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Key Points:
- Triple collocation is used to estimate the MSE of measurement system estimates
- We extend triple collocation to estimate the correlation coefficient
- The new approach requires no additional assumptions or computational burden

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Extended triple collocation: Estimating errors and correlation coefficients with respect to an unknown target

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Abstract Calibration and validation of geophysical measurement systems typically require knowledge of the "true" value of the target variable. However, the data considered to represent the "true" values often include their own measurement errors, biasing calibration, and validation results. Triple collocation (TC) can be used to estimate the root-mean-square-error (RMSE), using observations from three mutually independent, error-prone measurement systems. Here, we introduce Extended Triple Collocation (ETC): using exactly the same assumptions as TC, we derive an additional performance metric, the correlation coefficient of the measurement system with respect to the unknown target, ρ_{t,X_i}. We demonstrate that ρ_{t,X_i}^2 is the scaled, unbiased signal-to-noise ratio and provides a complementary perspective compared to the RMSE. We apply it to three collocated wind data sets. Since ETC is as easy to implement as TC, requires no additional assumptions, and provides an extra performance metric, it may be of interest in a wide range of geophysical disciplines.

1. Introduction

Geophysical measurement systems, such as *in-situ* sensor networks, satellites, and models, require calibration and validation. This requires comparison of their measurements with true observations of the target variable. A range of performance metrics exist to summarize this comparison, including the root-mean-square-error (RMSE) and correlation coefficient. No single metric can capture all relevant characteristics of the relationship between the measurement system and the target, which may include, but are not limited to, the measurement system's bias, noise, and sensitivity with respect to the target variable [*Entekhabi et al.*, 2010].

In practice, however, the data considered to represent the "true" observations are themselves imperfect due to their own measurement errors and differences in support scale. Triple collocation (TC) is a technique for estimating the unknown error standard deviations (or RMSEs) of three mutually independent measurement systems, without treating any one system as perfectly observed "truth" [*Stoffelen*, 1998]. It assumes a linear error model where errors are uncorrelated with each other and the target variable. TC has been used widely in oceanography to estimate errors in measurements of sea surface temperature [*Gentemann*, 2014; *O'Carroll et al.*, 2008], wind speed and stress [*Portabella and Stoffelen*, 2009; *Stoffelen*, 1998; *Vogelzang et al.*, 2011], and wave height [*Caires and Sterl*, 2003; *Janssen et al.*, 2007]. It has also been used in hydrology to estimate errors in measurements of precipitation [*Roebeling et al.*, 2012], fraction of absorbed photosynthetically active radiation [*D'Odorico et al.*, 2014], leaf area index [*Fang et al.*, 2012], and, particularly, soil moisture [*Anderson et al.*, 2012; *Dorigo et al.*, 2010; *Draper et al.*, 2013; *Hain et al.*, 2011; *Miralles et al.*, 2010; *Parinussa et al.*, 2011; *Scipal et al.*, 2008; *Su et al.*, 2014]. It has been applied in data assimilation [*Crow and van den Berg*, 2010] and can also be used to optimally rescale two measurement systems to a third reference system [*Stoffelen*, 1998; *Yilmaz and Crow*, 2013].

While TC is a powerful approach for estimating one metric of measurement system performance (RMSE), a suite of metrics are needed for calibration and validation. In this paper, we extend TC to also estimate the correlation coefficient of each measurement system with respect to the unknown target variable. We call this approach Extended Triple Collocation (ETC). ETC is simple to implement and adds no additional assumptions or computational cost to TC. In section 2, we review TC and introduce ETC, deriving an equation for the correlation coefficient from the assumptions of TC alone. We show that the correlation coefficients provide important insights into the fidelity of the measurement systems to the target variable beyond those provided by the RMSE, combining information on the measurement system's sensitivity and noise with information on the strength of the target signal. In section 3, we present a collocated data set of ocean surface wind measurements from buoys, satellite scatterometers, and a Numerical Weather Prediction (NWP) forecast model and apply ETC to it in section 4.

