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Triple collocation

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Contents

1 Introduction

Triple collocation is a method that is now widely used to characterize systematic biases and random errors in in-situ measurements, satellite observations and model fields. It attempts to segregate the measurement uncertainties, geophysical, spatial and temporal representation and sampling differences in the different data sets by an objective method.

In scientific literature often dual comparisons are provided for validation, verification and calibration. However, implicit assumptions are made that limit the accuracy of dual comparisons. A frequent and often biased assumption is that all errors are due to the system that is being tested against a reference system, that is in turn assumed perfect, but *Stoffelen* [1998] also refers to biases associated with regression and with error distributions. Problems with dual comparison, such as satellite data verification against in-situ measurements, may be caused by differences in:

- temporal and spatial representation (instantaneous versus hourly mean and for example local, average over a satellite footprint or NWP grid volume);
- geophysical representation (real winds versus equivalent neutral winds, bulk versus skin SST, etc.);
- spatial and temporal sampling (over a whole basin or only at in-situ stations, twice daily or sampled over full diurnal cycles);
- error distributions, including aspects of error amplitude and skewness.

These issues cannot be clearly resolved in dual comparisons, as scatter will be caused simultaneously by all issues above for both observing systems and there is no clear objective way to assign errors to one or the other. In other words, dual comparisons are really difficult to comprehend. *Stoffelen* [1998] formalizes some of these problems in his section 3 and Appendix A. This basically has driven the discovery of triple collocation.

In triple collocation, three (ideally) independent data sets are brought together, so three scatter plots can be made. The plot with the least scatter obviously denotes the two systems that agree most, while the worst scatter plot, indicates that the excluded and third measurement system is the best performing. Moreover, triple collocation provides the relative linear calibration (scaling) of the three systems. Also, assuming known (normal) error distributions and after mutual linear calibration (rescaling) of the distributions with the errors, matching of the cumulative PDF leads to higher order calibration as well (known as CDF matching). This is described in the original paper (*Stoffelen* [1998]) dealing with the triple collocation method and elaborating it for buoy, scatterometer and NWP wind data sets.

Following *Stoffelen* [1998], it has been and is being used in wind and stress comparisons [*Portabella and Stoffelen*, 2009; *Vogelzang et al.* , 2011] wave height comparison [*Caires and Sterl*, 2003; *Janssen et al.*,

2007], sea surface temperature (SST) [*O'Carroll et al.,* 2008], soil moisture [*Scipal et al.*, 2010]; *Delphine et al.*, 2011], ice drift [*Hwang and Lavergne*, 2010], precipitation analyses [*Roebeling et al.*, 2011], etc. Some of these authors consider the measurements as already properly calibrated and perform only random error estimation.

A limitation of the triple collocation method may be the fact that three independent measurement systems are needed that must deliver simultaneous collocated measurements. Collocation in space and time may be hard to achieve and it takes typically one year to gather enough data for successful application of the method. The method can moreover only be applied at those locations and times where triple collocation data is available. Usually this is limited by the availability of in-situ observation locations, i.e., similar to dual in-situ comparisons, and the satellite overpass times, i.e., twice a day for polar satellites in sun-synchronous orbits.

Another hurdle in application may be that the triple collocation method is felt difficult to comprehend. Where in dual comparisons often implicit assumptions are made on the error distributions (see above), in triple collocation explicit assumptions are needed on the random and systematic error distributions, i.e., a realistic error model needs to be defined and tested. The method has been described in the scientific literature [*Stoffelen*, 1998], but such a presentation must necessarily be very concise. Implementation of the method is tedious, since a more detailed description on text book level is missing. This report is intended to fill that gap.

This report gives a full description of the triple collocation error model, the derivation of the calibration coefficients and the measurement error variances, the assumptions needed in the triple collocation method, and its numerical implementation. Also attention is paid to the role of representation errors and the scale dependency of measurement errors.

2 Derivation

2.1 Definitions

In this chapter the following definitions hold:

Assume N measurements of a quantity α, denoted as $\alpha_i, i = 1,2,...,N$. The first moment of α, or its average, is denoted as M_α and satisfies

$$M_\alpha = <\alpha> = \frac{1}{N}\sum_{i=1}^{N}\alpha_i \quad , \tag{2.1}$$

where <> denotes statistical averaging. If there are also N measurements of a quantity β, the mixed second moment $M_{\alpha\beta}$ satisfies

$$M_{\alpha\beta} = <\alpha\beta> = \frac{1}{N}\sum_{i=1}^{N}\alpha_i\beta_i \quad . \tag{2.2}$$

In case $\beta = \alpha$ one obtains the ordinary second moment $M_{\alpha\alpha}$.

