and Sadegh, 2013; Gupta et al., 2012; Clark et al., 2011; de Vos et al., 2010; Gupta et al., 2008; Vrugt and Robinson, 2007; Liu and Gupta, 2007). This is mainly because the ultimate improvement in model forecasts is largely linked to uncertainties from: model parameters, initial states, input forcing data, and the model structure.

To address these sources of uncertainty, Gupta et al. (2008) have outlined a conceptual framework for diagnostic model evaluation, with the aim to determine which components/aspects of the model need improvement, together with guidance towards the kinds of model improvements needed. However, a crucial task in diagnostic model evaluation is the ability to identify and quantify model uncertainties which are specific to: state variables, parameters, input forcing data, and spatial variations in landscape properties. The model parameters, initial states, and input forcing data have direct impact on the internal dynamics of the model and its simulated output. The landscape spatial variabilities control the level of uncertainty for model parameters and initial states (Gupta et al., 2012), needed to account for sub-grid heterogeneity of vegetation and soil properties. To assess these uncertainty sources, suitable procedures are needed to separate and quantify the individual contributions that the various sources of uncertainty

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have on the simulated model output. Assessment of these specific uncertainties is needed to target where improvements are needed, and to better estimate the combined model uncertainty due to the individual uncertainties from model parameters, initial states, input forcing data, and model structure. Consequently, specific steps are needed towards the detection of model weaknesses, through the quantification of model uncertainty, conditioned on spatial variability in the landscape (e.g. vegetation and soil) properties.

This study assesses four crucial sources of uncertainty in land surface models, namely model parameters, initial states, input forcing data, and landscape spatial variability. Recent studies including Dumedah and Walker (2013) and Dumedah and Coulibaly (2013), have shown the capability of DA (based on the Evolutionary Data Assimilation – EDA) to quantify the level of convergence for model states and parameters. The convergence of model parameters and states, which was estimated across several time periods using the EDA, accounted for the spatial variations of the landscape using vegetation and soil properties data. The convergence level was estimated on a model parameter-by-parameter basis, and the corresponding uncertainty was due to the variability in the landscape properties. While the parameter-by-parameter evaluation is an important step to quantify the levels of convergence, the simulated model output is a product of the combined interaction between model parameters, initial states, and input forcing data, along with the model structure.

Therefore, an assessment of the combined uncertainty requires a DA approach, together with a multi-dimensional clustering to determine the dominant pathway(s) in model parameter space (i.e. decision space). The model parameter pathway, in this case, is a decision item representing a vector string connecting all model parameters, initial state variables, and forcing data uncertainties. Specifically, the parameter pathway incorporates the sum of all individual sources of uncertainty from model parameters, states, and input forcing data, which together approximate the overall uncertainty for a perfect model structure. In other words, when these individual uncertainties are estimated and accounted for, the remaining uncertainty is equivalent to the inadequacy (or loosely the error) associated with the model structure. As a result, this study accounts for and quantifies the uncertainty associated with the landscape properties, and the specific uncertainties for model parameters, initial states, and input forcing variables.

It is important to point out the crucial roles for both the DA procedure, and the clustering analysis. The DA procedure allows a continuous evaluation of the dynamics between the simulated output and the observation (in objective space) through time, along with the temporal changes in model parameters, states, and input forcing data (in decision space). In essence, the DA procedure facilitates a continuous monitoring of the changes in both objective and decision space, with the capability to study the model behavior in time. The temporal dimension of the DA approach is critical, because it facilitates the testing of the model, and its associated components under different input data and observation conditions. Also, the temporal dimension allows the DA procedure to be tested for consistency in time. However, to study the model behavior, clustering analysis was used to examine the temporal dynamics in decision space, which encompasses the four sources of uncertainty. Clustering analysis is an exploratory analytical approach with the capability to determine the degree of commonality either for a single variable or for multiple variables across sampling records. Clustering analysis is well suited to studying the model behavior in time, through assessment of the temporal dynamics for updated ensemble members obtained from the DA procedure.

The model uncertainty estimation procedure is illustrated with the Community Atmosphere Biosphere Land Exchange (CABLE) model for soil moisture estimation in the Yanco area in south-east Australia. The study assimilates the retrieved soil moisture from the Advanced Microwave Scanning Radiometer for the Earth Observing System (AMSR-E) into CABLE using the EDA approach. The clustering procedure was then performed on the updated ensemble members to derive the uncertainty for the various model components. The EDA is a formulation based on evolutionary strategy (Dumedah, 2012), with stochastic and adaptive capabilities suitable for addressing and learning about complex and indeterminate problems.

2. Materials and methods

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

The study is demonstrated for the Yanco area (shown in Fig. 1) in the western plains of New South Wales, Australia. The terrain in the Yanco area is flat, covered predominantly with grassland together with scattered irrigated crops. The main soil texture group is loam, along with few traces of clayey and sandy textured loams. Topographically, the area is formed by plains with domes, lunettes, and swampy depressions, separated by discontinuous low river ridges and with prior stream systems (McKenzie et al., 2000). The plains are traversed by stream valleys, and layered soil and sedimentary materials that are common at fairly shallow depths.

The soil moisture evolution was simulated using the Community Atmosphere Biosphere Land Exchange (CABLE) model (Wang et al., 2011; Kowalczyk et al., 2006). CABLE is a tiled model of sub-grid heterogeneity, capable of simulating water and energy fluxes between a vertical profile of soil layers, vegetation, and the atmosphere. The model has five main modules including: (i) radiation, (ii) canopy micrometeorology, (iii) surface flux, (iv) soil, and (v) ecosystem carbon. The radiation component accounts for the radiation transfer and absorption by the sunlit and shaded leaves, whereas the canopy micrometeorology estimates the surface roughness length, zero-plane displacement height, and aerodynamic conductance from the reference height to the air within canopy or to the soil surface (Wang et al., 2011). The surface module comprises the energy balance, transpiration, stomatal conductance and photosynthesis of sunlit and shaded leaves. The soil component accounts for the energy and water fluxes within and surface of the soil; and the ecosystem carbon module includes estimates for the respiration of stem, root and soil organic carbon decomposition (Wang et al., 2011). The CABLE model uses six fixed soil layer thicknesses of 2.2-cm, 5.8-cm, 15.4-cm, 40.9-cm, 108.5-cm and 287.2-cm respectively from top to bottom, with the movement of water between layers estimated using the Richards equation (Kowalczyk et al., 2006). Evaporation from bare soil is based on the Penman–Monteith calculation for potential evaporation which is then weighted by a water availability index based on soil moisture in the top soil layer (Wang et al., 2011; Kowalczyk et al., 2006).