2. Methods

2.1. Classical Triple Collocation

In this section, we review the derivation of the TC estimation equations. We begin with an affine error model relating measurements to a (geophysical) variable, a standard form used in the triple collocation literature [*Zwieback et al.*, 2012]:

$$X_i = X'_i + \varepsilon_i = \alpha_i + \beta_i t + \varepsilon_i \tag{1}$$

where the X_i ($i \in \{1, 2, 3\}$) are collocated measurement systems linearly related to the true underlying value t with additive random errors ε_i, respectively. They could represent, for instance, outputs from a model, a remotely sensed product, and point measurements from *in-situ* stations. X_i, X'_i, ε_i and t are all random variables. α_i and β_i are the ordinary least squares (OLS) intercepts and slopes, respectively.

The covariances between the different measurement systems are given by

$$\mathrm{Cov}\left(X_i, X_j\right) = \mathrm{E}\left(X_i X_j\right) - \mathrm{E}(X_i)\mathrm{E}\left(X_j\right) = \beta_i \beta_j \sigma_t^2 + \beta_i \mathrm{Cov}\left(t, \varepsilon_j\right) + \beta_j \mathrm{Cov}(t, \varepsilon_i) + \mathrm{Cov}\left(\varepsilon_i, \varepsilon_j\right) \tag{2}$$

where $\sigma_t^2 = \mathrm{Var}(t)$. We assume that the errors from the independent sources have zero mean ($E(\varepsilon_i) = 0$) and are uncorrelated with each other ($\mathrm{Cov}(\varepsilon_i, \varepsilon_j) = 0$, $i \neq j$) and with t ($\mathrm{Cov}(\varepsilon_i, t) = 0$). Using these assumptions, the two middle terms on the right-hand side are zero, and so is the last when $i \neq j$, so the equation reduces to

$$Q_{ij} \equiv \mathrm{Cov}\left(X_i, X_j\right) = \begin{cases} \beta_i \beta_j \sigma_t^2, & \text{for } i \neq j \\ {\beta_i}^2 \sigma_t^2 + {\sigma_{\varepsilon_i}}^2, & \text{for } i = j \end{cases} \tag{3}$$

where ${\sigma_{\varepsilon_i}}^2 = \mathrm{Var}(\varepsilon_i)$. Since there are six unique terms in the 3×3 covariance matrix (Q_{11}, Q_{12}, Q_{13}, Q_{22}, Q_{23}, Q_{33}), we have six equations but seven unknowns (β_1, β_2, β_3, σ_{ε_1}, σ_{ε_2}, σ_{ε_3}, σ_t); therefore, the system is underdetermined and there is no unique solution. However, if we forego solving for β_i and σ_t^2, and instead define a new variable $\theta_i = \beta_i \sigma_t$, we can write

$$Q_{ij} = \begin{cases} \theta_i \theta_j, & \text{for } i \neq j \\ \theta_i^2 + {\sigma_{\varepsilon_i}}^2, & \text{for } i = j \end{cases} \tag{4}$$

We now have six equations and six unknowns, and can solve the system. We obtain the TC estimation equation for RMSE,

$$\boldsymbol{\sigma_\varepsilon} = \begin{bmatrix} \sqrt{Q_{11} - \dfrac{Q_{12} Q_{13}}{Q_{23}}} \\ \sqrt{Q_{22} - \dfrac{Q_{12} Q_{23}}{Q_{13}}} \\ \sqrt{Q_{33} - \dfrac{Q_{13} Q_{23}}{Q_{12}}} \end{bmatrix} \tag{5}$$

We may also solve for θ_i, but this is not typically done in TC. We will show in the next section that θ_i contains useful information that forms the basis for ETC. Within the soil moisture community, triple collocation is often applied by calculating the covariances of two differences between products [e.g., *Scipal et al.*, 2008]. This is equivalent to deriving the parameters from the measurement system covariance equations as discussed here.

