On the solution of the multiple collocation problem

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Key points:

1. The general multiple collocation problem can be solved for both determined and overdetermined subsets of the covariance equations.
2. The least-squares solution of all covariance equations equals the average of the solutions of all determined subsets.
3. Results of quintuple collocation analysis are consistent with those of triple and quadruple collocation.

Index terms:

0520 (data analysis: algorithms and implementation)

4504 (air-sea interactions)

0560 (numerical solutions)

Keywords:

1. multiple collocation analysis
2. numerical solution
3. analytical solution
4. quadruple collocation analysis
5. quintuple collocation analysis
6. ocean vector surface winds

Abstract:

A new solution method is given for the general multiple collocation problem formulated in terms of the covariance equations. By a logarithmic transformation, the covariance equations reduce to ordinary linear equations that can be handled using standard methods. Solution by matrix inversion has the advantage that the analytical solutions can be reconstructed. The method can be applied to each determined or overdetermined subset of the covariance equations. It is demonstrated on quintuple collocations of ocean surface vectors winds obtained from buoys, three scatterometers and model forecasts, with representativeness errors estimated from differences in spatial variances. The results are in good agreement with those from quadruple collocation analyses reported elsewhere.

The average of the solutions from all determined subsets of the covariance equations equals the least-squares solution of all equations. The standard deviation of all solutions from determined subsets agrees with the accuracy found in earlier triple and quadruple collocation studies, but the difference between minimum and maximum value is much larger. It is shown that this is caused by increased statistical noise in more complex solutions. The averages of the error covariances are close to zero, with a few exceptions that may point at small deficiencies in the underlying error model. Precise accuracy estimates are needed to decide to what extent statistical noise explains the spreading in the results and what is the role of deficiencies in the underlying error model.

Plain language summary

When a quantity is measured with three independent measuring systems at (almost) the same time and place, it is possible to retrieve the relative calibration and the errors of the systems using a statistical technique named triple collocation. When more than three measuring systems are available, also error correlations can in principle be retrieved. In most cases there are more equations than unknowns, and the problem is solved in an approximate way. In this paper a new solution method is presented. It allows to solve all possible subsets of the problem, to retrieve the analytical solutions, and to study the statistics of the solutions. The method is applied to ocean surface wind components measured with five different systems (quintuple collocation): buoys, three satellite-borne scatterometers, and forecasts from a weather prediction model. The results are in good agreement with those from earlier triple and quadruple analyses, though the spreading in the results is larger. It is shown that this is due to the more complex solutions that are present in a quintuple collocation analysis, but not in quadruple or triple collocation. It is also shown that the underlying error model has good consistency.

1. Introduction

The triple collocation method was introduced by Stoffelen (1998) in order to assess the intercalibration coefficients and error variances of three systems observing ocean surface vector winds. It is an extension of regression analysis to three dimensions under the assumptions that linear calibration is sufficient, that the errors are independent of the measured value (also referred to as error orthogonality), and that the correlations in the errors of the observing systems are known or can be neglected. Triple collocation has been applied to a variety of geophysical parameters like ocean surface vector winds (Stoffelen, 1998; Vogelzang et al., 2011; Vogelzang and Stoffelen, 2021), ocean surface wind speed (Abdallah and De Chiara, 2017), ocean surface current (Danielson et al., 2018), sea surface salinity (Horeau et al., 2018), precipitation (Roebeling et al., 2012), soil moisture (e.g. Gruber et al., 2016), etc.

Stoffelen (1998) already realized that the assumption of uncorrelated errors is in most cases violated, because differences in the spatial and/or temporal resolutions between the observation systems give rise to representativeness errors which express themselves as error covariances, also in cases where the measurements are completely independent. Unfortunately the term representativeness error has different meanings in different communities (Gruber et al., 2020). In this paper we follow the meteorological convention and consider representativeness errors as caused by differences in resolution between the various systems, in order to distinguish them from error correlations caused by interdependence of the measurement system errors. Spatial representativeness errors can be estimated from spectral analysis (Stoffelen, 1998; Vogelzang et al., 2011), from constraints on the intercalibration (Lin et al., 2015), or from spatial analysis (Vogelzang et al., 2015). Another approach is to estimate spatial representativeness errors, or error covariances in general, using more than three observation systems. This is enabled by the increase of satellite observations, but can also be achieved by introducing instrumental variables, i.e., using model forecasts or hindcasts with different analysis times (Su et al., 2014; Abdallah and De Chiara, 2017; Danielson et al., 2018) or time-lagged variables (Crow et al., 2015). These developments led to so called extended collocation analyses, although that term has also been used by McColl et al. (2014) for a generalization of the correlation coefficient from linear regression to triple collocation.

