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Supporting Information for

Operational soil moisture data assimilation for improved continental water balance prediction

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Introduction

This document expands the description of data assimilation method and analysis increment mass redistribution (AIR). Specifically it covers:

- the method of linear transformation of the satellite soil moisture products over gauge-sparse region;
- the derivation of equation 4 from equation 1; and
- all the equations for AIR.

Text S1.

The observation operator that links AWRA model upper-layer soil water storage (S_o) state with the satellite soil moisture (SSM) is a linear transformation derived from temporal mean and variance matching between the two estimates. Mean and variance matching is an accepted practice of correcting systematic bias between model estimates and observations, and in our case map observations into state space for data assimilation. However, for regions of Australia with little, or no, rain gauge coverage, AWRA model S_o persist as zeros or very low values, reflecting a deficiency in the gauge-based analysis of daily rainfall used to drive model simulations. The result of mean and variance matching in these gauge-sparse areas will be to flatten the dynamics of SSM time series to zero.

To resolve this problem, and make full use of the SSM products to fill the modelling gap in gauge-sparse region of the continent, we derived a set of coefficients for the observation operator from the cells surrounding the gaps. We obtained the maximum SSM values through time and the derived 'slope' and 'intercept' from the observation model for each cell in neighboring region. Then we applied linear regression to estimate the correspond slope and intercept from the maximum SSM values in the rainfall gaps. This provided an observation model to transform the SSM in into water storage unit (mm) and ensures the assimilation can effectively impart spatial pattern of soil moisture over the sparsely gauged regions.

Text S2.

The generic form of the state updating equation for sequential data assimilation is given as:

$$\mathrm{X_t^a} = \mathrm{X_t^f} + \mathrm{K_t}[\mathrm{Y_t} - \mathrm{H}(\mathrm{X_t^f})],$$

where the terms are defined as for Eq. (1). In this study, there are two satellite soil moisture observations, transformed into model space (i.e. water storage) through the observation operator, denotes as Y_t^{SMAP} and Y_t^{SMOS}. Since the error variances of the SSM products are independent, we can therefore write the above as:

$$\mathrm{X_t^a} = \mathrm{X_t^f} + [K_{SMAP}, K_{SMOS}] \begin{bmatrix} Y_t^{SMAP} - \mathrm{X_t^f} \\ Y_t^{SMOS} - \mathrm{X_t^f} \end{bmatrix}$$

$$= (1 - K_{SMAP} - K_{SMOS})\mathrm{X_t^f} + K_{SMAP} Y_t^{SMAP} + K_{SMOS} Y_t^{SMOS}$$

$$= K_{AWRA}\mathrm{X_t^f} + K_{SMAP} Y_t^{SMAP} + K_{SMOS} Y_t^{SMOS},$$

where the gain factors are calculated as:

$$K_{AWRA} = \frac{\frac{1}{\sigma_x^2}}{\frac{1}{\sigma_x^2} + \frac{1}{\sigma_y^2} + \frac{1}{\sigma_z^2}}, K_{SMAP} = \frac{\frac{1}{\sigma_y^2}}{\frac{1}{\sigma_x^2} + \frac{1}{\sigma_y^2} + \frac{1}{\sigma_z^2}}, K_{SMOS} = \frac{\frac{1}{\sigma_z^2}}{\frac{1}{\sigma_x^2} + \frac{1}{\sigma_y^2} + \frac{1}{\sigma_z^2}}$$

respectively. The error variance σ^2 for each data set are obtained through the triple collocation (TC) methods, Eq (3).

Text S3.

The influence of the improved, or analysed, upper-layer soil water, S_0^a is only realized in the TC data assimilation once the model integrates to the next time step when the water balance is restored between model components. We proposed an analysis increment redistribution (AIR) modification to the TC data assimilation method (TC-AIR) as a way of maintaining water balance at each time step. The idea borrows from tangent linear modelling (TLM), where only relevant model components are modified to accommodate the increment. The following are the specific components of AWRA model which are relevant here (for greater detail see Frost et al., 2016) and are used in the AIR approach, and they includ the modifications necessary to impart the water balance constraint.

