

Kalman filters for assimilating near-surface observations in the Richards equation – Part 2: A dual filter approach for simultaneous retrieval of states and parameters
by Medina et al.

Reply to Referee#2

We thank Referee#2 for his/her comprehensive review. Below we provide our detailed answers to Referee's comments.

Ref#2

Why is the dual filter approach constructed with a SKF for the state update and a UKF for the parameters? I did read the authors' explanation on p.13332, lines 17-25, but this is not helpful.

Back to the drawing board:

- Non-linear state propagation model; (filter 1)
- Linear parameter propagation model; (filter 2)
- Non-linear or linear observation model; (applies to *both* filter 1 and 2)

*Could you please explain this: why use a *linear* filter (SKF) to deal with a *non-linear* state model, and use a *non-linear* filter (UKF) to deal with a *linear* parameter model? This is *independent* of the observation model (see also below).*

The UKF is in its core meant to deal with non-linearities in the propagation model, i.e. historically meant to get some good assessment of the dynamically evolving Pmatrix, which seems to be somewhat understood by the authors in line 15-17. All 'special' Kalman filters (also the UKF) are really designed to "sample" the mean and error covariances of dynamically propagated variables that need to be updated. The "sampling" is mainly done because the calculation of the background (a priori) error covariance is cumbersome with non-linear propagation models. So, I don't see why the UKF would be more beneficial than the SKF for parameter estimation (constant propagation model).

Reply

Here we recall some essential aspects of the dual approach applied to the specific case study in order to overcome Referee#2's concern.

In the dual filter a separate state-space representation is used for the states and the parameters.

The set of system equations for states can be written as:

$$\mathbf{x}_k = F(\mathbf{x}_{k-1}, \mathbf{u}_k, \mathbf{v}_k, \hat{\mathbf{w}}_{k-1}) \quad (1)$$

$$\mathbf{y}_k = H(\mathbf{x}_k, \mathbf{n}_k, \hat{\mathbf{w}}_{k-1}) \quad (2)$$

The set of system equations for parameters can be written as:

$$\mathbf{w}_k = \mathbf{w}_{k-1} + \mathbf{r}_{k-1} \quad (3)$$

$$\mathbf{y}_k = H(F(\hat{\mathbf{x}}_{k-1}, \mathbf{u}_k, \mathbf{v}_k, \mathbf{w}_{k-1}), \mathbf{n}_k, \mathbf{w}_k) \quad (4)$$

When the observation and state variables are identical (i.e., the $h-h$ and the $\theta-\theta$ retrieving modes) the operators H and F are both linear with respect to the states \mathbf{x}_k but F is non-linear with respect to the parameters \mathbf{w}_k , thus the observation equation of the parameter filter (Eq. 4) is non-linear.

Below we provide some details, examining the case of the $h-h$ retrieving mode.

The state propagation equation is linear as the Richards equation is integrated with a Crank Nicolson (CN) numerical scheme.

The governing soil water flow equation in its stochastic form is:

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right]}{\partial z} + v(t) \quad (\text{c\#2.1})$$

where $C(h) = \partial\theta/\partial h$ [1/L] represents the specific water capacity of the soil at pressure head h obtained by differentiating the soil water retention function $\theta(h)$, whereas $K(h)$ [L/T] represents the unsaturated hydraulic conductivity function. The functions $\theta(h)$ and $K(h)$ are described by the following non-hysteretic van Genuchten-Mualem (VGM; van Genuchten, 1980) relations, widely used in soil hydrology:

$$\theta(h) = \theta_r + (\theta_s - \theta_r) \left(1 + |\alpha h|^n\right)^{-m} \quad (34)$$

$$K(\theta) = K_s S_e^\lambda \left[1 - (1 - S_e^{1/m})^m\right]^2 \quad (35)$$

The corresponding discrete form of Eq. (c#2.1) according to the CN differential scheme for node i at time-step $k+1$ is for $i=2, \dots, N-1$:

$$\left(\frac{-K_k^{i-1/2}}{2\Delta z^i \Delta z^i}; \frac{C_k^i}{\Delta t_k} + \frac{K_k^{i-1/2}}{2\Delta z^i} + \frac{K_k^{i+1/2}}{2\Delta z^i}; \frac{-K_k^{i+1/2}}{2\Delta z^i \Delta z^i} \right) \begin{pmatrix} h_{k+1}^{i-1} \\ h_{k+1}^i \\ h_{k+1}^{i+1} \end{pmatrix} = \left(\frac{K_k^{i-1/2}}{2\Delta z^i \Delta z^i}; \frac{C_k^i}{\Delta t_k} - \frac{K_k^{i-1/2}}{2\Delta z^i} + \frac{K_k^{i+1/2}}{2\Delta z^i}; \frac{K_k^{i+1/2}}{2\Delta z^i \Delta z^i} \right) \begin{pmatrix} h_k^{i-1} \\ h_k^i \\ h_k^{i+1} \end{pmatrix} + \frac{K_k^{i-1} - K_k^{i+1}}{2\Delta z^i} + v_k^i \quad (c\#2.2)$$

