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Supplement of

An ensemble square root filter for the joint assimilation of surface soil moisture and leaf area index within the Land Data Assimilation System LDAS-Monde: application over the Euro-Mediterranean region

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In this supplementary material, we detail how the equations of the SEKF are derived in the context of patches and the ISBA land surface model.

1 Simplified Extended Kalman Filter

We first recall in this section the equations of the Simplified Extended Kalman Filter. Introduced by [1], the SEKF is a simplified version of the Extended Kalman Filter. It is a sequential approach aiming to give the estimation of the state \mathbf{x} of a system at various times. We denote by $n_{\mathbf{x}}$ the size of the state vector.

The SEKF is a two-steps algorithm. For a given time t_k , it provides a first estimate \mathbf{x}_k^f called the *forecast*

$$\mathbf{x}_k^f = \mathcal{M}_{k-1}(\mathbf{x}_{k-1}^a) \quad (\text{S1})$$

with \mathcal{M}_{k-1} a (nonlinear) model. The forecast step just aims to propagate the estimate \mathbf{x}_{k-1}^a at the last previous time t_{k-1} to the new time t_k .

This forecast is then corrected by using observations \mathbf{y}_k^o of the system with \mathbf{R}_k its associated error covariance matrix. We denote by $n_{\mathbf{y}}$ the size of \mathbf{y}_k^o . The observations are linked to the state through the (possibly nonlinear) observation operator \mathcal{H}_k . This correction step is called the *analysis* and provides a new estimate \mathbf{x}_k^a with

$$\mathbf{x}_k^a = \mathbf{x}_k^f + \mathbf{K}_k \left(\mathbf{y}_k^o - \mathcal{H}_k(\mathbf{x}_k^f) \right) \quad (\text{S2})$$

$$\mathbf{K}_k = \mathbf{B} \mathbf{J}_k^T (\mathbf{J}_k \mathbf{B} \mathbf{J}_k^T + \mathbf{R}_k)^{-1} \quad (\text{S3})$$

\mathbf{B} is a prescribed background error covariance matrix of size $n_{\mathbf{x}} \times n_{\mathbf{x}}$ and \mathbf{J}_k is a Jacobian matrix of size $n_{\mathbf{y}} \times n_{\mathbf{x}}$ defined as

$$\mathbf{J}_k = \frac{\partial \left(\mathcal{H}_k(\mathbf{x}_k^f) \right)}{\partial \mathbf{x}_{k-1}^a} = \frac{\partial \left(\mathcal{H}_k(\mathcal{M}_{k-1}(\mathbf{x}_{k-1}^a)) \right)}{\partial \mathbf{x}_{k-1}^a} \quad (\text{S4})$$

This Jacobian can be estimated using finite differences. In that case, we would need to run $n_{\mathbf{x}}$ perturbed model runs in addition to the model run used in the forecast step. If $n_{\mathbf{x}}$ is too big, computing \mathbf{J}_k with finite differences is unaffordable.

2 First assumption: linearity of the observation operator

We now assume that the observation operator meaning that $\mathcal{H}_k = \mathbf{H}_k$. This implies that the Jacobian matrix \mathbf{J}_k can be rewritten as

$$\mathbf{J}_k = \frac{\partial \left(\mathbf{H}_k \mathbf{x}_k^f \right)}{\partial \mathbf{x}_{k-1}^a} = \mathbf{H}_k \frac{\partial \mathbf{x}_k^f}{\partial \mathbf{x}_{k-1}^a} = \mathbf{H}_k \frac{\partial \left(\mathcal{M}_{k-1}(\mathbf{x}_{k-1}^a) \right)}{\partial \mathbf{x}_{k-1}^a} = \mathbf{H}_k \mathbf{M}_{k-1} \quad (\text{S5})$$

with \mathbf{M}_{k-1} the tangent linear operator of \mathcal{M}_{k-1} at \mathbf{x}_{k-1}^a .

