<u>Error propagation formulas to accompany:</u>

Seasonal partitioning of precipitation between streamflow and evapotranspiration, inferred from end-member splitting analysis

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xxsS1.1 Gaussian error propagation

In our paper, we calculate all uncertainties in derived quantities using Gaussian error propagation. Gaussian error propagation has found widespread application in many scientific disciplines, and for good reason: it is relatively straightforward to apply, its data requirements are modest, and its underlying assumptions are reasonable approximations for many real-world cases. Consider, for example, a function of several variables $z = f(w, x, y, \ldots)$. The Gaussian error propagation formula approximates the standard error in z as a function of the standard errors of each of the inputs, as follows:

$$\mathrm{SE}(z) \approx \sqrt{\left(\frac{\partial f}{\partial w}\mathrm{SE}(w)\right)^2 + \left(\frac{\partial f}{\partial x}\mathrm{SE}(x)\right)^2 + \left(\frac{\partial f}{\partial y}\mathrm{SE}(y)\right)^2 + \cdots} \quad , \qquad \text{(S1)}$$

where each of the terms includes an estimate of the uncertainty in each input (as expressed by its standard error), multiplied by z's sensitivity to that input, as expressed by the partial derivative of the function f, evaluated at the central estimates for all of the input variables (Kirchner, 2001).

Gaussian error propagation assumes that the uncertainties in each of the input variables are uncorrelated with one another. However, and contrary to what is sometimes claimed, it makes no assumption whatsoever concerning how those variables are distributed (Gauss, 1823); the term "Gaussian" refers to Carl Friedrich Gauss and not to the probability distribution that also bears his name. Gaussian error propagation also makes no specific assumption about the form of the function f, but of course the approximations implied by the derivatives will be more exact, the closer f is to a linear function of each of the input variables. In the special case where f is a linear function of all the input variables (as is the case for the weighted average in Eq. S4, below), Eq. (S1) will be exact rather than an approximation.

The assumption that the input uncertainties are independent will, particularly in the case of mass balances, often lead to somewhat conservative (i.e., somewhat too large) uncertainty estimates for the result z. For example, if we are solving for the mass balance $ET = P - Q$, and our estimates of the input uncertainties are obtained from the variability in water-year averages of P and Q, Eq. (S1) will overestimate the uncertainty in ET because all else equal, years with higher P will also tend to have higher Q, so part of the uncertainties in P and Q will tend to cancel each other out. Where the uncertainties in the inputs are correlated, and those correlations can themselves be estimated, a more accurate estimate of the uncertainty in z can be obtained using first-order, second-moment error propagation,

$$\mathrm{SE}(z) \approx \sqrt{\begin{array}{c} \left(\frac{\partial f}{\partial w}\mathrm{SE}(w)\right)^2 + \left(\frac{\partial f}{\partial x}\mathrm{SE}(x)\right)^2 + \left(\frac{\partial f}{\partial y}\mathrm{SE}(y)\right)^2 \\ + 2r_{wx}\left(\frac{\partial f}{\partial w}\mathrm{SE}(w)\right)\left(\frac{\partial f}{\partial x}\mathrm{SE}(x)\right) + 2r_{wy}\left(\frac{\partial f}{\partial w}\mathrm{SE}(w)\right)\left(\frac{\partial f}{\partial y}\mathrm{SE}(y)\right) \\ + 2r_{xy}\left(\frac{\partial f}{\partial x}\mathrm{SE}(x)\right)\left(\frac{\partial f}{\partial y}\mathrm{SE}(y)\right) + \cdots \end{array}} \quad , \qquad \text{(S2)}$$

where the correlation coefficients r_{xy} (etc.) express the correlations between the *uncertainties in the measurements or estimates* of the corresponding variables, which often will differ from the correlations between the variables themselves; see Kirchner (2001) for details. For the analysis presented here, the more complex approach of Eq. (S2) would provide little advantage over the simpler approach of Eq. (S1), because the most consequential uncertainties are those in the isotope measurements, which are not generally correlated with one another.

xxsS1.2 Standard errors of weighted averages

Weighted averages are widely used in isotope hydrology, and in environmental science more broadly. The formula for calculating the standard error of an *unweighted* average of n measurements y_i is well known:

$$\mathrm{SE}(\bar{y}) = \sqrt{\frac{\mathrm{var}(y)}{n}} \quad \text{where} \quad \mathrm{var}(y) = \frac{\sum(y_i - \bar{y})^2}{n}\,\frac{n}{n-1} \quad , \qquad \text{(S3)}$$

where the factor of $n/(n-1)$ corrects for the underestimation bias in the estimated variance as the degrees of freedom become small. (If, for example, one had only one measurement, y_i would equal $\bar{y}$, but the variance in y should be undefined, rather than zero. The factor of $n-1$ guarantees this result.)