The soil properties data were obtained from the Digital Atlas of Australian Soils (McKenzie et al., 2000), provided through the Australian Soil Resource Information System (ASRIS). ASRIS information on soil properties include soil texture classes, along with proportion of clay content, bulk density, and saturated hydraulic conductivity (McKenzie et al., 2000; McKenzie and Hook, 1992). The essential meteorological forcing data variables used in the CABLE model include short and long wave incoming radiation, air temperature, precipitation, wind speed, and specific humidity. The forcing data were obtained from weather monitoring stations at Griffith, Yanco (station Y3) and Coleambally, all shown in Fig. 1, with precipitation obtained from the 15 weather and soil moisture monitoring stations. Additionally, CABLE uses leaf area index (LAI)

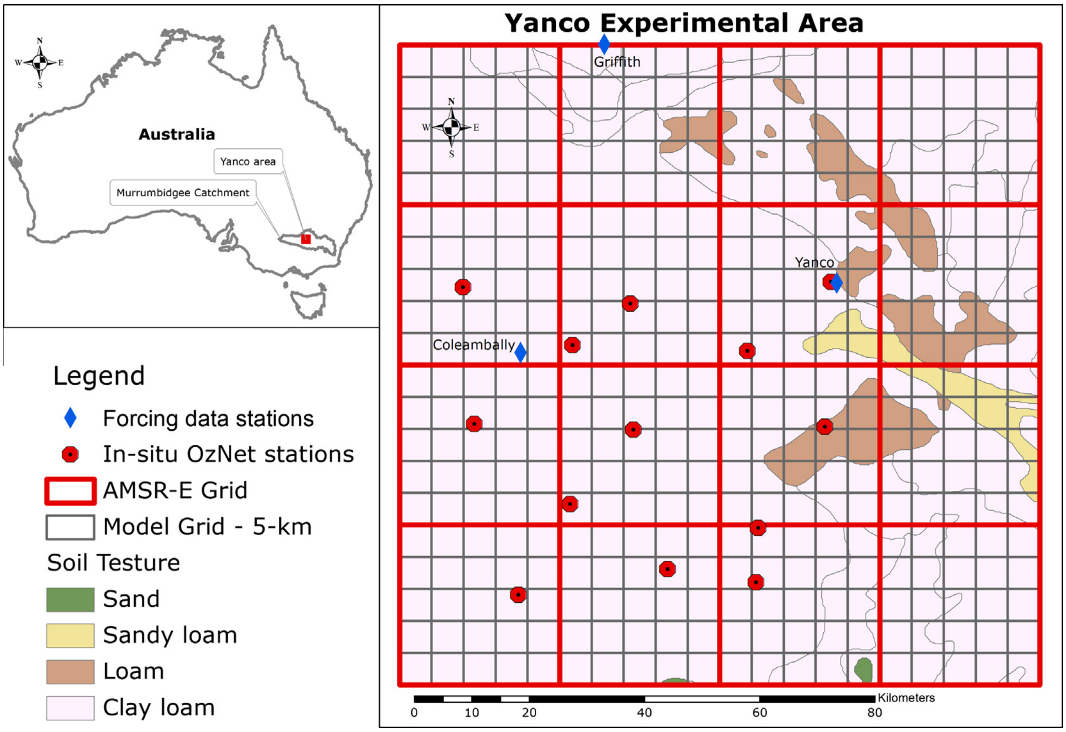

Fig. 1. The Yanco experimental area showing the forcing data stations, the in-situ OzNet soil moisture monitoring stations, the soil texture classes, the AMSR-E grid, and the 5-km model grid.

data to account for the energy balance partition between soil and vegetation surfaces, and to facilitate the estimation of water use by vegetation. The LAI data were obtained from the MYD15A2 Moderate Resolution Imaging Spectroradiometer (MODIS) data at 8-day temporal and 1-km spatial resolution. The model parameters and input forcing data were assigned to the 5-km modeling grid by using data from the nearest station for point-based data (e.g. forcing data), and data from overlapping areas for grid-based data (MODIS data). That is, the grid-based 1-km LAI data set was spatially averaged within each 5-km modeling grid. It is noted that the forcing data were at half-hourly interval, and as such, the modeling time step was conducted at the same temporal scale.

The observation soil moisture data used to drive the assimilation was the Land Parameter Retrieval Model (LPRM) derived soil moisture from AMSR-E (Owe et al., 2008). The AMSR-E LPRM derived soil moisture has been shown to provide improved soil moisture when compared to other algorithms (Crow et al., 2010). Additionally, the LPRM soil moisture data set has been validated under different physiographic conditions and widely used in several studies including Pipunic et al. (2011), Dumedah et al. (2011), Champagne et al. (2010), Gruhier et al. (2010), and Draper et al. (2009).

2.2. The evolutionary data assimilation strategy

Evolutionary algorithms are population based analytical methods which employ biological evolution and natural selection to address complex problems (Eiben and Smith, 2003; Coello Coello et al., 2002; Deb, 2001; Zitzler and Thiele, 1999). In evolutionary algorithms, a population of candidate members are allowed to compete based on evaluation conditions, after which the fittest (i.e. the most competitive) members are naturally selected and varied to reproduce new members for the population. The candidate members have both genotype information relating to their inherent or decision space properties, and phenotype information which is their expressed behavior in objective space (Eiben and Smith, 2003). As a result, the variation and reproduction of members are undertaken in genotype (or decision) space, while natural selection and competition between members occur in phenotype space. For a land surface model, the genotype represents a vector string of values which makeup the internal dynamics (states, parameters, input forcing data) of the model (Dumedah, 2012). A simplified representation of the genotype is presented in Fig. 2, where the land surface model components for parameters, initial states, and forcing data uncertainties are represented as a vector string of values. The resulting simulated model output is the expressed behavior of the model representing the phenotype. To assess the phenotype for multiple evaluation conditions, the concept of Pareto dominance (Zitzler et al., 2004; Deb, 2001; Goldberg, 1989) is usually employed to account for the multi-objective evaluation of candidate members.