A number of methods has been proposed to solve the multiple collocation problem for four or more observing systems. The methods depend on the spatial and temporal statistical properties of the quantity under consideration and on the availability of a calibration reference. The most popular one is to change variables, cast the problem in matrix form, and solve the resulting overdetermined system of equations using a least-squares method (Pierdicca et al., 2015; Gruber et al., 2016). This is equivalent to minimizing a quadratic cost function to the unknowns. A different approach has been followed by Vogelzang and Stoffelen (2021) for quadruple collocations. They solve each subset of four equations from the six off-diagonal covariance equations analytically. There are 15 such subsets, further referred to as models, of which 12 are soluble. The remaining two equations of each soluble model can be solved for two error covariances. The number of possibilities grows rapidly with the number of observing systems, and for quintuple collocation there are already 252 models. It is clear that the analytical solution of the problem becomes increasingly cumbersome and mathematically complex.

In this paper a new method is introduced for solving all possible models. The diagonal covariance equations establish the error variances of the observing systems, while a determined subset of the off-diagonal equations is solved for the calibration scalings and the common variance. By taking logarithms, this system of covariance equations is transformed into a set of ordinary linear equations, that can be solved using standard methods. The determinant of the system clearly indicates whether a solution exists. Solution by matrix inversion enables reconstruction of the analytical solutions and introduction of a quantity named complexity that gives the number of observed covariances that enter the analytical solution. The method proves to be fast and accurate, and can also be applied to any overdetermined subset of the covariance equations. Results are shown here for quintuple collocations of ocean vector surface winds, while up to octuple collocations have been tested (not shown here for brevity).

In section 2 the multiple collocation problem is formulated and the new solution method is introduced. It is applied to a quintuple collocation data set consisting of ocean surface vector winds observed by buoys, three different scatterometers (ASCAT-A, ASCAT-B, and ScatSat), and ECMWF model forecasts. Section 3 contains a short description of the data used and the representativeness errors that are estimated from differences in spatial variances. The results are presented and discussed in section 4. For comparison also least-squares and minimization solutions are calculated. The average of all models equals the least-squares solution and the minimization solution. The standard deviation over all models agrees with the accuracy estimated from triple collocation analyses, but the range is considerably larger. It is shown that this is caused by increased statistical noise in more complex solutions. The average error covariances are close to zero, indicating that deficiencies in the underlying error model may also play a role. The paper ends with the conclusions in section 5.

2 Multiple collocation formalism

Suppose we have a set of K collocated measurements made by n observation systems, $\left\{x_i^{(k)}\right\}$, with k the collocation index, $k = 1, \dots, K$, and i the observation system index, $i = 1, \dots, n$. Assuming that linear calibration is sufficient for intercalibration and omitting the collocation index k, we can pose the following simplified observation error model:

$x_i = a_i \left(t + \varepsilon_i\right) + b_i$ (1)

where t is the signal common to all observation systems (also referred to as the truth), a_i the calibration scaling, b_i the calibration bias, and ε_i a random measurement error with zero average and variance σ_i^2. It is assumed that ε_i is uncorrelated with the common signal t, $\langle t\varepsilon_i \rangle = 0$, where the brackets $\langle\ \rangle$ stand for averaging over all measurements k. In the literature this condition is also referred to as error orthogonality. Of course, the assumptions made on linearity and error orthogonality should be checked first by inspecting scatter plots. Note that x_i is an uncalibrated measurement while t is calibrated, so (1) actually constitutes an inverse calibration transformation.

Without loss of generality we can select the first observation system as calibration reference, so $a_1 = 1$ and $b_1 = 0$. By forming first and second moments from (1) and introducing covariances the general collocation problem can be cast in the form (McColl et al., 2014; Vogelzang and Stoffelen, 2021)

$b_i = M_i - a_i M_1$ (2)

with $M_i = \langle x_i \rangle$ the averages of the observations, and

$C_{\mathrm{ij}} = a_i a_j \left(T + e_{\mathrm{ij}}\right)$ (3)

with $C_{\mathrm{ij}} = M_{\mathrm{ij}} - M_i M_j$ the (co-)variances of the observations, $M_{\mathrm{ij}} = \langle x_i x_j \rangle$

the (mixed) second moments of the observations, $T = \langle t^2 \rangle - M_1^2$ the common variance, and $e_{\mathrm{ij}} = \langle \varepsilon_i \varepsilon_j \rangle$ the error covariances. Note that C_{ij} and e_{ij} are symmetric in their indices. Representativeness errors can be incorporated in the observed covariances by

$C_{\mathrm{ij}} \to C_{\mathrm{ij}} - \sum_{k=max(i,j)}^{n-1} r_k^2$ (4)

where r_k^2 is the representativeness error of system k with respect to system $k+1$, the systems assumed to be sorted to decreasing spatial resolution. Also error covariances known a priori can be included in this way.

At this point it must be emphasized that the approach outlined above is geared towards ocean surface vector winds. Their statistical properties in time and space are well studied. In particular, their spectra follow power laws, and the observing systems with highest resolution show the largest variations. Therefore buoy winds are widely accepted as calibration standard. This need not be the case for other quantities, and slightly different approaches have been developed to account for this. Nevertheless, much of what follows can be easily adapted to those approaches.