But what if we instead have a *weighted* average of the form

$$\bar{y}_{\mathrm{wtd}} = \frac{\sum w_i\, y_i}{\sum w_i} \quad , \qquad \text{(S4)}$$

where the individual weights w_i represent the precipitation or streamflow associated with each measurement y_i, or some other measure of the importance of each y_i as a component of the mean? Applying Gaussian error propagation to Eq. (S4), under the assumption that the uncertainties in the y_i's are independent and identically distributed, directly yields

$$\mathrm{SE}(\bar{y}_{\mathrm{wtd}}) = \sqrt{\frac{\sum w_i^2\ \mathrm{var}_{\mathrm{wtd}}(y)}{(\sum w_i)^2}} = \sqrt{\frac{\mathrm{var}_{\mathrm{wtd}}(y)}{n_{\mathrm{eff}}}} \quad , \qquad \text{(S5)}$$

where $\mathrm{var_{wtd}}(y)$ is a weighted estimate of the variance (i.e., the squared uncertainty) in each of the y_i, and n_{eff} is the effective sample size,

$$n_{\mathrm{eff}} = \frac{(\sum w_i)^2}{\sum w_i^2} \quad , \tag{S6}$$

a formula often attributed to Kish (1995). If all of the weights w_i are the same, n_{eff} will equal *n*. The more uneven the weights are, the smaller n_{eff} will be in relation to *n*; in the limiting case that all of the weight is contained in a single measurement, n_{eff} will equal 1.

The remaining issue is how to estimate the weighted variance. Intuition suggests that it must be a weighted average of the squared deviations of the individual y_i from $\bar{y}_{\mathrm{wtd}}$,

$$\mathrm{var_{wtd}}(y) = \frac{\sum w_i \, (y_i - \bar{y}_{\mathrm{wtd}})^2}{\sum w_i} \quad , \tag{S7}$$

and that is nearly correct. However, as the weights w_i become more and more uneven, $\bar{y}_{\mathrm{wtd}}$ will come closer and closer to the points that carry most of the weight, leading to a downward bias in $\mathrm{var_{wtd}}(y)$; in the limiting case that all of the weight is contained in a single measurement, $\bar{y}_{\mathrm{wtd}}$ will exactly equal that measurement and Eq. (S7) will return a weighted variance of zero. One can eliminate this bias using a degree-of-freedom correction similar to Eq. (S3), but with n_{eff} instead of *n* (see Galassi et al., 2016):

$$\mathrm{var_{wtd}}(y) = \frac{\sum w_i \, (y_i - \bar{y}_{\mathrm{wtd}})^2}{\sum w_i} \, \frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1} = \frac{\sum w_i \, (y_i - \bar{y}_{\mathrm{wtd}})^2}{\sum w_i} \, \frac{(\sum w_i)^2}{(\sum w_i)^2 - \sum w_i^2} \quad . \tag{S8}$$

Combining Eqs. (S8) and (S5) yields the standard error of the weighted average $\bar{y}_{\mathrm{wtd}}$:

$$\mathrm{SE}(\bar{y}_{\mathrm{wtd}}) = \sqrt{\frac{\frac{\sum w_i \, (y_i - \bar{y}_{\mathrm{wtd}})^2}{\sum w_i} \, \frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1}}{n_{\mathrm{eff}}}} = \sqrt{\frac{\sum w_i \, (y_i - \bar{y}_{\mathrm{wtd}})^2}{\sum w_i} \, \frac{\sum w_i^2}{(\sum w_i)^2 - \sum w_i^2}} \quad . \tag{S9}$$

We have used Eq. (S9) to estimate the uncertainties in the weighted-average isotopic compositions of the end-members and mixtures, because Monte Carlo benchmark tests have shown that it accurately estimates the root-mean-square error in weighted averages across widely varying conditions (Kirchner, 2006).