For nodes $i=1$ and $i=N$ the discrete forms at time-step $k+1$ are:

$$\left(\frac{C_k^1}{\Delta t_k} + \frac{K_k^{1+1/2}}{2\Delta z^1 \Delta z^1}; \frac{-K_k^{1+1/2}}{\Delta z^1 \Delta z^1} \right) \begin{pmatrix} h_{k+1}^1 \\ h_{k+1}^2 \end{pmatrix} = \left(\frac{C_k^1}{\Delta t_k} - \frac{K_k^{1+1/2}}{2\Delta z^1 \Delta z^1}; \frac{K_k^{1+1/2}}{2\Delta z^1 \Delta z^1} \right) \begin{pmatrix} h_k^1 \\ h_k^2 \end{pmatrix} + \frac{q^1 - K_k^{1+1/2}}{\Delta z^1} + v_k^1 \quad (c\#2.3)$$

$$\left(\frac{-K_k^{N-1/2}}{\Delta z^N \Delta z^i}; \frac{C_k^N}{\Delta t_k} + \frac{K_k^{N-1/2}}{2\Delta z^N \Delta z^i} \right) \begin{pmatrix} h_{k+1}^N \\ h_{k+1}^{N+1} \end{pmatrix} = \left(\frac{K_k^{N-1/2}}{2\Delta z^N \Delta z^i}; \frac{C_k^N}{\Delta t_k} - \frac{K_k^{N-1/2}}{2\Delta z^N \Delta z^i} \right) \begin{pmatrix} h_k^N \\ h_k^{N+1} \end{pmatrix} + \frac{K_k^{N-1/2} - q^N}{\Delta z^N} + v_k^N \quad (c\#2.4)$$

The forecasting equation of the system state \mathbf{x}_k , coinciding with the matric pressure head ($x_k^i = h_k^i$), can be obtained by combining the discrete equations written for all N nodes in the following linear state-space form:

$$\hat{\mathbf{x}}_{k+1}^- = \mathbf{A}_k^{-1} \mathbf{B}_k \mathbf{x}_k + \mathbf{A}_k^{-1} \mathbf{g}_k + \mathbf{A}_k^{-1} \mathbf{v}_k \quad (c\#2.5)$$

where \mathbf{A}_k is the tri-diagonal matrix obtained by assembling the terms in the first parenthesis on the right hand-side of Eqs. (c#2.2-2.4), \mathbf{B}_k is the tri-diagonal matrix obtained by assembling the terms in the first parenthesis on the left hand-side of Eqs. (c#2.2-2.4). The term \mathbf{g}_k is a vector obtained by assembling the source terms on the right hand-side of Eqs. (c#2.2-2.4) which are independent from the process noise.

Please note that Eq. (c#2.5) is linear with respect to the state \mathbf{x}_k but it is non-linear with respect to the parameter vector \mathbf{w} (which in our study is defined by K_s , α and n), due to the non-linearity of Eqs. (34) and (35).

Although we believe these concepts can be derived from Sections 2 and 3, we will improve the manuscript to avoid any misunderstanding.

Ref#2

Probably related to this problem, I could not follow section 5.4. re. the observation operator (btw, also check on inconsistent bold and italic H for non-linear H in this section).

Line 15, p.13353: why think about inverting soil moisture to pressure? When assimilating soil moisture in the “theta-h retrieving mode”, one should convert the state h to soil moisture observation predictions (with the forward observation operator), and calculate the soil moisture innovation: not invert soil moisture. The Kalman gain will transform the soil moisture innovations into pressure increments. Why consider a linearization of the observation operator here (p.13354, Line 1)?

Reply

We realize that the misunderstanding is related to the last sentence in p.13353, L. 25-27. The last part of this sentence “*obtained by simple inversion of the soil water retention curve*” is contextually wrong and should be removed. Sorry for this. It was taken from an old version of this manuscript with a different structure. The sentence wanted to explain how the soil moisture data being assimilated in the θ - h mode were obtained in this synthetic experiment: by transforming the “true” pressure heads by means of the soil water retention curve with the “true” parameters.

