HadSST.4.0.0.0 Product User Guide

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October 29, 2019

Citation: Kennedy, J.J., Rayner, N.A., Atkinson, C.P., and Killick, R.E. (2019). An ensemble data set of sea surface temperature change from 1850: the Met Office Hadley Centre HadSST.4.0.0.0 data set. Journal of Geophysical Research: Atmospheres, 124. https://doi.org/10.1029/2018JD029867

EMERGENCY ONE PAGE QUICK START GUIDE FOR HadSST.4.0.0.0

HadSST.4.0.0.0 is the Met Office Hadley Centre Sea-surface temperature anomaly data set. Anomalies are expressed relative to the 1961-1990 average. The data have been adjusted to minimize the effect of systematic errors associated with instrumentation changes and are representative of SST measured at a depth of 20cm. The data set is presented on an equi-rectangular 5° latitude by 5° longitude monthly grid from January 1850 to December 2018.

Uncertainty in the data is presented using a combined approach. Uncertainty in the bias adjustments is presented as an ensemble of interchangeable realisations. Uncertainty arising from local measurement errors and local sampling errors are presented as gridded fields. Uncertainties associated with correlated measurement errors are presented as error-covariance matrices. These can be combined to give uncertainty estimates for derived quantities such as the global mean temperature.

HadSST.4.0.0.0 is based on ICOADS release 3.0.0 (1850-2014, [2]) and ICOADS release 3.0.1 (2015-present). In addition it uses drifting buoy observations from CMEMS.

What products are available?

The basic time series products are:

- Global average SST anomaly with uncertainties, link
- Regional average SST anomalies with uncertainties, link

The basic gridded products are:

- Grid of median SST anomalies calculated from the ensemble, monthly 1850-present, link
- Grids of bias-adjusted SST anomalies for the 200 ensemble members, monthly 1850-present, link
- Grid of estimated uncertainties arising from all sources, monthly 1850-present, link

There are other products including individual components of uncertainty, error covariances (for propagating uncertainty properly) and counts of numbers of observations.

How do I obtain the data?

Data are available from http://www.metoffice.gov.uk/hadobs/hadsst4/ and specific links are given above.

How do I read the HadSST.4.0.0.0 data?

The time series data are stored in csv (Comma Separated Value) files which can be read by a wide variety of tools including Excel.

The gridded data are stored in NetCDF format files. NetCDF files are a platform-independent, self-describing binary format and there are a number of common tools (Section 3.2) that can be used to access the data. Some basic python code is provided in Section 4 to show worked examples of reading the data and performing some simple calculations and processing.

What tools are available for these products?

Some basic python code is provided in Section 4 to show worked examples of reading the data and performing some simple calculations and processing.

How to cite the data set

Kennedy, J.J., Rayner, N.A., Atkinson, C.P., and Killick, R.E. (2019). An ensemble data set of sea surface temperature change from 1850: the Met Office Hadley Centre HadSST.4.0.0.0 data set. Journal of Geophysical Research: Atmospheres, 124. https://doi.org/10.1029/2018JD029867

Further information and contact

For further help please read the rest of the document. The paper describing the data set is the best place to find the technical details. Updated diagnostics are available from http://www.metoffice.gov.uk/hadobs/hadsst4/. For further enquiries contact john.kennedy@metoffice.gov.uk. Data set updates will be tweeted from @metofficeHadOBS

Contents

1 Getting started with HadSST.4.0.0.0

This section describes some basic information about the HadSST.4.0.0.0 data set. HadSST.4.0.0.0 is a data set of sea-surface temperature anomalies. The data have been adjusted to minimize the effect of instrumentation changes. The data are presented on a regular 5°latitude by 5° longitude grid for each month from January 1850. Uncertainty estimates associated with measurement and sampling limitations are also provided. Uncertainty in the bias adjustments are represented by the use of an ensemble; there are 200 versions of the data set making different assumptions about the biases. The data set is not globally-complete and there is little processing to smooth the fields beyond averaging the data onto a regular grid.

1.1 How do I get the data?

Data are available from http://www.metoffice.gov.uk/hadobs/hadsst4/data where checksums for the files can also be found. There are time series files in csv format and gridded fields of SST anomalies, uncertainty information and numbers of observations in NetCDF format.

1.1.1 Time series data

The time series data are in csv (Comma Separated Value) format. There are monthly and annual series:

- Global annual mean SST anomaly series: HadSST.4.0.0.0_annual_GLOBE.csv
- Global monthly mean SST anomaly series: HadSST.4.0.0.0_monthly_GLOBE.csv
- Northern hemisphere annual mean SST anomaly series: HadSST.4.0.0.0_annual_NHEM.csv
- Northern hemisphere monthly mean SST anomaly series: HadSST.4.0.0.0_monthly_NHEM.csv
- Northern hemisphere annual mean SST anomaly series: HadSST.4.0.0.0_annual_SHEM.csv
- Northern hemisphere monthly mean SST anomaly series: HadSST.4.0.0.0_monthly_SHEM.csv

1.1.2 Gridded data

The gridded data are in NetCDF format. There are a number of different files. The most commonly used files are:

- Grid of median SST anomalies calculated from the ensemble, monthly 1850-present, link
- Grids of bias-adjusted SST anomalies for the 200 ensemble members, monthly 1850-present, link
- Grid of estimated uncertainties arising from all sources, monthly 1850-present, link

Additional information is provided in the following files:

- Grid of measurement and sampling uncertainty, monthly 1850-present, link
- Grid of uncorrelated measurement uncertainty, monthly 1850-present,link
- Grid of correlated measurement uncertainty, monthly 1850-present,link
- Grid of sampling uncertainty, monthly 1850-present,link
- Grid of number of observations, monthly 1850-present,link
- Grid of number of super obserations, monthly 1850-present,link
- Error covariance matrices, monthly 1850-present,link

1.2 How do I use the data?

The data are in NetCDF format, which is a standard data format for climate data. Furthermore, the data files are CF compliant which means that the metadata in the files is in a standardised format. The structure of the data files is described in more detail in Section 3. Some example code for reading and processing the data is found in Section 4. The gridded data are stored in a 3-dimensional array, with dimensions of time x longitude x latitude. There are 72 longitude points and 36 latitude points. The 72 longitude points represent grid cells with centres running from $-177.5°$E to $+177.5°$E. The 36 latitude points represent grid cells with centres running from $-87.5°$N to $+87.5°$N.