The EDA employs the multi-objective evolutionary strategy based on the Non-dominated Sorting Genetic Algorithm – II (NSGA-II) developed by Deb et al. (2002), in a DA approach that merges the simulated model output with observation data. The reproduction and variation of new members is conducted using crossover and mutation operators that are stochastic, allowing the generation of diverse members for evaluation. Crossover allows the sharing of genotype information between competitive members, and ensures that new observational data do not overly drive the assimilation procedure (Dumedah and Coulibaly, 2013; Dumedah, 2012; Dumedah and Coulibaly, 2012a). The crossover operation has the capability to retain quality elements of the genotype for future assimilation time periods. The diversity in genotype space for population members is maintained by mutation operation which perturbs the genetic makeup of members. In phenotype space, diversity between members is achieved through a crowding operation, by replacing crowded members with similarly competitive members (Eiben and Smith, 2003; Deb et al., 2002; Coello Coello et al., 2002). Additional information on the operators in

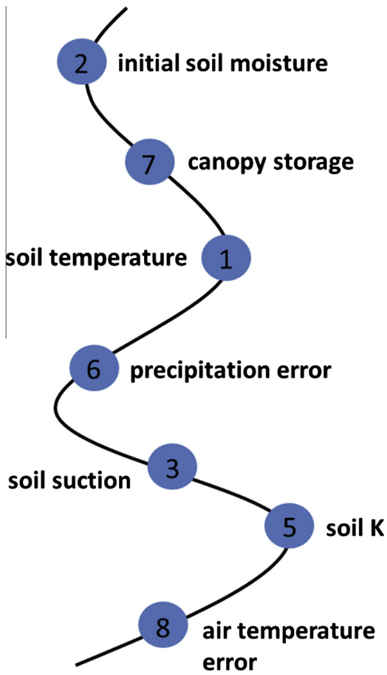

Fig. 2. A simplified genotype for a land surface model presented as a vector string of values for model parameters, state variables, and forcing data uncertainties representing a parameter pathway in decision space. The vector string indicates the genotype information for a candidate member of a population in the evolutionary strategy.

multi-objective evolutionary algorithms can be found in several sources including Dumedah (2012), Zitzler et al. (2004), Eiben and Smith (2003), Deb (2001), and Zitzler and Thiele (1999).

The EDA procedure implemented in this study follows Dumedah and Walker (2013) and Dumedah (2012). The EDA procedure begins by generating an initial population obtained by perturbing model parameters, states, and input forcing data. The population members are applied into CABLE to generate the ensemble predictions forward in time. A corresponding number of observation ensemble members are generated based on the AMSR-E observation soil moisture and its associated uncertainty. The population members are evaluated by using the ensemble predictions and observations to determine the absolute difference (according to Eq. (1)), and the cost function (in Eq. (2)).

$$AbsDiff = |y_i - y_{o,i}| \tag{1}$$

where y_i is the simulated soil moisture from a population member; $y_{o,i}$ is the observed soil moisture from an observation ensemble member.

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

where $y_{b,i}$ is the background (i.e., forecasted) soil moisture for the ith data point; σ_b^2 is the variance for the background soil moisture; σ_o^2 is the variance for the observation soil moisture; y_i represents the analysis (i.e., the searched) soil moisture for ith data point which minimizes $J(\hat{y}_i)$; and t is the number of data points or the time (note that $t = 1$ in this case for sequential assimilation).

The high performing members with optimal compromise between the simulated output and the observation are selected and varied to determine new members for the population. This complete cycle comprising evaluation, selection and variation of members, and reproduction of new members constitutes one cycle of a generation. Consequently, the ensemble members undergo evolution within a population, whereas the population as a unit undergoes evolution across several generations. At the referenced generation when population members have been evolved across several generations, the final evolved members are chosen to represent the updated members. The updated members, in this case, are a subset of all members that have been evaluated at the current assimilation time step. The evolution procedure is repeated to determine the updated members for each assimilation time step. It is noted that updated members were seeded between assimilation time steps, and also applied to make model forecasts forward in time for subsequent assimilation time steps.

2.3. Evolutionary data assimilation approach for model uncertainty estimation

In the EDA approach, updated ensemble members for each assimilation time step were obtained as a subset of several members which have been evaluated and evolved over numerous generations at each assimilation time period. It is noted that the genotype information for previous assimilation time steps were seeded and shared with future assimilation time periods. The procedure to seed updated members for future time periods is an established evolutionary strategy, elitism (Zitzler et al., 2004; Eiben and Smith, 2003; Deb, 2001), allowing competition between old and new population members with the capacity to retain quality members for future generations. The uncertainties in the simulated output and the observation were accounted for through the cost function and the absolute bias in phenotype space. Accordingly, the changes in genotype space measure the temporal changes of the updated members which is indicative of the internal dynamics of the model, needed for the optimal compromise between the model and the observation.

It is important to emphasize the unique nature of the updated ensemble members obtained from the EDA procedure. The updated members are equally competitive, in the sense that each member provides a unique tradeoff between the simulated output and the observation. Based on the evaluation conditions, the updated members were not dominated by other members, that is, they are fitter than all other members which have been evaluated at each assimilation time period. For a given assimilation time period, the updated members represent the optimal model dynamics (in terms of parameters, states, and input forcing data), chosen from among several scenarios, to best merge the simulated output to the observation with the least tradeoff. Given these unique properties of the updated ensemble members obtained from the EDA, it is crucial to assess the model behavior, the tradeoffs, the model-observation dynamics, and the dynamics in genotype space through time with the potential to learn about the various components of the model.

In genotype space, the updated ensemble members can be examined in two different phases: (i) convergence, and (ii) parameter pathway evaluations. The convergence analysis evaluates the updated members using clustering analysis on a parameter-by-parameter basis across all assimilation time steps, to obtain the level of convergence achieved for each parameter. The estimation of convergence for model parameters, states, and input forcing uncertainty follows the procedure outlined in Dumedah and Walker (2013). For the updated members, the sub-string of the genotype comprising model parameters and states represent the landscape properties from the model standpoint. Consequently, their clustering across time is equivalent to the spatial variations in the landscape properties data. That is, the convergence estimate approximates the spatial variation in the landscape properties data in concert with the model-observation dynamics.