Equations (2) and (3) completely define the multiple collocation problem for error model (1). Once the calibration scalings a_i are known, the calibration biases b_i follow from (2). The remaining unknowns, in particular the essential unknowns (the calibration scalings a_i, the error variances $\sigma_i^2 = e_{\mathrm{ii}}$, and the common variance T), must be obtained from the covariance equations (3).

For triple collocation, $n = 3$, there are six equations. Setting the off-diagonal error covariances e_{ij} to zero, the covariance equations can be solved analytically for the essential unknowns. For quadruple and higher-order collocations there are more equations than essential unknowns: the number of equations is $n(n+1)/2$ while the number of essential unknowns equals $2n$. The common approach is to solve (3) as an overdetermined system with a least-squares method by introducing new variables $y_k = a_i a_j T$ if the error covariance e_{ij} is neglected or $y_k = a_i a_j \left(T + e_{\mathrm{ij}}\right)$ if it is included as unknown and writing the covariance equations in matrix-vector form as Ay $= \mathbf{b}$ with $b_k = C_{\mathrm{ij}}$ and $\mathbf{A}$ a matrix with elements zero or one (Gruber et al., 2016). The solution reads

$\mathbf{y} = \left(\mathbf{A}^T\mathbf{A}\right)^{-1}\mathbf{A}^T\mathbf{b}$ (5)

provided the inverse of $\mathbf{A}^T\mathbf{A}$ exists. In cases where no calibration reference is selected, also the error variances are included in the variables (e.g., Gruber et al., 2016).

The n error variances σ_i^2 only appear in the n diagonal covariance equations, so these are easily calculated when a_i and T are known. The remaining $n(n-1)/2$ off-diagonal covariance equations only contain the essential variables a_i and T plus the error covariances e_{ij}. For quadruple collocations, Vogelzang and Stoffelen (2021) take all possible combinations of determined subsets of off-diagonal covariance equations, neglect the error covariances, and solve each set analytically. There are 15 possible combinations, further referred to as models, of which 12 have a solution. Besides the essential unknowns each model also yields two error covariances from the remaining two covariance equations that were not used to solve a_i and T. The spread in the model solutions is considered as an indication of how accurate the underlying error model (1) describes the data. The number of models grows rapidly with the number of observing systems, see table 1 in the next section. For quintuple collocation there are already 252 models, and analytical solution is practically impossible.

Taking a closer look at the covariance equations with the error covariances neglected, one sees that the unknowns a_i and T appear as a product on one side and the coefficients C_{ij}, calculated from the data, on the other. By taking logarithms on both sides, the unknowns are separated and the equations reduce to an ordinary system of linear equations. Suppose a selection of n off-diagonal covariance equations $\left\{C_{\mathrm{ij}}^{(m)} = a_i a_j T\right\}$ with $j > i$ has been made, labeled with index $m = 1, \ldots, n$. Setting $z_1 = \ln T$, $z_m = \ln a_m$ for $m = 2, \ldots, n$, and $d_m = \ln C_{\mathrm{ij}}^{(m)}$, the off-diagonal covariances read in matrix-vector notation

$\mathrm{Dz} = \mathbf{d}$ (6)

where the matrix $\mathbf{D}$ has for each row the value 1 in the first column, $D_{m1} = 1$, and one or two additional values 1 in the remaining columns, $D_{\mathrm{mi}} = 1$ if $i > 1$, and $D_{\mathrm{mj}} = 1$. All other elements of $\mathbf{D}$ are zero. The determinant of $\mathbf{D}$ can thus only take integer values, the zero value indicating that system (6) has no solution. The calibration scalings a_m are generally close to 1, so their logarithms are around 0, and the observed covariances C_{ij} are nonnegative, also when representativeness errors are taken into account. Therefore the problem (6) is well posed and can be solved numerically with standard methods.

In this work the inverse of $\mathbf{D}$ is calculated using Gaussian elimination, and the solution reads $\mathbf{z} = \mathbf{D}^{-1}\mathbf{d}$. This has the advantage that the analytical solution can be reconstructed, since in components

$z_m = \sum_{k=1}^{n} D_{\mathrm{mk}}^{-1} d_k$ (7)

which implies that after exponentiating

$T = \prod_{k=1}^{n} \left(C_{\mathrm{ij}}^{(k)}\right)^{D_{1k}^{-1}}$ (8)

$a_m = \prod_{k=1}^{n} \left(C_{\mathrm{ij}}^{(k)}\right)^{D_{\mathrm{mk}}^{-1}}, \quad m > 1$ (9)

so the analytical solutions for the common variance T and the calibration scalings a_m are products of observed covariances raised to a power determined by the components of $\mathbf{D}^{-1}$. The error variances are given by $\sigma_m^2 = C_{\mathrm{mm}} - a_m^2 T$, and from (8) and (9) it follows that

$\sigma_1^2 = C_{11} - \prod_{k=1}^{n} \left(C_{\mathrm{ij}}^{(k)}\right)^{(D_{1k}^{-1})}$ (10)

$\sigma_m^2 = C_{\mathrm{mm}} - \prod_{k=1}^{n} \left(C_{\mathrm{ij}}^{(k)}\right)^{\left(D_{1k}^{-1}+2D_{\mathrm{mk}}^{-1}\right)}, \quad m > 1$ (11)

Note that in (11) factors may cancel in the exponent.