1.2.1 Dos and Donts of using the data

Do - be aware that there are gaps in the data and that there can be considerable “noise” in less-well-observed grid cells. Auxiliary products like the uncertainty estimates and the number of observations files can provide useful additional information for identifying grid cells in which the uncertainty is likely to be large.

Do - use the uncertainty information (see next section). It will help you to understand the relative reliability of the data as this changes markedly over time and in different places.

Don’t - compare HadSST.4.0.0.0 to globally complete SST analyses without taking into account the gaps in the data. Data coverage can affect the comparability of two data sets.

Do - send us feedback when you use the data to john.kennedy@metoffice.gov.uk.

1.3 How do I use the uncertainty estimates?

The uncertainty analysis is one of the more complex parts of using HadSST.4.0.0.0. The following information provides a basic guide to using the uncertainty information provided with the data set. Every effort has been made to make this process as painless as possible, but it can still be somewhat painful. It is worth it though.

The uncertainty has been broken down into three separate components, which have different degrees of correlation. The separate components need to be propagated individually through any calculation and combined at the end to get an estimate of the overall uncertainty. The three components are:

1. Uncorrelated measurement and sampling error component, provided as gridded fields on the same 5x5x1-month grid as the SST anomalies. They represent uncertainties arising from uncorrelated measurement errors and local under sampling. In most cases the uncertainty for this kind of error can be propagated analytically.
2. Simply-correlated measurement error component, provided as an error-covariance matrix. The error-covariance matrices represent errors such as individual ship biases that can be represented by an error-covariance matrix. In many cases the uncertainty for this kind of error can be propagated analytically.
3. The spread of the 200 members of the ensemble represents the uncertainty in the bias adjustments. The ensemble represents errors with complex correlation structures. In most cases, the uncertainty associated with this kind of error cannot be propagated analytically, which is why we use an ensemble.

Each of these components should be propagated separately through any calculation and then combined at the end

1.3.1 Propagating uncertainty associated with uncorrelated errors

Propagation of uncertainties associated with uncorrelated errors are relatively easy to deal with using the standard propagation of errors formula. If the SST anomalies are being processed through a function $f(x_1, x_{2,}..., x_n)$where $x_1, x_2...x_n$are the gridded SST anomalies with uncertainties $\sigma_1, \sigma_2...\sigma_n$then the uncertainty in f, $\sigma_f$is given by

$$\sigma_f^2 = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i}\right)^2 \sigma_i^2 \tag{1}$$

So, for a weighted average, such as the global average where the area of each grid cell is $w_i$then

$$f = \sum_{i=1}^{n} w_i x_i \tag{2}$$

and the uncertainty in the global average arising from uncorrelated errors is given by:

$$\sigma_f^2 = \sum_{i=1}^{n} w_i^2 \sigma_i^2 \tag{3}$$

If there are multiple steps in the processing then the uncertainty can often be propagated through each step separately. For example, if we want to calculate an annual global average we can take the uncertainties in the twelve monthly global averages, call them σ_{month}, and combine them like so:

$$\sigma_{annual}^2 = \sum_{month=Jan}^{Dec} \left(\frac{1}{12}\right)^2 \sigma_{month}^2 \tag{4}$$

Care must be taken though because if data values are used more than once in the calculation, then errors in different parts of the calculation will become correlated and these simple formulae won't work.

1.3.2 Propagating uncertainty associated with simply-correlated errors

The propagation of uncertainty associated with simply-correlated errors is slightly more complex than for uncorrelated errors. For an error-covariance matrix E the uncertainty in f would be

$$\sigma_f^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \left(\frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} E_{ij} \right) \tag{5}$$

so for our example above of the global average, the uncertainty in f would become

$$\sigma_f^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j E_{ij} \tag{6}$$

A more compact way of writing this (and calculating it) is to use vector and matrix notation. If we have a vector of weights w then the uncertainty in f becomes simply:

$$\sigma_f^2 = \mathbf{w} E \mathbf{w}^{\mathbf{T}} \tag{7}$$

Unlike the case of uncorrelated errors, it is usually not so simple to propagate simply-correlated errors through multiple processing steps. There are, however, a number of approaches.

