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A generalized Gaussian distribution based uncertainty sampling approach and its application in actual evapotranspiration assimilation

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ABSTRACT

It is extremely important for ensemble based actual evapotranspiration assimilation (AETA) to accurately sample the uncertainties. Traditionally, the perturbing ensemble is sampled from one prescribed multivariate normal distribution (MND). However, MND is under-represented in capturing the non-MND uncertainties caused by the nonlinear integration of land surface models while these hypernormal uncertainties can be better characterized by generalized Gaussian distribution (GGD) which takes MND as the special case. In this paper, one novel GGD based uncertainty sampling approach is outlined to create one hypernormal ensemble for the purpose of better improving land surface models with observation. With this sampling method, various assimilation methods can be tested in a common equation form. Experimental results on Noah LSM show that the outlined method is more powerful than MND in reducing the misfit between model forecasts and observations in terms of actual evapotranspiration, skin temperature, and soil moisture/ temperature in the 1st layer, and also indicate that the energy and water balances constrain ensemble based assimilation to simultaneously optimize all state and diagnostic variables. Overall evaluation expounds that the outlined approach is a better alternative than the traditional MND method for seizing assimilation uncertainties, and it can serve as a useful tool for optimizing hydrological models with data assimilation.

1. Introduction

As the nature feedback of land surface water to atmosphere, actual evapotranspiration (AET) bridges the water and energy balances by allocating energy in geosphere, biosphere and hydrosphere to reflect the interaction between land surface processes and climate change (Xu et al., 2011). As a core subprocess in water and energy cycles, accurately estimating AET has important scientific and practical significances for drought prediction (Li et al., 2016; Xiong et al., 2015), crop yield estimation (Kukal and Irmak, 2016; Jiang et al., 2016), irrigation and drainage (Güçlü et al., 2017; Liu et al., 2016), and water resources management (Jarihani et al., 2015; Billah et al., 2015; Renzullo et al., 2008; Xu et al., 2011). Land surface models (LSMs) can forecast AET continuously both temporally and spatially but with greater uncertainties compared with in situ observations or remote sensing retrievals due to coarse meteorological forcing, unrepresentative model parameters, incomplete model parameterization, and/or inaccurate model initial field et al. (Meng et al., 2009). Data assimilation (DA) aims at producing a statistically optimal and kinetically consistent forecast trajectory by integrating the certainties of model forecasts and observations according to their inherent uncertainties to correct model state variables and parameters within the framework of Bayesian inference (Reichle, 2008). Hence, it is crucial for the success of actual evapotranspiration assimilation (AETA) to specify the uncertainty statistics of the observations and state field (Petrie and Bannister, 2011; Chen et al., 2015).

Currently, ensemble KF (EnKF) (Evensen, 1994) based methods have been becoming the mainstream because they have two attractive advantages: (1) model independence avoids adjoint models; and (2) time-dependence can provide high order moments of errors by the uncertainty flow (Xue and Zhang, 2014). These methods mainly include variance localization/reduced/inflation EnKF (Han and Li, 2008), ensemble adjustment/transform/ square root KF (Vrugt et al., 2013), double EnKF (Houtekamer and Mitchell, 2001, 1998), particle filter (PF) (Doucet and Johansen, 2011), unscented Kalman Filter (KF) (van der Merwe et al., 2000), sampling importance resampling PF (Arulampalam et al., 2002), regularised PF (Musso et al., 2001), etc. Later, EnKF is also coupled into four dimensional variational DA (4Dvar), such as ensemble 4Dvar (En4DVar) (Liu et al., 2009), proper orthogonal decomposition En4DVar (PODEn4DVar) (Tian et al., 2011), 4Dvar EnKF

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(4DLETKF) (Hunt et al., 2004), auto-tuned DA (Crow and Yilmaz, 2014). In such cases when LSMs and observation operators are both linear and the uncertainties follow multivariate normal distribution (MND), KF as the analytic solution of DA can achieve the best effect (Wikle and Berliner, 2007). When the two assumptions do not hold, KF based methods represent the uncertainties of state variables using perturbing samples produced from given probability density functions (pdfs), then replace background error covariance matrix by the sample covariance matrix (Li et al., 2014).

In practice, because it is difficult to know the accurate a priori pdfs of the uncertainties in advance, KF based DA methods usually assume the pdfs of the uncertainties follow MND (Storto, 2016), which will cause nonnegligible DA bias since the true pdfs will never be MND (Murphy and Godsill, 2016). Despite the assumption is right at the beginning of DA, the MND will be transformed into non-MND due to the nonlinear integration of LSMs, hence, MND is usually not a good choice for sampling the uncertainties because it cannot accommodate the hypernormal pdfs arising in DA, then probably results in suboptimal DA results (Bishop, 2016). PF-like methods do not require the pdf types of uncertainties, but the improper selection of the proposal pdfs will lead to particle degradation, and may also introduce additional uncertainties (Bocquet et al., 2010), moreover, they are scarcely evaluated in the case of non-MND (Han and Li, 2008; Moradkhani et al., 2012). Therefore, how to accurately designate the pdfs of the uncertainties has become the bottleneck of DA further advance though many DA systems and methods have been developed. To more accurately and representatively sample the uncertainty, non-MNDs should be covered (Bishop, 2016; Bocquet et al., 2010; Murphy and Godsill, 2016; Moradkhani et al., 2012).

