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THREE-WAY ERROR ANALYSIS BETWEEN AATSR, AMSR-E AND IN SITU SEA SURFACE TEMPERATURE OBSERVATIONS.

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ABSTRACT

Using co-locations of three different observation types of sea surface temperatures (SSTs) gives enough information to enable the standard deviation of error on each observation type to be derived. SSTs derived from the Advanced Along-Track Scanning Radiometer (AATSR) and Advanced Microwave Scanning Radiometer (AMSR-E) instruments are used, along with SST observations from buoys. Various assumptions are made within the error theory including that the errors are not correlated, which should be the case for three independent data sources. An attempt is made to show that this assumption is valid and also that the covariances between the observations due to representativity error are negligible. Overall, the AATSR observations are shown to have a very small standard deviation of error of 0.16K, whilst the buoy SSTs have an error of 0.23K and the AMSR-E SST observations have an error of 0.42K.

1. INTRODUCTION

Sea surface temperatures (SSTs) derived from satellite-borne instruments have some advantages over traditional in situ SST measurements from buoys and ships. Firstly they provide a global coverage important in regions with sparse in situ observations. Secondly satellite instruments can potentially give well-calibrated, accurate skin SST measurements with global and temporal consistency not possible from in situ measurements. Satellite datasets are also beginning to span long enough time periods to start being able to detect long term drifts in SST. However, it is important to understand the error characteristics of these data.

This study investigates the errors in SST observations from three different sources: firstly, infra-red SSTs from the Advanced Along-Track Scanning Radiometer (AATSR); secondly microwave SST observations from the Advanced Microwave Scanning Radiometer (AMSR-E); and finally in situ SST observations from drifting and moored buoys. A three-way analysis is performed where all three SST types are co-located using data during the whole of 2003. These three observation types are complementary, with each having its own strengths and weaknesses.

In situ SST measurements are affected by the varying depth of measurement according to buoy type. Also, the lack of maintenance of in situ instruments, mainly affecting drifting buoys, contributes to variations in the accuracy of in situ SST observations. Errors related to satellite-derived SST observations include cloud contamination and inadequacies of the retrieval process. Microwave SST retrievals can be obtained in areas that are cloudy, though not those that are precipitating, which provides a better coverage than the infra-red sensors.

An additional issue, applicable to all three observation types is to consider the depth at which the observation is actually representative. For in situ observations we generally assume the depth to be around 1 metre, although this will vary. Infra-red satellite observations retrieve the radiative skin SST which is only 1 micron thick, whilst microwave satellite observations retrieve an SST a couple of millimeters below the skin layer of the ocean. In the analyses we consider these differences and correct for them where possible.

The three SST observation types are co-located, and statistics of the differences between pairs of observation types at a time are computed. The standard deviations are used within a statistical method to calculate the error of each observation type, assuming un-correlated errors. A number of experiments are performed, using slightly different co-location criteria to assess whether the results are robust and therefore whether the various assumptions made are justified.

2. DESCRIPTION OF SEA SURFACE TEMPERATURE DATASETS

2.1 Advanced Along-Track Scanning Radiometer

The Advanced Along Track Scanning Radiometer (AATSR) was launched upon the sun-synchronous ENVISAT in March 2002. AATSR has 3 infra-red channels centred in the atmospheric windows at 3.7µm, 10.8µm and 12µm plus channels in the visible/near infrared part of the spectrum used for cloud detection. The instrument has an inclined conical scan which enables it to make observations of the surface from two different angles, nadir and forward views (~55º), within a few minutes of each other, allowing for effective correction of atmospheric absorption and aerosol. The instrument is designed to produce *dual-view* SST retrievals to better than 0.3K accuracy in the

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derived SST and to give a long-term stability of better than 0.1K/decade. The AATSR instrument continues the data collection of high-quality dual-view SSTs begun by ATSR-1 and ATSR-2 upon the European Remote Sensing satellites: ERS-1 and ERS-2 launched in 1991 and 1995 respectively.

The measurements are most closely related to the radiative skin temperature (skin SST) which is usually cooler than the sub-skin by more than 0.1K. Two types of dual-view skin SST retrieval are possible: those using all 3 infra-red channels (hereafter D3) during the night-only due to the solar contribution to the 3.7µm channel during the day, and retrievals using just the 10.8µm and 12µm channels (hereafter D2) during both day and night. The AATSR data used for this study are supplied as an averaged clear sky radiance product to a spatial resolution of 1/6 degree, although 1km resolution data are available from AATSR. In this study D3 retrievals have been used which are expected to be the most accurate retrievals due to the availability of the extra shortwave infra-red channel.