First, one can combine the separate calculation steps. For example, if you want to calculate the uncertainty in the difference between the northern hemisphere average and the southern hemisphere average then one can combine the two calculations into one where

$$f = \sum_{i=1}^{n} w_i x_i - \sum_{i=1}^{n} v_i x_i = \sum_{i=1}^{n} (w_i - v_i) x_i \tag{8}$$

where $w_i$is the weight a grid box gets in the northern hemisphere average (and zero for any grid box in the southern hemisphere) and v_i is the weight given to grid box i in the southern hemisphere average (again, zero for any grid box in the northern hemisphere). The uncertainty in f is then

$$\sigma_f^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} (w_i - v_i)(w_j - v_j) E_{ij} \tag{9}$$

or, using vector and matrix notation,

$$\sigma_f^2 = (\mathbf{w} - \mathbf{v}) E (\mathbf{w} - \mathbf{v})^T \tag{10}$$

An alternative approach is to draw samples from a multi-variate Gaussian distribution with mean zero and covariance set equal to the error-covariance matrix. These samples can then be added to the SST anomalies to generate an ensemble and the techniques used in the next section to deal with ensembles can be employed to propagate the uncertainty. Sampling from a multi-variate Gaussian distribution is relatively easy to do in two steps:

1. Calculate the Cholesky decomposition A of HEH^T, where E is the error covariance matrix and H is a matrix, consisting of 1s and 0s that selects out the n non-missing data points.

2. Draw n independent standard normal values and put them into a vector z
3. Calculate $x = Az$. The vector x will now contain a sample of n correlated errors which can be added to the n SST anomalies.
4. Repeat steps 2 and 3 to build up an ensemble.

This method can be combined with samples drawn from the uncorrelated error component and the ensemble to propagate all error types simultaneously.

Temporal averaging is tricky because, as yet, there are no error covariances which describe the temporal relationship of simply-correlated errors.

1.3.3 Propagating uncertainty using the ensemble

In many ways this is the simplest of the three types of error to deal with. If we have n ensemble members then we can calculate the uncertainty on f by calculating f for each ensemble member. The uncertainty on f is then, simply, the standard deviation of the n values of f. It is as simple as that. One can also calculate other uncertainty measures such as quantiles, by calculating quantiles of the n values of f.

Although the method for propagating uncertainty using the ensemble is simple, its usefulness is limited by the size of the ensemble and the distribution of the ensemble members. Although 200 ensemble members is a reasonable number for calculating a standard deviation, it might not be enough for calculating extreme quantiles - such as the 99th percentile - or calculations that rely on events in the tails of the distribution. In all cases, it is sensible to look at the output distribution before performing calculations on it.

1.3.4 Combing the propagated uncertainty components

The three uncertainty components are independent of one another, so the three uncertainty components can be combined by squaring the three individual values, adding them together and then taking the square root.

$$\sigma_{total} = \sqrt{\sigma^2_{uncorrelated} + \sigma^2_{simply-correlated} + \sigma^2_{ensemble}} \tag{11}$$

1.3.5 Caveats

The uncertainty analysis for HadSST.4.0.0.0 has some know deficiencies.

1. The error-covariance matrices can only be calculated where we have callsigns for ships. At some times (for example, the 1860s) there is very little call sign information and so the simply-correlated error component will generally be under-estimated.
2. Currently, there is no mechanism for the correct combination of simply-correlated errors from month to month. To do this analytically would require very large covariance matrices. There are various approximations that can be made. For example, assuming that errors are correlated within one year, but uncorrelated between years.
3. The ensemble likely underestimates the uncertainty arising from residual bias adjustments. In particular it does not represent structural uncertainty arising from fundamental choices made in the dataset construction process. We recommend that any analysis be repeated using a different SST data set.
4. As with any analysis there are likely unknown unknowns. If you have feedback on the uncertainty information or how it is provided, please let us know (john.kennedy@metoffice.gov.uk).

1.4 Basic data statistics

Some simple diagnostics are shown in Figure 1. The number of SST observations has increased from around 2 to 12 thousand per month in the period 1850-1880 to between 0.5 and 1.8 *million* per month in the period 2000-present. The number of super-observations (which counts the number of 1 degree 5 day grid cells containing data) has also increased over the same period. However, in contrast to straight counts of observations, the number of super observations peaked between 1965 and 1990 when the VOS fleet was at its peak. There are drops in the numbers of observations and super observations during both