The covariance $C_{\alpha\beta}$ is defined as

$$C_{\alpha\beta} = M_{\alpha\beta} - M_\alpha M_\beta \quad . \tag{2.3}$$

In case $\beta = \alpha$ equation (2.3) yields the variance of α, $C_{\alpha\alpha} = \sigma_\alpha^2$.

2.2 Error model

2.2.1 Calibration and measurement errors

Suppose three measurement systems X, Y, and Z, giving collocated measurements (x, y, z) of the same quantity t. Supposing that system X is the reference system with respect to which systems Y and Z are to be calibrated. Suppose also that linear calibration is sufficient for the whole range of values under consideration, and that the reference system is free of bias (i.e., there are no systematic errors or these are corrected for). The measurements then satisfy

$$\begin{aligned} x &= t + \varepsilon_x \\ y &= b_y + a_y(t + \varepsilon_y) \\ z &= b_z + a_z(t + \varepsilon_z) \end{aligned} \quad , \tag{2.4}$$

where t is the common part of the signal (sometimes referred to as "truth") and ε_α, $\alpha = x, y, z$ the true random error in each measurement. These random measurement error components are assumed unbiased,

$$< \varepsilon_\alpha >= 0 \quad , \quad \alpha = x, y, z \quad . \tag{2.5}$$

It is assumed that the error variances are constant over the whole range of values under consideration, so

$$< \varepsilon_\alpha^2 >= \sigma_\alpha^2 \quad , \quad \alpha = x, y, z \quad . \tag{2.6}$$

Further, it is assumed that the errors are independent of the common signal t, so

$$< \varepsilon_\alpha t >=< \varepsilon_\alpha >< t > \quad , \quad \alpha = x, y, z \quad , \tag{2.7}$$

which yields zero due to (2.5).

2.2.2 Representation error

The true or calibrated measurement errors are also assumed uncorrelated,

$$< \varepsilon_\alpha \varepsilon_\beta >= 0 \quad , \quad \alpha, \beta = x, y, z \quad , \tag{2.8}$$

unless common representation errors play a role. Suppose that system Z has a much coarser resolution than system Y and that system Y has coarser resolution than system X. High resolution signal that is common to X and Y will not be detectable for system Z and therefore be regarded as error. It can be represented as a correlated error between X and Y, so

$$< \varepsilon_x \varepsilon_y >= r^2 \quad , \tag{2.9}$$

with r^2 the variance of the representation error, i.e., the signal in X and Y that is not detected by Z. The other error correlations are zero according to (2.8). It is noted that coarse resolution may refer to spatial or temporal resolution, but there may also be geophysical representation issues that make systems X and Y look more alike while system Z lacks certain geophysical sensitivity. For example, for SST two systems X and Y could measure skin temperatures and a third system Z bulk temperature. X and Y then measure signal that is lacking in Z, and therefore $< \varepsilon_x \varepsilon_y > \neq 0$.

Note that with this procedure, the error model (2.4) gives the measurement error variances at the scale of the coarse observations made by system Z. It will be shown in section 2.4 how the measurement error variances at the scale of the intermediate resolution system Y can be obtained as well. In chapter 3 the concept of scale-dependent errors will be elaborated further, together with procedures to obtain the representation error.

2.3 Calibration coefficients and error variances

Forming the first statistical moments of (2.4) yields

$$\begin{aligned} M_x &= < t > + < \varepsilon_x > \\ M_y &= b_y + a_y\left(< t > + < \varepsilon_y > \right) \\ M_z &= b_z + a_z\left(< t > + < \varepsilon_z > \right) \end{aligned} \quad . \tag{2.10}$$

The first moments of the random measurement errors all equal zero by (2.5). The first equation of (2.10) therefore yields $M_x = < t >$ and can be used to eliminate $< t >$ from the others. This results in

$$\begin{aligned} b_y &= M_y - a_y M_x \\ b_z &= M_z - a_z M_x \end{aligned} \quad . \tag{2.11}$$

The ordinary second-order moments of (2.4) are

$$\begin{aligned} M_{xx} &= < t^2 > + 2 < t\varepsilon_x > + < \varepsilon_x^2 > \\ M_{yy} &= a_y^2 < t^2 > + b_y^2 + a_y^2 < \varepsilon_y^2 > + 2a_y b_y < t > + 2a_y^2 < t\varepsilon_y > + 2b_y a_y < \varepsilon_y > \\ M_{zz} &= a_z^2 < t^2 > + b_z^2 + a_z^2 < \varepsilon_z^2 > + 2a_z b_z < t > + 2a_z^2 < t\varepsilon_z > + 2b_z a_z < \varepsilon_z > \end{aligned} \quad . \tag{2.12}$$