The AATSR skin SSTs used in this study have been processed to a pseudo-bulk SST using the Fairall model (Fairall et al, 1996). The bulk SST is the temperature of the ocean at around 1metre in depth and is more representative of the overall heat capacity of the upper layers of the ocean. Further information on applying a skin effect model to (A)ATSR skin SSTs can be found in Horrocks et al. (2003). Figure 1 shows an example of night-time AATSR bulk (D3) SSTs for July 2003.

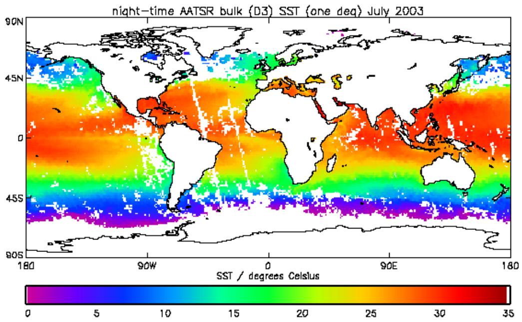

Figure 1. Monthly mean map of night-time AATSR bulk (D3) SSTs for July 2003

2.2 In situ observations

In this study, in situ SST observations have been obtained by extracting global moored and drifting buoy SST measurements obtained via the Global Telecommunications System. The buoy SSTs are co-located to the AATSR 10 arc minute cell within a 3 hour time window to provide an AATSR-buoy matchup dataset. AATSR validation results against in situ SSTs and other SST datasets can be found in O’Carroll et al. (2006).

2.3 Advanced Microwave Scanning Radiometer

The Advance Microwave Sounding Radiometer (AMSR-E) instrument is onboard the sun-synchronous AQUA satellite which was launched in May 2002. The instrument was provided to NASA by the National Space Development Agency of Japan (NASDA). Global, daily, version 4 AMSR-E products of SST, wind speed, atmospheric water vapour, cloud water and rain rate were obtained at 0.25° spatial resolution. Note that since the release of AMSR-E version 5 products, some of the results presented in this paper have been re-checked using the new version and found to be very similar. The ability of AMSR-E to view the surface through non-precipitating clouds is a major advantage over traditional cloud-free infra-red measurements of SST. Details of the AMSR SST algorithm are given in Wentz & Meissner (2000). The global SSTs have been retrieved as daily averaged files from the Remote Sensing Systems (RSS) Website http://www.ssmi.com. The microwave-derived SSTs are representative of a depth of a few millimetres. RSS have applied a method to correct for a flaw in the AMSR-E calibration where a problem in the design of the AMSR-E hot reference load within the calibration system causes large thermal gradients to develop with the hot load. More details can be found in documents available from the RSS website. It should be noted that RSS have applied bias corrections to the AMSR-E SSTs (more information available from http://www.ssmi.com), but that the resultant SSTs remain representative of the same depth. Figure 2 shows an example of AMSR-E SSTs for July 2003.

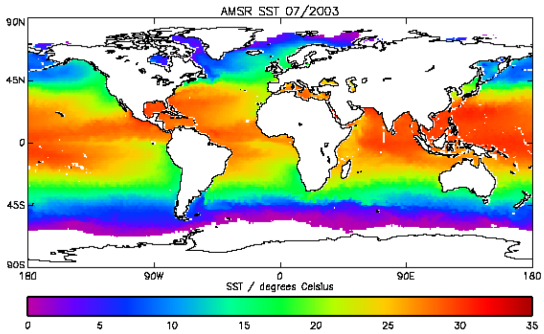

Figure 2. Monthly mean map of AMSR-E SSTs for July 2003 averaged to 1-degree spatial resolution

3. Method of comparison

The AATSR bulk SSTs for 2003 used in this study have been previously validated against buoy SSTs (Watts et al, 2004). A matchup database between AATSR SSTs and buoy SSTs was produced containing co-located observations. The matchup criteria were that the co-located observations occur within 3 hours of each other, and the buoy SSTs were located within the AATSR 10 arc minute grid. Throughout 2003, over 16000 day and night-time matchups between AATSR SSTs and buoy SSTs were obtained. A map of their distribution is shown in figure 3.