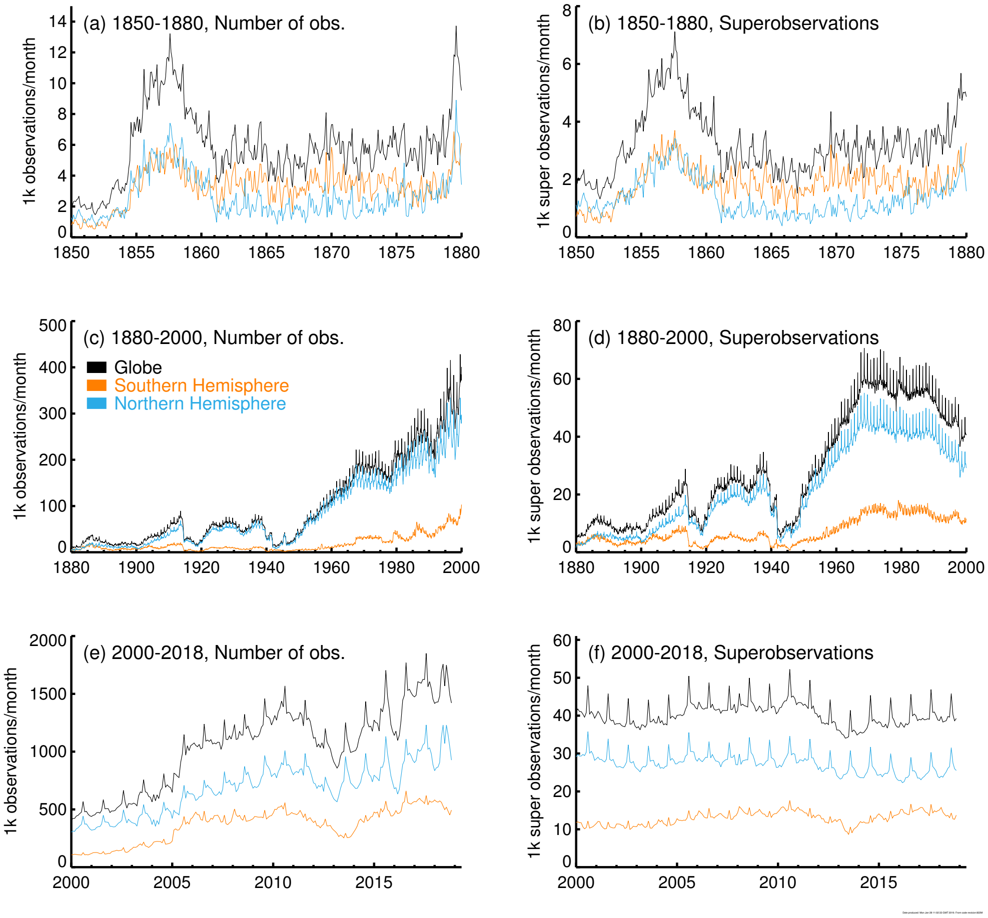

Figure 1: Number of SST observations (left column) and super-observations (right column) for three different periods: (a) and (b) 1850-1880; (c) and (d) 1880-2000; and (e) and (f) 2000-2018. A “super-observation” is a populated 1° 5-day grid cell. Moored buoys make large numbers of observations, but contribute relatively few super observations as they make all their measurements in the same 1° grid cell.

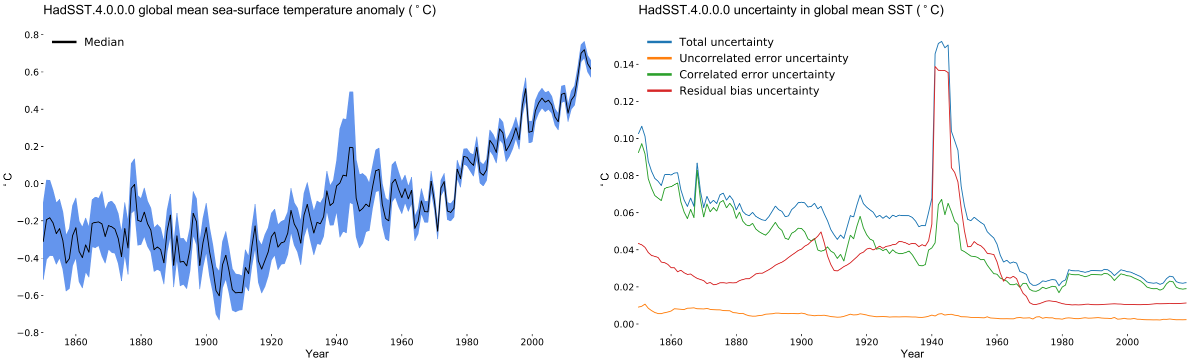

Figure 2: (left) Global mean sea-surface temperature anomaly (relative to the 1961-1990) median (black) and uncertainty range (blue shading). (right) Estiamted uncertainty in the global mean and breakdown of the uncertainty components.

World Wars. There is a seasonal cycle in the number of observations, with more during northern hemisphere summer months. In particular, August has large numbers of observations. This is partly due to the extra pentad in August.

Figure 2 shows the global mean SST and its uncertainty along with a breakdown of the uncertainty into individual components. The overall change in global mean SST is a long-term increase. There were two periods of more rapid warming - 1900-1940 and 1975-present - separated by a period with little change in temperature 1945-1975. Uncertainties typically get larger the further back in time one goes. The major exception to this general rule is the period of the Second World War where uncertainties are estimated to be much higher because of reduced shipping and undocumented changes in the way measurements were made.

1.5 Contact us

If you have further questions about the HadSST.4.0.0.0 data set, please contact us at john.kennedy@metoffice.gov.uk.

1.6 FAQ

1.6.1 Is HadSST.4.0.0.0 the data set for me?

There are a number of different SST data sets available covering different periods and intended for a variety of purposes. Table 1 lists strengths and weaknesses of the HadSST.4.0.0.0 data set.

Dataset	Gridded?	Resolution	Infilled?	Uncertainty?	Updates?	Smoothed?	Ensemble?	Start	Adjusted?
HadSST.4.0.0.0	Y	5°monthly		Y	Y		Y	1850	Y
HadISST1	Y	1°monthly	Y		Y	Y		1870	Y
ERSSTv5	Y	2°monthly	Y	Y	Y	Y	Y	1854	Y
COBE SST 2	Y	1°daily	Y			Y		1850	Y
ICOADS	Y	2°monthly			Y				

Table 1: Dataset characteristic comparison table

1.6.2 What anomaly period have you used?

Anomalies are calculated as temperature differences from the 1961-1990 period. Note that in the calculation of the anomalies, an estimate of the climatological bias is also calculated and removed (see the paper for details). Combining the anomalies with an SST climatology will typically lead to biased SSTs unless the climatology has been specifically bias adjusted.

