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# An alternate and robust approach to calibration for the estimation of land surface model parameters based on remotely sensed observations

Guido D. Salvucci<sup>1</sup> and Dara Entekhabi<sup>2</sup>

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[1] Atmospheric models include land surface parameterizations of heat and moisture fluxes. Most parameterizations derive from early models of layered soil and vegetation canopy that account for liquid, vapor and heat diffusion, radiation processes, and surface turbulence. The number of parameters in these models ranges roughly from 10 to 50. Some parameters are known to vary over a small range and/or not significantly impact predictions. Others are highly influential (e.g., Leaf Area Index), but are currently well estimated from satellite data. Many parameters, however, are highly influential, vary over a large dynamic range, cannot be estimated from satellite data, and cannot be readily upscaled from *in-situ* measurements. For such parameters (e.g., maximum stomatal conductance and soil hydraulic conductivity), values are assigned based on look-up tables sorted by land cover and soil texture. Here we present a method for estimating these parameters by minimizing a measure of nonstationarity of model-predicted moisture state variable tendencies. This method has advantages over calibration: 1) it does not require flux data (e.g., evapotranspiration); and 2) the tendency terms are evaluated at the model grid and thus yield parameters that are effective for that scale. The method is demonstrated with the Noah Land Surface Model, using remotely-sensed soil moisture, at a site in California. Preliminary results indicate that the method is robust and performs better than both: 1) calibration to soil moisture observations, which can lead to large, compensating errors in drainage and evaporation; and 2) minimizing the sum of squares of innovations of soil moisture updates. **Citation:** Salvucci, G. D., and D. Entekhabi (2011), An alternate and robust approach to calibration for the estimation of land surface model parameters based on remotely sensed observations, *Geophys. Res. Lett.*, 38, L16404, doi:10.1029/2011GL048366.

## 1. Introduction

[2] Most land surface models embedded within climate and weather models (Noah LSM, SIB, MOSAIC, CLM etc) are broadly similar, having been derived from early work in layered models of soil and vegetation canopy that account for liquid, vapor and heat diffusion, radiation processes, and boundary layer turbulence. Values for free parameters in these models (e.g., the maximum stomatal conductance, the

ratio of heat to momentum roughness lengths, and soil hydraulic conductivity) are typically assigned based on look-up tables sorted by dominant land cover and soil classifications. The values in these tables [e.g., *Dorman and Sellers*, 1989] are typically based on a few field or laboratory measurements, or in some cases, educated guesses.

[3] In a recent paper [*Sun et al.*, 2011], we have presented a method for estimating land surface model parameters by maximizing a measure [*Salvucci*, 2001] of stationarity of model predicted tendencies (the time derivative of land surface moisture and temperature states with time). The measure is formed by conditionally averaging the tendency term by the state, which *Salvucci* [2001] showed to be zero for stationary systems. This measure has distinct advantages over calibration metrics. The model tendency terms are evaluated at the relevant scale with measured forcing (e.g., precipitation, wind, radiation) and measured state variables (e.g., remotely-sensed surface soil moisture and temperature). Lack of stationarity in the resulting tendency terms arise from structural model error and mis-specification of parameters. Minimizing the lack of stationarity thus estimates land surface parameters that are consistent with the measured forcings, at the appropriate scale.

[4] The proposed method is an alternative to calibration based on fitting model simulated time series of soil moisture and/or measured fluxes to observations [e.g., *Scott et al.*, 2000; *Gupta et al.*, 1999; *Hogue et al.*, 2005]. The main strength of the proposed method is that it does not require measurements of the actual surface fluxes (e.g., latent and sensible heat flux, soil water drainage or capillary rise) for calibration. Such measurements are too scarce (even with the advent of the FLUXNET network [*Baldocchi et al.*, 2001]) to use for estimating continuous maps of surface parameters. As by *Sun et al.* [2011], the method was demonstrated at FLUXNET sites, using a land surface model similar to the Noah LSM [*Ek et al.*, 2003], but simplified to a single soil layer. Here the tendency terms is calculated directly from the current version of the Noah LSM (public release version 2.7.1) ensuring that the resulting parameter estimates are compatible with the NOAA WRF model and are applicable to atmospheric models that employ the Noah LSM.

