Ref#1

Equation 4: This is not the expression for the gain that I have seen in many paper on data assimilation, for example De Lannoy et al., Reichle et al., etc. Please further explain or correct. I hope the formula has been applied correctly.

Reply

First, we noticed that there is a minor editing error on the right hand side of Eq. (4). The correct form is the following:

$$\mathbf{K}_{k} = E\left[\left(\mathbf{x}_{k} - \hat{\mathbf{x}}_{k}^{-}\right)\left(\mathbf{y}_{k} - \hat{\mathbf{y}}_{k}^{-}\right)^{T}\right] E\left[\left(\mathbf{y}_{k} - \hat{\mathbf{y}}_{k}^{-}\right)\left(\mathbf{y}_{k} - \hat{\mathbf{y}}_{k}^{-}\right)^{T}\right]^{-1} = \mathbf{P}_{\mathbf{x}\mathbf{y},k}^{-} \left[\mathbf{P}_{\mathbf{y},k}^{-}\right]^{-1}$$
(Eq. 4)

Ref#1 refers to the more common expression of the Kalman gain:

$$\mathbf{K}_{k} = \mathbf{P}_{\mathbf{x}_{k}}^{-} \mathbf{H}_{k}^{T} \left(\mathbf{H}_{k} \mathbf{P}_{\mathbf{x}_{k}}^{-} \mathbf{H}_{k}^{T} + \mathbf{R}_{k} \right)^{-1}$$
(c.#1_1)

The expression of Eq. (c.1#1) is equivalent to Eq. (4). Reminding that

$$\mathbf{y}_k = \mathbf{H}\mathbf{x}_k + \mathbf{n}_k \tag{c.#1_2}$$

the covariance matrices $\mathbf{P}_{xy,k}^-$ and $\mathbf{P}_{y,k}^-$ can be expressed as follows

$$\mathbf{P}_{\mathbf{x}\mathbf{y},k}^{-} = E\left[\left(\mathbf{x}_{k} - \hat{\mathbf{x}}_{k}^{-}\right)\left(\mathbf{y}_{k} - \hat{\mathbf{y}}_{k}^{-}\right)^{T}\right] = \mathbf{P}_{\mathbf{x}_{k}}^{-} \mathbf{H}$$
(c.#1_3)

$$\mathbf{P}_{\mathbf{y},k}^{-} = E\left[\left(\mathbf{y}_{k} - \hat{\mathbf{y}}_{k}^{-}\right)\left(\mathbf{y}_{k} - \hat{\mathbf{y}}_{k}^{-}\right)^{T}\right] = \left(\mathbf{H}_{k}\mathbf{P}_{\mathbf{x}_{k}}^{-}\mathbf{H}_{k}^{T} + \mathbf{R}_{k}\right)$$
(c.#1_4)

Eq. (c.#1_1) can be then obtained by combining (c.#1_3) and (c.#1_4).

<u>Ref#1</u>

Equation 5: Again, this equation is different from the equation in other papers on EKF. Same remark regarding the application.

Reply

Ref#1 refers to the expression:

$$\mathbf{P}_{\mathbf{x}_{k}} = \left(\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k}\right)\mathbf{P}_{\mathbf{x}_{k}}^{-} = \mathbf{P}_{\mathbf{x}_{k}}^{-} - \mathbf{K}_{k}\mathbf{H}_{k}\mathbf{P}_{\mathbf{x}_{k}}^{-}$$
(c.#1_5)

This expression is equivalent to Eq. (5), which we repeat here for the sake of clarity: $\mathbf{P}_{x,k} = \mathbf{P}_{x,k}^{-} - \mathbf{K}_{k} \mathbf{P}_{y,k}^{-} \mathbf{K}_{k}^{T}$ (Eq. 5)