This can be simplified by application of (2.4)-(2.9) and by using $M_x = < t >$ to

$$\begin{aligned} M_{xx} &= < t^2 > + \sigma_x^2 \\ M_{yy} &= a_y^2 < t^2 > + b_y^2 + a_y^2 \sigma_y^2 + 2a_y b_y M_x \\ M_{zz} &= a_z^2 < t^2 > + b_z^2 + a_z^2 \sigma_z^2 + 2a_z b_z M_x \end{aligned} \quad , \tag{2.13}$$

Now b_y and b_z can be eliminated from (2.13) using (2.11). A little algebra and introduction of the covariances (2.3) results in

$$\begin{aligned} C_{xx} &= < t^2 > - M_x^2 + \sigma_x^2 \\ C_{yy} &= a_y^2\left(< t^2 > - M_x^2 + \sigma_y^2 \right) \\ C_{zz} &= a_z^2\left(< t^2 > - M_x^2 + \sigma_z^2 \right) \end{aligned} \quad . \tag{2.14}$$

In the same way the mixed second order moments of (2.4) read

$$\begin{aligned} M_{xy} &= a_y < t^2 > + b_y < t > + a_y < t\varepsilon_y > + a_y < t\varepsilon_x > + b_y < \varepsilon_x > + a_y < \varepsilon_x \varepsilon_y > \\ M_{yz} &= a_y a_z < t^2 > + a_y b_z < t > + a_y a_z < t\varepsilon_z > + a_z b_y < t > + b_y b_z + b_y a_z < \varepsilon_z > + \\ &\quad + a_z a_y < t\varepsilon_y > + b_z a_y < \varepsilon_y > + a_y a_z < \varepsilon_y \varepsilon_z > \\ M_{zx} &= a_z < t^2 > + b_z < t > + a_z < t\varepsilon_z > + a_z < t\varepsilon_x > + b_z < \varepsilon_x > + a_z < \varepsilon_z \varepsilon_x > \end{aligned} \quad . \tag{2.15}$$

This can be simplified using (2.4)-(2.9) and $M_x = < t >$ to

$$\begin{aligned} M_{xy} &= a_y < t^2 > + b_y M_x + a_y r^2 \\ M_{yz} &= a_y a_z < t^2 > + a_y b_z M_x + a_z b_y M_x + b_y b_z \\ M_{zx} &= a_z < t^2 > + b_z M_x \end{aligned} \quad , \tag{2.16}$$

where, according to (2.9), we assumed that system Z has coarser resolution than systems X and Y. Again,

b_y and b_z can be eliminated from (2.16) using (2.11). A little algebra and introduction of the covariances (2.3) results in

$$\begin{aligned} C_{xy} &= a_y\left(< t^2 > -M_x^2 + r^2\right) \\ C_{yz} &= a_y a_z\left(< t^2 > -M_x^2\right) \\ C_{zx} &= a_z\left(< t^2 > -M_x^2\right) \end{aligned} \quad . \tag{2.17}$$

Eliminating a_y and a_z from the second equation in (2.17) using the first and third, respectively, yields

$$< t^2 > -M_x^2 + r^2 = \frac{C_{zx}C_{xy}}{C_{yz}} \quad . \tag{2.18}$$

Substituting (2.18) back into (2.17) yields

$$a_y = \frac{C_{yz}}{C_{zx}} \quad , \quad a_z = \frac{C_{yz}}{C_{xy} - a_y r^2} \quad . \tag{2.19}$$

Substituting (2.18) and (2.19) into (2.14) and solving for the error variances yields

$$\sigma_x^2 = C_{xx} - \frac{C_{zx}\left(C_{xy} - a_y r^2\right)}{C_{yz}} \quad , \quad \sigma_y^2 = C_{yy} - \frac{\left(C_{xy} - a_y r^2\right)C_{yz}}{C_{zx}} \quad , \quad \sigma_z^2 = C_{zz} - \frac{C_{yz}C_{zx}}{\left(C_{xy} - a_y r^2\right)} \quad . \tag{2.20}$$

This completes the derivation of the calibration coefficients and measurement error variances of the calibrated data with the triple collocation method. However, the actual implementation of the method makes use of a slightly different formulation. Moreover, there are two other issues that receive further attention:

1. If the representation error plays a role, the error variances are with respect to the system with coarsest resolution;
2. The representation error variance is valid for the calibrated data, not for the raw data. However, note that $a_y r^2$ is a scaled representation error that may be determined from the raw Y data.

These issues will be addressed in the next sections.