In practice, "representativeness errors" may exist due to differences in support scale between measurement systems, causing subtle cross correlations between the errors such that $\mathrm{Cov}\left(\varepsilon_i, \varepsilon_j\right) = r_{ij}^2 > 0$. This introduces additional unknowns into the problem, rendering it underdetermined. To avoid this, the representativeness error has been ignored in many studies that use TC, often without justification. However, if an estimate for r_{ij}^2

exists, it can be easily subtracted from Q_{ij}. For wind measurements, r_{ij}^2 can be estimated using assumptions about the wind spectra [*Stoffelen*, 1998; *Vogelzang et al.*, 2011], but little is known about the representativeness error for other target variables.

If we are willing to treat one of the measurement systems as a reference with known calibration (i.e., known α and β), we can reduce the number of unknowns and solve for the remaining unknowns without introducing θ_i. Without loss of generality, assume X_1 is the reference system and has been perfectly calibrated to t so that $\alpha_1 = 0$ and $\beta_1 = 1$. Then we have

$$\begin{aligned} \beta_2 &= \frac{Q_{23}}{Q_{13}}, \;\; \beta_3 = \frac{Q_{23}}{Q_{12}} \\ \alpha_2 &= \overline{X_2} - \beta_2\overline{X_1}, \;\; \alpha_3 = \overline{X_3} - \beta_3\overline{X_1} \end{aligned} \tag{6}$$

where the overbars denote sample means. The system is often solved iteratively, incorporating an outlier detection and removal process. This is very important since covariance matrix estimates are highly sensitive to outliers. In many studies, the measurement systems are rescaled before applying TC, and it is presumed that $\beta_1 = \beta_2 = \beta_3 = 1$ and $\alpha_1 = \alpha_2 = \alpha_3 = 0$, simplifying the TC estimation equation to

$$\boldsymbol{\sigma_\varepsilon} = \begin{bmatrix} \sqrt{Q_{11} - Q_{12}} \\ \sqrt{Q_{22} - Q_{12}} \\ \sqrt{Q_{33} - Q_{13}} \end{bmatrix} \tag{7}$$

Note, however, that this approach should be used with caution. Naively rescaling the measurement systems (e.g., by matching their temporal variances) and applying this simplified estimation equation will deliver biased RMSE estimates, since error estimation and calibration are fundamentally intertwined [*Stoffelen*, 1998]. In practice, consistent estimates of calibration parameters and error estimates can be obtained by solving the equations iteratively (see *Vogelzang and Stoffelen* [2012] for more details), since triple collocation achieves the optimal rescaling [*Yilmaz and Crow*, 2013]. In this study we calculate RMSEs using equation (5) rather than rescaling and using equation (7).

2.2. Extended Triple Collocation

In this section, we show that θ_i can be used to solve for the correlation coefficients of the measurement systems with respect to the unknown truth. We demonstrate that the correlation coefficient contains useful information beyond that provided by the RMSE. Recall that for OLS,

$$\beta_i = \rho_{t,X_i}\frac{\sqrt{Q_{ii}}}{\sigma_t} \tag{8}$$

where ρ_{t,X_i} is the correlation coefficient between t and X_i. Note that this relation can also be obtained directly from (1) using the standard definitions of correlation and covariance. We emphasize that the independent variable t is the true underlying value and not subject to measurement error, so the OLS framework is valid. If there are errors in the measurement of t that are not captured by the error model (1), then the OLS slope will be biased and a new error model will be required [*Cornbleet and Gochman*, 1979; *Deming*, 1943]. Overcoming these biases was, in fact, the original motivation for the development of triple collocation, rather than the estimation of RMSEs [*Stoffelen*, 1998].

The key insight of ETC is that, from equation (8), we obtain $\theta_i = \rho_{t,X_i}\sqrt{Q_{ii}}$. Since $\sqrt{Q_{ii}}$ is already estimated from the data, and since we can solve for θ_i using equation (4), we can solve for ρ_{t,X_i}. We obtain the new ETC estimation equation

$$\boldsymbol{\rho_{t,X}} = \pm \begin{bmatrix} \sqrt{\dfrac{Q_{12}Q_{13}}{Q_{11}Q_{23}}} \\ \operatorname{sign}(Q_{13}Q_{23})\sqrt{\dfrac{Q_{12}Q_{23}}{Q_{22}Q_{13}}} \\ \operatorname{sign}(Q_{12}Q_{23})\sqrt{\dfrac{Q_{13}Q_{23}}{Q_{33}Q_{12}}} \end{bmatrix} \tag{9}$$

where the ρ_{t,X_i} are correct up to a sign ambiguity. In practice, the measurement systems will almost always be expected to be positively correlated to the unobserved truth.