We did precisely what the referee suggests: dealing with a nonlinear observation operator with the help of the UKF, as indicated in p.13354, Line 1.

Yes, in p.13354, Line 1, the observation operator H should not be indicated in bold.

The statement in *Line 15, p.13353* is simply aimed to alert against what could be a wrong strategy: converting the “observed” surface soil moisture θ in pressure heads by means of the soil water retention function with the current estimate of soil hydraulic parameters. In case of the θ - h retrieving mode, the operator H (i.e., the soil water retention function) is non-linear and thus the non-linear propagation of the observation error through the non-linear H cannot be eluded.

Ref#2

Earlier publications have shown that simultaneous state and parameter estimation may not always be a good idea (Vrugt et al; Moradkhani et al) and in fact, the authors give a hint in the same direction by showing how K_s would not converge. The reason for these unsatisfactory parameter estimation results is the lack of ‘observability’ of the system to which the filter is applied. I would tone down the statement that the “dual filter is suitable for simultaneous retrieving of soil moisture and ... parameters” and instead recognize possible convergence issues. Another (secondary) issue is the underlying assumption of entirely independent state and parameter errors in a parallel dual formulation. Please mention this in the theoretical part and maybe provide a reflection on this. Unless these 2 issues are resolved (not for this paper; in general), I personally don’t think that combined state and parameter estimation can be truly successful.

Reply

We consider that effectively there is a lack of *observability*, but mainly due to the very narrow range covered by the state variables in the considered experiment, which does not prove the unsuitability of the approach.

This drawback is reflected in the manuscript (p. 13349, L.10): *Several authors evidenced the limitations for a successful estimation of VGM parameters, as imposed by the narrow variability of naturally occurring boundary conditions (Scharnagl et al., 2011; Vrugt et al., 2001, 2002). A wide range of soil moisture states is required to reliably constraining the soil hydraulic functions.*

Vrugt et al. (2003) states that “*experiments that yield a wide range of water contents or pressure heads are beneficial for parameter estimation studies, since the measurements then contain independent information for most of the parameters. This increases the identifiability of the parameters and enhances the likelihood of uniqueness of the final parameter estimates.*” He also shows that the maximum sensitivity of the parameters α and n occurs at high pressure head values in fine-textured soil. According to his work, good indentifiability of n in clay soil demands pressure values well beyond -10^4 cm. In our case we worked with a clay loam soil, covering a limited range of pressure heads (see Fig. 1 in the manuscript).

We also believe that a main factor affecting the parameter identifiability is the strong parameter correlation. The issues related to the correlation between VGM parameters are widely documented (e.g., Romano and Santini, 1999; van Dam, 2000; Vrugt at al., 2003). Van Dam (2000), for example, reports correlation values between α , n and K_s very close to -1 for a one-step outflow experiment. Romano and Santini report correlation values whose absolute values are higher than 0.714. Vrugt at al. (2003) show high correlation between α and n , particularly in fine-textured soils. Given these considerations, we sincerely believe that the indentifiability problems have, at most, a minor relation with the adopted dual formulation.

The theoretically expected superiority of the joint approach is not always supported by practical applications. Nelson (2000) states: “*the resulting system of state-space equations (using the joint approach) is highly nonlinear, even for linear models. Several authors have reported convergence problems with this approach (Nelson and Stear, 1976; Ljung, 1979).*”

Similarly Liu and Gupta (2007) reports: *a joint approach could produce "process unstable and intractable because of complex interactions between states and parameters in nonlinear dynamic systems (Todini, 1978a, 1978b). In addition, since parameters generally vary much more slowly than the system states, unstable problems may also result from the fact that both model states and parameters are updated at each observation time step in this method."*

These issues (the complex interactions between retrieved states and parameters and the marked differences in their variability patterns) are even more relevant under the adopted (yet necessary) strategy involving the parameter transformation with the help of a sigmoidal function.

Ref#2

1) Need correct mathematical expressions, and far more diligent explanations

Reply

We will verify all mathematical expressions, providing diligent explanations of the symbols.

Ref#2

*a) The SKF is designed for linear systems with *additive* and *zero mean* noise.*

Reply

Yes, however one has to account for the continuous nature of the original stochastic differential equations. As illustrated in Eqs. (c#2.1-2.5), the additive zero mean noise should be added prior the numerical integration of the differential stochastic equation, as done, for example, by Katul et al. (1993), Enthekabi et al. (1994) and Reichle et al. (2002). Maybeck (1979) provides many details about these formal aspects.