	HadSST.4.0.0.0	HadSST.3.1.1.0	HadSST2	HadISST1.1
Resolution	Monthly, 5°	Monthly, 5°	Monthly, 5°	Monthly, 1°
Time span	1850-present	1850-2018	1850-2014	1870-present
Base data set	ICOADS.3.0.0	ICOADS.2.5.1	ICOADS.2.1	Met Office Marine Data Bank
Satellite data used	Partly: satellite data are used to estimate covariance structures	No	No	Yes
Data completeness	Gaps where there are no data	Gaps where there are no data	Gaps where there are no data	Globally complete
Data processing	Simple gridding	Simple gridding	Simple gridding	EOF-based reconstruction
Bias adjustments	Yes, 1850-present, space- and time-varying ERI adjustment, buoy-ship adjustment	Yes, 1850-present, fixed ERI adjustment	Yes, 1850-1941, bucket corrections only	Yes, 1870-1941, bucket corrections only
Uncertainty	ensemble + error covariance + fields	ensemble +fields	fields	none
Citation	[10]	[8, 9]	[16]	[17]
Known issues	None	Recent trends are underestimated because of constant ERI bias	No bias adjustments after 1941	No bias adjustments after 1941, suspected cold bias from late 1990s onwards

Table 2: Comparison with earlier versions of HadSST and HadISST.

1.6.3 Where do the observations come from?

Individual SST reports are sourced from the International Comprehensive Ocean-Atmosphere Data Set (ICOADS) release 3.0.0 (1850-2014) and 3.0.1 (2015-present). In addition, drifting buoy data were obtained from the Copernicus project. From January 2016 onwards, the Copernicus drifting buoys were used in place of the drifting buoys in ICOADS.3.0.1. ICOADS comprises a diverse range of data sources, provided in a consistent format with extensive (though incomplete) metadata.

International Comprehensive Ocean-Atmosphere Data Set (ICOADS) Release 3, Individual Observations. Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory.

Drifting buoy data were collected and made freely available by the Copernicus project and the programs that contribute to it. Data downloaded from here.

In addition subsurface profile data from HadIOD.1.2.0.0 were used as reference data set for the calculation of the bias adjustments.

1.6.4 How does HadSST.4.0.0.0 differ from HadSST.3.0.0.0 and HadISST?

Key differences between different generations of HadSST and HadISST are summarized in Table 2. Note that HadSST.4.0.0.0 is the recommended member of the HadSST family for current use.

1.6.5 Why are there 200 different data sets?

The 200 data sets are known as ’the ensemble’. The differences between the members of ’the ensemble’ represent uncertainties in the bias adjustment scheme. The errors associated with residual biases have complex long-term correlations and an ensemble is the only practical way to express them. Briefly, uncertain parameters in the bias adjustment algorithm are varied within their plausible ranges to generate a range of different bias adjustments. Some of the uncertain parameters are things like what fraction of measurements with no metadata are assigned to particular measurement types. More details are given in the paper.

1.6.6 How to cite the data?

Kennedy, J.J., Rayner, N.A., Atkinson, C.P., and Killick, R.E. (2019). An ensemble data set of sea surface temperature change from 1850: the Met Office Hadley Centre HadSST.4.0.0.0 data set. Journal of Geophysical Research: Atmospheres, 124. https://doi.org/10.1029/2018JD029867

1.6.7 There are gaps in the data, what can I do?

It is possible to process data with gaps in, but the gaps must be considered during the processing. For example, when comparing datasets, it can be helpful to reduce the data sets to their common coverage so that a direct comparison can be made.

There are alternative products that you can use, in which the gaps have been filled by various methods. Long-term analyses include HadISST1 ([17]), ERSSTv5 ([6]) and COBE-SST-2 ([4]). There are a large number of analyses that cover the satellite era including the SST CCI analysis product. One thing to note about infilled products is that there are still areas where the data are more uncertain either due to lack of observations or because of limitations of the infilling techniques. Some recent papers comparing different data sets and their uncertainties are [12, 11].

2 Using the time series files

2.1 File names

The filenames for the time series files follow a simple pattern: HadSST.4.0.0.0_annual_RRRR.csv where RRRR is the region identifier. The regions are described in the following table.

Region (RRRR)	Nice name	lat-lon extents W,S,E,N
GLOBE	Globe	-180, -90, 180, 90
SHEM	Southern Hemisphere	-180, -90, 180, 0
NHEM	Northern Hemisphere	-180, 0, 180, 90
TROP	Tropics	-180, -20, 180, 20

2.2 Tools that can be used

CSV files are simple text files and can be opened and read by any software that can process simple text files. They can be read and processed by a large number of different tools including Excel and Libre Open Office. In Python there are dedicated standard csv file readers as well as a number of packages that can read and process CSV.

2.3 Contents of the time series files

The files are csv (Comma Separated Value) files and the columns are described in the following Table.

Column Name	Description; variable type	Units
year	Year; integer	
month	Month; integer	
anomaly	SST anomaly relative to 1961-1990; floating point	K
total_uncertainty	Uncertainty combining all sources of uncertainty: uncorrelated measurement error, sampling error, correlated measurement error and residual bias uncertainty; floating point	K
uncorrelated_uncertainty	1σ Uncertainty from uncorrelated measurement errors and sampling errors; floating point	K
correlated_uncertainty	1σ Uncertainty arising from correlated measurement errors; floating point	K
bias_uncertainty	1σ residual bias uncertainty; floating point	K
coverage_uncertainty	1σuncertainty arising from errors due to large-scale coverage limitations; floating point	K
lower_bound_95pct_bias_uncertainty_range	2.5%limit of the ensemble spread; floating point	K
upper_bound_95pct_bias_uncertainty_range	97.5% limit of the ensemble spread; floating point	K

3 Using the gridded data files

3.1 File names

Filenames for the different data types are given in the following table.