[5] Below we demonstrate the method at the Vaira Ranch Ameriflux site [*Ryu et al.*, 2008] using field measured atmospheric forcing and remotely sensed soil moisture (AMSR-E derived LPRM [*Owe et al.*, 2008] product) and Leaf Area Index (MODIS level 4 product available through the USGS Land Processes Distributed Active Archive Center). To keep the parameter estimation manageable for large scale applica-

<sup>1</sup>Departments of Earth Sciences and Geography and Environment, Boston University, Boston, Massachusetts, USA.

<sup>2</sup>Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA.

tions, we start with default soil and vegetation parameters sets and then further refine key parameters within these sets.

## 2. Methodology

[6] The basic idea presented here, by *Salvucci* [2001] and by *Sun et al.* [2011] is as follows: Using conditional averaging, the relation between soil moisture and precipitation ( $P$ ) can be studied in place of the relation between soil moisture and evapotranspiration ( $ET$ ), and drainage plus runoff ( $D+RO$ , which we will here denote as  $Q$ ). The benefit of doing this is that very few long term and/or spatially distributed data sets exist for evapotranspiration and drainage, but many exist for precipitation and soil moisture. Furthermore precipitation and indices of surface soil moisture can be estimated from satellite data with global coverage. To accomplish this we apply conditional averaging to the water balance equation for soil water storage ( $\forall$ ) per unit area of land:  $\frac{d\forall}{dt} = P - ET - Q$ , and exploit the condition that  $E\left[\frac{d\forall}{dt}|\forall\right] = 0$  for stationary systems. As a first step, we review the derivation of this property.

### 2.1. Conditional Averaging of the Water Balance Equation

[7] *Salvucci* [2001] demonstrated (through mathematical derivation, monte-carlo studies, and observed data sets) that  $E\left[\frac{d\forall}{dt}|\forall\right] = 0$ . There are a few complementary ways to see why this is so. The simplest is to note that if  $E\left[\frac{d\forall}{dt}|\forall\right]$  depended on  $\forall$ , and an estimate of this dependence were approximated through a polynomial-series regression function (e.g., say  $E\left[\frac{d\forall}{dt}|\forall\right] = a + b\forall + c\forall^2 + \dots$ ), then each of the coefficients ( $a-c, \dots$ ) could be found using least squares regression by solving a set of equations whose right-hand side involved the terms  $E\left[\forall^n \frac{d\forall}{dt}\right]$  for  $n = 0$  to 2 (in this example). But each of these terms can be re-written, using the chain rule as  $\frac{1}{n+1}E\left[\frac{d\forall^{n+1}}{dt}\right]$ . Stationarity of the statistical moments of  $\forall$ , however, requires that these all be zero, thus the estimates of the coefficients are zero, demonstrating  $E\left[\frac{d\forall}{dt}|\forall\right] = 0$ .

[8] Another way to demonstrate this key result is to consider representing  $\forall$  as a Fourier series. The rate of change of  $\forall$  would then be another series (with sines replaced by cosines and vice-versa), which, because of the orthogonality of the trigonometric series, will be uncorrelated with  $\forall$ . Finally, it can also be seen from a sampling perspective. For a time series of  $\forall$ , if  $\forall$  is stationary, then for any level of  $\forall$  (e.g., the 75th percentile, which we denote  $\forall_{75}$ ), the difference between the number of upcrossings (from  $\forall$  less than  $\forall_{75}$  to greater) and downcrossings ( $\forall_t > \forall_{75} > \forall_{t+dt}$ ) will be at most one. Taking these crossings as samplings of  $\frac{d\forall}{dt}$ , they balance in the long term mean. Note that all of the above statements remain valid in the presence of a seasonal cycle (in fact, it is even more straightforward to demonstrate for the seasonal cycle of  $\forall$  since both  $\forall$  and  $\frac{d\forall}{dt}$  can be represented by deterministic Fourier components, and they by definition will be orthogonal).