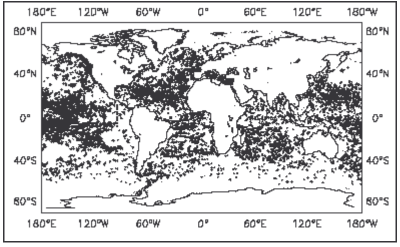

Figure 3. Distribution of AATSR/buoy matchups throughout 2003

These co-located observations were then compared to daily AMSR-E SSTs at 0.25degree spatial resolution. The AATSR SST locations were then matched to the nearest AMSR-E SST cell within which the AATSR/buoy matchup would be located.

Before statistics on the differences were calculated between these three-way daily matchups, various quality control processes were performed on the observations. Only night-time AATSR observations were used to reduce the effect of diurnal warming on the observations. In addition, a thermocline flag contained within the AATSR/buoy matchup database was interrogated to see if a diurnal thermocline, created in scenarios of high insolation and low wind speed, was likely. This thermocline flag was created in the initial processing of the AATSR observations at the Met Office within which a diurnal thermocline model is run based on Kantha and Clayson (1994), although this procedure is only relevant during the day.

The AATSR skin SSTs contained within the matchups are bias-corrected before use. The bias-correction is calculated by observing the difference between night-time AATSR skin SSTs and the buoy SSTs which have been converted to a buoy ‘skin’ SST using the Fairall model (Horrocks et. al., 2003). The time difference between the selected co-located observations is less than 1 hour. The derived bias correction to be applied to the D3 AATSR skin SSTs is -0.21K. The bulk SSTs are then computed from the bias corrected skin SSTs.

A statistical analysis is performed on these quality controlled AATSR/buoy/AMSR matchups. The differences between the co-located AATSR and buoy SSTs are computed and the mean difference and standard deviation of all the differences assessed using a 3-sigma standard deviation test to remove outliers. The same method is applied to derive the mean difference and standard deviation between the buoy and AMSR-E SSTs, and also the AATSR and AMSR-E SSTs.

Six different experiments were performed with slightly different areas, AATSR/buoy matchup criteria, and use of buoy types, as defined in table 1. When dividing the matchups spatially, 2 different global regions have been used: region 1 (0º to 90ºN latitude, 0º to 180ºW longitude), and region 2 (-90ºS to 0º latitude, 0º to 180ºE longitude). By selecting these different experiment types we can observe whether the error analysis is consistent through these different regions and matchup criteria. In addition, the method of co-location was slightly altered, recorded as experiments 7 and 8, in which the rest of the criteria remained the same as experiment 1. For these additional two experiments, 4 AMSR-E SSTs were used for each point of each co-located grid box and interpolated to either the AATSR location (experiment 7) or the buoy location (experiment 8).

Expt.	Details of matchup scheme
1	Global, 3 hour AATSR/buoy matchup cutoff, moored and drifting buoys
2	Global, 3 hour matchup cutoff, moored buoys only
3	Global, 3 hour matchup cutoff, drifting buoys only
4	Global, 1 hour AATSR/buoy matchup cutoff, moored and drifting buoys
5	Region 1, 3 hour matchup cutoff, moored and drifting buoys
6	Region 2, 3 hour AATSR/buoy matchup cutoff, moored and drifting buoys
7	As experiment 1, but AMSR-E SSTs interpolated to AATSR location
8	As experiment 1, but AMSR-E SSTs interpolated to buoy location

Table 1. Definitions of subsets of the AATSR/buoy/AMSRE matchups from which statistics are calculated.

4. THEORY OF ERROR ANALYSIS

In Appendix A, we derive a set of simultaneous equations for estimating the error variances, σ_i^2, for observation type i (where i = 1, 2 or 3) for an ensemble of collocations of observation triplets:

$$\begin{aligned}\sigma_1^2 &= \tfrac{1}{2}(V_{12} + V_{31} - V_{23}) + (r_{12}\sigma_1\sigma_2 + r_{31}\sigma_3\sigma_1 - r_{23}\sigma_2\sigma_3),\\ \sigma_2^2 &= \tfrac{1}{2}(V_{23} + V_{12} - V_{31}) + (r_{23}\sigma_2\sigma_3 + r_{12}\sigma_1\sigma_2 - r_{31}\sigma_3\sigma_1),\\ \sigma_3^2 &= \tfrac{1}{2}(V_{31} + V_{23} - V_{12}) + (r_{31}\sigma_3\sigma_1 + r_{23}\sigma_2\sigma_3 - r_{12}\sigma_1\sigma_2),\end{aligned} \quad (1)$$

where V_{ij} is the variance of the difference between observation types i and j, and r_{ij} is the correlation of error between observation types i and j.