Following this assumption, the analysis step of the SEKF is now:

$$\mathbf{x}_k^a = \mathbf{x}_k^f + \mathbf{K}_k \left(\mathbf{y}_k^o - \mathbf{H}_k \mathbf{x}_k^f \right) \quad (\text{S6})$$

$$\mathbf{K}_k = \mathbf{B} \left(\mathbf{H}_k \mathbf{M}_{k-1} \right)^T \left(\left(\mathbf{H}_k \mathbf{M}_{k-1} \right) \mathbf{B} \left(\mathbf{H}_k \mathbf{M}_{k-1} \right)^T + \mathbf{R}_k \right)^{-1} \quad (\text{S7})$$

3 The case of LDAS-Monde, ISBA and patches

Until now, we have not assumed anything regarding the spatial distribution of state variables and observations.

The ISBA land surface model involved in LDAS-Monde owns features that can help to simplify the SEKF. They are:

- At grid cell level: ISBA only consider vertical diffusion for soil moisture and temperature and vegetations variables of different grid cells do not interact with each other.
- Each grid cell of ISBA is divided into 12 different patches representing different types of vegetation. To each patch p is associated a patch fraction $\alpha_{[p]}$ representing the proportion of the type of vegetation associated to patch p in the grid cell.
- At patch level: variables (vegetation, soil moisture, soil temperature, ...) of different patches do not interact with each other.

Second assumption: Observations are available at ISBA grid cell level and no spatial covariances are taken into account in LDAS-Monde.

Following this second assumption, equations (S6) and (S7) can be applied directly at a grid cell level. This allows an easy parallelisation of the SEKF analysis using domain decomposition.

Now we split the control vector \mathbf{x} into 12 vectors $\mathbf{x}_{[p]}$, $p = 1, \dots, 12$, each containing only control variables relative to that particular patch. It means we have 12 LAI variables (one for each patch), 12 SM2 variables (soil moisture in layer 2, 1-4 cm depth), etc. \mathbf{x} can be written as the concatenation of these 12 vectors:

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_{[1]} \\ \mathbf{x}_{[2]} \\ \vdots \\ \mathbf{x}_{[12]} \end{pmatrix} \quad (\text{S8})$$

While control variables are available at patch level, observations are available at grid cell level. It means that variables at patch level need to be aggregated to grid cell level to obtain observation equivalents.

Third assumption: The observation operator \mathbf{H}_k aggregates control variables at patch level averaging them with patch fractions as weights:

$$\mathbf{H}_k \mathbf{x} = \sum_{j=1}^{12} \alpha_{[j]} \tilde{\mathbf{H}}_k \mathbf{x}_{[j]} \quad (\text{S9})$$

$\tilde{\mathbf{H}}_k$ is a matrix selecting directly the observed variable (either LAI and/or SM2) meaning that $\tilde{\mathbf{H}}$ is full of 0 and 1.

Following the third assumption, the observation operator \mathbf{H}_k can also be rewritten as:

$$\mathbf{H}_k = \left(\alpha_{[1]} \tilde{\mathbf{H}}_k \quad \alpha_{[2]} \tilde{\mathbf{H}}_k \quad \dots \quad \alpha_{[12]} \tilde{\mathbf{H}}_k \right) \quad (\text{S10})$$

Since variables of different patches do not interact with each other in ISBA, it also simplifies the Jacobian matrix \mathbf{M}_{k-1} making it block-diagonal as follows:

$$\mathbf{M}_{k-1} = \begin{pmatrix} \mathbf{M}_{[1],k-1} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_{[2],k-1} & & \vdots \\ \vdots & & \ddots & \mathbf{0} \\ \mathbf{0} & \dots & \mathbf{0} & \mathbf{M}_{[12],k-1} \end{pmatrix} \quad (\text{S11})$$

It leads that $\mathbf{H}_k \mathbf{M}_{k-1}$ can be now written as:

$$\mathbf{H}_k \mathbf{M}_{k-1} = \left(\alpha_{[1]} \tilde{\mathbf{H}}_k \mathbf{M}_{[1],k-1} \quad \alpha_{[2]} \tilde{\mathbf{H}}_k \mathbf{M}_{[2],k-1} \quad \dots \quad \alpha_{[12]} \tilde{\mathbf{H}}_k \mathbf{M}_{[12],k-1} \right) \quad (\text{S12})$$

Fourth assumption: No covariances between patches are taken into account in LDAS-Monde.