Filename	Sec.	Variable	Notes
HadSST.4.0.0.0_median.nc	3.3.1	SST anomaly	Median of the 200 member ensemble
HadSST.4.0.0.0_unadjusted.nc	3.3.2	SST anomaly	Unadjusted, biased SST anomalies
HadSST.4.0.0.0_ensemble_member_EEEE.nc	3.3.3	SST anomaly	EEEE is the ensemble number in the range [1,200]
HadSST.4.0.0.0_number_of_observations.nc	3.3.4	Ob count	Number of observations contributing to grid cell averages
HadSST.4.0.0.0_number_of_superobservations.nc	3.3.5	Ob count	Number of superobservations contributing to grid cell averages
HadSST.4.0.0.0_total_uncertainty.nc	3.3.6	Uncertainty	Combined uncertainty in the grid cell average SST anomaly including uncertainties associated with residual bias errors, uncorrelated measurement errors, correlated measurement errors and sampling
HadSST.4.0.0.0_measurement_and_sampling_uncertainty.nc	3.3.7	Uncertainty	Combined uncertainty in the grid cell average SST anomaly including uncertainties associated with uncorrelated measurement errors, correlated measurement errors and sampling. This does NOT include uncertainty associated with residual biases.
HadSST.4.0.0.0_uncorrelated_measurement_uncertainty.nc	3.3.8	Uncertainty	Uncertainty arising from uncorrelated measurement errors
HadSST.4.0.0.0_correlated_measurement_uncertainty.nc	3.3.9	Uncertainty	Uncertainty arising from correlated measurement errors
HadSST.4.0.0.0_sampling_uncertainty.nc	3.3.10	Uncertainty	Uncertainty arising from sampling errors

3.2 Tools that can be used to work with data files

A list of software tools that work with NetCDF files is maintained by UCAR https://www.unidata.ucar.edu/software/netcdf/software.html). Some simple tools for viewing and manipulating NetCDF files in Linux include:

- ncdump: provided with the NetCDF library, produces a text rendering of a NetCDF file (Unidata at UCAR).
- Climate Data Operators (CDO)s: a set of command line utilities for performing operations on NetCDF files including concatenation, editing and mathematics (https://code.mpimet.mpg.de/projects/cdo).
- ncview: a program to produce graphical displays of the contents of NetCDF files. More information can be found here. A more complete list can be found here.

In addition, packages are available in most commonly-used scientific programming languages for reading and working with NetCDF files. For example, in Python there are numerous packages including:

- netCDF4 - this basic package provides functionality to read NetCDF files and extract metadata.
- Iris - developed by the Met Office, Iris provides functionality to read, write and process files in a variety of formats including NetCDF. Some example snippets of code using Iris to process HadSST.4.0.0.0 are provided in Section 4.

There are a number of packages in R that can be used to process NetCDF files:

- ncdf4: https://cran.r-project.org/web/packages/ncdf4/index.html
- raster: https://cran.r-project.org/web/packages/raster/index.html
- rcdo: https://github.com/r4ecology/rcdo
- RNetCDF: https://cran.r-project.org/web/packages/RNetCDF/index.html
- CM SAF R tools: https://www.mdpi.com/2220-9964/8/3/109

3.3 Contents of data files

Each of the regular NetCDF file contains metadata and data. The metadata are compliant with the CF-1.5 convention. The majority of files have the same basic structure with the following coordinates (The exception are the error covariances described in Section 3.3.11).

coordinate	size	Description	Notes
time	unlimited	days since 1850-01-01T00:00:00Z gregorian calendar	Start and end dates for each month are stored in time_bnds
latitude	36	degrees_north	Grid cell boundaries are stored in latitude_bnds
longitude	72	degrees_east	Grid cell boundaries are stored in longitude_bnds

3.3.1 SST anomalies: HadSST.4.0.0.0_median.nc

This file contains the median SST anomalies The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	sea_water_temperature_anomaly	
tos:long_name	Sea water temperature anomaly at a depth of 20cm	
tos:var_name	tos	
tos:units	K	
global:title	Ensemble-median sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.2 SST anomalies: HadSST.4.0.0.0_unadjusted.nc

This file contains the unadjusted SST anomalies The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	sea_water_temperature_anomaly	
tos:long_name	Unadjusted, biased sea water temperature anomaly at a depth of 20cm	
tos:var_name	tos	
tos:units	K	
global:title	Unadjusted, biased sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.3 SST anomalies: HadSST.4.0.0.0_ensemble_member_EEEE.nc

The 200 ensemble members are stored in a zip file. Unzipping the file produces 200 data sets in the same format. The files contain the ensemble of SST anomaly data sets, where EEEE is the ensemble member number running from 1 to 200 The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	sea_water_temperature_anomaly	
tos:long_name	Sea water temperature anomaly at a depth of 20cm	
tos:var_name	tos	
tos:units	K	
global:title	Single ensemble member of sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.4 SST anomalies: HadSST.4.0.0.0_number_of_observations.nc

This file contains the numbers of observations contributing the grid cell average SST anomalies. The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	None	
tos:long_name	Number of observations contributing to sea water temperature anomaly	
tos:var_name	numobs	
tos:units	1	
global:title	Number of observations contributing to sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.5 SST anomalies: HadSST.4.0.0.0_number_of_superobservations.nc

This file contains the numbers of super-observations contributing the grid cell average SST anomalies. The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	None	
tos:long_name	Number of superobservations contributing to sea water temperature anomaly	
tos:var_name	numsuperobs	
tos:units	1	
global:title	Number of superobservations contributing to sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.6 SST anomalies: HadSST.4.0.0.0_total_uncertainty.nc

This file contains the total uncertainties, combining bias, measurement and sampling uncertainty in the SST anomalies. The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	sea_water_temperature_anomaly standard_error	
tos:long_name	one-sigma total uncertainty in sea water temperature anomaly	
tos:var_name	tos_unc	
tos:units	K	
global:title	Total uncertainty in sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.7 SST anomalies: HadSST.4.0.0.0_measurement_and_sampling_uncertainty.nc