Readers should be aware, however, that many statistical software packages will calculate a different weighted standard error, which is based on different assumptions and yields very different behavior. Specifically, the weighted standard error that is calculated by many software packages assumes that the weights w_i are equal to the inverse of the variances of the individual measurements y_i, and thus that the points with greater weight are more precisely known than the ones with less weight. (A slightly different starting point, namely that each of the y_i is itself an average of w_i individual measurements with equal variance, leads to the same assumption). Under those assumptions (which usually do not apply to the typical weighted averages used in hydrology, and in environmental science more generally), using inverse-variance weights w_i in Eq. (S4) yields a maximum likelihood estimate of $\bar{y}_{\mathrm{wtd}}$, with a standard error of

$$\mathrm{SE}'(\bar{y}_{\mathrm{wtd}}) = \sqrt{\frac{\mathrm{var}'_{\mathrm{wtd}}(y)}{n}} \quad , \qquad \text{where} \quad \mathrm{var}'_{\mathrm{wtd}}(y) = \frac{\sum w_i \, (y_i - \bar{y}_{\mathrm{wtd}})^2}{\sum w_i} \, \frac{n}{n-1} \quad . \qquad \text{(S10)}$$

Readers will notice that Eq. (S10) has the same form as Eq. (S9), but with n in place of n_{eff}. This difference is crucial. As the weights w_i become more uneven, uncertainty estimates derived from Eq. (S9) will increase, as they should, because with fewer points exerting significant influence on the average, the uncertainty in the average must grow. But under exactly the same conditions, uncertainty estimates derived from Eq. (S10) *will become smaller, not larger*. In the limiting case of a single y_i that carries all the weight in the data set, with the other points having no weight at all, Eq. (S10) will return a standard error of *zero*, whereas Eq. (S9) will return a standard error of infinity.

Weighted averages that are commonly encountered in environmental science (such as volume-weighted means in precipitation or streamflow) are consistent with the assumptions underlying Eq. (S9) but not Eq. (S10). Monte Carlo benchmark tests show that uncertainties in these averages *will be underestimated by Eq. (S10), potentially by large factors*, but will be correctly estimated by Eq. (S9) (Kirchner, 2006). Thus it is important for environmental scientists to determine – using benchmark tests if necessary – which standard error calculations their software is actually performing.

xxsS2.1 Uncertainty in end-member mixing fractions

Applying Gaussian error propagation to the end-member mixing formula (Eq. 11) yields

$$\mathrm{SE}\left(f_{\mathrm{Q_s \leftarrow P_s}}\right) = \sqrt{\left(\frac{\partial f_{\mathrm{Q_s \leftarrow P_s}}}{\partial \bar{\delta}_{\mathrm{Q_s}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{Q_s}}\right)\right)^2 + \left(\frac{\partial f_{\mathrm{Q_s \leftarrow P_s}}}{\partial \bar{\delta}_{\mathrm{P_s}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{P_s}}\right)\right)^2 + \left(\frac{\partial f_{\mathrm{Q_s \leftarrow P_s}}}{\partial \bar{\delta}_{\mathrm{P_w}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{P_w}}\right)\right)^2} \quad , \qquad \text{(S11)}$$

and writing out the partial derivatives gives (see also Genereux, 1998)

$$\mathrm{SE}\left(f_{\mathrm{Q_s \leftarrow P_s}}\right) = \sqrt{\left(\frac{\mathrm{SE}\left(\bar{\delta}_{\mathrm{Q_s}}\right)}{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}}\right)^2 + \left(-\frac{\bar{\delta}_{\mathrm{Q_s}} - \bar{\delta}_{\mathrm{P_w}}}{\left(\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}\right)^2} \mathrm{SE}\left(\bar{\delta}_{\mathrm{P_s}}\right)\right)^2 + \left(\frac{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{Q_s}}}{\left(\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}\right)^2} \mathrm{SE}\left(\bar{\delta}_{\mathrm{P_w}}\right)\right)^2} \quad . \qquad \text{(S12)}$$