[9] Now, if we return to the water balance equation:

$$\frac{d\forall}{dt} = P - ET - Q \quad (1)$$

and take the conditional average with respect to  $\forall$ , i.e.:

$$E\left[\frac{d\forall}{dt}|\forall\right] = E[P|\forall] - E[ET|\forall] - E[Q|\forall] \quad (2)$$

and then invoke the stationarity condition  $E\left[\frac{d\forall}{dt}|\forall\right] = 0$ , and rearrange, we find:

$$E[P|\forall] = E[ET|\forall] + E[Q|\forall] \quad (3)$$

### 2.2. Adaptation of Method for Estimating Noah LSM Parameters

[10] Our previous application of the stationarity-based parameter estimation was in the context of a relatively simple land surface model. In that model [*Sun et al.*, 2011], there was a single root zone moisture storage, and the fluxes of evapotranspiration, drainage, runoff and capillary rise to the root zone were parameterized based on that single storage state.

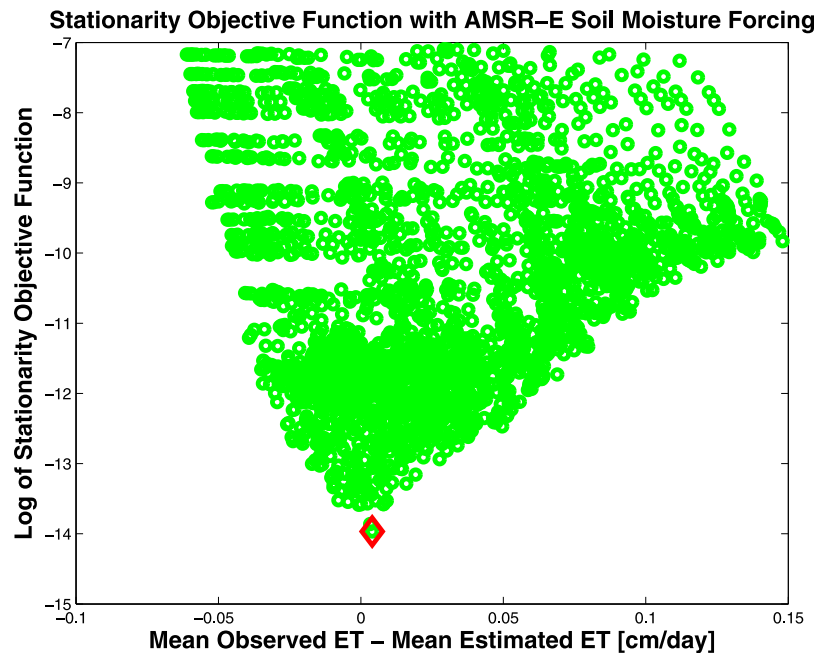
[11] The challenge here is to apply the same concepts to a modern, multi-layer soil-vegetation-atmosphere transfer model, complete with canopy retention and evaporation, soil water redistribution, bare soil evaporation and transpiration, and snowpack physics. The significant difference is that the fluxes in this case depend on both the (observable) surface states, and also on deeper-layer, unobserved, moisture and temperature states. The solution we demonstrate below is simply to integrate the LSM forward in time, but update the surface states (here, soil moisture) when data are available (e.g., at satellite crossing time). Below we do this with a hard-update, but future work will assess if a data assimilation approach will improve results enough to justify the added complexity and computation required.

[12] The updated soil moisture is the (observable) top soil layer (nominally 10 cm in the community version Noah LSM). The input into the layer is thus liquid precipitation net of canopy storage plus snow melt, and the outputs are root zone extraction from this layer, bare soil evaporation, and flow to and from the soil layer below. However, when evaluating the stationarity of the system using equation (3), we take  $\forall$  to be the total storage integrated over all layers, and the fluxes to be defined by that choice. The basic idea behind the parameter estimation strategy is that the Noah LSM parameters most consistent with the observed forcing and state-variables will be those for which  $E\left[\frac{d\forall}{dt}|\forall\right] = 0$  for the model run with periodic updates to the surface state.

[13] As is illustrated in an example below, if the parameters are not consistent with the forcings and measured states, the model dynamics will drift, violating the stationarity condition. When this happens, the conditionally-averaged tendency terms are not zero, and instead reflect the moisture-dependent errors in the fluxes (or temperature-dependent errors when evaluating the heat storage tendency terms). This can be seen by re-writing equation (2) in terms of modeled fluxes (denoted with an asterisk superscript), and subtracting equation (3), yielding an estimate of the moisture-dependent error  $\varepsilon$ :

$$E[\varepsilon|\forall] \equiv E\{[(ET^* - ET) + (Q^* - Q)]|\forall\} \cong E\left[\frac{d\forall^*}{dt}|\forall^*\right] \quad (4)$$