Given that the dynamics between the simulated output and the observation is optimally compromised in phenotype space, the associated changes in genotype space need evaluation. Accordingly, the persistent temporal clustering for the individual model parameters in genotype space represents the spatial variations in landscape properties, needed to obtain the compromised merging between the simulated output and the observation. It is noted that the convergence estimate is the minimum uncertainty needed for each model parameter, and state variable, to obtain a consistently optimal compromise between the model and observation across all assimilation time periods. As a result, the estimated convergence levels approximate the minimum threshold for landscape spatial variability, within which to obtain the optimal merger between the simulated output and the observation across the assimilation time periods.

It is noteworthy that the temporal changes in model parameters are due to a selection from among several parameter scenarios, derived from a spatially varied landscape. That is, the temporal changes in model parameters were mainly in response to spatial variations in the landscape, rather than the fluctuations in meteorological forcing data. In concert with the landscape data, the ensemble of model parameter values are equally valid because they represent a natural mix of landscape properties. In brief, the landscape is spatially varied in a way that is best represented with an ensemble of model parameter values. Therefore, given the spatial variations in the landscape, the estimated convergence represents the corresponding optimal uncertainty in model states and parameters from the model standpoint. The combined EDA and clustering procedure is capable to determine the optimal uncertainty in model parameters and states needed to account for a given spatial variation in the landscape.

In the parameter pathway analysis, the updated members are examined using multi-dimensional clustering to determine the persistent parameter pathway in decision space. The updated members for each assimilation time step represent the optimal values for model parameters, state variables, and the forcing data uncertainties. The multi-dimensional clustering of these updated members across all assimilation time steps determines the overall optimal parameter pathway, and therefore the individual uncertainties for model parameters, states, and input forcing variables. That is, given a perfect model structure, the estimated parameter pathway approximates the uncertainty for each model parameter, state variable, and input forcing data uncertainty. The estimated parameter pathway represents the minimum uncertainty interval within which to obtain a consistently optimal compromise in phenotype space across all time periods. The significance of the estimated parameter pathways lies in the monitoring of model components, which are intricately linked through the updated members, and their temporal persistence under different input data, states and observation conditions.

It is noted that the clustering analysis performed for both convergence and parameter pathway evaluations provides an interval for model parameters, state variables, and forcing data uncertainties. The clustering performed in both cases explored the degree of commonality across assimilation time periods: for each parameter at a time in the convergence case, and simultaneously for all parameters in a multi-dimensional approach for the parameter pathway case. The significance of the estimated clusters is due to their persistence across the assimilation time periods, supported by the level of commonality between the individual time steps. Consequently, this uncertainty estimation procedure accounts for the inaccuracies due to changes in observation and input forcing data under different time periods, and the associated model response with respect to these changes. It is important to point out that other analytical classifiers can be used to assess the distribution of the updated ensemble members, and that the choice of cluster analysis should not be thought of as the norm. The rationale for the use of clustering (Dumedah et al., 2010) is, if and only if, a pattern of clustering is observed following the 'knee' testing procedure outlined in Thorndike (1953).

The convergence and parameter pathway evaluations estimate specific uncertainties for landscape spatial variability, model parameters, initial states, and input forcing variables. These uncertainty estimates represent significant error sources for a perfect model structure, and it is assumed that the remaining uncertainty in the simulated model output is due to model physics.

2.4. Setup of model and data assimilation runs

The EDA procedure was used to assimilate the AMSR-E derived soil moisture into CABLE at a daily time step from July 1, 2006 to June 31, 2007. A population of 40 members was evolved across 5 generations, with 20 updated members selected for each assimilation time step. That is, for each assimilation time step an ensemble of 200 (i.e. 40×5) members were evaluated after which 20 optimal ones were selected as the updated members. The initial population members were generated based on the uncertainty intervals for model parameters, states, and input forcing variables in Table 1. For subsequent population members and assimilation time steps, the uncertainty values for model parameters, states, and forcing variables were derived from the population members, with the uncertainties constrained to the lower and upper bounds found in Table 1. It is noted that the original values for model parameters and states were determined by soil and land cover data in concert with the CABLE model. Using these original values, the model parameters were perturbed using a relative measure, such that an ensemble value for a model parameter is always relative to the original model parameter value determined from the landscape properties data. Similarly, the input forcing variables were perturbed using a relative measure. The state variables were also perturbed using a relative measure from their updated values.

The observation uncertainty used for the AMSR-E derived soil moisture was set to 0.05-m^3/m^3 (Pipunic et al., 2011), whereas the simulated soil moisture uncertainty was derived adaptively from the updated population members. It is important to point out that the simulated soil moisture for the first layer (i.e., top 2.2-cm) in CABLE were used in the evaluation against the observation AMSR-E soil moisture, since the AMSR-E observation is equivalent to the top $\sim$2-cm soil moisture. Following the standard NSGA-II implementation, a crossover probability of 0.8 and a mutation probability of $1/m$ (where m is the number of variables) were used to perturb and reproduce new population members.

3. Results and discussion

3.1. Evaluation of the updated soil moisture

A typical evaluation of the assimilation procedure is the comparison of its updated estimates against the open loop estimate and some 'truth' estimates. The open loop soil moisture was determined by using CABLE input values, which are randomly selected from the minimum and maximum bounds of model parameters, initial states, and forcing variables in Table 1. The soil moisture comparison between the open loop and the updated estimate is shown in Fig. 3, where the AMSR-E is taken as the truth estimate for the surface layer. The assimilation procedure has improved upon the open loop estimates with reductions in both root mean square error (RMSE) and bias by 0.066 m^3/m^3 and 0.063 m^3/m^3 respectively. These improvements amount to about 60% reduction in RMSE and about 70% reduction in bias. Usually, an increased accuracy in the updated estimate of the surface soil moisture relative to the assimilated observations is expected against the open loop estimate, so additional evaluation of the updated estimate is

Table 1
Description of model parameters, initial states and input forcing variables for the CABLE model. These model parameter intervals were estimated in concert with land cover, soil and meteorological forcing data in the Yanco area.