The number of observed covariances contributing to a solution will be denoted as its complexity γ. For the common variance and the calibration scalings the complexities are

$\gamma(T) = \sum_{k=1}^{n} \left|D_{1k}^{-1}\right|$ (12)

$\gamma\left(a_m\right) = \sum_{k=1}^{n} \left|D_{\mathrm{mk}}^{-1}\right|, \quad m > 1$ (13)

The calibration scalings are composed of an even number of observed covariances, as many in the numerator as in the denominator, since their values are of order one. The common variance is composed of an odd number of observed covariances, one more in the numerator than in the denominator. The definition of complexity is extended for the error variances as the complexity of $a_m^2 T$ and reads

$\gamma\left(\sigma_1^2\right) = \gamma(T) = \sum_{k=1}^{n} \left|D_{1k}^{-1}\right|$ (14)

$\gamma\left(\sigma_m^2\right) = \gamma\left(a_m^2 T\right) = \sum_{k=1}^{n} \left|D_{1k}^{-1} + 2D_{\mathrm{mk}}^{-1}\right|$ (15)

The error variances have odd complexity.

The same logarithmic transformation can also be applied to all off-diagonal covariance equations and solved with the least-squares method, having the advantage that the solution is given directly in the logarithms of the basic unknowns rather than combinations of them. The complexities of the solutions are defined in the same manner as (12) - (15), except that $\mathbf{D}^{-1}$ is to be replaced by $\left(\mathbf{D}^T\mathbf{D}\right)^{-1}\mathbf{D}^T$ because it is no longer a square matrix and that the summation is over all $n(n-1)/2$ off-diagonal covariance equations. If the number of equations permits, also error covariances can be included by adding extra variables $z_m = log(T + e_{\mathrm{ij}})$ with $m > n$. Similarly, the scaling of system 1 can be included if no calibration reference is selected.

A solution method equivalent to the least-squares solution is minimizing a quadratic cost function J defined as

$J = \sum_{i=1}^{n} \sum_{j=i+1}^{n} \left(a_i a_j T - C_{\mathrm{ij}}\right)^2$ (16)

to a_i and T using a standard conjugate-gradient method. In this work the quasi-Newton routine named LBFGS written by J. Nocedal is used (Liu and Nocedal, 1989).

3 Data and representativeness errors

A quintuple collocation analysis has been performed with the data used by Vogelzang and Stoffelen (2021). The quadruple collocation files of buoy (b), ASCAT-B (B) or ASCAT-A (A), ScatSat (S), and ECMWF (E), were combined into one bBASE quintuple collocation file with 2454 collocations. The reader is referred to Vogelzang and Stoffelen (2021) for a description of these data. The maximum time difference was set to 1 hour, because of the 50 minutes time difference between ASCAT-A and ASCAT-B, while the maximum distance between buoy location and scatterometer grid center was 25 km.

In general, the representativeness errors can't be retrieved from the error covariances. The number of off-diagonal covariance equations is $n_{\text{od}} = n(n-1)/2$, so the number of error covariances that can be retrieved is $n_{\text{ec}} = n_{\text{od}} - n = n(n-3)/2$. The number of representativeness errors is $n_{\text{re}} = \frac{(n-1)(n-2)}{2} = n_{\text{ec}}+1$, so there is always one off-diagonal covariance equation lacking. This can be circumvented when the two coarsest resolution systems have the same spatial and temporal resolution. In the case considered here one could try ECMWF forecasts with different analysis time. However, as already remarked in (Vogelzang and Stoffelen, 2021) this would introduce an additional error covariance between the two forecasts, and the resulting model has no solution.

As a consequence, the representativeness errors must be estimated in a different way. In this study they are obtained from differences in spatial variance as a function of separation distance (scale). Figure 1 shows the difference in spatial variance $V(s) = V_{\text{scat}}(s) - V_{\text{ECMWF}}(s)$, as a function of scale s for ASCAT-B, ASCAT-A, and ScatSat. Figure 1 is the same as Figure 2 in (Vogelzang and Stoffelen, 2021). In the terminology of equation (4), the ScatSat representativeness error with respect to the ECMWF model, r_4^2, is defined as $r_4^2 = V_{\text{ScatSat}}(s) - V_{\text{ECMWF}}(s)$, the height of the dotted curve. The representativeness error r_3^2 of ASCAT-A relative to ScatSat equals the vertical distance between the dotted curve and the solid curve, and that of ASCAT-B relative to ASCAT-A, r_2^2 by the vertical distance between the dashed and the solid curve. The representativeness error of ASCAT-B relative to the ECMWF background equals $r_2^2+r_3^2+r_4^2$, the height of the dashed curve in Figure 1. The representativeness errors increase with scale. Previous work indicated that the optimum scale for calculating the representativeness errors is about 200 km for the zonal wind component u and about 100 km for the meridional wind component v. Note that both correspond to a spatial representativeness wind vector component variance of about 0.3 $\text{m}^2\ \text{s}^{-2}$ for the ASCATs,