Minimizing the error term (and thus estimating model parameters), can thus be accomplished by calculating the right-hand side of equation (4). The model tendency term  $\left(\frac{d\forall^*}{dt}\right)$  is readily extracted from the LSM (for those familiar



**Figure 1.** Demonstration of the stationarity-objective function calculated for the Vaira Ranch Ameriflux site using the AMSR-E based LPRM [Owe *et al.*, 2008] remotely sensed soil moisture forcing for the top layer of the Noah LSM. The green circles correspond to the log of the objective function (equation (5)) for approximately 2500 different parameter sets. The parameter set for which the Noah LSM model output is most consistent with the meteorological forcing and observed soil moisture yields the lowest stationarity-objective function (red diamond). Note that the bias between the measured ET at Vaira ranch and the model simulated ET for this stationarity-chosen parameter set is close to zero, demonstrating the potential of the proposed methodology. The root-mean square error of the daily-averaged ET for the chosen parameter set is approximately 0.04 cm/day (12 watts/square meter) and the mean bias is less than 0.005 cm/day (1.5 watts/square meter).

with the Noah LSM, the *SRT* subroutine calculates the tendency implicitly for use in the tri-diagonal system of equations for time stepping). The tendency term is then saved, and after the integration (e.g., 5 years of integration, exclusive of spin -up), the mean value of  $\frac{d\psi^*}{dt}$  is calculated in each of ten “bins” of  $\psi^*$ , thus forming an estimate of conditionally-averaged tendency  $E\left[\frac{d\psi^*}{dt}\middle|\psi^*\right]$ .

[14] In order to better equalize the variance of  $\frac{d\psi^*}{dt}$  in each bin, we first transform the storage variable using a cumulative-distribution function mapping [Calheiros and Zawadzki, 1987], as has been done previously for soil moisture [e.g., Saleem and Salvucci, 2002; Reichle and Koster, 2004], and we normalize  $\frac{d\psi^*}{dt}$  by its standard deviation ( $\sigma$ ). The former insures that the same number of values is used in each bin when calculating the conditional-mean tendency, and the latter insures that low variance model runs are not preferred over high variance runs. The stationarity-objective function can thus be written as:

$$OBJ_{stationarity} = \sum_{i=1}^{Nbins} \left( E \left[ \frac{d\psi^*}{dt} / \sigma \left( \frac{d\psi^*}{dt} \right) \right]_i \right)^2 \quad (5)$$

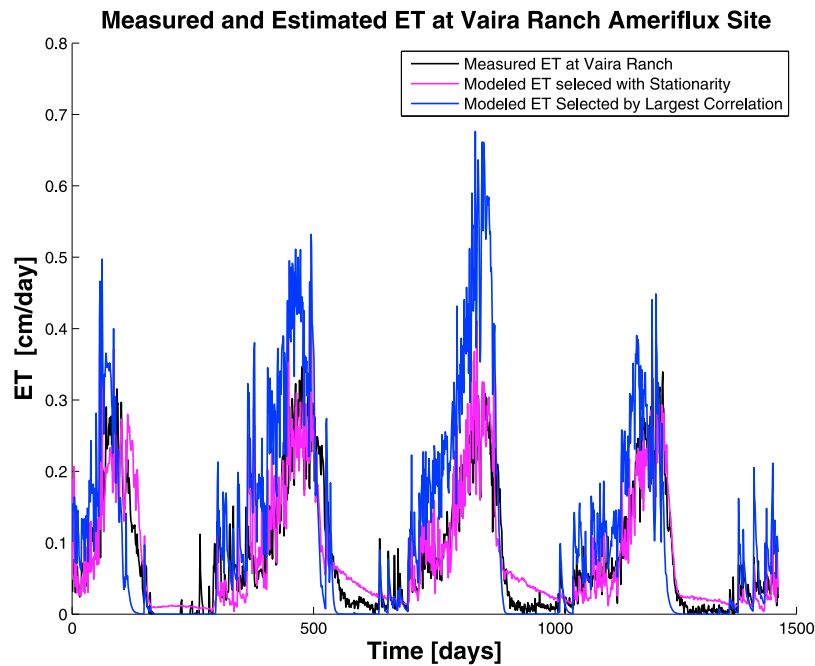
Also note that because in every time step the model conserves mass at all layers (to within the numerics of the model), the conditionally-averaged tendency term is equal (to within the natural statistical variability of  $\psi$ ) to the conditionally-averaged innovations (the soil moisture update required to nudge the system to the observed moisture). However, the objective function (5) is not the same, and is not proportional