Parameter	Description	Interval (%)
Model parameters		
clay	Fraction of soil which is clay (–)	±10
sand	Fraction of soil which is sand (–)	±10
silt	Fraction of soil which is silt (–)	±10
froot	Fraction of roots in each soil layer (–)	±10
albsoil	Snow free shortwave soil reflectance fraction (–)	±10
bch	Parameter b, Campbell eqn 1985 (–)	±10
css	Heat capacity of soil minerals (J/kg/C)	±10
hyds	Hydraulic conductivity at saturation (m/s)	±10
rhosoil	Density of soil minerals (kg/m^3)	±10
sucs	Suction at saturation (m)	±10
sfc	Fraction of soil volume which is water at field capacity (–)	±10
ssat	Fraction of soil volume which is water at saturation (–)	±10
swilt	Fraction of soil volume which is water at wilting point (–)	±10
Meteorological forcing variables		
SWdown	Downward shortwave radiation (W/m^2)	±10
LWdown	Downward longwave radiation (W/m^2)	±10
Tair	Near surface air temperature (K)	±10
Qair	Near surface specific humidity (kg/kg)	±10
Rainf	Rainfall rate (mm/s)	±10
Wind	Surface wind speed (m/s)	±10
LAI	Leaf area index (m^2/m^2)	±10
Model state variables		
SoilMoist	Average layer soil moisture (m^3/m^3)	Updated
SoilTemp	Average layer soil temperature (K)	Updated
CanopInt	Canopy intercepted water storage (kg/m^2)	Updated

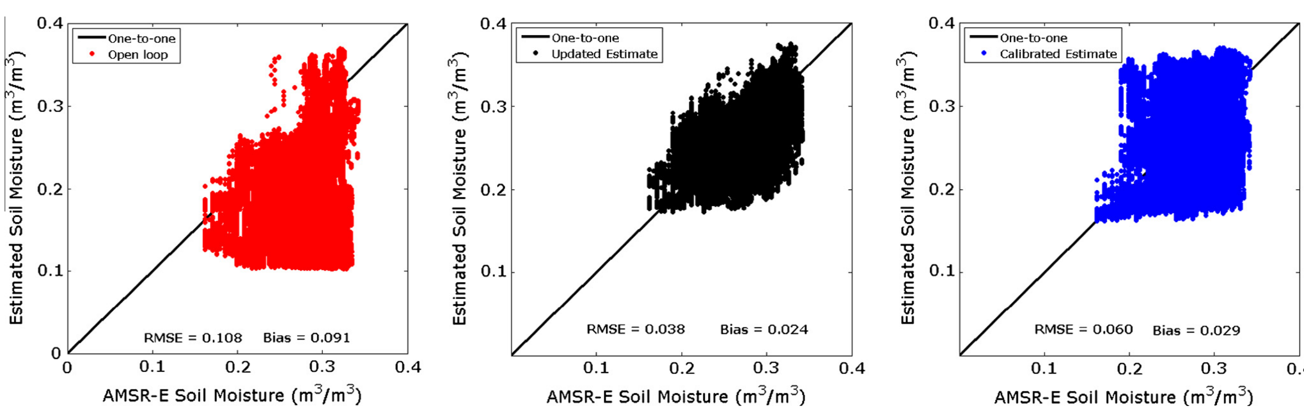

Fig. 3. Soil moisture comparison between the open loop, the updated and the calibrated estimates for all grids at the surface soil layer.

needed. A calibration procedure has been undertaken to match the AMSR-E soil moisture to the model estimates from CABLE. The calibrated soil moisture estimates are compared to the updated estimates in Fig. 3. The calibration procedure also improved upon the open loop estimation, yet its accuracy is not up to those obtained from the updated estimate. The calibration and the updated estimates have similar bias values, whereas a superior RMSE was obtained for the updated estimate with a reduction of about 37%.

Additionally, the assimilation procedure was assessed by comparing the updated estimates to OzNet in-situ soil moisture in Fig. 4. The OzNet comparison to the AMSR-E soil moisture (in the left-hand panel) shows an inaccurate temporal relationship between the two data sets. This inaccurate temporal accuracy is reflected in the OzNet soil moisture comparison to the updated estimate, with a slightly improved RMSE and bias values in comparison to the AMSR-E data. The calibrated estimate, which is based on the matching between the OzNet in-situ soil moisture and the CABLE model estimate is shown in the right-hand panel (in Fig. 4). The comparisons show that the calibration and the updated estimates have similar evaluation accuracies in both RMSE and bias values. That is, the updated estimate is no worse than the inaccuracy that exists between the OzNet and AMSR-E data sets, and has an accuracy comparable to those obtained from the calibration estimate.

3.2. Estimation of minimum uncertainty due to landscape spatial variation

To estimate the minimum uncertainty for model parameters and states needed to account for the landscape spatial variations, the parameter-by-parameter clustering described in Section 2.3 was performed on all the updated members to determine the dominant clusters. The updated members comprise an archive of all ensemble members obtained for each assimilation time step. The estimated dominant clusters were used to represent convergence

