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Fluxpart: Open source software for partitioning carbon dioxide and water vapor fluxes

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ABSTRACT

The eddy covariance method is regularly used for measuring gas fluxes over agricultural fields and natural ecosystems. For many applications, it is desirable to partition the measured fluxes into constitutive components: the water vapor flux into transpiration and direct evaporation components, and the carbon dioxide flux into photosynthesis and respiration components. The flux variance similarity (FVS) partitioning method is based on flux variance similarity relationships and correlation analyses of high-frequency eddy covariance data (Scanlon and Sahu, 2008; Scanlon and Kustas, 2010, 2012). The FVS method is relatively complex computationally, and that complexity has likely been an impediment to greater use and testing of the procedure. In this work, we present a new algebraic solution to the key computational task in the partitioning algorithm, which significantly simplifies the FVS method. We also introduce Fluxpart, a free and open source Python 3 module that implements the FVS partitioning procedure. Example flux partitioning calculations are presented.

1. Introduction

The eddy covariance method is routinely used to measure gas fluxes over agricultural fields and other landscapes (Baldocchi, 2014). Greater insight into the functioning of agroecosystems is possible if the measured gas fluxes can be separated into their constitutive components: the water vapor flux into transpiration and direct evaporation components, and the carbon dioxide flux into photosynthesis and respiration components.

General information about flux partitioning can be found in the other articles of this special issue, as well as the recent reviews by Kool et al. (2014) and Anderson et al. (2017b). The focus of this paper is the flux variance similarity (FVS) partitioning method of Scanlon et al., a procedure based on flux variance similarity relationships and correlation analyses of eddy covariance data (Scanlon and Sahu, 2008; Scanlon and Kustas, 2010, 2012). The FVS method is gaining in popularity as evidenced by a number of recent publications (e.g. Palatella et al., 2014; Sulman et al., 2016; Wang et al., 2016; Anderson et al., 2017a). However, wider testing and adoption has been hindered by the relative difficulty of implementing the method, which requires complex and computationally intensive processing and analysis of high-frequency eddy covariance data.

We have two objectives. First, we examine some computational aspects of the FVS partitioning algorithm, and introduce a new algebraic method for the key computational task in the procedure, eliminating the need for more complicated numerical calculations. Second, we introduce Fluxpart, a free and open source Python 3 module intended to permit wider use, testing, and development of the FVS partitioning procedure. Example calculations with Fluxpart are presented.

2. Background

The FVS flux partitioning method has been described at length in the literature (Scanlon and Sahu, 2008; Scanlon and Kustas, 2010; Palatella et al., 2014). We present here a brief overview.

Monin-Obukhov similarity theory implies that high-frequency time series for scalars, such as the water vapor (q) and carbon dioxide (c) concentrations, will exhibit perfect correlation when measured at the same point within a homogeneous atmospheric layer (Monin and Obukhov, 1954; Scanlon and Sahu, 2008). Actual measured correlations may deviate from this prediction for several reasons, including the presence of multiple, distinct source/sinks for the scalar quantities within the layer (Scanlon and Albertson, 2001; Scanlon and Sahu, 2008). Flux variance similarity and perfect correlation may exist for concentrations associated with a single source/sink, but the superposition of fluxes from multiple source/sinks degrades the overall correlation.

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In the case of q and c, one source/sink arises from the exchange of q and c across leaf stomata during transpiration and photosynthesis, and a second from non-stomatal direct evaporation and respiration. If only transpiration and photosynthesis occur, similarity theory predicts $\rho_{q,c} = -1$ (a negative correlation because transpiration acts as a q source and photosynthesis as a c sink). Conversely, if only evaporation and respiration occur, theory predicts $\rho_{q,c} = 1$ (evaporation and respiration being sources for q and c, respectively).