to, the sums of squares of innovations. By conditioning on moisture, (5) detects, and can thus minimize, structural (i.e., moisture-dependent) errors, whereas the sum of squares of innovations cannot. The proposed method is thus distinct from methods that simultaneously assimilate observations and estimate parameters through minimization of innovations [e.g., Caparrini *et al.*, 2004].

[15] The procedure described above is repeated for each trial parameter set. Specifically, the model is integrated (with soil moisture updating), and the objective function (equation (5)) is evaluated, for each of the seven basic soil texture groups, the two most reasonable a priori estimates of vegetation class, and a set of adjusted parameters within each of these default groups. The parameters that are further adjusted within the groupings are the maximum stomatal conductance, the saturated hydraulic conductivity, and the exponent of the bare soil evaporation efficiency function (a power law model in Noah). Adjusting these refined parameters in four to eight increments over a reasonable range of values (for each default soil texture class and two vegetation classes) requires approximately 2500 model runs.

### 2.3. Example of Methodology

[16] In this example, we apply the method to the Vaira Ranch data set of the Ameriflux network [Ryu *et al.*, 2008] where measured evaporation flux data is available for verification. The site is located in California (N38.4067/W120.9507, elevation 129m). The soil type is rocky silt-loam. The site is a grazed C3 grassland opening in a region of oak/grass savanna. The climate is Mediterranean. Forcing



**Figure 2.** Time series of daily-averaged measured ET (black line) and the daily-averaged ET produced by the Noah LSM with the parameters chosen via the stationarity objective function (magenta line). The root mean square error of the stationarity-chosen modeled ET flux is 0.04 cm/day (about 12 watts/square meter). The anomaly correlation at one day lag is approximately 0.5, indicating the presence of persistent, structural error. Considering that the stationarity-objective function does not use measured ET fluxes, i.e., it is only based on forcing and surface soil moisture state, this is a significant result. The blue line corresponds to the parameter set for which the simulated surface soil moisture demonstrated the largest rank-correlation with the AMSR-E soil moisture. It is severely biased.

and validation data from 2003 to 2007 are used in the analysis. In this application, the Noah model was forced with half-hourly Ameriflux-observed meteorological data (wind speed, air temperature, humidity, pressure, downwelling longwave and shortwave radiation, and precipitation), and remotely-sensed surface soil moisture from the AMSR-E derived LPRM data set [Owe *et al.*, 2008]. For broader applications (i.e., beyond testing the method at Ameriflux sites), we suggest using the North American Land Data Assimilation System (<http://www.emc.ncep.noaa.gov/mmb/nldas/>) for gridded values of the required forcing data (including merged gauge-radar precipitation estimates).