Table 1. Scatterometer Products[a]

Product	Grid Size (km)	r_u^2 (m^2s^{-2})	r_v^2 (m^2s^{-2})	N
ASCAT-12.5	12.5	0.63	1.00	32,317
ASCAT-25	25	0.49	0.69	54,187
SeaWinds-KNMI	25	1.28	0.44	76,947

[a]The scatterometer products and values used are identical to those used in *Vogelzang et al.* [2011]. N is the number of collocated triplets available for each product. r_u^2 and r_v^2 are the estimated representativeness errors in the u and v wind component measurements, respectively.

The correlation coefficients provide important new information about the performance of the measurement systems. For the given error model (1), it can be shown that

$$\rho_{t,X_i}^2 = \frac{\beta_i^2\sigma_t^2}{\beta_i^2\sigma_t^2 + \sigma_{\varepsilon_i}^2} = \frac{\mathrm{SNR_{ub}}}{\mathrm{SNR_{ub}} + 1} \tag{10}$$

where we define $\mathrm{SNR_{ub}} = \frac{Var(X_i')}{Var(\varepsilon_i)} = \frac{\beta_i^2\sigma_t^2}{\sigma_{\varepsilon_i}^2}$ to be the unbiased signal-to-noise-ratio (in contrast, the standard signal-to-noise ratio is $\mathrm{SNR} = \frac{E(X_i'^2)}{Var(\varepsilon_i)}$). The squared correlation coefficient therefore is the unbiased signal-to-noise ratio, scaled between 0 and 1. It combines information about (i) the sensitivity of the measurement system β, (ii) the variability of the signal σ_t^2, and (iii) the variability of the measurement error σ_ε^2. In contrast, standard triple collocation only directly estimates (iii). Note that, while TC returns an estimate for (i), this is estimated with respect to a reference measurement system. Its intended purpose is for calibration against that reference measurement system, not as an estimate of the true system sensitivity. Therefore, ρ_{t,X_i}^2 contains useful additional information relevant to measurement system validation that is not included in $\sigma_{\varepsilon_i}^2$. This is clear from the fact that, for a fixed MSE, ρ_{t,X_i}^2 may take any value between 0 and 1, its full range. This makes intuitive sense: a given noise level may be too high for a low-sensitivity system measuring a weak signal but acceptable for a high-sensitivity system measuring a strong signal.

We note that ρ_{t,X_i}^2 is closely related to the fRMSE metric defined in *Draper et al*. [2013] as $\mathrm{fRMSE} = \frac{\sigma_{\varepsilon_i}}{\sqrt{Q_{ii}}}$. They are both measures of relative similarity that isolate phase differences between two signals. Furthermore, it is apparent that $\mathrm{fRMSE} = \frac{\sigma_{\varepsilon_i}}{\sqrt{Q_{ii}}} = \sqrt{\frac{\sigma_{\varepsilon_i}^2}{\beta_i^2\sigma_t^2+\sigma_{\varepsilon_i}^2}} = \sqrt{1-\rho_{t,X_i}^2}$ from equations (3) and (10) and therefore yields identical performance rankings compared to those obtained using ρ_{t,X_i}^2. However, in contrast to the fRMSE, the correlation coefficient has been used in many validation studies spanning several decades [e.g., *Jackson et al*. [2012], *Mo et al*. [1982], and *Owe et al*. [1992]).