Scanlon and Sahu (2008) note that one may think of evaporation and respiration as contaminating the transpiration and photosynthesis fluxes, driving the q–c correlation away from the expected $\rho_{q,c} = -1$. The premise of the FVS technique is that an analysis of the degree of that contamination can be used to infer the relative amounts of stomatal and non-stomatal fluxes present.

More specifically, Scanlon and Sahu (2008) propose the following partitioning analysis. The water vapor concentration, carbon dioxide concentration, and vertical wind velocity (w) measured at a point on an eddy covariance tower can each be decomposed as

$$q = \langle q \rangle + q' \tag{1a}$$

$$c = \langle c \rangle + c' \tag{1b}$$

$$w = \langle w \rangle + w' \tag{1c}$$

where angle brackets indicate the temporal mean over a short interval (e.g., 15–60 min) and the prime indicates the fluctuation from the mean.

According to the conventional eddy covariance method, the water vapor and CO_2 fluxes for the interval are, respectively,

$$F_q = \langle w'q' \rangle \tag{2a}$$

$$F_c = \langle w'c' \rangle \tag{2b}$$

The gas concentration fluctuations and fluxes can be further decomposed into components regulated by stomatal and non-stomatal controls:

$$q' = q_e' + q_t' \tag{3a}$$

$$c' = c_r' + c_p' \tag{3b}$$

$$F_q = F_{q_e} + F_{q_t} = \langle w'q_e' \rangle + \langle w'q_t' \rangle \tag{4a}$$

$$F_c = F_{c_r} + F_{c_p} = \langle w'c_r' \rangle + \langle w'c_p' \rangle \tag{4b}$$

where q_e' and q_t' are the water vapor concentration fluctuations associated with non-stomatal (evaporation) and stomatal (transpiration) controls, respectively; c_r' and c_p' are the CO_2 concentration fluctuations associated with non-stomatal (respiration) and stomatal (photosynthesis) controls, respectively; and F_{q_e}, F_{q_t}, F_{c_r}, and F_{c_p} are the corresponding flux components. The FVS partitioning method is applicable only when the photosynthesis CO_2 flux is directed downward and the other fluxes are upward,

$$F_{c_p} < 0 \tag{5a}$$

$$F_{c_r},\ F_{q_t},\ F_{q_e} > 0 \tag{5b}$$

Scanlon and Sahu (2008) assume that the transfer efficiencies of the stomatal-controlled scalars are greater than those of the non-stomatal scalars, which leads to the following approximations for the scalar correlations (Bink and Meesters, 1997; Katul and Hsieh, 1997)

$$\rho_{q_t,q_e} \approx \frac{\rho_{w,q_e}}{\rho_{w,q_t}} = \frac{\langle w'q_e' \rangle}{\langle w'q_t' \rangle}\frac{\sigma_{q_t}}{\sigma_{q_e}} \tag{6a}$$

$$\rho_{c_p,c_r} \approx \frac{\rho_{w,c_r}}{\rho_{w,c_p}} = \frac{\langle w'c_r' \rangle}{\langle w'c_p' \rangle}\frac{\sigma_{cp}}{\sigma_{c_r}} \tag{6b}$$

where σ indicates the standard deviation over the averaging interval. These definitions and approximations allowed Scanlon and Sahu (2008) to derive a series of equations that can be used to calculate the constituent flux components. As discussed by Palatella et al. (2014), the main computational task in this procedure involves solving two simultaneous nonlinear equations that can be expressed more compactly than originally presented by Scanlon and Sahu (2008). Similarly to Palatella et al. (2014), we formulate this two-equation system as

$$W\frac{\langle w'q' \rangle}{\langle w'c' \rangle}\left(\frac{\langle w'c_r' \rangle}{\langle w'c_p' \rangle} + 1\right) = \left(\frac{\langle w'q_e' \rangle}{\langle w'q_t' \rangle} + 1\right) \tag{7a}$$