If the errors in the 3 observation types are uncorrelated, then $r_{ij} = 0$ for all $i \neq j$, and so (1) becomes:

$$\begin{aligned}\sigma_1 &= \{\tfrac{1}{2}(V_{12} + V_{31} - V_{23})\}^{\frac{1}{2}},\\ \sigma_2 &= \{\tfrac{1}{2}(V_{23} + V_{12} - V_{31})\}^{\frac{1}{2}},\\ \sigma_3 &= \{\tfrac{1}{2}(V_{31} + V_{23} - V_{12})\}^{\frac{1}{2}}.\end{aligned} \quad (2)$$

For (2) to be a reasonable approximation to (1), we require that the covariances of error between the observation types are small relative to the error variances. The validity of this approximation is not obvious, for the reasons discussed in the Appendix. We will proceed in Section 5 by tentatively making this assumption, and we will discuss its implications in Section 6.

5. ERROR ANALYSIS

The statistics of differences between AATSR, buoy and AMSR-E SSTs are presented in table 2 for the experiments 1 to 8 as described in table 1. The results show that the mean AATSR bulk (D3) SSTs minus buoy SSTs are close to zero for all experiments. This is expected for the mean difference as the AATSR SSTs have been bias corrected with respect to buoy SSTs. The standard deviation of their differences is also very low at 0.27-0.30K.

The AMSR-E SSTs are 0.02K cooler than the AATSR bulk (D3) SSTs and the buoy SSTs for experiment 1, and similar results are obtained for the remaining experiments. AMSR-E measures a sub-surface SST so it is expected that AMSR-E SSTs should be cooler than the 'bulk' SST measurements. Both measurement types have been bias-corrected leading to a near zero difference.

		AATSR bulk D3–AMSRE SST (K)		**Buoy – AMSRE SST (K)**		**AATSR D3 bulk–buoy SST (K)**	
	Num	**Mean diff**	**Stan. Dev.**	**Mean diff**	**Stan. Dev.**	**Mean diff**	**Stan. dev.**
1	2970	0.02	0.45	0.02	0.48	0.00	0.28
2	228	0.02	0.53	0.02	0.57	0.00	0.27
3	2844	0.03	0.44	0.02	0.48	0.01	0.28
4	2135	0.02	0.47	0.02	0.50	-0.02	0.27
5	1001	0.03	0.45	0.06	0.51	-0.03	0.30
6	664	0.00	0.42	0.00	0.50	0.00	0.27
7	2706	0.02	0.45	0.02	0.48	0.00	0.27
8	2600	0.03	0.45	0.02	0.48	0.00	0.28

Table 2. Statistics on mean differences between AATSR, buoy and AMSR-E SSTs for 2003.

By inserting the standard deviations presented in Table 2 into equations 2, we can calculate the standard deviation of error on each observation type, for each different experiment. These errors are presented in table 3. For experiment 1, the errors on the AATSR bulk (D3) SSTs are at ~0.16K, increasing to ~0.23K for the buoy SSTs and again to ~0.42K for the AMSR-E SSTs. All the experiments have errors broadly consistent with each other, suggesting that the assumption that all errors are uncorrelated is quite good. The smallest error on the AATSR SSTs is estimated for experiment 2 at 0.12K and increases to its maximum of 0.16K for experiments 1, 6 and 8.

	Derived standard deviation of error for each observation type (K)		
Experiment	**AATSR bulk(D3) SST**	**Buoy SST**	**AMSR-E SST**
1	0.16	0.23	0.42
2	0.12	0.24	0.51
3	0.14	0.24	0.42
4	0.15	0.23	0.45
5	0.13	0.27	0.43
6	0.16	0.22	0.45
7	0.15	0.22	0.42
8	0.16	0.23	0.42

Table 3. Derived standard deviation of error on each observation type for 2003 according to experiment type.