3. Wind Data

In this section, we describe the buoy, NWP, and scatterometer wind products used in this study as a case study for ETC. TC was originally designed for application to wind velocities [*Stoffelen*, 1998], and this target variable more closely matches the assumptions of TC compared to other variables such as soil moisture [*Yilmaz and Crow*, 2014]. Unlike other target variables, reasonable estimates of the representativeness error also exist [*Stoffelen*, 1998; *Vogelzang et al*., 2011]. We use the same collocated triplets as in *Vogelzang et al*. [2011] and refer the reader to this study for more detail on the data used; for completeness, we give a brief description here. Three different scatterometer products are used. Wind retrievals from EUMETSAT's C-band Advanced SCATterometer (ASCAT) are processed to generate two different products: the 12.5 km resolution ASCAT-12.5 product and the 25 km resolution ASCAT-25 product. Retrievals from the SeaWinds sensor on board QuickSCAT are processed to generate the 25 km resolution SeaWinds-KNMI product. *Vogelzang et al*. [2011] consider a fourth product, SeaWinds-NOAA, processed by the National Oceanic and Atmospheric Administration. This product exhibited anomalous behavior compared to the others and is omitted from this study. Table 1 gives further details on the scatterometer products used, including their grid size, representativeness errors, and number of observations available that were also collocated with a buoy and NWP measurement. The very large sample sizes (much larger than the recommended value of ~500 given by *Zwieback et al*. [2012]) ensure precise ETC estimates.

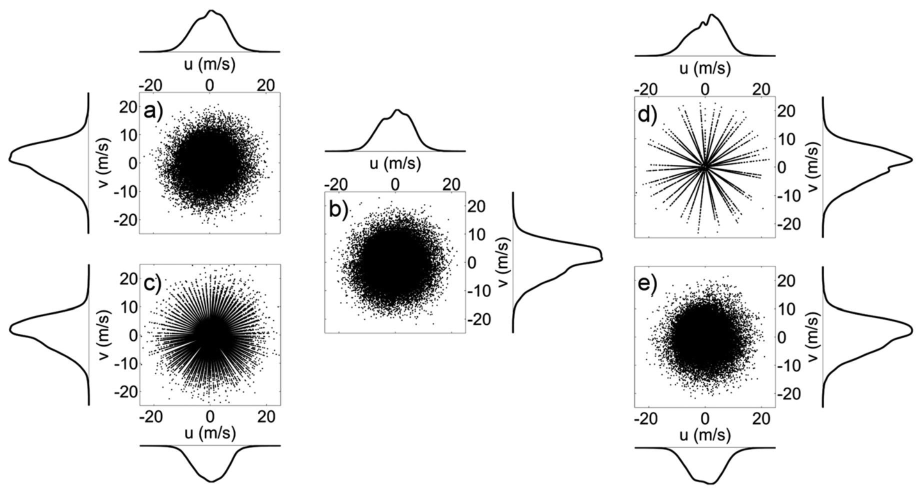

Figure 1. Scatter plots and kernel-density-estimated marginal distributions (on the same axes) for the wind data used in this study, where *u* is the zonal wind velocity and *v* is the meridional wind velocity. Plots for scatterometer products correspond to (a) Advanced SCATterometer (ASCAT)-12.5, (b) ASCAT-25, and (c) SeaWinds-KNMI. Plots for (d) buoys and (e) Numerical Weather Prediction (NWP) products are also shown. The marginal distributions are all approximately normal for all products used.

Quality-controlled buoy data are taken from the European Center for Medium-range Weather Forecasting (ECMWF) Meteorological Archival and Retrieval System. The NWP forecasts are also obtained from the ECMWF. Collocated buoy-scatterometer-NWP triplets are obtained for the period 1 November 2007 to 30 November 2009, except for those including the ASCAT-12.5 product, where the period is 1 October 2008 to 30 November 2009. The study domain is largely restricted to the tropics and the coasts of Europe and North America, due to a lack of reliable buoy observations outside these regions. The data are plotted in Figure 1. Note that for each data set, the marginal distributions are approximately Gaussian, although Gaussian data are not required for TC or ETC (indeed, TC has frequently been applied to non-Gaussian data such as soil moisture). Gaussianity does, however, ensure that the RMSE is well defined and assists in interpretation. The block correlations in the SeaWinds-KNMI and buoy data are due to binning in those data sets.