$$W\rho_{q,c}\sigma_q\sigma_c\sigma_{c_p}^{-2} = 1 + \frac{\langle w'c_r' \rangle}{\langle w'c_p' \rangle} + \frac{\langle w'q_e' \rangle}{\langle w'q_t' \rangle} + \rho_{c_p,c_r}^{-2}\frac{\langle w'c_r' \rangle}{\langle w'c_p' \rangle}\frac{\langle w'q_e' \rangle}{\langle w'q_t' \rangle} \tag{7b}$$

where:

$$\frac{\langle w'q_e' \rangle}{\langle w'q_t' \rangle} = -\rho_{c_p,c_r}^2 + \rho_{c_p,c_r}^2\sqrt{1 - \rho_{c_p,c_r}^{-2}(1 - W^2\sigma_q^2/\sigma_{c_p}^2)} \tag{8a}$$

$$\frac{\langle w'c_r' \rangle}{\langle w'c_p' \rangle} = -\rho_{c_p,c_r}^2 \pm \rho_{c_p,c_r}^2\sqrt{1 - \rho_{c_p,c_r}^{-2}(1 - \sigma_c^2/\sigma_{c_p}^2)} \tag{8b}$$

Note that Eq. (7) has two branches due the presence of the plus–minus operator in Eq. (8b). Eq. (8a) would similarly have two branches except that the "minus" branch can be ruled out since it can never satisfy the required $\langle w'q_e' \rangle / \langle w'q_t' \rangle > 0$

The system contains five parameters that are known directly from eddy covariance data and three unknown parameters. The known parameters are: $F_q = \langle w'q' \rangle$ and $F_c = \langle w'c' \rangle$, the water vapor and CO_2 fluxes, respectively; σ_q^2 and σ_c^2, the variances of the water vapor and CO_2 concentrations, respectively; and $\rho_{q,c}$, the correlation coefficient for the water vapor and CO_2 concentrations. The free parameters are: $\sigma_{c_p}^2$, the variance of the photosynthesis CO_2 concentration; ρ_{c_p,c_r}, the correlation coefficient for the photosynthesis and respiration CO_2 concentrations; and W, the leaf-level water use efficiency. The latter is defined

$$W = \frac{\langle w'c_p' \rangle}{\langle w'q_t' \rangle} \tag{9}$$

By definition or by physical reasoning, it is required that $-1 < \rho_{c_p,c_r} < 0$, $\sigma_{c_p}^2 > 0$, and $W < 0$ (Scanlon and Sahu, 2008). If a value for W is known from leaf-level measurements or can be otherwise estimated (see Scanlon and Sahu, 2008, Appendix A), then Eq. (7) can be solved for the remaining unknowns, $\sigma_{c_p}^2$ and ρ_{c_p,c_r} (explained in greater detail in the next section). The flux components are then given by

$$F_{c_p} = \langle w'c' \rangle / \left(\frac{\langle w'c_r' \rangle}{\langle w'c_p' \rangle} + 1\right) \tag{10a}$$

$$F_{c_r} = F_c - F_{c_p} \tag{10b}$$

$$F_{q_t} = F_{c_p}/W \tag{10c}$$

$$F_{q_e} = F_q - F_{q_t} \tag{10d}$$

The partitioning procedure does not always produce a result because a solution to Eq. (7) may not exist or the solution may be nonphysical (that is, the obtained values for either $\sigma_{c_p}^2$ or ρ_{c_p,c_r} may be invalid, or the obtained flux components may violate the directional requirements in Eq. (5)). No solution for a given time interval or series of intervals may be the correct outcome. For example, meteorological conditions may be incompatible with the theory or assumptions underlying the FVS method. On the other hand, Scanlon and Sahu (2008) found that, in some instances, the root cause of failure may be the presence of large-scale eddies that affect flux variance similarity relationships but do not contribute significantly to fluxes. They therefore proposed retrying failed analyses after filtering the high-frequency q, c, and w time series data to remove large-scale (low-frequency)