2.5 Analysis of the calibrated data

The measurement error variances for the calibrated data are obtained from error model (2.4). Suppose that one has an estimate of the calibration coefficients a_α and $b_\alpha, \alpha = x, y$. The calibrated measurements $\bar{x}$, $\bar{y}$, and $\bar{z}$ are given by

$$\begin{aligned} \bar{x} &= x \\ \bar{y} &= \frac{y - b_y}{a_y} \\ \bar{z} &= \frac{z - b_z}{a_z} \end{aligned} \quad . \tag{2.21}$$

Note that no errors are involved in (2.21), because it just gives the inverse of the linear calibration as it is performed on the raw data. Now the triple collocation error model (2.4) can be applied to the calibrated data. The model is solved the same way as in section 2.3 under the same assumptions. The results are

$$\bar{b}_y = \overline{M}_y - \bar{a}_y \overline{M}_x \quad , \quad \bar{b}_z = \overline{M}_z - \bar{a}_z \overline{M}_x \quad ,$$

$$\bar{a}_y = \frac{\overline{C}_{yz}}{\overline{C}_{zx}} \quad , \quad \bar{a}_z = \frac{\overline{C}_{yz}}{\overline{C}_{xy} - \bar{a}_y r^2} \quad , \tag{2.22}$$

$$\bar{\sigma}_x^2 = \overline{C}_{xx} - \frac{\overline{C}_{zx}\left(\overline{C}_{xy} - \bar{a}_y r^2\right)}{\overline{C}_{yz}} \quad , \quad \bar{\sigma}_y^2 = \overline{C}_{yy} - \frac{\left(\overline{C}_{xy} - \bar{a}_y r^2\right)\overline{C}_{yz}}{\overline{C}_{zx}} \quad , \quad \bar{\sigma}_z^2 = \overline{C}_{zz} - \frac{\overline{C}_{yz}\overline{C}_{zx}}{\left(\overline{C}_{xy} - \bar{a}_y r^2\right)} \quad ,$$

where the bar indicates that all quantities are for calibrated values. Note that the representation error has been defined with respect to the calibrated data.

If the values of the calibration coefficients a_α and $b_\alpha, \alpha = x, y$ are correct, then the measurements $\bar{x}$, $\bar{y}$, and $\bar{z}$ are properly calibrated and we must obtain

$$\begin{aligned} \bar{b}_y &= \bar{b}_z = 0 \\ \bar{a}_y &= \bar{a}_z = 1 \end{aligned} \quad . \tag{2.23}$$

Using (2.22) the relation $\bar{a}_y = \bar{a}_z = 1$ leads to $\overline{C}_{zx} = \overline{C}_{yz} = \left(\overline{C}_{xy} - r^2\right)$, and the error variances for calibrated data reduce to

$$\bar{\sigma}_x^2 = \overline{C}_{xx} - \overline{C}_{xy} + r^2 \quad , \quad \bar{\sigma}_y^2 = \overline{C}_{yy} - \overline{C}_{xy} + r^2 \quad , \quad \bar{\sigma}_z^2 = \overline{C}_{zz} - \overline{C}_{xy} + r^2 \quad . \tag{2.24}$$

Equation (2.24) is valid with respect to the system with coarsest resolution, say system Z. The equations in this section can be solved iteratively on a computer. More details are given in chapter 4.

2.4 Resolution

If all three measurement systems have roughly the same resolution then the representation error $r^2 = 0$ and the equations for calibration coefficients and measurement error variances further simplify. When the representation error plays a role, then the results of the previous section apply to the system with coarsest

resolution, because the representation error has been taken into account as an error correlation between the two systems with higher resolution.

Suppose that system Z has coarsest resolution. It is easy to obtain the error variances with respect to the system with intermediate resolution: just subtract the representation error variance r^2 from σ_x^2 and σ_y^2, since it represents part of the common resolved signal in X and Y. System Z does not resolve this part of the signal and error variance r^2 should be added to σ_z^2. Now the signal detected by systems X and Y but not by Z is counted as measurement error of system Z (lack of resolution) and as signal of X and Y. Denoting the error standard deviation at intermediate resolution by $\hat{\sigma}_\alpha, \alpha = x, y, z$, one has

$$\begin{aligned} \hat{\sigma}_x^2 &= \overline{C}_{xx} - \overline{C}_{xy} \\ \hat{\sigma}_y^2 &= \overline{C}_{yy} - \overline{C}_{xy} \\ \hat{\sigma}_z^2 &= C_{zz} - \overline{C}_{xz} + r^2 \end{aligned} \quad . \tag{2.25}$$

Suppose now that system X has much finer resolution than system Y. Equations (2.25) then gives the measurement error variances with respect to the resolution of Y. It is not possible to say something on the measurement error variances at the finest resolution of system X, unless additional assumptions are made on the measurement error distributions. For example, if X is a calibrated local in-situ measurement system, then the measurement error may be known. This could be used to compute a temporal or spatial representation error for Y and Z, such that the errors of X, Y and Z in representing a local in-situ measurement may be estimated.