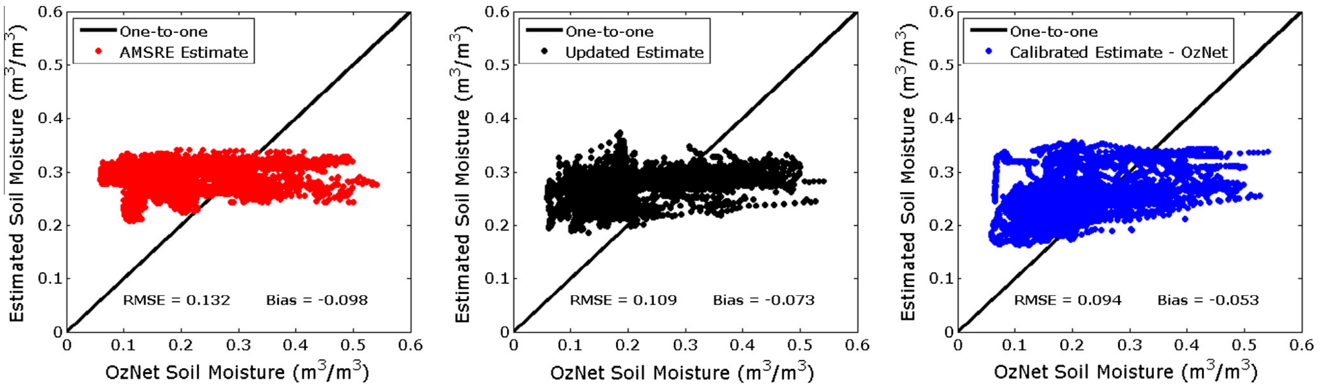

Fig. 4. OzNet in-situ soil moisture comparison to the AMSR-E, the updated estimate, and the calibrated estimate based on OzNet data for all model grids overlapping the 13 OzNet monitoring stations in the Yanco area.

estimates for model parameter and states, which in turn, were equated to the minimum uncertainty required from the model standpoint to accommodate the spatial variations in the landscape. A test of clustering according to the knee approach (Thorndike, 1953), was performed for each variable in decision space, and the suitable number of clusters was selected to group the parameter values. The selected cluster for each parameter and their centroid, minimum and maximum bounds, and their coverage of the entire decision space are presented in Table 2. The coverage, in this case, is a frequency based estimate which was determined as the ratio of the number of members in the largest membership cluster to the total number of updated members available across all assimilation time steps. This frequency based estimate of the coverage is equivalent to the level of convergence attained for each model parameter (Dumedah and Walker, 2013).

The clustering results show that the number of cluster groups range between 4 and 8, with 80% of the parameters having a coverage greater than 50%. The plot of the dominant cluster bounds, and the updated bound in relation to the initial bound for all decision variables are shown in Fig. 5. The updated bound represents the minimum and maximum values obtained for each updated decision variable across all assimilation time steps. It is noted that even though the updated bound is presented as a continuous interval, the frequency of values within this interval is not uniformly distributed. Given that the updated ensemble is a selected subset of all evaluated members, the intervals for individual model parameters, states and forcing variables are unique. The proportion of the area covered by the updated bound as a percentage of the original bound is 75%, indicating a 25% reduction in the search space of the original bound. However, the dominant cluster bound has further reduced the original bound by 76%. The proportion of the area covered by the dominant cluster as a percentage of the updated bound is about 30%, representing a 70% reduction of the search area covered by the updated bound. In general, an overall clustering of 6 groups was found to have a frequency based coverage of about 56%, with a 70% reduction of the updated bound. The estimated values of the dominant cluster bound are equivalent to the minimum uncertainty needed from the model standpoint to account for the landscape spatial variations.

3.3. Estimation of the minimum uncertainty for model components

While the individual uncertainties that account for landscape spatial variations in the above section are important, the simulated soil moisture from the model is subject to the simultaneous interactions from all model components. Consequently, the uncertainties for model parameters, states and input forcing data were quantified through a multi-dimensional clustering analysis of the

Table 2
Dominant intervals for model parameters, initial states, and input forcing variables, represented by the largest membership clusters. The definition of the coverage in genotype (or parameter) space is given by number of clustering groups, their centroids and lower and upper bounds. The coverage is expressed in percentage, with a maximum value of 100 representing a perfectly converged cluster and a value close to zero represents a sensitive cluster.

Parameter	Clusters	Centroid	Lower bound	Upper bound	Coverage (%)
clay	7	−0.0343	−0.0556	−0.0156	50.45
sand	8	0.0046	−0.0112	0.0110	44.58
silt	6	0.0058	−0.0112	0.0199	59.11
froot	7	−0.0322	−0.0556	−0.0156	44.30
albsoil	4	−0.0069	−0.0556	0.0199	73.94
bch	5	−0.0048	−0.0556	0.0199	79.21
css	6	0.0041	−0.0112	0.0199	51.81
hyds	5	−0.0171	−0.0556	0.0110	72.54
rhosoil	5	−0.0072	−0.0556	0.0199	61.66
sfc	4	−0.0209	−0.0556	0.0199	68.05
ssat	6	−0.0145	−0.0556	0.0110	65.31
sucs	6	−0.0111	−0.0556	0.0199	70.73
swilt	6	−0.0301	−0.0556	−0.0156	55.24
SWdown	5	−0.0752	−0.0867	−0.0600	42.18
LWdown	8	−0.0749	−0.0867	−0.0600	35.19
Tair	5	0.0348	−0.0023	0.0598	43.15
Qair	7	0.0919	0.0643	0.0998	74.70
Rainf	5	0.0837	0.0643	0.0998	49.53
Wind	7	0.0900	0.0643	0.0998	57.78
LAI	5	0.0901	0.0643	0.0998	32.90

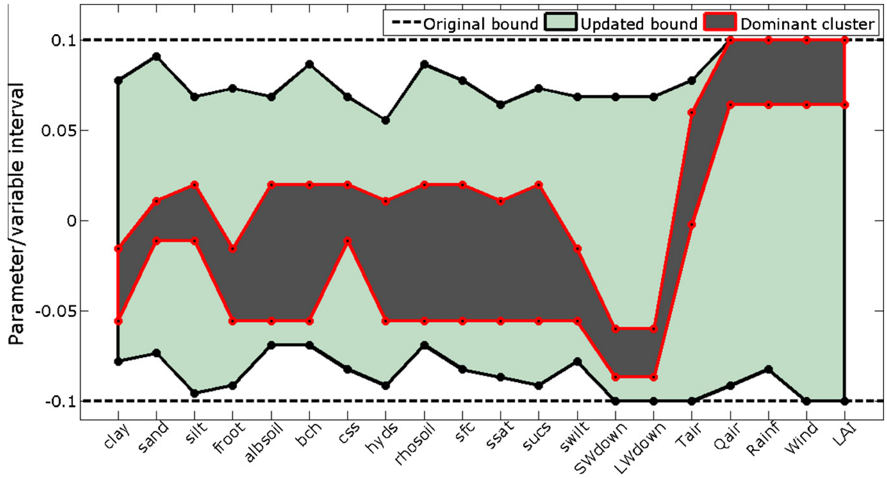

Fig. 5. Model parameter/variable intervals showing the original intervals, the updated bound obtained from the EDA procedure, and the dominant clusters obtained through the assessment of the updated members in genotype space.

updated members, as described in Section 2.3, to determine the optimal parameter pathway. It is worth emphasizing that the parameter pathway analysis accounts for the inter-connectedness of model components, together with the temporal persistence of parameter values across the assimilation time steps. Using the knee approach (Thorndike, 1953) for the test of clustering, the appropriate number of cluster groups was found to be 8, with an overall frequency based coverage of 50%. The largest membership cluster found was used to represent the dominant parameter pathway (or simply, the dominant pathway), and is shown in Fig. 6.