This file contains the uncertainties combining measurement and sampling uncertainty in the SST anomalies. It does not include uncertainty arising from residual biases that remain after adjustment. It is intended to be used in conjunction with the ensemble. The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	sea_water_temperature_anomaly standard_error	
tos:long_name	one-sigma uncertainty associated with measurement and sampling errors in sea water temperature anomaly	
tos:var_name	tos_unc	
tos:units	K	
global:title	Measurement and sampling uncertainty in sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.8 SST anomalies: HadSST.4.0.0.0_uncorrelated_measurement_uncertainty.nc

This file contains estimated uncertainties associated with uncorrelated measurement errors in the gridded SST anomalies. The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	sea_water_temperature_anomaly standard_error	
tos:long_name	one-sigma uncertainty associated with uncorrelated measurement errors in sea water temperature anomaly	
tos:var_name	tos_unc	
tos:units	K	
global:title	Uncorrelated measurement error uncertainty in sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.9 SST anomalies: HadSST.4.0.0.0_correlated_measurement_uncertainty.nc

This file contains estimated uncertainties associated with simply-correlated measurement errors in the gridded SST anomalies. Note that the error covariance matrices give a more complete description of this uncertainty component including spatial covariance of the errors. The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	sea_water_temperature_anomaly standard_error	
tos:long_name	one-sigma uncertainty associated with correlated measurement errors in sea water temperature anomaly	
tos:var_name	tos_unc	
tos:units	K	
global:title	Correlated measurement error uncertainty in sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.10 SST anomalies: HadSST.4.0.0.0_sampling_uncertainty.nc

This file contains estimated sampling uncertainties in the gridded SST anomalies. The variable names and attributes are given in the following table

Variable:attribute	Value	Notes
tos:standard_name	sea_water_temperature_anomaly standard_error	
tos:long_name	one-sigma uncertainty associated with sampling errors in sea water temperature anomaly	
tos:var_name	tos_unc	
tos:units	K	
global:title	Uncorrelated sampling error uncertainty in sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

3.3.11 Error covariances: HadSST.4.0.0.0_error_covariance_YYYYMM.nc

These files contain the error covariances describing the spatial covariance of the simply-correlated errors in the grid cell average SST anomalies. There is one error covariance matrix per month with YYYY referring to the year and MM to the month. The coordinates are different from the other files and are given in the following table.

coordinate	Description	Notes
location_index_1	location_index_1	The location index is an index which assigns a unique value to each of the 2592 5° grid cells in the regular grids. The latitudes and longitudes of the indices are given in the variables latitude_vector_1 and longitude_vector_1
location_index_2	location_index_2	The location index is an index which assigns a unique value to each of the 2592 5° grid cells in the regular grids. The latitudes and longitudes of the indices are given in the variables latitude_vector_2 and longitude_vector_2

The location indices can be aligned with latitudes and longitudes within the other files using the Latitude_vector and longitude_vector variables. The key variables and attributes are as follows:

Variable:attribute	Value	Notes
tos_cov:standard_name	sea_water_temperature_anomaly standard_error	
tos_cov:long_name	Error covariance of sea water temperature anomaly at a depth of 20cm	
tos_cov:units	K2 (K^2)	This is Kelvin squared as the error covariances are variances rather than standard deviations
tos_cov:cell_methods		Not specified
global:title	Error covariance of sea-surface temperature anomalies from the HadSST.4.0.0.0 data set	

4 Worked examples

4.1 Calculate global mean SST time series

Read data and calculate a global mean SST anomaly series from 1850 to present using the Iris package in Python.

```
import iris
import numpy as np
import matplotlib.pyplot as plt
import iris.analysis.cartography

anoms = iris.load_cube('HadSST.4.0.0.0_median.nc')
grid_areas = iris.analysis.cartography.area_weights(anoms)
timeseries = anoms.collapsed(['longitude', 'latitude'],
                             iris.analysis.MEAN, weights=grid_areas)

plt.plot(timeseries.data)
plt.show()
```