One can also re-cast Eq. (S12) in a slightly simpler form by dividing both sides by $f_{\mathrm{Q_s \leftarrow P_s}}$, yielding

$$\frac{\mathrm{SE}\left(f_{\mathrm{Q_s \leftarrow P_s}}\right)}{f_{\mathrm{Q_s \leftarrow P_s}}} = \sqrt{\left(\frac{\mathrm{SE}\left(\bar{\delta}_{\mathrm{Q_s}}\right)}{\bar{\delta}_{\mathrm{Q_s}} - \bar{\delta}_{\mathrm{P_w}}}\right)^2 + \left(\frac{\mathrm{SE}\left(\bar{\delta}_{\mathrm{P_s}}\right)}{\bar{\delta}_{\mathrm{P_w}} - \bar{\delta}_{\mathrm{P_s}}}\right)^2 + \left(f_{\mathrm{Q_s \leftarrow P_w}} \frac{\mathrm{SE}\left(\bar{\delta}_{\mathrm{P_w}}\right)}{\bar{\delta}_{\mathrm{Q_s}} - \bar{\delta}_{\mathrm{P_w}}}\right)^2} \quad , \qquad \text{(S13)}$$

where $f_{\mathrm{Q_s \leftarrow P_w}} = 1 - f_{\mathrm{Q_s \leftarrow P_s}}$. Error propagation equations of the form of (S13) have the advantage that one can readily assess whether each of the contributing uncertainties is large or small. For example, the uncertainty in $\bar{\delta}_{\mathrm{Q_s}}$ is "large" (in the sense that it leads to a large percentage uncertainty in $f_{\mathrm{Q_s \leftarrow P_s}}$) if it is large compared to $\bar{\delta}_{\mathrm{Q_s}} - \bar{\delta}_{\mathrm{P_w}}$. Appropriate substitution of variables will yield analogous error propagation formulas for the other end-member mixing fractions ($f_{\mathrm{Q_s \leftarrow P_w}}$, $f_{\mathrm{Q_w \leftarrow P_s}}$, $f_{\mathrm{Q_w \leftarrow P_w}}$, $f_{\mathrm{Q \leftarrow P_s}}$, and $f_{\mathrm{Q \leftarrow P_w}}$).

xxsS2.2 Uncertainty in end-member splitting proportions

One can estimate the uncertainty in the fraction of summer precipitation becoming summer streamflow, $\eta_{\mathrm{P_s \to Q_s}}$, by applying Gaussian error propagation to Eq. (22):

$$\mathrm{SE}\left(\eta_{\mathrm{P_s \to Q_s}}\right) = \sqrt{\begin{array}{c}\left(\frac{\partial \eta_{\mathrm{P_s \to Q_s}}}{\partial \bar{\delta}_{\mathrm{Q_s}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{Q_s}}\right)\right)^2 + \left(\frac{\partial \eta_{\mathrm{P_s \to Q_s}}}{\partial \bar{\delta}_{\mathrm{P_s}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{P_s}}\right)\right)^2 + \left(\frac{\partial \eta_{\mathrm{P_s \to Q_s}}}{\partial \bar{\delta}_{\mathrm{P_w}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{P_w}}\right)\right)^2 \\ + \left(\frac{\partial \eta_{\mathrm{P_s \to Q_s}}}{\partial Q_{\mathrm{s}}} \mathrm{SE}(Q_{\mathrm{s}})\right)^2 + \left(\frac{\partial \eta_{\mathrm{P_s \to Q_s}}}{\partial P_{\mathrm{s}}} \mathrm{SE}(P_{\mathrm{s}})\right)^2\end{array}} \quad . \qquad \text{(S14)}$$

Writing out the partial derivatives and simplifying terms, in particular by substituting $\eta_{\mathrm{P_s \to Q_s}}$ itself for $\frac{Q_{\mathrm{s}}}{P_{\mathrm{s}}} \frac{\bar{\delta}_{\mathrm{Q_s}} - \bar{\delta}_{\mathrm{P_w}}}{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}}$, gives the result

$$\mathrm{SE}\left(\eta_{\mathrm{P_s \to Q_s}}\right) = \sqrt{\begin{array}{c}\left(\frac{\eta_{\mathrm{P_s \to Q_s}}}{\bar{\delta}_{\mathrm{Q_s}} - \bar{\delta}_{\mathrm{P_w}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{Q_s}}\right)\right)^2 + \left(\frac{\eta_{\mathrm{P_s \to Q_s}}}{\bar{\delta}_{\mathrm{P_w}} - \bar{\delta}_{\mathrm{P_s}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{P_s}}\right)\right)^2 + \left(\frac{Q_{\mathrm{s}}}{P_{\mathrm{s}}} \frac{f_{\mathrm{Q_s \leftarrow P_w}}}{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}} \mathrm{SE}\left(\bar{\delta}_{\mathrm{P_w}}\right)\right)^2 \\ + \left(\frac{\eta_{\mathrm{P_s \to Q_s}}}{Q_{\mathrm{s}}} \mathrm{SE}(Q_{\mathrm{s}})\right)^2 + \left(-\frac{\eta_{\mathrm{P_s \to Q_s}}}{P_{\mathrm{s}}} \mathrm{SE}(P_{\mathrm{s}})\right)^2\end{array}} \quad . \qquad \text{(S15)}$$