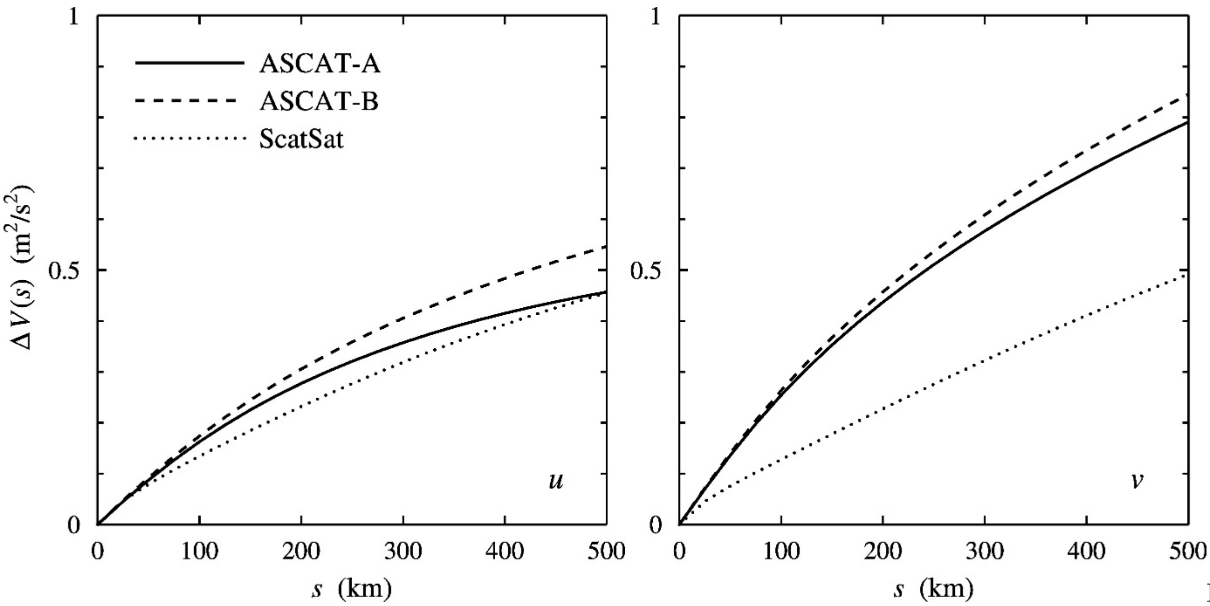


Figure 1. Difference between the spatial variance of ASCAT-A, ASCAT-B, and ScatSat and that of ECMWF, $V(s)$, as a function of s for the zonal and meridional wind components, u and v.

4 Results and discussion

As a check, the numerical solutions, calculated in double precision, were compared to the analytical ones for the quadruple collocations in (Vogelzang and Stoffelen, 2021) and were found to agree to at least six decimal places.

4.1 Number of solvable models

Table 1 gives the number of observing systems, n, the number of off-diagonal covariance equations, the number of models, and the number of solvable and unsolvable models obtained from (6). The number of models, n_m, satisfies

$$n_m = \binom{n(n-1)/2}{n} \quad (17)$$

The fraction of solvable models decreases from 80% for quadruple collocation to about 23% for nonuple collocations, but still the number of solvable models increases rapidly.

Observing systems	Off-diagonal equations	Models	Solvable	Unsolvable

Observing systems	Off-diagonal equations	Models	Solvable	Unsolvable

Table 1 Number of observing systems, number of equations, number of models, and number of solvable and unsolvable models.