Ref#2

- Eq.10-11: $R_{v0} = E[v_0 v_0]$, etc. Also, what is the overline (as opposed to hat) in these equations? Please explain symbols when they are used for the first time.

Reply

We will be more diligent in explaining symbols and notations. We used the notations employed by Wan and Nelson (2001) and van de Merwe, (2004), indicating with “ $\hat{\cdot}$ ” (e.g., \hat{x}_k) the posterior mean and with “ $\bar{\cdot}$ ” (e.g., \bar{x}_k) the a priori predicted mean.

Ref#2

Eq. 12-13 are out of place for a SKF: v should be additive (while at is, turn the italic F into a linear matrix), and thus the second term in Eq. 13 should not have the $F.F^T$ around R_v . Likewise: n should be additive for a SKF (take out in eq. 15, which BTW is an awkward mix of a linear H -matrix which receives non-linear arguments), and thus the $H.H^T$ around R_n in Eq. 14 are out of place.

Reply

As illustrated in Eqs. (c#2.1-2.5), to ensure physical consistency in the time-dependency during the formulation of the dynamic state space model, one has to account (either implicitly or explicitly) for the continuous-time dynamic models, as done, for example, by Katul et al. (1993), Enthekabi et al. (1994) and Reichle et al. (2002). When passing from the continuous formulation to the equivalent

discrete-time system model, the zero-mean white Gaussian noise normally appears multiplied by a term, necessarily proportional to the computational time-step. Otherwise it is necessary to resort to an artificial normalization of the error (see Walker (1999), Chapter 6, pp. 6.26).

Maybeck (1979) provides many details about these formal aspects.

We will provide a detailed and more accurate description of the SKF algorithm. Following Eqs. (c#2.2-2.5) reported above, the a priori estimate of the covariance matrix is calculated as follows:

$$\mathbf{P}_{x,k}^- = \mathbf{A}_k^{-1} \mathbf{B}_k \mathbf{P}_{x,k-1} (\mathbf{A}_k^{-1} \mathbf{B}_k)^T + \mathbf{A}_k^{-1} \mathbf{R}_{v,k} (\mathbf{A}_k^{-1})^T \quad (\text{c\#2.6})$$

We agree that the matrices H and H^T around R_n in Eq. (14) can be removed without loss of generality.

Ref#2

Eq.1-2 + Eq.3-4: for clarity, maybe mention explicitly in the text that the posterior parameter estimate is passed into the Eq. 1-2 for state propagation and that the posterior state estimate is passed into the Eq. 4 to calculate the observation prediction. Line 7, p.13334: nhat-symbol does not show up between the quotes.

Reply

We will follow the suggestion. Some editing errors occur.

Ref#2

Eq. 7: the observation error covariance is missing in this equation? What is ntilde referring to? Line 19, p.13334 suggests that this $P_{\tilde{y}}$ would be the auto-covariance of the observation prediction error. Yet the observation predictions are \hat{y} and do not include the observation error. Eq. 7 could only be right if $P_{\tilde{y}}$ is the innovation covariance, which is not mentioned as such, and needs explanation to be understood by an average reader.

Reply

Yes, $\mathbf{P}_{\tilde{y},k}$ indicates the innovation covariance. It will be declared in the text for clearness. An explicit description of Eq. (7) is the following:

$$\mathbf{K}_k^w = E \left[(\mathbf{w}_k - \hat{\mathbf{w}}_k^-) (\mathbf{y}_k - \hat{\mathbf{y}}_k^-)^T \right] E \left[(\mathbf{y}_k - \hat{\mathbf{y}}_k^-) (\mathbf{y}_k - \hat{\mathbf{y}}_k^-)^T \right]^{-1} = \mathbf{P}_{w\tilde{y},k}^- \left[\mathbf{P}_{\tilde{y},k}^- \right]^{-1} \quad (7)$$

See that we also fix an imprecision on the original expression by adding the tilde in $\mathbf{P}_{w\tilde{y},k}^-$

Ref#2

*Also note that the error covariances are meant to be *cross*-covariance (could include correlations between errors in different variables) and not *auto*-covariance. Along the same lines: throughout the entire paper, it is suggested that there are multi-dimensional observation (and observation prediction) error matrices, while I believe only scalar observations are assimilated. Either replace the matrices or state clear upfront that these are 1-dimensional entries.*

Reply

The observations refer to more than one node, as done by Walker (2001). Only when the observation depth is equal to 0.5 cm the observation is a single scalar value.