Dividing both sides by $\eta_{\mathrm{P_s \to Q_s}}$ yields the error propagation formula in an even simpler ratio form,

$$\frac{\mathrm{SE}\left(\eta_{\mathrm{P_s \to Q_s}}\right)}{\eta_{\mathrm{P_s \to Q_s}}} = \sqrt{\begin{array}{c}\left(\frac{\mathrm{SE}\left(\bar{\delta}_{\mathrm{Q_s}}\right)}{\bar{\delta}_{\mathrm{Q_s}} - \bar{\delta}_{\mathrm{P_w}}}\right)^2 + \left(\frac{\mathrm{SE}\left(\bar{\delta}_{\mathrm{P_s}}\right)}{\bar{\delta}_{\mathrm{P_w}} - \bar{\delta}_{\mathrm{P_s}}}\right)^2 + \left(\frac{f_{\mathrm{Q_s \leftarrow P_w}}}{f_{\mathrm{Q_s \leftarrow P_s}}} \frac{\mathrm{SE}\left(\bar{\delta}_{\mathrm{P_w}}\right)}{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}}\right)^2 \\ + \left(\frac{\mathrm{SE}(Q_{\mathrm{s}})}{Q_{\mathrm{s}}}\right)^2 + \left(-\frac{\mathrm{SE}(P_{\mathrm{s}})}{P_{\mathrm{s}}}\right)^2\end{array}} \quad . \qquad \text{(S16)}$$

If one has already evaluated the uncertainty in $f_{\mathrm{Q_s \leftarrow P_s}}$, the uncertainty in the end-member splitting proportion $\eta_{\mathrm{P_s \to Q_s}}$ can be even more straightforwardly expressed as

$$\frac{\mathrm{SE}\left(\eta_{\mathrm{P_s \to Q_s}}\right)}{\eta_{\mathrm{P_s \to Q_s}}} = \sqrt{\left(\frac{\mathrm{SE}\left(f_{\mathrm{Q_s \leftarrow P_s}}\right)}{f_{\mathrm{Q_s \leftarrow P_s}}}\right)^2 + \left(\frac{\mathrm{SE}(Q_{\mathrm{s}})}{Q_{\mathrm{s}}}\right)^2 + \left(-\frac{\mathrm{SE}(P_{\mathrm{s}})}{P_{\mathrm{s}}}\right)^2} \quad . \qquad \text{(S17)}$$

Appropriate substitution of variables will yield analogous error propagation formulas for the other end-member splitting proportions ($\eta_{\mathrm{P_s \to Q_w}}$, $\eta_{\mathrm{P_s \to Q}}$, $\eta_{\mathrm{P_w \to Q_s}}$, $\eta_{\mathrm{P_w \to Q_w}}$, and $\eta_{\mathrm{P_w \to Q}}$). Because $\eta_{\mathrm{P_s \to ET}} = 1 - \eta_{\mathrm{P_s \to Q}}$, the uncertainty in $\eta_{\mathrm{P_s \to ET}}$ will equal the uncertainty in $\eta_{\mathrm{P_s \to Q}}$; likewise the uncertainty in $\eta_{\mathrm{P_w \to ET}}$ will equal the uncertainty in $\eta_{\mathrm{P_w \to Q}}$.