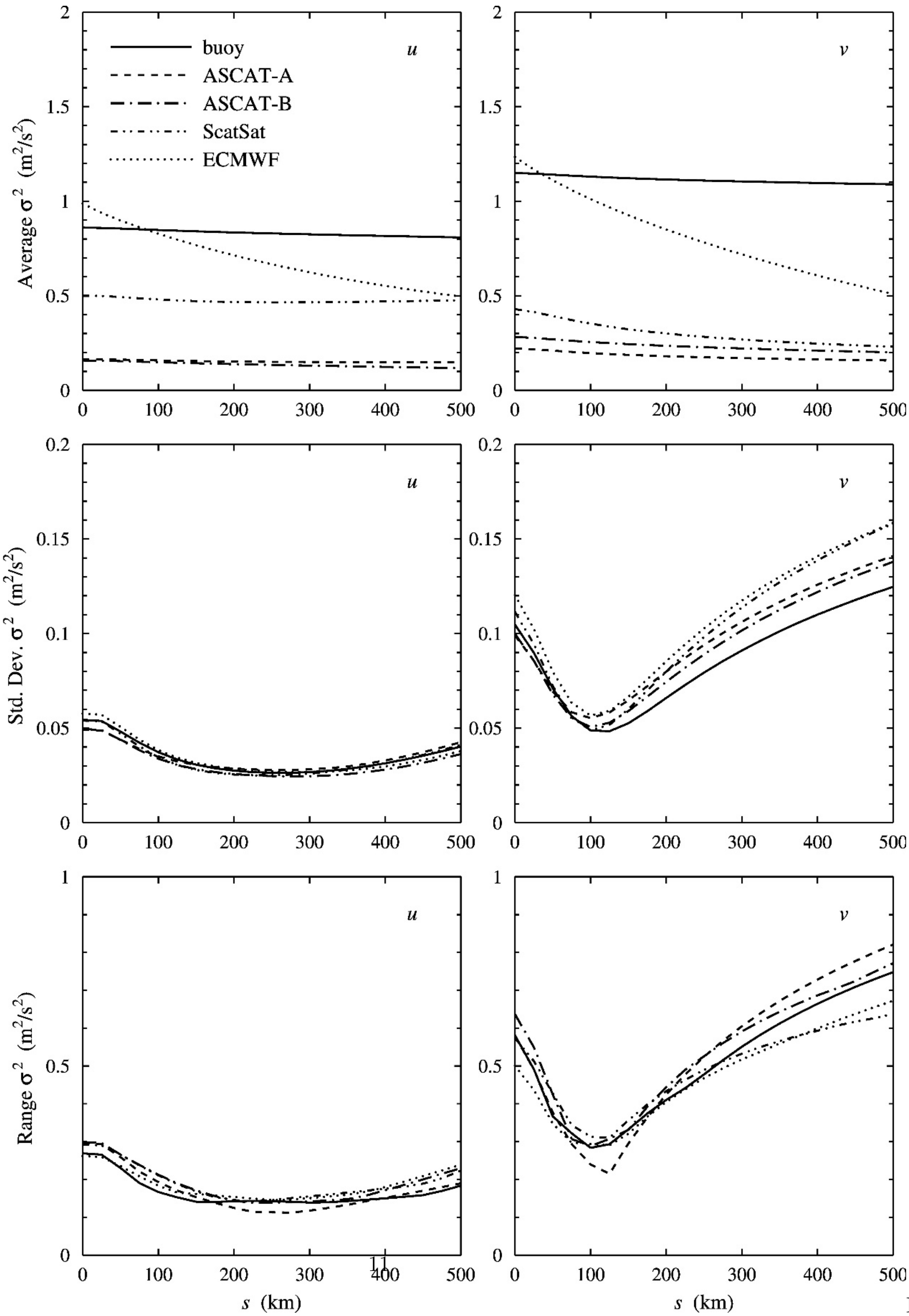
Table 1 shows that there are 162 solvable models for quintuple collocations. As for quadruple collocations, different models lead to different solutions, so it makes little sense to present them all. Therefore only statistical results will be shown.

4.2 Error variances

Figure 2 shows statistical results over all models as a function of the scale at which the representativeness errors are calculated. The top panel of Figure 2 shows the average error variances, σ^2, for buoys, ASCAT-A, ASCAT-B, ScatSat, and ECMWF. The middle panels show the standard deviation in the error variances, and the bottom panels the range in the error variances (highest value minus lowest value). The left hand panels are for the zonal wind component u; the right hand panels for the meridional wind component v.

The average error variances in Figure 2 differ little (in the second or higher decimal) from those obtained with the least-squares solution of all off-diagonal covariance equations. The least-squares solution differs only in the third or higher decimal from the minimization solution of (16), as may be expected. This is a strong indication that the average over all models is equivalent to the least-squares solution, and that the spreading between the models can be interpreted as a measure of accuracy of the underlying error model and/or statistical noise caused by the sample size.

The value of the representativeness error affects the average error variances of ECMWF and ScatSat (top panels of Figure 2): these error variances decrease with increasing scale (increasing representativeness error). For ScatSat there is little effect in u, because there ScatSat has almost the same representativeness error as ASCAT, see Figure 1.



buoy
ASCAT-A
ASCAT-B
ScatSat
ECMWF
u
v
Average σ^2 (m^2/s^2)
Std. Dev. σ^2 (m^2/s^2)
Range σ^2 (m^2/s^2)
s (km)

Figure

2. Results for error variances as a function of scale for bBASE collocations. Top panels: average error variance of each system; middle panels: standard deviation of error variances; bottom panels: range in error variance.

The effect of representativeness error is clearly visible in the standard deviation and the range of the observation error variances for all five observation systems, notably in v. In u the standard deviation and the range are smallest at scales around 200 km, in v at scales slightly larger than 100 km. This agrees with the results from the quadruple collocation analyses in (Vogelzang and Stoffelen, 2021). The standard deviation in the error variances (middle panels of Figure 2) is around 0.025 m^2s^{-2} for u and around 0.055 m^2s^{-2} for v, which agrees with the accuracy in the error variance estimated from triple collocation analyses (Vogelzang and Stoffelen, 2021). Note that the standard deviation in the error variance is about the same for all observation systems involved.