Up to now, there have been some explorations about the application of non-MND pdfs to DA. Cohn (1997) performed a logarithm transformation on state variables and observations under lognormal statistics, which transformed linear observation operator to be nonlinear. Simon and Bertino (2009) switched state variables between non-MND and MND with (inverse) numerical anamorphosis functions while correlation considered anamorphosis functions were intricate. Bulygina and Gupta (2009) conjectured the uncertainty structure of hydrological models by Bayesian DA with pre-assumed pdfs. Bocquet et al. (2010) generalized the techniques of tackling the problem beyond normality, and stated the difficulties to be circumvented. Pires et al. (2010) diagnosed the sources and impacts of the innovation nonnormality under the case of additive errors. Lei and Bickel (2011) debiased EnKF to forecast ensemble with the desired pdf but the collapse problem of PF had not yet been tackled. Ebtehaj and Foufoula (2011) recovered the non-normal states of geophysical processes via wavelet sparse regularization. Song et al. (2012) constructed one lognormal distribution based cost function by only applying the logarithm transform to these variables mapped to observation space.

Nakano (2014) hybridized ensemble transform KF and importance sampling PF for assimilating non-normal observations, but it was not effective when the ensemble deviated from the true state. Yen et al. (2014) examined the significance of multisource uncertainties in controlling and reducing the predictive errors of watershed behavior. Metref et al. (2014) proposed one multivariate rank histogram method to yield a fully nonparametric transform for ensemble DA, which was just tested with an idealized Lorenz 63 model not a realistic one. Bishop (2016) featured the uncertainty pdfs of semi-positive-definite variables into Gamma, inverse-Gamma and normality for optimizing ensemble production. Storto (2016) relaxed the pdfs to be heavier-tailed than normality for assimilating observations with poor quality however the minimization at first exhibited a low score. Attia et al. (2016) proposed a cluster Hamiltonian Monte Carlo sampling filter for non-normal DA while the sampling efficiency would be reduced by the local ensemble with an improper size. Key results for these studies are summarized in Table 1. Although these methods dissect the contribution of the uncertainties of various pdfs on DA, they cannot act as a general method to estimate and control hypernormal uncertainties due to their complex causes and diverse forms.

To capture these hypernormal uncertainties in DA, this paper has three objectives: (1) a novel sampling method is outlined based on generalized Gaussian distribution (GGD); (2) with the GGD samples created, three traditional assimilation methods are unified into a common DA equation; and (3) the outlined method is tested through two assimilation experiments. The outlined method is founded on the simulation technique (Nardon and Pianca, 2006; Song, 2006; Yu et al., 2012). Unlike above ways, it needs neither space transform nor specific hypothesis since GGD is one pdf of universival significance, so it can also manage the propagation of MND errors during nonlinear LSM integration because MND is one special case of GGD.

2. Theoretical background

2.1. The MND uncertainty sampling approach

Under the central limit theorem, MND can be used to approximate and derive some famous pdfs, such as lognormal/t/F distributions. The traditional sampling approach used in most ensemble based DA methods produces the perturbing ensemble of state field with the Monte Carlo method from one given a priori MND of the uncertainties.

The MND in n dimensions has pdf as:

$$f(Z) = \frac{1}{\sqrt{(2\pi)^n |\sum|}} \exp\left\{ -\frac{1}{2}(z-\mu)^{\mathrm{T}} \sum^{-1} (z-\mu) \right\} \tag{1}$$

The steps of generating a multivariate normal random vector Z include (Kroese, 2011):

1) Derive the Cholesky decomposition $\Sigma = AA^{\mathrm{T}}$.
2) Generate independent identically uniform distributed U_1, $U_2 \sim \mathrm{U}(0, 1)$.
3) Return two independent standard ND variables, X and Y:

$$\begin{aligned} X &= \sqrt{-2\ln U_1}\cos(2\pi U_2) \\ Y &= \sqrt{-2\ln U_1}\sin(2\pi U_2) \end{aligned} \tag{2}$$

4) Select one of X and Y as Z_1 according to acceptance-rejection with an exponential proposal distribution which gives an acceptance probability of $\sqrt{\pi/(2e)} \approx 0.76$.
5) Go to step 2) until obtain n standard ND variables, and let Z_s=(Z_1,. . ., Z_n).
6) Output $Z = \mu + AZ_s$. This affine transformation can give a MND variable with mean vector μ and covariance matrix Σ.

Even if the uncertainty is subject to MND at the beginning of DA, nonlinear LSMs will also deform it into non-normality by nonlinear integral, as shown by the example in Fig. 1. In Fig. 1a, the ensembles used to perturb skin temperature and soil temperature in the first layer are sampled from two NDs, and hence the graphs of the ensembles and the NDs are exactly matched. However, after a period of DA, the uncertainties of the two state variables obviously deviate from NDs, as shown in Fig. 1b. In such case, the ensemble sampled from ND cannot reflect the actual random behaviors of state variables, and will result in incorrect KF updating gain.