xxsS2.3 Uncertainty in seasonal origins of evapotranspiration

One can estimate the uncertainty in the fraction of ET originating from summer precipitation, $f_{\mathrm{ET \leftarrow P_s}}$, by applying Gaussian error propagation to Eq. 18:

$$\mathrm{SE}(f_{\mathrm{ET}\leftarrow \mathrm{P_s}}) = \sqrt{\begin{aligned}&\left(\frac{\partial f_{\mathrm{ET}\leftarrow \mathrm{P_s}}}{\partial \bar{\delta}_{\mathrm{P_s}}}\mathrm{SE}(\bar{\delta}_{\mathrm{P_s}})\right)^2 + \left(\frac{\partial f_{\mathrm{ET}\leftarrow \mathrm{P_s}}}{\partial \bar{\delta}_{\mathrm{P_w}}}\mathrm{SE}(\bar{\delta}_{\mathrm{P_w}})\right)^2 + \left(\frac{\partial f_{\mathrm{ET}\leftarrow \mathrm{P_s}}}{\partial \bar{\delta}_{\mathrm{Q}}}\mathrm{SE}(\bar{\delta}_{\mathrm{Q}})\right)^2 \\ &+ \left(\frac{\partial f_{\mathrm{ET}\leftarrow \mathrm{P_s}}}{\partial P_{\mathrm{s}}}\mathrm{SE}(P_{\mathrm{s}})\right)^2 + \left(\frac{\partial f_{\mathrm{ET}\leftarrow \mathrm{P_w}}}{\partial P_{\mathrm{w}}}\mathrm{SE}(P_{\mathrm{w}})\right)^2 + \left(\frac{\partial f_{\mathrm{ET}\leftarrow \mathrm{P_s}}}{\partial Q}\mathrm{SE}(Q)\right)^2\end{aligned}} \quad . \qquad \text{(S18)}$$

Writing out the partial derivatives gives the result

$$\mathrm{SE}(f_{\mathrm{ET}\leftarrow \mathrm{P_s}}) = \sqrt{\begin{aligned}&\left(\frac{Q}{ET}\frac{\bar{\delta}_{\mathrm{Q}} - \bar{\delta}_{\mathrm{P_w}}}{(\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}})^2}\mathrm{SE}(\bar{\delta}_{\mathrm{P_s}})\right)^2 + \left(\frac{Q}{ET}\frac{\bar{\delta}_{\mathrm{Q}} - \bar{\delta}_{\mathrm{P_s}}}{(\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}})^2}\mathrm{SE}(\bar{\delta}_{\mathrm{P_w}})\right)^2 + \left(\frac{Q}{ET}\frac{\mathrm{SE}(\bar{\delta}_{\mathrm{Q}})}{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}}\right)^2 \\ &+ \left(\left(\frac{1}{ET} - \frac{P_{\mathrm{s}} - Q\, f_{\mathrm{Q}\leftarrow \mathrm{P_s}}}{ET^2}\right)\mathrm{SE}(P_{\mathrm{s}})\right)^2 + \left(-\frac{P_{\mathrm{s}} - Q\, f_{\mathrm{Q}\leftarrow \mathrm{P_s}}}{ET^2}\mathrm{SE}(P_{\mathrm{w}})\right)^2 \\ &+ \left(\left(-\frac{f_{\mathrm{Q}\leftarrow \mathrm{P_s}}}{ET} + \frac{P_{\mathrm{s}} - Q\, f_{\mathrm{Q}\leftarrow \mathrm{P_s}}}{ET^2}\right)\mathrm{SE}(Q)\right)^2\end{aligned}} \quad , \qquad \text{(S19)}$$

where $ET = P_{\mathrm{s}} + P_{\mathrm{w}} - Q$ and $f_{\mathrm{Q}\leftarrow \mathrm{P_s}} = (\bar{\delta}_{\mathrm{Q}} - \bar{\delta}_{\mathrm{P_w}})/(\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}})$. Equation (S19) can be simplified somewhat to yield

$$\mathrm{SE}(f_{\mathrm{ET}\leftarrow \mathrm{P_s}}) = \sqrt{\begin{aligned}&\left(\frac{Q\, f_{\mathrm{Q}\leftarrow \mathrm{P_s}}}{ET}\frac{\mathrm{SE}(\bar{\delta}_{\mathrm{P_s}})}{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}}\right)^2 + \left(\frac{Q\, f_{\mathrm{Q}\leftarrow \mathrm{P_w}}}{ET}\frac{\mathrm{SE}(\bar{\delta}_{\mathrm{P_w}})}{\bar{\delta}_{\mathrm{P_w}} - \bar{\delta}_{\mathrm{P_s}}}\right)^2 + \left(\frac{Q}{ET}\frac{\mathrm{SE}(\bar{\delta}_{\mathrm{Q}})}{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{P_w}}}\right)^2 \\ &+ \left(\frac{f_{\mathrm{ET}\leftarrow \mathrm{P_w}}}{ET}\mathrm{SE}(P_{\mathrm{s}})\right)^2 + \left(-\frac{f_{\mathrm{ET}\leftarrow \mathrm{P_s}}}{ET}\mathrm{SE}(P_{\mathrm{w}})\right)^2 \\ &+ \left(\frac{f_{\mathrm{ET}\leftarrow \mathrm{P_s}} - f_{\mathrm{Q}\leftarrow \mathrm{P_s}}}{ET}\mathrm{SE}(Q)\right)^2\end{aligned}} \quad , \qquad \text{(S20)}$$