It is easy to verify that $\mathbf{K}_{k}\mathbf{P}_{yk}^{-}\mathbf{K}_{k}^{T} = \mathbf{K}_{k}\mathbf{H}_{k}\mathbf{P}_{\mathbf{x}_{k}}^{-}$:

$$\mathbf{K}_{k}\mathbf{H}_{k}\mathbf{P}_{\mathbf{x}_{k}}^{-} = \mathbf{K}_{k}\mathbf{P}_{\mathbf{y},k}^{-}\left(\mathbf{P}_{\mathbf{y},k}^{-}\right)^{-1}\mathbf{H}_{k}\mathbf{P}_{\mathbf{x}_{k}}^{-} = \mathbf{K}_{k}\mathbf{P}_{\mathbf{y},k}^{-}\left\{\left(\mathbf{H}_{k}\mathbf{P}_{\mathbf{x}_{k}}^{-}\right)^{T}\left[\left(\mathbf{P}_{\mathbf{y},k}^{-}\right)^{-1}\right]^{T}\right\}^{T} = \mathbf{K}_{k}\left\{\mathbf{P}_{\mathbf{y},k}^{-}\left(\mathbf{P}_{\mathbf{x}_{k}}^{-}\right)^{T}\left(\mathbf{H}_{k}\right)^{T}\left[\left(\mathbf{P}_{\mathbf{y},k}^{-}\right)^{-1}\right]^{T}\right\}^{T}$$

$$(c.\#1_{6})$$

Since $\mathbf{P}_{\mathbf{x}_k}^-$ and $(\mathbf{P}_{\mathbf{y},k}^-)^{-1}$ are symmetric matrices, they do not change with the transpose operator and hence:

$$\mathbf{K}_{k}\mathbf{H}_{k}\mathbf{P}_{\mathbf{x}_{k}}^{-} = \mathbf{K}_{k}\mathbf{P}_{\mathbf{y},k}^{-} \left[\left(\mathbf{P}_{\mathbf{x}_{k}}^{-}\right) \left(\mathbf{H}_{k}\right)^{T} \left(\mathbf{P}_{\mathbf{y},k}^{-}\right)^{-1} \right]^{T} = \mathbf{K}_{k}\mathbf{P}_{\mathbf{y},k}^{-} \left(\mathbf{K}_{k}\right)^{T}$$
(c.#1_7)

The expressions employed for \mathbf{K}_{k} (Eq. 4) and $\mathbf{P}_{\mathbf{x}_{k}}$ (Eq. 5) are equal to those employed by van der Merwe (2004). Alternative expressions can be found in the literature, as reported for instance by Grewal and Andrews (2008).

<u>Ref.#1</u>

Beginning of section 2.1. Looking at literature I would argue that the ensemble Kalman filter is the most widely used version of the KF for nonlinear settings. Please either prove the statement or correct.

Reply

We agree with Ref.#1. We suggest changing lines 16-17 of page 13297 as follows: "Within the general framework of the Kalman Filter, the Extended Kalman Filter (EKF) has been the first approach suggested for dealing with nonlinearity."

<u>Ref.#1</u>

Equation 18 is unclear. $\hat{\mathbf{x}}_{k-1}^{a}$ is multiplied to itself. Please explain or correct.

Reply

This is an editing error, we are sorry for this. A space is missing between the vectors. This is correct form of Eq. (18):

$$\mathcal{X}_{k-1}^{a} = \begin{bmatrix} \hat{\boldsymbol{x}}_{k-1}^{a} & \hat{\boldsymbol{x}}_{k-1}^{a} + \sqrt{\gamma \mathbf{P}_{\boldsymbol{x},k-1}^{a}} & \hat{\boldsymbol{x}}_{k-1}^{a} - \sqrt{\gamma \mathbf{P}_{\boldsymbol{x},k-1}^{a}} \end{bmatrix}$$
(Eq. 18)

<u>Ref.#1</u>

The explanation between equations 33 and 36 is unclear. This needs more explanation. **Reply**

We agree with Ref.#1: this part needs more comments. We also noticed a formal error in Eq. (35). We suggest modifying this part as follows:

"The same effect is achieved with the SKF-CN algorithm, where the dynamic equation assumes the following equation:

$$\mathbf{A}_{\left(K^{k},C^{k},z,t\right)}\boldsymbol{x}^{k+1} = \mathbf{B}_{\left(K^{k},C^{k},z,t\right)}\left(\boldsymbol{x}^{k}+\boldsymbol{v}^{k}\right) + \boldsymbol{f}_{\left(K^{k},K^{k},\mathcal{Q}top,\mathcal{Q}bot,z,t\right)}$$
(33)