The multi-dimensional clustering result shows that the area covered by the dominant pathway as a percentage of the original bound is about 32%, indicating a 68% reduction in the original search area. The area covered by the dominant pathway expressed as a percentage of the updated bound is 38%, representing a 62% reduction in the search area of the updated bound. The estimated dominant pathway represents the temporally stable values for model parameters, states, and forcing data uncertainties, which have remained persistent across all the assimilation time steps. The estimated values of the dominant pathway are equivalent to the minimum uncertainties needed for the individual model parameters, states, and input forcing variables to obtain a comparable estimate of the updated soil moisture across all the assimilation time steps.

To assess the robustness of the estimated dominant pathway, an ensemble of 20 members was generated based on the dominant pathway and applied into CABLE to estimate the soil moisture. The rational for this estimation was to compare the estimated soil moisture from the dominant pathway to the updated soil moisture obtained through the assimilation procedure. The AMSR-E soil moisture comparison to the estimate from the dominant pathway is shown in Fig. 7, with the updated estimate shown earlier in Fig. 3. The soil moisture comparison shows that the accuracy decline from the updated estimate to the dominant pathway estimate is about 47% ($\ll$0.02 m^3/m^3) based on the RMSE, together with an improved estimate of bias in the dominant pathway output.

Additionally, the dominant pathway estimate is evaluated against the OzNet in-situ soil moisture in Fig. 8, with the calibrated and updated estimates shown earlier in Fig. 4. In this case, the dominant pathway improved the estimated soil moisture when compared with the calibrated and updated estimates, based on both the RMSE and bias values. When compared with the calibrated estimate, the dominant pathway estimate has reduced the RMSE value by 17%, and the bias value by 57%. A higher accuracy increase was found when compared to the updated estimate, with a 28% and 68% decline in RMSE and bias respectively from the dominant pathway estimate. The higher soil moisture estimation

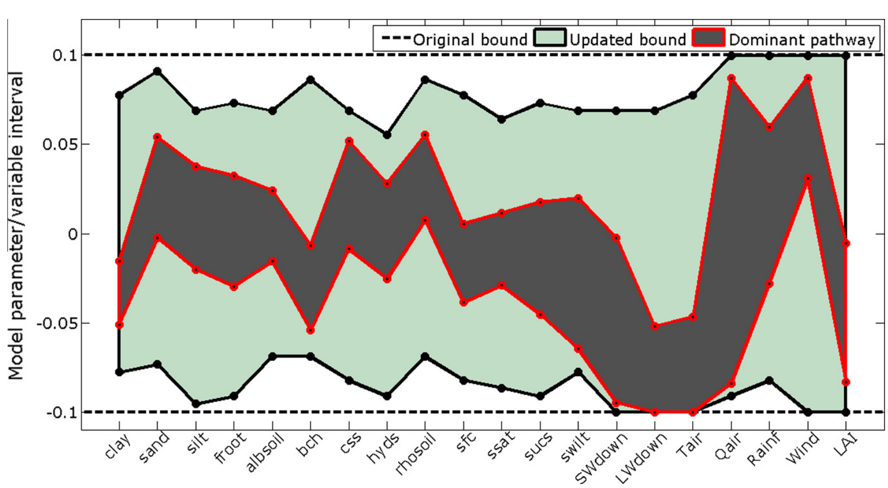

Fig. 6. Model parameter/variable intervals showing the original intervals, the updated bound obtained from the EDA procedure, and the dominant parameter pathway obtained through the assessment of the updated members in genotype space.

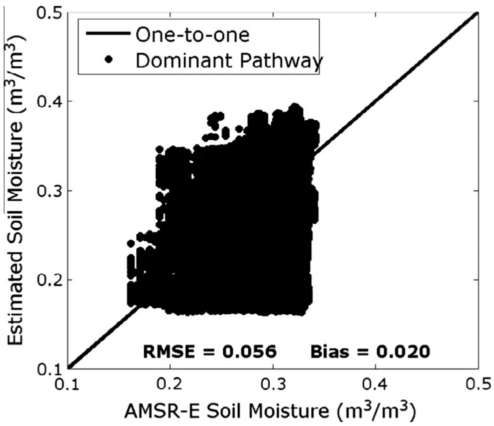

Fig. 7. Comparison between the AMSR-E soil moisture and the estimate from the dominant pathway.

accuracy from the dominant pathway demonstrates its high prediction potential given its small number of ensemble membership and limited uncertainty interval.

3.4. Significance and implication of findings

The predictive potential demonstrated through the improved soil moisture estimates obtained from the assimilation procedure and its dominant pathway is important. But the key findings of this study are focused on learning about the land surface model from decision space while using the model predictions in objective space only as a guide. The EDA approach has uniquely facilitated this learning process, providing updated members which capture the model dynamics both in decision space and objective space through time. The EDA being a natural union between the evolutionary strategy and temporal updating of data assimilation, accommodates the simultaneous interactions between model components and their persistence through time. But the key potential of the EDA contribution lies in the assessment of its updated members, mainly in decision space. While the updated membership is massive with several strings of values, some of which may be redundant at certain time periods, their inclusion is important to maintain the adaptive nature of the updated ensemble with the capability to accommodate changing environment (landscape, climate, etc) conditions.