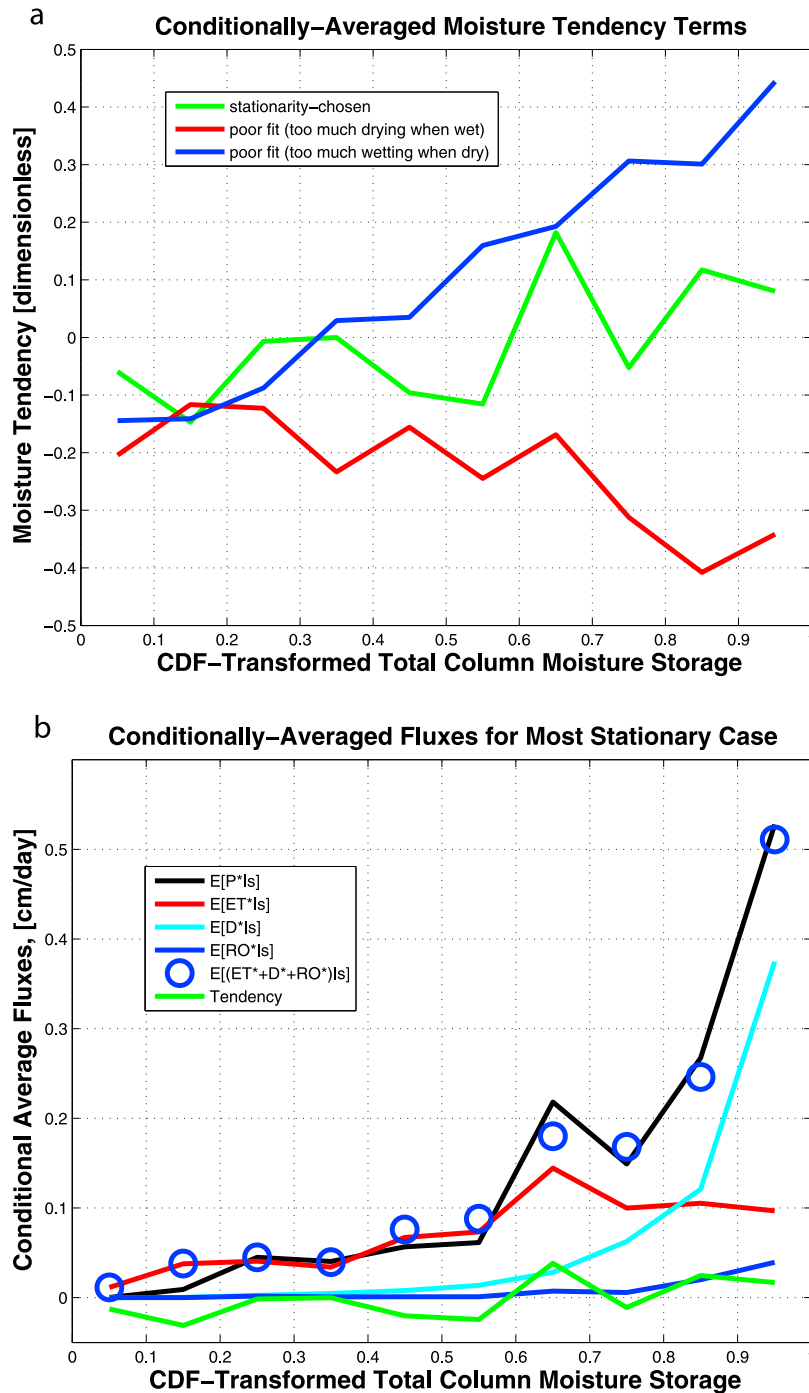
[17] To illustrate the capability of the method in a simple way, Figure 1 plots the log of the stationarity-objective function (5) against the bias of the estimated  $ET$  (i.e., the model-estimated  $ET$  minus the observed  $ET$ ), for approximately 2500 parameter sets. Note that the methodology chooses a parameter set minimizing (5) which produces a modeled mean  $ET$  very close to the measured value (red diamond, Figure 1). The chosen parameters corresponded to a silty loam with a conductivity of  $3.5E-6$  meters/sec, a bare soil evaporation efficiency exponent of 5, and a maximum stomatal conductance of 5 mm/sec.

[18] The key point to remember here is that the proposed parameter estimation method does not use measurements of turbulent fluxes (such as evapotranspiration). It indirectly estimates these fluxes by selecting model parameters for which the measured forcings (e.g., precipitation) and states (e.g., soil moisture) are in statistical equilibrium with the model's moisture tendency.

[19] In Figure 2, we plot the corresponding time series of (daily-averaged) measured (black lines) and modeled (magenta lines)  $ET$ . With the parameters estimated by the proposed stationarity-objective function, the model does a convincing job of capturing the seasonal and synoptic dynamics of  $ET$ . The blue lines of Figure 2 are discussed in section 2.4.