Coherently with Eq.1, in Eq. (33) the system noise \mathbf{v}_k is adopted in such way that it drives the dynamic system through the nonlinear state transition function F, which is fully defined by $\mathbf{A}_k^{-1}\mathbf{B}_k$. As a result, the dynamic system operator affects the a priori estimate of the covariance matrix by acting simultaneously on both the state covariance (\mathbf{P}_{xk}) and the noise covariance (\mathbf{Q}_k) matrices:

$$\hat{\mathbf{P}}_{\boldsymbol{x},k+I}^{-} = \left(\mathbf{A}_{k}^{-1}\mathbf{B}_{k}\right)\mathbf{P}_{\boldsymbol{x},k}\left(\mathbf{A}_{k}^{-1}\mathbf{B}_{k}\right)^{T} + \left(\mathbf{A}_{k}^{-1}\mathbf{B}_{k}\right)\mathbf{Q}_{k}\left(\mathbf{A}_{k}^{-1}\mathbf{B}_{k}\right)^{T}$$
(34)

As anticipated above, the SKF_v-CN algorithm by Walker et al. (2001) differs from the SKF-CN algorithm, since in SKF_v-CN the system noise is directly added to the a priori estimate of the current system state:

$$\boldsymbol{x}^{k+1} = \boldsymbol{A}_{(\kappa^{k}, c^{k}, z, z)}^{-1} \boldsymbol{B}_{(\kappa^{k}, c^{k}, z, z)} \boldsymbol{x}^{k} + \boldsymbol{A}_{(\kappa^{k}, c^{k}, z, z)}^{-1} f_{(\kappa^{k}, \kappa^{k}, Qtop, Qbot, z, z)} + \boldsymbol{v}^{k}$$
(35)

Thus the noise covariance matrix (\mathbf{Q}_k) directly contributes to the a priori estimate of the covariance matrix, without being transformed by the dynamic operator:

$$\hat{\mathbf{P}}_{\boldsymbol{x},k+l}^{-} = \left(\mathbf{A}_{k}^{-1}\mathbf{B}_{k}\right)\mathbf{P}_{\boldsymbol{x},k}\left(\mathbf{A}_{k}^{-1}\mathbf{B}_{k}\right)^{T} + \mathbf{Q}_{k}$$
(36)

These differences between SKF_v -CN and SKF-CN in the way of treating the system noise v^k are scarcely transcendent in the domain of a few hours of simulation, but become important when the frequency of the observations significantly decreases to one every several days, as could be in practical circumstances."

<u>Ref.#1</u>

We need more explanation on how the principal components are calculated in section 4.5. **Reply**

We also agree on this remark. We suggest modifying the initial part of section 4.5 as follows: "The dynamic evolution of the system state covariance has been explored by examining the relative change in the variance explained by the first two principal components of the state covariance matrix. The principal component analysis has been done by singular value decomposition of the state covariance matrix. Fig. 6 shows how the variances explained by the first two principal components (PC) of the state covariance evolve, considering the simulations during the first 24 hours for pressure head assimilations, and 72 hours for soil water content assimilations, with two different initial state covariance matrices, 10^3 cm² and 10^4 cm². Figs. 6a) and 6b) shows the evolution of the explained variance with the application of SKF_v-EX and SKF_v-CN schemes, respectively."

Ref.#1 minor remarks

Reply

We thank Ref.#1 for the suggested corrections. We will change the text according to these remarks.

For what concerns the request

"- Page 13308 line 13: please name some operational applications of this kind of model."

we recall that the Crank-Nicolson (CN) finite difference scheme has been very often applied to numerically solve the Richards equation (e.g. Romano et al., 1998). Moreover, and with a view to the analysis carried out in the third paper of this work, the CN scheme has been implemented to determine the soil hydraulic properties through inversion of laboratory evaporation experiments and drainage field tests (e.g., Romano, 1993; Romano and Santini, 1999).

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