This assumption leads to a block diagonal \mathbf{B} matrix that can be defined as:

$$\mathbf{B} = \begin{pmatrix} \tilde{\mathbf{B}} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{B}} & & \vdots \\ \vdots & & \ddots & \mathbf{0} \\ \mathbf{0} & \dots & \mathbf{0} & \tilde{\mathbf{B}} \end{pmatrix} \quad (\text{S13})$$

with $\tilde{\mathbf{B}}$ the prescribed covariance matrix for control variables within a patch. In practice $\tilde{\mathbf{B}}$ is taken diagonal.

Using this new definition of \mathbf{B} and equation (S12), $\mathbf{B} (\mathbf{H}_k \mathbf{M}_{k-1})^T$ can be written as:

$$\mathbf{B} (\mathbf{H}_k \mathbf{M}_{k-1})^T = \begin{pmatrix} \alpha_{[1]} \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[1],k-1} \right)^T \\ \alpha_{[2]} \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[2],k-1} \right)^T \\ \vdots \\ \alpha_{[12]} \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[12],k-1} \right)^T \end{pmatrix} \quad (\text{S14})$$

and

$$(\mathbf{H}_k \mathbf{M}_{k-1}) \mathbf{B} (\mathbf{H}_k \mathbf{M}_{k-1})^T = \sum_{j=1}^{12} \alpha_{[j]}^2 \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right) \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right)^T \quad (\text{S15})$$

Using equations (S14) and (S15) into (S7), it gives for the gain matrix:

$$\mathbf{K}_k = \begin{pmatrix} \alpha_{[1]} \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[1],k-1} \right)^T \left(\sum_{j=1}^{12} \alpha_{[j]}^2 \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right) \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right)^T + \mathbf{R}_k \right)^{-1} \\ \alpha_{[2]} \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[2],k-1} \right)^T \left(\sum_{j=1}^{12} \alpha_{[j]}^2 \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right) \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right)^T + \mathbf{R}_k \right)^{-1} \\ \vdots \\ \alpha_{[12]} \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[12],k-1} \right)^T \left(\sum_{j=1}^{12} \alpha_{[j]}^2 \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right) \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right)^T + \mathbf{R}_k \right)^{-1} \end{pmatrix} \quad (\text{S16})$$

Using this formulation of the gain matrix and equation (S10) into equation (S6), it leads to the following equations for the analysis in each patch p :

$$\mathbf{x}_{[p],k}^a = \mathbf{x}_{[p],k}^f + \mathbf{K}_{[p],k} \left(\mathbf{y}_k^o - \sum_{j=1}^{12} \alpha_{[j]} \tilde{\mathbf{H}}_k \mathbf{x}_{[j],k}^f \right) \quad (\text{S17})$$

$$\mathbf{K}_{[p],k} = \alpha_{[p]} \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[p],k-1} \right)^T \left(\sum_{j=1}^{12} \alpha_{[j]}^2 \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right) \tilde{\mathbf{B}} \left(\tilde{\mathbf{H}}_k \mathbf{M}_{[j],k-1} \right)^T + \mathbf{R}_k \right)^{-1} \quad (\text{S18})$$

These two equations are equivalent to equations (3) and (4) of the manuscript.

In practice, we do not compute $\mathbf{M}_{[p],k-1}$ but directly $\tilde{\mathbf{H}}_k \mathbf{M}_{[p],k-1}$ using finite differences.

References

- [1] J.-F. Mahfouf, K. Bergaoui, C. Draper, C. Bouyssel, F. Taillefer and L. Taseva, A comparison of two offline soil analysis schemes for assimilation of screen-level observations, *J. Geophys. Res.*, 114, D08105, doi: 10.1029/2008JD011077, 2009.