The range in the quintuple collocation results (bottom panels in Figure 2) is much larger than the standard deviation: at the minimum about 0.15 m^2s^{-2} for u and about 0.3 m^2s^{-2} for v. It may exceed the size of the error variance of ASCAT-A and ASCAT-B, indicating that some models give negative error variances for these instruments. Incompleteness of the error model (1) may play a role. The scatterometer data may have retrieval problems, and in particular Ku-band scatterometers like ScatSat are known to have wind direction biases that will affect a collocation analysis (e.g., Ebuchi, 1999; Wang et al., 2017). The ECMWF model is known to have biases in wind speed and direction too (Belmonte and Stoffelen, 2019). Error orthogonality is hard to check and might be violated. However, triple collocation analyses of all sensor combinations in the dataset did not show such strong outliers.

4.3 Statistical noise

A more likely cause for the large spreading in the error variances in Figure 2 is statistical noise in the observed covariances C_{ij} which leads to larger errors in solutions with higher complexity γ. For triple collocation all error variances have $\gamma = 3$, while for quadruple collocation there are error variances with $\gamma = 5$, as can be inferred from the equations in Appendix A of (Vogelzang and Stoffelen, 2021). For quintuple collocation also error variances with $\gamma = 7$ occur. Table 2 shows the statistics of the error variances of the zonal wind component u with representativeness errors evaluated at a scale of 200 km for complexities 3, 5, and 7. The subscripts in the first column indicate the observation system, while the bottom row gives N, the number of models in the complexity class.

Table 2 shows that the average error variance is the same for each complexity class, but that the standard deviation and the range increase with complexity. The results for the meridional wind component v follow the same pattern and are not shown here. This implies that higher-order collocation analyses may produce results that are less accurate than triple collocation analyses, provided, of course, that the error covariances from representativeness and/or error correlation are well known.

	average (m^2s^{-2})	standard deviation (m^2s^{-2})	range (m^2s^{-2})					
	$\gamma = 3$	$\gamma = 5$	$\gamma = 7$	$\gamma = 3$	$\gamma = 5$	$\gamma = 7$	$\gamma = 3$	$\gamma = 5$
σ_b^2	0.835	0.835	0.835	0.020	0.033	0.041	0.051	0.115
σ_A^2	0.152	0.152	0.152	0.021	0.035	0.041	0.071	0.102
σ_B^2	0.139	0.138	0.138	0.017	0.030	0.046	0.051	0.118
σ_S^2	0.467	0.467	0.467	0.016	0.030	0.050	0.044	0.115
σ_E^2	0.714	0.714	0.714	0.021	0.035	0.042	0.053	0.126
N	90	60	12	90	60	12	90	60

Table 2. Average error variance, its standard deviation, and its range of the zonal wind component u with representativeness errors evaluated at 200 km for complexity 3, 5, and 7.

4.4 Error covariances

Figure 3 shows the average error covariances, represented by the dot, and their standard deviation, indicated by the error bars, for the zonal wind component u (left hand panel) and the meridional wind component v (right hand panel) with representativeness errors evaluated at a scale of 200 km for u and 100 km for v. Error covariances set to zero to solve the covariances were, of course, excluded. Each average is over 81 values - the additional error covariances appear distributed evenly over the solvable models. The standard deviations of the average error covariances show the same dependency on the scale as the error variances in Figure 2, with minimum spreading at a scale of about 200 km for u and about 100 km for v.