For our scatterometer application, system X corresponds to moored buoys, system Y to the scatterometer, and system Z to the NWP background. The triple collocation method enables us to calculate error variances at the scales resolved by the NWP background and at the scale of the scatterometer, which scales have our main interest.

2.6 Resume

The triple collocation method requires the following assumptions:

1. Linear calibration is sufficient over the whole range of measurement values;
2. The reference measurement values are unbiased and calibrated;
3. The random measurement errors have constant variance over the whole range of calibrated measurement values;
4. The measurement errors are uncorrelated with each other (except for representation errors);
5. The random measurement errors are uncorrelated with the geophysical signal.

Under these assumptions the calibration coefficients and measurement error variances are given in terms of the first and second order statistical moments as

$$b_y = M_y - a_y M_x \quad , \quad b_z = M_z - a_z M_x \quad ,$$

$$a_y = \frac{C_{yz}}{C_{zx}} \quad , \quad a_z = \frac{C_{yz}}{C_{xy} - a_y r^2} \quad ,$$

$$\sigma_x^2 = C_{xx} - \frac{C_{zx}\left(C_{xy} - a_y r^2\right)}{C_{yz}} \quad , \quad \sigma_y^2 = C_{yy} - \frac{\left(C_{xy} - a_y r^2\right)C_{yz}}{C_{zx}} \quad , \quad \sigma_z^2 = C_{zz} - \frac{C_{yz}C_{zx}}{\left(C_{xy} - a_y r^2\right)} \quad ,$$

where system Z has coarser resolution than the other systems, resulting in a representation error of r^2. These results hold with respect to the resolution of system Z and are valid for the uncalibrated data.

The error variances with respect to the system with medium resolution, which may be either X or Y, is obtained by subtracting the representation error from σ_x^2 and σ_y^2, and adding it to σ_z^2. Within the triple collocation method it is not possible to retrieve the measurement error variances with respect to the system with finest resolution (if any), unless additional assumptions on the error distributions are made.

The error variances with respect to the calibrated data are found by implicitly solving the triple collocation error model. When the calibration coefficients a_α and $b_\alpha, \alpha = x, y$ are correctly estimated, the error variances are

$$\overline{\sigma}_x^2 = \overline{C}_{xx} - \overline{C}_{xy} + r^2 \quad , \quad \overline{\sigma}_y^2 = \overline{C}_{yy} - \overline{C}_{xy} + r^2 \quad , \quad \overline{\sigma}_z^2 = \overline{C}_{zz} - \overline{C}_{xy} + r^2 \quad ,$$

with the bars indicating that the corresponding quantity is for calibrated data. Note that the error variances with respect to the system of medium resolution (underlined) are independent of the representation error for the two systems with finer resolution (X and Y)

$$\underline{\overline{\sigma}}_x^2 = \overline{C}_{xx} - \overline{C}_{xy} \quad , \quad \underline{\overline{\sigma}}_y^2 = \overline{C}_{yy} - \overline{C}_{xy} \quad , \quad \underline{\overline{\sigma}}_z^2 = \overline{C}_{zz} - \overline{C}_{xz} + r^2 \quad .$$

3 Representation errors

3.1 Resolution and representation errors

Geophysical data originate from a variety of sources: in-situ measurements, satellite observations, and model predictions. Each type has its own geophysical, spatial and temporal characteristics: in-situ data are representative of a point whereas satellite and model data give a value that is representative for some area. Geophysical in-situ data are often presented as time averaged (for instance the wind speed and direction which is commonly given as average over 10 minutes or 1 hour), while satellite data are almost instantaneous. NWP models compute a new time step every 10 or 20 minutes and will represent temporal scales at about 5-7 times this time step [*Skamarock*, 2004].

For wind calibration, some authors use the assumption of frozen turbulence, called Taylor's hypothesis [*Taylor*, 1921; *Richardson*, 1926], to manipulate (in-situ) data sets in order to reduce spatial resolution to match a comparison data set. We note that this is not a very accurate method of obtaining a certain spatial resolution. At a wind speed of 8 m/s, one would thus average 3600 s or one hour to match a satellite footprint of ~30 km. When averaging over one hour one would however obtain an effective resolution of ~15 km at 4 m/s, but only ~60 km at 16 m/s. Extreme high winds thus would be severely smoothed, while low winds would not be smoothed much. Spatial and temporal smoothing of a field change the PDF, because extreme high values will become less frequent. Therefore, calibration or regression with respect to a temporally smoothed data set will tend to follow the extreme values and be representative for a coarser resolution than anticipated. Temporal smoothing of transient fields in order to reduce spatial resolution is thus prone to rather complex error characteristics. Following Kolmogorov's hypothesis [*Kolmogorov*, 1941], it appears more attractive to model small-scale variability through a representativeness error [*Stoffelen*, 1998].