We use the ASCAT Wind Data Processor (AWDP) triple collocation scheme described in *Vogelzang and Stoffelen* [2012, available at http://research.metoffice.gov.uk/research/interproj/nwpsaf/scatterometer/TripleCollocation_NWPSAF_TR_KN_021_v1_0.pdf], updated to also calculate correlation coefficients. The scheme solves iteratively for the RMSEs and correlation coefficients and includes quality control and outlier detection and removal steps. We subtract out representativeness errors (Table 1) calculated in [*Vogelzang et al*., 2011] and estimate 95% confidence intervals using bootstrapping [*Efron and Tibshirani*, 1994] with $N = 100$ replicates. We perform the analysis with buoy-scatterometer-NWP forecast triplets three separate times, using a different scatterometer product each time. In all analyses, the buoy data are used as the reference data set, for consistency with *Vogelzang et al*. [2011]. However, the choice of reference system only impacts the estimates of α_i and β_i (not shown), not our estimates of σ_{ε_i} and $\rho^2_{t,\,X_i}$.

4. Results and Discussion

Figure 2 shows the ETC estimates of *u*, *v* RMSE and correlation coefficient for the buoy, NWP, and various scatterometer products. The RMSE estimates are all low and the correlation coefficients are all high. They are consistent with reasonable guesses for β and σ_t^2. As an example, consider the ETC estimates of scatterometer *u* RMSE $\sigma_\varepsilon(u) = 1.05\ m\ s^{-1}$ and correlation coefficient $\rho_{t,X}(u) = 0.985$, estimated using ASCAT-12.5 scatterometer data (we use the mean of the bootstrapped replicates here). Substituting into equation (10), and assuming $\beta \approx 1$, we obtain $\sigma_t \approx 6$. While the true value of σ_t is unknown, this estimate appears very reasonable given the marginal distribution of *u* in Figure 1a.

The results demonstrate the importance of using a validation metric that combines measures of noise and sensitivity, rather than noise alone. Focusing on the scatterometer ETC estimates, we see that, for *u*, the