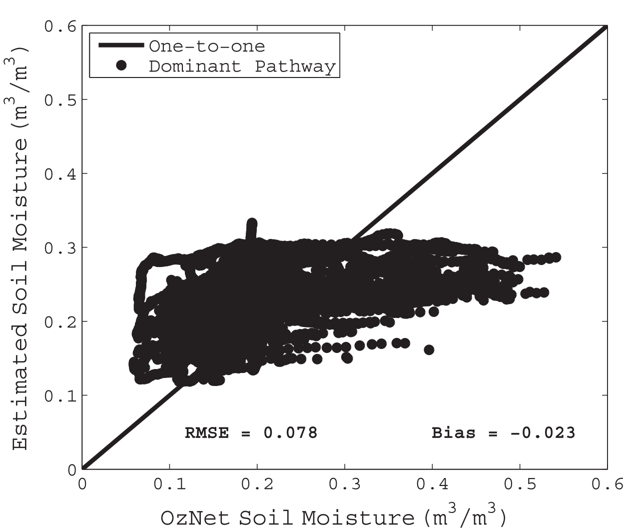

Fig. 8. OzNet in-situ soil moisture comparison to the estimate from dominant pathway for all model grids overlapping the 13 OzNet monitoring stations in the Yanco area.

The assessment of the updated members in decision space through clustering analysis quantified the minimum uncertainty needed from the model standpoint to accommodate the spatial variations in the landscape. While this uncertainty is usually ignored or not accounted for in the past, our findings showed the significance of considering this inaccuracy in the diagnosis of model uncertainty. Additionally, the evaluation of the updated members demonstrates the need for finding robust pathways in decision space, instead of single scenarios of parameter values. Our findings in the dominant pathway illustrate that values for model parameters, states, and forcing data uncertainty can be temporally persistent over several assimilation time periods, with the potential for trading-space-for-time (Troch et al., 2009) analysis. Moreover, the assessment of the updated members showed how the individual model parameters, states and input forcing variables respond from the model standpoint to changes in observation data. For example, the model response to precipitation data was to increase rainfall input when accounting for landscape spatial variations, but when considered in relation to other parameters, the model response was to moderate/reduce the rainfall input. Another distinct example is the model response to LAI data; the model needed more vegetation cover to account for the landscape spatial variations whereas the dominant pathway analysis showed that less vegetation cover is needed when considered in relation to other parameters.

Additionally, it is noted that the uncertainty intervals for the individual model parameters, states and forcing variables represent their sensitivity levels in accordance with the definition of robustness in Willink (2008), Ross et al. (2008), and Deb and Gupta (2006). That is, smaller uncertainty intervals represent highly sensitive parameters, where small changes in their uncertainty values will produce considerable model response in the soil moisture output. The larger uncertainty intervals signify robust parameters, where small changes in their uncertainty values will not cause considerable changes in the simulated soil moisture. When accounting for the spatial variability of the landscape, all the forcing variables were found to be sensitive in comparison to the model parameters and states. Since the landscape properties are more closely linked to model parameters and states, their uncertainty intervals were much larger, thus incorporating the different aspects of the landscape properties. In the dominant pathway evaluation, the uncertainty intervals were mostly found to be robust mainly because these intervals focused on the interconnectedness of all model components.

Furthermore, our findings showed that the path towards the diagnosis of model inaccuracy is not straightforward, and that frameworks are needed to study the model dynamics, particularly in decision space, and for the quantification uncertainties in relation to both individual and combined impacts of model components. The EDA approach and the subsequent assessment of its updated members have been shown to quantify uncertainties for model components, with the potential to steer future research towards further diagnosis of model weakness.

4. Summary and conclusion

This study has examined the uncertainties associated with model parameters, initial states, input forcing variables, and landscape spatial variations for the CABLE land surface model in a soil moisture estimation for the Yanco area in south-east Australia. The uncertainties for the model components were assessed by assimilating the LPRM retrieved soil moisture from the AMSR-E into the CABLE model through the EDA approach. The comparison of the updated soil moisture to both open loop and calibrated estimates showed improved estimation accuracy from the EDA procedure. When the updated members were compiled in decision space across all assimilation time periods, it was found to cover 75% of the original uncertainty bound, indicating a 25% reduction in the original uncertainty interval.

The updated ensemble members were analyzed mainly in decision space through clustering analysis to quantify the uncertainties for specific model components. The assessment of the updated members in decision space was performed in two phases: (i) in a one-dimensional parameter-by-parameter clustering to assess the uncertainty associated with landscape spatial variations, and (ii) in a multi-dimensional clustering to determine the temporally persistent parameter pathway with dominant coverage in decision space. The findings from the parameter-by-parameter clustering analysis showed that the overall minimum uncertainty needed from the model standpoint to account for the landscape spatial variability was 24% of the original uncertainty bound and 30% of the updated bound, representing a search space reduction of 76% and 70% for the original and updated bounds respectively. Moreover, it was found that the model parameters and initial states were generally more robust in comparison to forcing variables when accounting for the spatial variability of the landscape.

The estimated dominant pathway was found to cover 32% of the original uncertainty bound and 38% of the updated bound, representing a search area reduction of 68% and 62% for the original and updated bounds respectively. The temporal persistence of the dominant pathway showed its robustness level, with small changes in the uncertainty bound for individual parameters, resulting in less dramatic (or minor) changes in the model response. Additional evaluation of the dominant pathway showed that its estimated soil moisture can reproduce (or approximate) the updated estimate with a RMSE smaller than 0.02 m^3/m^3 and with superior bias estimate. When evaluated against OzNet in-situ soil moisture, the dominant pathway estimate of soil moisture was found to be more accurate than both the calibrated and the updated estimates. Thus, the dominant pathway is reasonably representative in both: (i) decision (or genotype) space representing a 38% area coverage and a 50% frequency based coverage of the updated bound, and (ii) objective (or phenotype) space approximating the updated soil moisture with comparable accuracy levels.

These findings are significant and provide solid steps towards integrated assessment of the weaknesses in land surface prediction models. Moreover they point to both a diagnostic and a prediction potential of the EDA approach, providing an assessment of its updated ensemble membership. It is important that future studies develop additional techniques to assess the updated members, with the capability to identify landmarks in decision space. Additional methodologies are needed for the assessment of the updated membership to map out unique pathways which are associated with specific model response in objective space, for example, model response to extreme weather conditions, extreme changes in the landscape or landuse change.

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