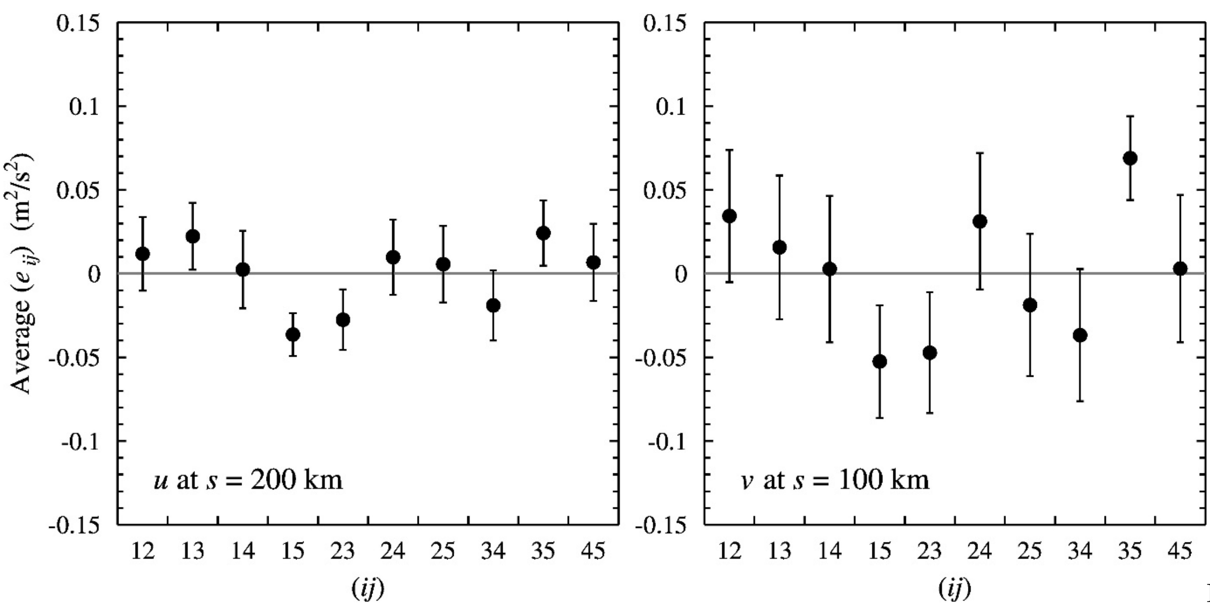


Figure 3. Average error covariances and their standard deviation.

Figure 3 shows that the averaged error covariances all lie around zero, with a standard deviation that is of the same order of magnitude as the average value. For both u and v e_{15} (buoy - ECMWF) and e_{23} (ASCAT-B - ASCAT-A) show a negative covariance, and e_{35} (ASCAT-A - ECMWF) a positive one. It is not plausible that the values of e_{15} and e_{23} are caused by correlated errors between buoys and ECMWF forecast or between ASCAT-B and ASCAT-A, as one would expect positive values. Averaged error covariance e_{35} is positive, but if this were caused by error correlations between ASCAT-A and ECMWF, one also expects a similar error covariance e_{25} between ASCAT-B and ECMWF. It is therefore more likely that the nonzero averaged error covariances are caused by deficiencies in the underlying error model (1) or by statistical noise. Since the differences from zero are small, well within three times the standard deviation, the error model shows good consistency.

To decide to what extent statistical noise is responsible for the spread in the results and what is the role of the error model, it is necessary to have good estimates of the statistical accuracy of the solutions, taking properly into account the correlations between the covariances. This is not a trivial problem that falls outside the scope of this study but is being investigated further.

Finally, it is worth mentioning that the determinant of $\mathbf{D}^T\mathbf{D}$ in the least-squares solution equals the number of soluble models for quadruple and quintuple collocations. In the determined case the matrix $\mathbf{D}^{-1}$ has only integer elements, in the overdetermined case $\left(\mathbf{D}^T\mathbf{D}\right)^{-1}\mathbf{D}^T$ also contains rational numbers. The complexities of the least-squares solutions are 3 for the common variance and 2 for the calibration coefficients, yet the analytical solutions are rather complicated as they involve square, cubic, and 6^{th} roots.

5. Conclusions

In this paper a new method for solving the multiple collocation problem is presented. The method is fast and accurate, and can easily be applied to quintuple collocations. Some preliminary tests show that up to and including octuple collocations can be handled within reasonable computation time. The method allows reconstruction of the analytical solutions and can be used for both determined and overdetermined subsets of the covariance equations.

The method is applied to a quintuple collocation dataset of ocean surface vector winds measured by buoys, three scatterometers, and ECMWF forecasts. The results show good consistency with triple and quadruple collocation analyses of the same data. The average over all solutions from determined subsets is almost equal to the least-squares solution and the solution obtained from minimizing a quadratic cost function. The standard deviation over all solutions agrees with the accuracy estimated from triple collocation analyses. The standard deviation and the range are smallest when representativeness errors from differences in spatial variances are taken into account, evaluated at a scale of 200 km for u and 100 km for v. This agrees with findings from quadruple collocations, showing that proper inclusion of representativeness errors increases the consistency of the underlying error model. The spreading in the results, however, is much larger than in triple and quadruple collocation analyses. This is most likely caused by an increase of statistical noise due to more complex solutions. The averaged error covariances are close to zero with a few exceptions that may be caused by incompleteness of the underlying error model. Further research is needed to determine the precise roles of statistical noise and imperfections in the underlying error model in the spreading of the results. The method introduced here may help to avoid unnecessary complex solutions and thus reduce the effect of statistical noise.

Acknowledgments, Samples, and Data

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The ASCAT-A, ASCAT-B, and ScatSat data can be obtained from the EUMETSAT archive www.eumetsat.int/website/home/Data/DataDelivery/EUMETSATDataCentre (BUFR or NetCDF format). The ASCAT data can also be obtained from the Physical Oceanography Distributed Active Archive Centre podaac.jpl.nasa.gov (NetCDF format only). The ECMWF NWP forecasts are part of the scatterometer data. The quadruple collocation data from which the quintuple collocation data set was formed can be obtained with doi 10.21944 from doi.org/10.21944/quad_coll_data.

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