We have neglected terms involving the correlation of errors between different observations in equation 2 (discussed further in Appendix A). We need to assess whether this has an impact on the sizes of derived errors. For example, if we define the truth on the scale of the buoy observations, then there is no representativity error for buoys and so $r_{12} = r_{23} = 0$ where the subscripts refer to 1=AATSR, 2=buoys and 3=AMSR-E. Examining equation 1 with such knowledge, we can argue that r_{31} must be positive, and so the σ_1^2 will be under-estimated, but σ_3^2 will be under-estimated by the same amount.

This analysis shows that we need to be confident that the assumption whereby the potential covariances of error between the observations is neglected in order for the results to stand. In order to test this assumption we can analyse the error of representativeness by changing the method of co-location between the observation pairings. This has been done by two similar methods. For the main experiments (1 to 6) the AMSR-E observations are co-located to the nearest 1/6 degree grid box of the AATSR/buoy matchup. However, for experiments 7 and 8, 4 AMSR-E observations are taken surrounding the AATSR/matchups cell and interpolated firstly to the AATSR observation location (experiment 7), and secondly to the buoy observation location (experiment 8). Compiling the same difference statistics as for the other experiments, gives an error of 0.15K on the AATSR observations for experiment 7 and 0.16K for experiment 8, which are close to the error on AATSR of 0.16K of experiment 1. Additionally the derived errors of buoy SSTs and AMSR-E SSTs for experiment 7 and 8 support those derived from experiment 1. These results indicate that the error of representivity is small, and so it is a reasonable assumption to ignore the covariances of errors between the observations when deriving equation 2.

6. CONCLUSIONS

Overall the standard deviation of error on night-time AATSR bulk (D3) SST observations for 2003 was evaluated at 0.16K, whilst the error on the co-located buoy SSTs was 0.23K and for AMSR-E SSTs 0.42K. Varying the co-location criteria whilst analysing the observation errors produce similar values of error throughout for each observation type, giving confidence in the results and that the assumption that the errors are not correlated is valid. As the characteristics of the ATSR-1/ATSR-2 and AATSR series of instruments are similar, there is good reason to assume that the complete (A)ATSR time series has a similar accuracy with the exception of the ATSR-1 data after the loss of the 3.7µm channel.

On a global scale the differences between night-time AATSR bulk (D3) SST observations and night-time AMSR-E SSTs varies mainly between ±0.5K. However at around 45ºN the AATSR SSTs are cooler than AMSR-E SSTs by up to 2K, whilst at around 45ºS the AATSR SSTs are warmer than AMSR-E SSTs by up to 2K. These patterns are currently unexplained.

The error analysis shows how the AATSR SST retrievals are of the highest accuracy, followed by the in situ SST observations and then the AMSR-E SST observations. However, the AMSR-E SST observations do have the advantage of being able to view through cloud giving better coverage. As most centres are aiming towards compiling SST analyses using both infra-red and microwave SST sources as well as in situ data it is essential to gain knowledge of the error characteristics of each measurement type.

Acknowledgements

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APPENDIX A. ERROR ANALYSIS FOR THREE-WAY COLLOCATION STATISTICS

A.1 Basic theory

In this section, we develop the theory relevant to the analysis of statistics of differences between collocated observations of three different types.

The error in observation x_i, of type i, can be expressed as

$$x_i = x_T + b_i + \varepsilon_i, \qquad \text{(A.1)}$$

where x_T, is the true value of variable x,
b_i is the bias (mean error) in the observation,
and ε_i, is the random error in the observation (which, by definition, has zero mean but may be non-Gaussian).

We shall return below to the non-trivial question of what we mean by the "true value of the variable". For the present we will only assume that we have a consistent definition of the true value for comparison with each observation.

For a set of 3 collocated observations, of types i=1, 2 and 3, we can write a corresponding set of equations for their errors:

$$\begin{aligned} x_1 &= x_T + b_1 + \varepsilon_1, \\ x_2 &= x_T + b_2 + \varepsilon_2, \\ x_3 &= x_T + b_3 + \varepsilon_3. \end{aligned} \qquad \text{(A.2)}$$

Now consider each set of 3 of observations as 3 sets of pairs. The difference between observations i and j is given by:

$x_i - x_j = b_i - b_j + \varepsilon_i - \varepsilon_j$. (A.3)

For an ensemble of such sets of observations, the mean difference between observations of type i and j is:

$b_{ij} = \bar{x}_i - \bar{x}_j = b_i - b_j$ (A.4)

and the variance of the difference between these two observation types is:

$V_{ij} = \{(\bar{x}_i - \bar{x}_j) - (\bar{b}_i - \bar{b}_j)\}^2 = \{\bar{\varepsilon}_i - \bar{\varepsilon}_j\}^2 = \bar{\varepsilon}_i^2 + \bar{\varepsilon}_j^2 - 2\,\overline{\varepsilon_i \varepsilon_j}$ (A.5)

Therefore

$V_{ij} = \sigma_i^2 + \sigma_j^2 - 2\, r_{ij}\, \sigma_i\, \sigma_j$, (A.6)

where σ_i^2 is the variance of the error in observation type i, and r_{ij} is the correlation of error between types i and j.