Spatial satellite and model data are produced at different resolutions. With both temporal and spatial resolution the true resolution of a measurement system is meant, i.e., the size of the smallest detail discernible with that system in resp. time and space. In most cases this resolution is coarser than the grid size on which the product is presented.

As noted earlier, coarse resolution may refer to spatial or temporal resolution as described above, but there may also be geophysical representation issues that make systems X and Y look more alike while where system Z lacks certain geophysical sensitivity. For example, for SST two systems X and Y could measure skin temperatures and a third system Z the bulk temperature. X and Y then measure signal that is lacking in Z, and therefore in triple collocation $< \varepsilon_x \varepsilon_y > \neq 0$. Another example may exist in soil wetness

from a NWP model, where the geophysical representation in the NWP model lacks local soil characteristics.

The difference in resolution between various data types becomes important when intercomparing data or when assimilating observed data into numerical prediction models. It gives rise to representation errors, also referred to as error of representativeness. The term error may be a bit misleading, because the representation error is not a real error but originates from merging data at different resolution. Moreover, its role depends on the point of view that one takes.

Suppose, again, three measurement systems X, Y, and Z, and three resolution classes: coarse or low resolution (L), medium resolution (M), and fine or high resolution (H). Suppose further that the resolution class is given as subscript to the system, and that we have the situation $\{X_H, Y_M, Z_L\}$. For the case of wind scatterometry this corresponds to X_H being the buoy measurements, Y_M the scatterometer observations, and Z_L the NWP model background. The highest resolution scale seen by system X_H will, of course, be missed by systems Y_M and Z_L. Medium scales will be seen by systems X_H and Y_M, but also be missed by system Z_L. From the point of view of X_H the other two systems have a hopelessly blurred view of reality. In case of comparison to and verification of system Y_M the high resolution details seen by X_H is unwanted variance and treated as error, while system Z_L misses medium resolution details that are important for the verification of Y_M. In case of verification of system Z_L all medium and high resolution details is unwanted variance and treated as error. In particular, the medium resolution part resolved by X_H and Y_M will appear as a correlated error in case of Z_L verification or calibration and will add to the error correlation $< \varepsilon_x \varepsilon_y >$.

The triple collocation method uses the common signal of $\{X_H, Y_M, Z_L\}$ and thus the measurement error variances are specified at the lowest resolution. It is important to include the representation error variance r^2 into the error model. Not only does it affect the results (the representation error is of the same order of magnitude as the measurement errors in the case of wind scatterometry), but it also offers the possibility to obtain the measurement errors at the medium resolution by subtracting r^2 as common X_H and Y_M signal variance from σ_x^2 and σ_y^2, as discussed in section 2.5. The representation variance r^2 should in this case be added to error σ_z^2 since system Z_L cannot resolve this signal. The system X_H measurement error at medium resolution, $\hat{\sigma}_x$ as specified in (2.25), contains geophysical signal that is resolved by system X_H, but not by the other systems, denoted r_x^2. While error $\hat{\sigma}_x$ is retrieved from the triple collocation method, we would need further information on the local measurement errors, $\sigma_{M,x}$, to obtain an estimate of the additional geophysical variance resolved by X_H, this is $\hat{\sigma}_x^2 = \sigma_{M,x}^2 + r_x^2$.

The argument can be repeated for other resolutions of the three measurement systems. For instance, *O'Connor et al.* [2008] discuss the case $\{X_H, Y_M, Z_M\}$ with X_H in-situ sea surface temperature

measurements and Y_M and Z_M satellite observations. In this case $<\varepsilon_x\varepsilon_y>=0$ as there is no common temperature signal of Y_M and X_H not resolved by Z_M. Table 3.1 summarizes a number of cases. All other cases follow from interchanging the roles of X, Y, and Z, and the fact that representation errors do not play a role when all three systems have the same resolution.

Resolution			Representation error		
X	**Y**	**Z**	$<\varepsilon_x\varepsilon_y>$	$<\varepsilon_y\varepsilon_z>$	$<\varepsilon_z\varepsilon_x>$
H	H	M/L	r^2	0	0
H	M	L	r^2	0	0
H	M	M	0	0	0
H/M	L	L	0	0	0

Table 3.1 Contribution of the representation error r^2 to the error covariances for various resolution cases

3.2 Calculation methods

In the literature several methods are described for calculating representation errors. Which method can be used depends, of course, on data availability.