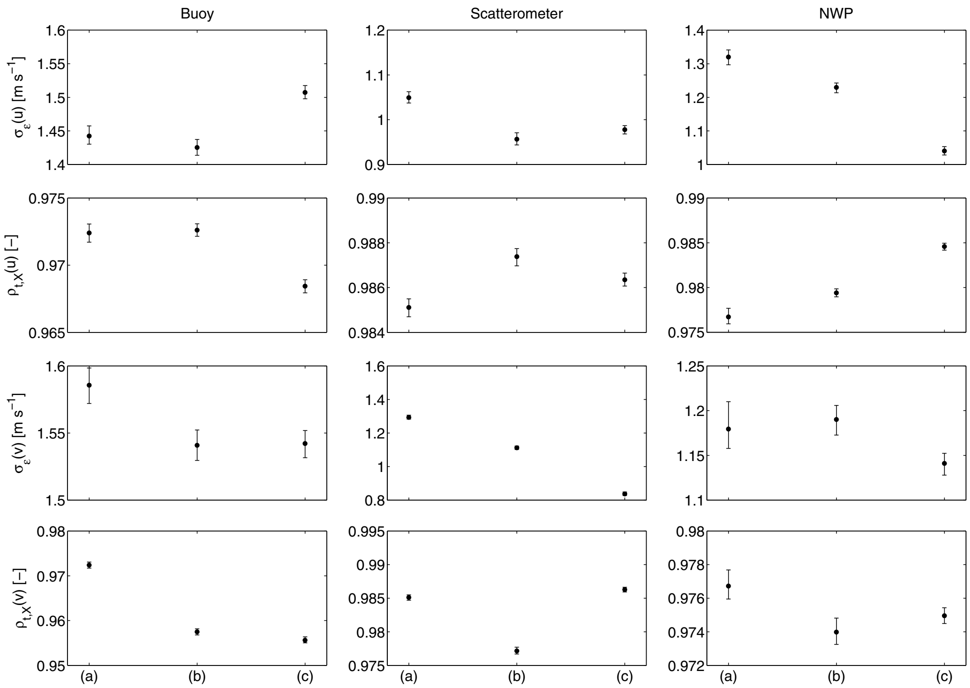

Figure 2. (Rows 1 and 3): Triple collocation estimates of the root-mean-square-errors (RMSEs) for *u* ($\sigma_\varepsilon(u)$) and *v* ($\sigma_\varepsilon(v)$) for the buoy, scatterometer, and NWP products, respectively, calculated using equation (5). The analysis is performed with buoy-scatterometer-NWP forecast triplets three separate times, using a different scatterometer product each time. (a) ASCAT-12.5, (b) ASCAT-25, and (c) SeaWinds-KNMI). (Rows 2 and 4): Extended triple collocation estimates of the correlation coefficient for *u* ($\rho_{t,X}(u)$) and *v* ($\rho_{t,X}(v)$) for the buoy, scatterometer, and NWP products, respectively, calculated using equation (9). Bootstrap estimates ($N = 100$ replicates) of the 95% confidence intervals are shown for each estimate. The bootstrapped sample means of $\sigma_\varepsilon(u)$ and $\sigma_\varepsilon(v)$ are identical to the values given in Table 4 of *Vogelzang et al.* [2011].

highest correlation coefficients correspond to the lowest RMSEs and vice versa. Since σ_t does not vary between scatterometer products, this suggests that differences in noise dominate differences in sensitivity between products. For *v*, however, this is not the case: ASCAT-12.5 has the highest RMSE but does not have the lowest correlation coefficient. This suggests that, while ASCAT-12.5 estimates of *v* are noisier than those of ASCAT-25, ASCAT-12.5 has a greater $\mathrm{SNR}_{\mathrm{ub}}$ because it is more sensitive to the signal, *v*, although it may also be an artifact caused by incorrect assumptions in the error model (1). In this case study, the differences in noise and sensitivity between products are relatively small. However, it is easy to imagine scenarios where validating multiple satellite products on the basis of RMSE alone, compared to a combination of RMSE and correlation coefficient, could yield very different interpretations of their relative performances.

ETC builds on TC but also inherits its weaknesses. Using different scatterometer products, we would expect the ETC estimates of buoy RMSEs and correlation coefficients to remain identical; similarly, for the NWP estimates. While the differences are small, they are too large to be explained by sampling error (particularly for the NWP estimates) and are likely due to subtle violations of the error model's assumptions or inaccurate corrections for representativeness errors. If the error model given in (1) is not valid, the estimates of RMSE and correlation coefficient will be biased. The results are particularly sensitive to the assumption of independent errors between buoy, scatterometer, and NWP estimates. However, these are all preexisting weaknesses in TC and not unique to ETC. ETC uses exactly the same assumptions as TC.

5. Conclusions

Triple collocation is a powerful and popular technique for calibrating and validating measurement system estimates of geophysical target variables. In this paper, we introduced ETC: using exactly the same error model and assumptions as TC, we derived the correlation coefficient of each measurement system with respect to the unknown target variable. We demonstrated that ETC's correlation coefficient provides useful insights into the correspondence between the measurement system estimates and the target variable, beyond those provided by TC's RMSE estimate. By integrating information on the measurement system's sensitivity to the target variable, measurement noise, and the variability of the target variable itself, the correlation coefficient provides a complementary (and sometimes, very different) perspective to that of the RMSE when validating measurement systems. In particular, the measurement noise (estimated by the RMSE) is much more informative when interpreted relative to the observed signal: for instance, a small amount of measurement noise, in absolute terms, may still be of concern if the measurement system is relatively insensitive to the target variable, and/or the target signal is weak [*Entekhabi et al.*, 2010]. Since ETC uses exactly the same assumptions as TC, it appears that it may also facilitate the estimation of correlation coefficients in recent generalizations of TC from $n = 3$ measurement systems to $n \geq 3$ [*Zwieback et al.*, 2012] and, in cases where the target variable has sufficient temporal autocorrelation, $n = 2$ [*Su et al.*, 2014]. Finally, since ETC is as easy to implement as TC, requires no additional assumptions, and provides estimates of two complementary performance metrics instead of one, we suggest that it may be of interest to practitioners in a wide range of geophysical disciplines.

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