Stating (A.6) explicitly for the 3 sets of observation pairs:

$V_{12} = \sigma_1^2 + \sigma_2^2 - 2\, r_{12}\sigma_1\sigma_2$,
$V_{23} = \sigma_2^2 + \sigma_3^2 - 2\, r_{23}\sigma_2\sigma_3$,
$V_{31} = \sigma_3^2 + \sigma_1^2 - 2\, r_{31}\sigma_3\sigma_1$. (A.7)

The 3 simultaneous equations (A.7) can be solved to give the variance of error in each observation type:

$\sigma_1^2 = ½\,(V_{12} + V_{31} - V_{23}) + (r_{12}\sigma_1\sigma_2 + r_{31}\sigma_3\sigma_1 - r_{23}\sigma_2\sigma_3)$,
$\sigma_2^2 = ½\,(V_{23} + V_{12} - V_{31}) + (r_{23}\sigma_2\sigma_3 + r_{12}\sigma_1\sigma_2 - r_{31}\sigma_3\sigma_1)$,
$\sigma_3^2 = ½\,(V_{31} + V_{23} - V_{12}) + (r_{31}\sigma_3\sigma_1 + r_{23}\sigma_2\sigma_3 - r_{12}\sigma_1\sigma_2)$.
(A.8)

If the errors in the 3 observation types are uncorrelated, then $r_{ij} = 0$ for all $i \neq j$, and so (A.8) becomes:

$\sigma_1^2 = ½\,(V_{12} + V_{31} - V_{23})$,
$\sigma_2^2 = ½\,(V_{23} + V_{12} - V_{31})$,
$\sigma_3^2 = ½\,(V_{31} + V_{23} - V_{12})$. (A.9)

This allows us to estimate the error variance in the 3 different observations types from the observation difference statistics. However, the validity and accuracy of this method depends crucially on the assumption of the independence of errors, which is examined further in the following section.

A.2 Some comments on the concept of the "true value" of a variable and on the correlation of observation error

Equation (A.9) is potentially very powerful, because it offers a method of separating out the (usually elusive) error variances of different observations types given statistics of the observation differences, which are easily obtained from samples of real data. However, the equation is also problematic, because it suggests that this separation can be done without defining carefully what we mean by the error in each observation, i.e. what we mean by the "true value" of the variable. If, as in this paper, we are concerned with observations of a geophysical variable made by three different measurement techniques, then we might expect that our estimate of the error variance for observations made using any of these techniques should be dependent on how we define the true value, e.g. whether it is a point value or an areal average. Yet equation (A.9) suggests that we do not have to define it.

The resolution of this paradox lies in the step from (A.8) to (A.9), where we neglect the potential covariances of error between the observations. For the measurement errors themselves, it is usually reasonable to assume that the errors in measurements made by totally independent techniques will be truly independent. However this is not the only source of error. We must also consider the "error of representativeness", which captures the difference between the value of the variable on the space/time scale on which it is actually measured and its value on the space/time scale on which we wish to analyse it. For a single observation, the latter scale can be chosen arbitrarily, but whenever we wish to compare two observations then it must be taken into account.

As we change our definition of the true value of the variable, so we change the value of the error variance of the observation. However, we also change the values of the error covariances between observations, and in such a way that equation (A.8) continues to hold whatever our definition of the true value might be.

Thus equation (A.8) will always be valid, but equation (A.9) will only be a reasonable approximation to it in certain circumstances; our ability to step between (A.8) and (A.9) assumes that we are using a space/time scale for the "true value" which, although we may avoid defining it precisely, is such that the covariances of the errors of representativeness on this scale are negligible when compared with the error variances. In this paper, we proceed tentatively on the assumption that these covariances are negligible, but also make analyses to determine if this assumption is valid.