Ref#2

*c) Eq. 16: The Kalman filter *differs* very much from eq. 16. The Kalman filter includes in its very nature the information about the background or prior state (in this case: prior parameter estimate).*

Reply

Van Der Merwe (2004) demonstrates that the UKF parameter estimation algorithm is equivalent to a maximum posterior likelihood estimate of the underlying parameters under a Gaussian posterior (and noise distribution). He provides an optimization perspective of the sigma point Kalman filter estimation, similarly to what Nelson (2000) and Wan and Nelson (2001) do for the dual extended Kalman filter methods.

Nevertheless, we prefer to remove Lines 1-5, page 13346, including Eq. (16); it is scarcely relevant and creates confusion.

Ref#2

*Line 5, p.13336: R_e : noise parameter covariance?? This should definitely be called something in observation space, *NOT* in parameter space. Yet, the parameter error covariance *should* show up in a second term that penalizes the background (the term that is forgotten in Eq. 16, as mentioned above). And, it will be artificial noise later in this paper, but up to this point, the artificial nature of the experiment is not mentioned in the state estimation, so please keep it general, as in previous sections.*

Reply

Yes, you are right, R_e refers to observation covariance as employed in Eq. (26):

$$\mathbf{P}_{\bar{y},k} = \sum_{i=0}^{2L} \mu_i^{(c)} (\mathcal{Y}_{i,k|k-1} - \hat{y}_k^-) (\mathcal{Y}_{i,k|k-1} - \hat{y}_k^-)^T + \mathbf{R}_{e,k} \quad (26)$$

The term “artificial” indicates that the choice of this variance is related to practical, and not only physical, criteria, as it affects convergence and tracking performances. The influence of the initial parameter covariances is discussed in section 5.5.

Reply

Line 15, p.13337: R_r : this cannot be called innovation covariances (innovations are in obs space)?? R_r has to be in parameter space.

Ref#2

Yes, R_r is the time-varying covariance of the “artificial” process noise applied to the parameter space.

Ref#2

Eq. 24-29: the use of z in superscript, tildes and hats is not consistent, please check thoroughly.

Reply

We are sorry. We will do that, thank you.

Ref#2

2) P.13332: is the UKF still ‘novel’? It is more than 10 years old?

Reply

We will remove “novel”, thank you.

Ref#2

3) Eq. 40 and eq. 41 should not use the same g -symbol for different things

Reply

We will check notations and symbols throughout the paper.

Ref#2

4) Line 14, p13342, introduce acronym VGM before using it

5) P.13344: line 11: : : : daily *precipitation* series

Reply

Thank you, we will apply these changes.

Ref#2

P.13344: line 18: not true: infiltration increases the state correlations – what you may want to say is that the correlations are made temporally variable

Reply

Referee#2 refers to the sentence:

“The inclusion of a rainfall pattern allows for evaluating the dual filter performance during continuous wetting and drying processes taking place in the soil profile. In mathematical terms, it also reduces the state correlations along the profile, thus making the synthetic study a more representative stress test of the overall retrieving process as compared with a constant top boundary condition as in Entekhabi et al. (1994) and Walker et al. (2001).”

According to Walker (1999) the ability of the Kalman Filter to make adjustments to the entire profile is highly dependent on the correlation between the states of adjacent nodes. What we wanted to say is that the occurrence of wet and dry periods might reduce these correlations with respect to those found in a pure evaporative process (as in Entekhabi et al. (1994) and Walker et al. (2001)). Anyway, it is true, as the Referee#2 says, that the signs of the correlation change with time and that the time-variation of the correlation is more marked. This makes the state and parameter retrieval more challenging than in the case of a pure evaporative process.

Ref#2

6) P. 13345: line 14: Montzka is the wrong reference for this. Please use Kerr et al 2010 if you refer to 3-day repeat for SMOS.

Reply

We will change this reference, thank you.

Ref#2

Line 28: I still understand that scalars are assimilated, so how could there be a diagonal matrix?

Reply

The observations refer to more than one node. Only when the observation depth is equal to 0.5 cm the observation is a single scalar value.

Ref#2

7) P. 13346 line 16: standard deviation across the profile?; say explicitly that $N_{nod} = 27$.

Reply

We will do this, thank you.

Ref#2

8) Please check the text thoroughly for grammar/spelling errors; e.g. L25, p13330, Soil water dynamic*s* *are* ...; L 10, p. 13351is able to f*i*nd...

Reply

We will do this, thank you.

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