Stoffelen [1998] and *Portabella and Stoffelen* [2009] obtain the representation error by considering the variance spectra of NWP background and scatterometer observations. They assume a scatterometer wind spectrum of $ck^{-5/3}$ [*Lindborg*, 1999]. The constant c is determined by requiring that the scatterometer spectrum equals the NWP spectrum at a certain spatial frequency k_{sep}, corresponding to a spatial scale of the order of 1000 km. Then the representation error equals the difference between the two spectra integrated from k_{sep} to the highest spatial frequency k_{max}, corresponding to the smallest scales in the spectrum.

Vogelzang et al. [2011] refine this approach by using observed scatterometer wind spectra rather than a theoretical $k^{-5/3}$ form. This is applied to various operational scatterometer wind products, and consistent results are obtained for k_{sep} corresponding to a spatial scale of 800 km.

Janssen et al. [2007] do not consider representation errors, but extend the number of datasets to five by using various NWP model results (first guess, analysis, and hindcast) that contain different levels of assimilation. The additional sets give rise to additional equations, allowing one to solve for six error correlations. However, error correlations between satellite observations (from altimeter) and in-situ (buoy) measurements are neglected, so basically the representation error is assumed to be zero.

O'Connor et al. [2008] discuss the effect of representation errors on the error correlations, but give no estimate for the magnitude of the representation errors.

4 Implementation

Calculation of the first and second moments needed for the triple collocation model must be done with some care, since notably the second moments are sensitive for outliers in the data set. Outliers may be caused by anomalous geophysical conditions. For example, for scatterometers one may think of excessive sub-WVC wind variability, e.g., at the passage of a front or caused by a large convective downburst, or, particularly for Ku-band scatterometers, blurring of the ocean wind signature by rain. Most of these conditions are removed in a quality control step, but some outlier may remain due to a non-perfect probability of detection. Outliers also exist in in-situ data for various reasons, e.g., due to salting or icing conditions. To avoid problems caused by outliers it is better to filter them out, for instance by rejecting all data that lie away more than a specified times the standard deviation from the expected value. However, whether or not some measurement must be classified as outlier depends not only on the selection criterion, but also on the calibration, since the calibration determines the expected value of some measurement relative to the reference measurement value.

It is clear that this problem is best solved in an iterative scheme as shown in figure 4.1. Adopting the formalism of section 2.5 one starts with an initial estimate of the calibration coefficients, $a_y^{(0)}$, $a_z^{(0)}$, $b_y^{(0)}$, and $b_z^{(0)}$, as well as for the expected distances from the calibration line, $d_{xy}^{(0)}$, $d_{yz}^{(0)}$ and $d_{zx}^{(0)}$. For scatterometer applications good results are obtained with the values

$$b_y^{(0)} = b_z^{(0)} = 0 \quad ,$$

$$a_y^{(0)} = a_z^{(0)} = 1 \quad ,$$

$$d_{xy}^{(0)} = d_{yz}^{(0)} = d_{zx}^{(0)} = 9\,\mathrm{m^2 s^{-2}}$$

Now the iterative scheme starts to solve the triple collocation model. The next step is to go through all collocated triplets, calculate the calibrated triplets $(\bar{x}_j, \bar{y}_j, \bar{z}_j)$, with j the triplet number. The triplet is rejected if any of the conditions

$$\bar{\delta}_j^{xy} > 16 d_{xy}^{(0)} \quad ,$$

$$\bar{\delta}_j^{yz} > 16 d_{yz}^{(0)} \quad ,$$

$$\bar{\delta}_j^{zx} > 16 d_{zx}^{(0)} \quad ,$$

holds (this is called the 4σ test, but is it written here in quadratic form). If the triplet is accepted, the f irst and second moments of the calibrated wind components are updated.