where $f_{\mathrm{Q}\leftarrow \mathrm{P_w}} = 1 - f_{\mathrm{Q}\leftarrow \mathrm{P_s}} = (\bar{\delta}_{\mathrm{Q}} - \bar{\delta}_{\mathrm{P_s}})/(\bar{\delta}_{\mathrm{P_w}} - \bar{\delta}_{\mathrm{P_s}})$ and $f_{\mathrm{ET}\leftarrow \mathrm{P_w}} = 1 - f_{\mathrm{ET}\leftarrow \mathrm{P_s}}$. Appropriate substitution of variables will yield a similar error propagation formula for $f_{\mathrm{ET}\leftarrow \mathrm{P_w}}$.

xxsS2.4 Uncertainty in inferred isotopic composition of evapotranspiration

One can estimate the uncertainty in the isotopic composition of ET, $\bar{\delta}_{\mathrm{ET}}$, by applying Gaussian error propagation to Eq. 21:

$$\mathrm{SE}(\bar{\delta}_{\mathrm{ET}}) = \sqrt{\begin{aligned}&\left(\frac{\partial \bar{\delta}_{\mathrm{ET}}}{\partial \bar{\delta}_{\mathrm{P_s}}}\mathrm{SE}(\bar{\delta}_{\mathrm{P_s}})\right)^2 + \left(\frac{\partial \bar{\delta}_{\mathrm{ET}}}{\partial \bar{\delta}_{\mathrm{P_w}}}\mathrm{SE}(\bar{\delta}_{\mathrm{P_w}})\right)^2 + \left(\frac{\partial \bar{\delta}_{\mathrm{ET}}}{\partial \bar{\delta}_{\mathrm{Q}}}\mathrm{SE}(\bar{\delta}_{\mathrm{Q}})\right)^2 \\ &+ \left(\frac{\partial \bar{\delta}_{\mathrm{ET}}}{\partial P_{\mathrm{s}}}\mathrm{SE}(P_{\mathrm{s}})\right)^2 + \left(\frac{\partial \bar{\delta}_{\mathrm{ET}}}{\partial P_{\mathrm{w}}}\mathrm{SE}(P_{\mathrm{w}})\right)^2 + \left(\frac{\partial \bar{\delta}_{\mathrm{ET}}}{\partial Q}\mathrm{SE}(Q)\right)^2\end{aligned}} \quad . \qquad \text{(S21)}$$

Writing out the partial derivatives and simplifying terms gives the result

$$\mathrm{SE}(\bar{\delta}_{\mathrm{ET}}) = \sqrt{\begin{aligned}&\left(\frac{P_{\mathrm{s}}}{ET}\mathrm{SE}(\bar{\delta}_{\mathrm{P_s}})\right)^2 + \left(\frac{P_{\mathrm{w}}}{ET}\mathrm{SE}(\bar{\delta}_{\mathrm{P_w}})\right)^2 + \left(\frac{-Q}{ET}\mathrm{SE}(\bar{\delta}_{\mathrm{Q}})\right)^2 \\ &+\left(\frac{\bar{\delta}_{\mathrm{P_s}} - \bar{\delta}_{\mathrm{ET}}}{ET}\mathrm{SE}(P_{\mathrm{s}})\right)^2 + \left(\frac{\bar{\delta}_{\mathrm{P_w}} - \bar{\delta}_{\mathrm{ET}}}{ET}\mathrm{SE}(P_{\mathrm{w}})\right)^2 + \left(\frac{\bar{\delta}_{\mathrm{ET}} - \bar{\delta}_{\mathrm{Q}}}{ET}\mathrm{SE}(Q)\right)^2\end{aligned}} \quad . \qquad \text{(S22)}$$

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