[20] To best understand how the stationarity-based method discriminates among the various parameters, we plot in Figure 3a the conditionally averaged tendency term  $E\left[\frac{dV^*}{dt}\middle|V^*\right]$  for ten bins and for 3 parameter sets: The chosen set, and two non-optimal sets (one producing too much ET and too little drainage and runoff (blue line), and the other producing too much ET, drainage, and runoff (red line)). Note that all three are approximately in water balance. But the two sub-optimal cases show trends in  $E\left[\frac{dV^*}{dt}\middle|V^*\right]$ . As discussed in

the methodology section,  $E\left[\frac{dV^*}{dt}\middle|V^*\right]$  must approach zero (to within statistical fluctuation) for natural, stationary systems, in each bin. The trends in  $E\left[\frac{dV^*}{dt}\middle|V^*\right]$  apparent in the red and blue off-optimal cases are indicative of moisture dependent errors due to poor parameter choice (see equation (4)). The right panel (Figure 3b) shows the conditionally-averaged fluxes that contribute to the change in total column moisture storage. For clarity, only the optimal case is plotted. The net of the precipitation (black), deep drainage (cyan), surface runoff (blue), and evapotranspiration (red), forms the tendency term (green). The tendency term is the same as is plotted in Figure 3a. To be more precise, the plotted conditionally



**Figure 3.** (a) Demonstration of conditionally-averaged tendency term for chosen (green), and sub-optimal (red and blue) parameter sets. (b) The fluxes which form the tendency term, plotted for the optimal case. The green line is the same in each panel, and corresponds to the black line minus the blue circles of Figure 3b.

averaged precipitation is actually the precipitation net of canopy and snow storage, and augmented by snowmelt. Likewise, the plotted conditionally-averaged ET is bare soil evaporation plus transpiration from all soil layers (i.e., it does not include direct canopy evaporation). These are the fluxes which form the tendency of soil moisture storage.

[21] We assess the robustness of the results with respect to forcing measurement errors. In this test, 20% random noise is added to the precipitation forcing, and the estimation procedure is repeated four times. In each case, the root-

mean-square error stayed under 15 watts/square meter, and the bias stayed within +/-3 watts per square meter. The stationarity method thus appears, at this point, robust to forcing errors.

**2.4. Comparison of Proposed Stationarity-Method and a Soil Moisture Calibration Approach**

[22] For comparison, we estimated the Noah parameters by maximizing the correlation of simulated and measured soil moisture, i.e., single-criteria soil moisture calibration.

Previous studies [e.g., Gupta *et al.*, 1999] indicated that single-criteria fitting, for example to soil moisture, is not robust. In essence, such a single-criteria fit could yield a predicted trace of soil moisture that is well correlated with the observed values, but poorly correlated with the fluxes, due to compensations between drainage, runoff and evapotranspiration. For Vaira Ranch, we find similar results to Gupta *et al.* [1999]. The parameter set yielding the best-correlated time series of soil moisture yields a highly biased and poor estimate of *ET*. This prediction of *ET* is plotted as the blue line in Figure 2. Note that in this comparison, the model was not updated with observed soil moisture during the model integration.

[23] We also tested whether simply minimizing the total sum of squares of innovations (the updates required to force the Noah LSM top node moisture to match the observed moisture at the observation times) could be used to estimate the parameters. Similar to the results of soil moisture calibration, model parameters leading to large biases (and large root mean square error) were selected. It appears that the key distinction is in the soil moisture conditional averaging of the tendency (or the innovation). This is the step that identifies the systematic (as opposed to random) errors in fluxes, and thus leads to robust parameter estimation.

### 3. Summary and Conclusions

[24] We conclude from these preliminary experiments that the stationarity-objective function is robust and that it extracts more information about the system, and thus yields better parameter estimates, than solely calibrating to soil moisture or minimizing the sum of squares of innovations. More information is extracted because the data are analyzed in a way that highlights the covariance of the forcings and responses, and their moisture dependence. Thus, a soil parameter set that is too “sandy”, for example, will drain too much at (relatively) large moisture, and thus have a different correlation with precipitation (and thus non-vanishing conditionally-averaged tendency), than the proper soil, even though it might (through a compensation of reduced evapotranspiration), yield a highly correlated time series of soil moisture and small innovations.

[25] As has been pointed out in previous studies [Gupta *et al.*, 1999; Hogue *et al.*, 2005], it should be noted that parameter values estimated by any optimization method, including that proposed here, do not have universal validity. For example, the values can and will change if: 1) different land surface models are forced with the same data; 2) subsets of parameters are allowed to vary while others are held constant; 3) different subsets of training data are used; and 4) the numerical resolution (vertical or horizontal) is altered.

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D. Entekhabi, Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139, USA.

G. D. Salvucci, Department of Earth Sciences, Boston University, 675 Commonwealth Ave., Boston, MA 02215, USA. (gdsalvuc@bu.edu)