If all triplets have been processed, the values for the error variances and calibration coefficients are calculated from (2.23). The calibration coefficients are updated according to

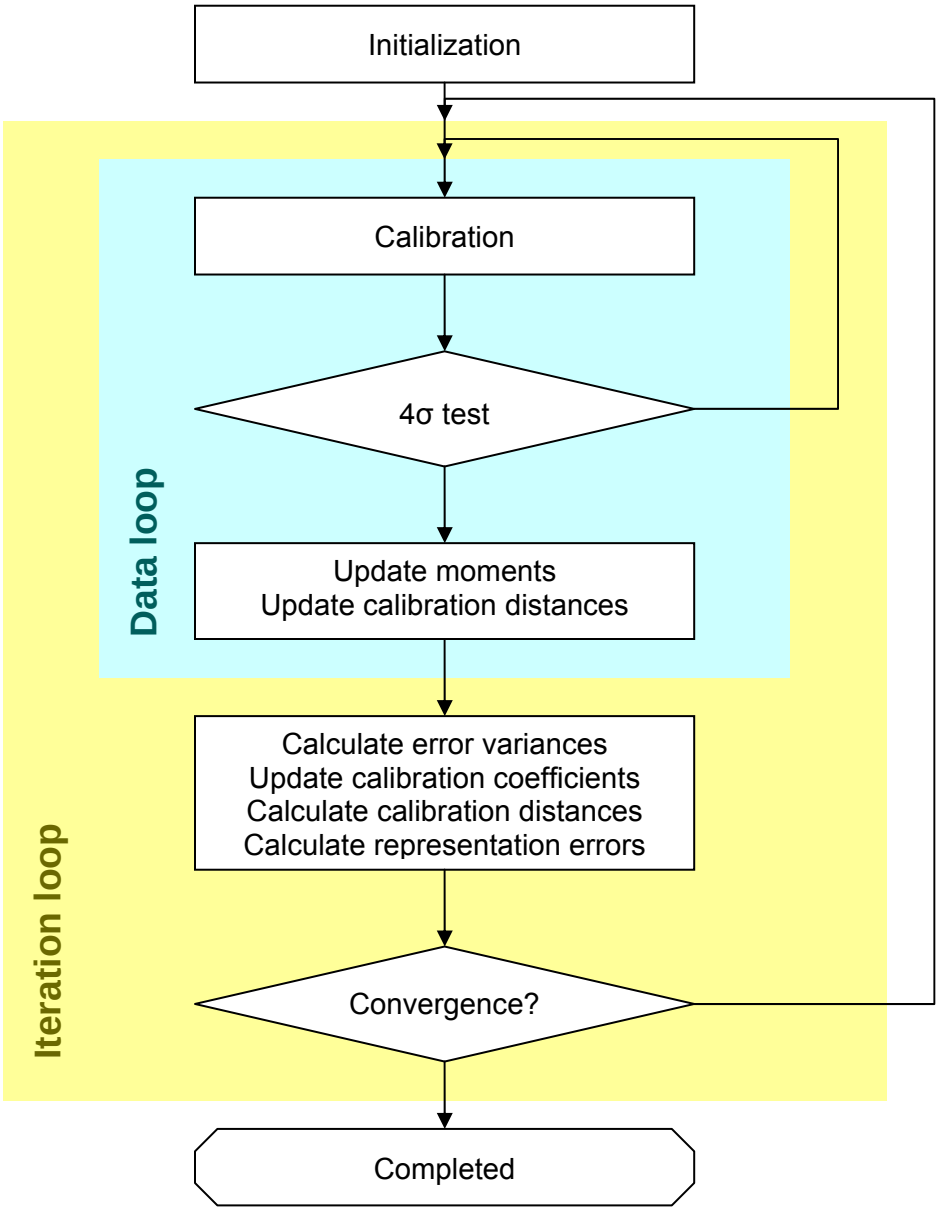

Figure 4.1 Flow chart for triple collocation algorithm.

$$a_\alpha^{(i+1)} = \frac{a_\alpha^{(i)}}{\overline{a}_\alpha} \quad , \quad \alpha = y,z \quad ,$$

$$b_\alpha^{(i+1)} = b_\alpha^{(i)} + \overline{b}_\alpha \quad , \quad \alpha = y,z \quad ,$$

with i the iteration number. The expected distances to the calibration line are set equal to the sum of the estimated error covariances

$$d_{xy}^{(i+1)} = \overline{\sigma}_x^2 + \overline{\sigma}_y^2 , \quad d_{yz}^{(i+1)} = \overline{\sigma}_y^2 + \overline{\sigma}_z^2 , \quad d_{zx}^{(i+1)} = \overline{\sigma}_z^2 + \overline{\sigma}_x^2$$

For normal unbiased random error distributions, only one in 15,787 data points would fall outside the 4-sigma range for each of the three differences in the triple collocation data set. Since these data points would be far away from the diagonal, one might want to check their contribution to the estimated errors and calibration. In this respect we note that one distance of $4\,\overline{\sigma}_x$ in 15,787 points adds 0.1% to the variance and thus 0.2% to the estimated standard error, i.e., is likely to be negligible in the context of the assumptions in the error model used for triple collocation.

Now the next iteration can be started, unless the calibration coefficients have converged.

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