The analysis increments after the data assimilation can be calculated as:

$$\Delta S_0 = S_0^a - S_0^f,$$

where S_0^a denotes the analysed upper-layer soil water storage and S_0^f denotes the forecast, or initial estimate. The change in S_0 affects the drainage to the lower-layer soil water storage (D_0) and interflow draining laterally from the top soil layer (Q_{I0}). The corresponding change in drainage to lower-layer soil water storage from the increment ΔS_0 is calculated as:

$$\Delta D_0 = (1-\beta_0)k_{0sat}[\left(\frac{S_0^a}{S0max}\right)^2 - \left(\frac{S_0^f}{S0max}\right)^2],$$

$$\Delta Q_{I0} = \beta_0 k_{0sat}[\left(\frac{S_0^a}{S0max}\right)^2 - \left(\frac{S_0^f}{S0max}\right)^2],$$

where the $k_{0\mathrm{sat}}$ and $S0max$ are model parameters representing the saturated hydraulic conductivity and maximum storage of the upper soil layer, respectively. The proportion of overall top layer drainage that is lateral drainage (β_0) given as:

$$\beta_0 = \tanh\,(k_\beta \beta \frac{S_0^a}{S0max})\tanh\,(k_\zeta (\frac{k_{0sat}}{k_{ssat}} - 1)\frac{S_0^a}{S0max}),$$

where β and k_β are the slope radians and scaling factor, and k_ζ is a scaling factor for the ratio of saturated hydraulic conductivity. The revised lower-layer soil water storage S_s^a is then determined as:

$$S_s^a = S_s^f + \Delta D_0.$$

The change in S_s will lead to the change in the shallow soil water storage (D_s) and lateral interflow (Q_{Is}). The soil water storage at lower layer is thus updated as:

$$S_d^a = S_s^a + \Delta D_s.$$

Similarly, the groundwater storage S_g will be adjusted with the increment of deep soil layer drainage.

The total runoff (Q_{tot}^a) should be updated as:

$$Q_{tot}^{a} = (1 - e^{-k_r})(S_r^f + Q_{tot}^f + \Delta Q_{Is} + \Delta Q_{I0}),$$

where k_r is a routing delay factor.

The surface water storage S_r should be updated accordingly as:

$$S_r^a = S_r^f + \Delta Q_{Is} + \Delta Q_{I0} - \Delta Q_{tot}.$$

The total evapotranspiration change (ΔE_{tot}) caused by the changes in S_0 and S_s can be updated as follow:

$$\Delta E_{tot} = \delta E_s * \Delta S_0 + \delta E_t * \Delta S_s,$$

where the E_s is the evaporation flux from the surface soil store (S_0) and E_t is the total actual plant transpiration. The term δE_s is given as

$$\delta E_s = (1 - f_{sat}) E_{t\_rem} \delta f_{soile},$$

where f_{soile} is relative soil evaporation and f_{sat} is the fraction of the grid cell that is saturated, and

$$E_{t\_rem} = E_0 - (E_t - \delta E_t)\ ,$$

The term δE_t is from the changes in root-water uptake from shallow and deep soil layers as

$$\delta E_t = \delta U_s + \delta U_d,$$

with

$$\delta U_s = \delta U_{smax} \frac{\max\,(abs(\delta U_{smax}, \delta U_{dmax}))}{\delta U_{smax} + \delta U_{dmax}}$$

$$\delta U_d = \delta U_{dmax} \frac{\max\,(abs(\delta U_{smax}, \delta U_{dmax}))}{\delta U_{smax} + \delta U_{dmax}}$$

$\delta U_{smax} = \frac{U_{s0}}{w_{slim}} \delta w_s$, $\delta U_{dmax} = \frac{U_{d0}}{w_{dlim}} \delta w_d$, where U_{smax} and U_{dmax} are the maximum root water uptake from the shallow soil store and from deep soil store. w_{slim} and $w_{dlim}$is the water-limiting relative water content from the *shallow and deep* soil layer.

Finally,

$\delta f_{soile} = \frac{f_{soilmax}}{w_{0lim}} \delta w_0$, where $f_{soilmax}$ is the scaling factor corresponding to unlimited soil water supply, with

$\delta w_0 = \frac{1}{S_{0max}}$, $\delta w_s = \frac{1}{S_{smax}}$, and $\delta w_d = \frac{1}{S_{dmax}}$,

where the w_z is the relative soil wetness of layer *z, i.e.* either 0, s or d.

Frost, A.J., Ramchurn, A. and Smith, A., (2016). The bureau's operational AWRA landscape (AWRA-L) Model. *Bureau of Meteorology Technical Report*.