4.2 Calculate monthly area average and uncertainty

Read anomalies and uncertainties and the ensemble and calculate the global average for January 1850 with an estimate of its uncertainty.

```
import iris
import numpy as np
import matplotlib.pyplot as plt
import iris.analysis.cartography

anoms = iris.load_cube('HadSST.4.0.0.0_median.nc')

uncorrelated_unc = iris.load_cube('HadSST.4.0.0.0_uncorrelated_measurement_uncertainty.nc')
sampling_unc = iris.load_cube('HadSST.4.0.0.0_sampling_uncertainty.nc')

covariance = iris.load_cube('HadSST.4.0.0.0_error_covariance_185001.nc')

#combine the uncorrelated-measurement-error and sampling uncertainties
m_and_s_unc = uncorrelated_unc*uncorrelated_unc + sampling_unc*sampling_unc
m_and_s_unc = iris.analysis.maths.exponentiate(m_and_s_unc, 0.5)

fill_value = 9.96921e+36

#extract latitudes to a 2-d array and convert to relative areas
latitude = anoms.coord('latitude').points
latitude_field = np.zeros((36, 72))
for i in range(0,36): latitude_field[i,:] = latitude[i]
area_field = np.cos(latitude_field * np.pi / 180.)

#form a vector from the anomaly field
anoms_1d = np.reshape(anoms.data[0,:,:],(2592,1))
anoms_1d = anoms_1d.data

#form a vector from the measurement and sampling uncertainty
unc_1d = np.reshape(m_and_s_unc.data[0,:,:],(2592,1))
unc_1d = unc_1d.data

#form a vector from the area field
areas_1d = np.reshape(area_field.data,(2592,1))

#where there are missing data in the anomaly field, set the areas to zero
areas_1d[anoms_1d == fill_value] = 0.0
unc_1d[anoms_1d == fill_value] = 0.0
anoms_1d[anoms_1d == fill_value] = 0.0

#convert the measurement and sampling uncertainty to a diagaonal covariance
#matrix and add to the covariance
covariance2 = np.diag(np.reshape(unc_1d*unc_1d,(2592)))
covariance = covariance + covariance2

#turn the areas into gridcell weights for the area average calculation
areas_1d = areas_1d/sum(areas_1d)

#calculate the area average
area_average = sum(anoms_1d * areas_1d) / sum(areas_1d)
area_average = area_average[0]

#calculate the uncertainty in the area average. Have to do this in two stages
#using numpy matrix multiplication
area_average_uncertainty_pre = np.matmul(covariance.data,areas_1d)
area_average_uncertainty_sq = np.matmul(np.matrix.transpose(areas_1d),
                                        area_average_uncertainty_pre)
area_average_uncertainty = np.sqrt(area_average_uncertainty_sq.data)[0][0]

#read ensemble and extract 1st timestep for each member
ensemble = iris.load('HadSST.4.0.0.0_ensemble_member_*.nc')
for i in range(0,200): ensemble[i] = ensemble[i][0:1]

#calculate the global area average timeseries for each ensemble member
#the time series only has one time step though
ensemble_gmt = np.zeros((200))
for i in range(0,200):
    grid_areas = iris.analysis.cartography.area_weights(ensemble[i])
```

```
    ts = ensemble[i].collapsed(['longitude', 'latitude'],
                              iris.analysis.MEAN, weights=grid_areas)
    ensemble_gmt[i] = ts.data[0]

bias_unc = np.std(ensemble_gmt)

area_average_uncertainty_sq += bias_unc*bias_unc
area_average_uncertainty = np.sqrt(area_average_uncertainty_sq.data)[0][0]

print('Global mean Jan 1850: {:4.2f} +- {:4.2f}'.format(area_average,
                                                        area_average_uncertainty))
```

5 Dataset Characteristics

In this section we show how HadSST.4.0.0.0 compares to a number of other marine temperature and instrumentally homogeneous [3] data sets. The comparisons and discussion are also in the HadSST.4.0.0.0 paper [10].

5.1 Intercomparisons with other SST datasets

A comparison to ERSSTv4 [5], ERSSTv5 [6], COBE-SST-2 [4] and HadSST.3.1.0.0 [8, 9] is shown in Figure 3. Also shown are the unadjusted data. A comparison of trends is shown in Figure 4. The principal effect of adjustments to HadSST.4.0.0.0 and all of the other data sets is to reduce the long-term warming relative to the unadjusted data. The adjusted data sets show good agreement on the overall long-term evolution of global and hemispheric SSTs, but there are minor differences in the rate of warming at different times.

The adjustments applied in each of the three data sets decrease the overall temperature change seen from the nineteenth century (and especially since 1900) relative to the unadjusted data. Of the three data sets, HadSST.4.0.0.0 has a marginally higher trend from 1900 (estimated using ordinary least squares) but the difference between the trends in the three data sets is not larger than the estimated uncertainty (estimated using the ensemble with each ensemble member additionally perturbed by a sample from the measurement and sampling errors). ERSSTv4 and COBE-SST-2 warm at a similar rate to the unadjusted data from the 1940s, 50s and 60s, but HadSST.4.0.0.0 warms somewhat faster than the other data sets due to the adjustments applied to account for the general decline in ERI biases over that period. From start dates in 1970, 1980 and 1990, COBE-SST-2 warms faster than the unadjusted data and, from 1980 and 1990, faster than either HadSST.4.0.0.0 or ERSSTv4 by a significant margin.

From 2000-2012, the rates of warming in all three data sets are very similar and consistent within their uncertainty ranges. All three warm faster than the unadjusted data, which has a trend close to zero. During this period, there are two important factors. First, there is a large increase in the relatively cooler drifting buoy measurements and, second, there is a decrease in the average ship bias. The analysis of HadSST.4.0.0.0 supports ERSSTv4 and ERSSTv5 in this period ([7]) and is consistent with instrumentally homogeneous reference series, supporting the analysis of [3].

5.2 Comparison to other long records

Over longer periods, it is necessary to use other data sets for comparison. We use two data sets here. The first is HadNMAT.2.0.1.0 ([13]) which is a data set of Nighttime Marine Air Temperatures (NMAT). Anomalies in NMAT are thought to closely track anomalies in SST over long periods and large scales (see [5] for an example using climate models). The second is based on oceanographic profiles from HadIOD.1.2.0.0, excluding Argo ([1]) and adjusted using the [14] adjustments for MBTs and XBTs.

In order to make a direct comparison between HadSST.4.0.0.0 and HadIOD.1.2.0.0, anomalies from HadSST.4.0.0.0 were adjusted using the absolute bias rather than the relative bias so that the SSTs could be directly compared. Anomalies were then calculated for both data sets using an unadjusted climatology. However, HadSST.4.0.0.0 is not then directly comparable to HadNMAT.2.0.1.0 as HadNMAT.2.0.1.0 is provided as actuals or relative to its own adjusted 1961-1990 climatology and not relative to a biased SST climatology. This will lead to a constant annual offset between the SST and NMAT series, which is approximately the size of the average climatological bias in the SST. Consequently, we shifted HadNMAT.2.0.1.0 by 0.15°C in Figure 5. The offset was chosen by eye to approximately align the two series; none of the conclusions depend on the choice of offset.

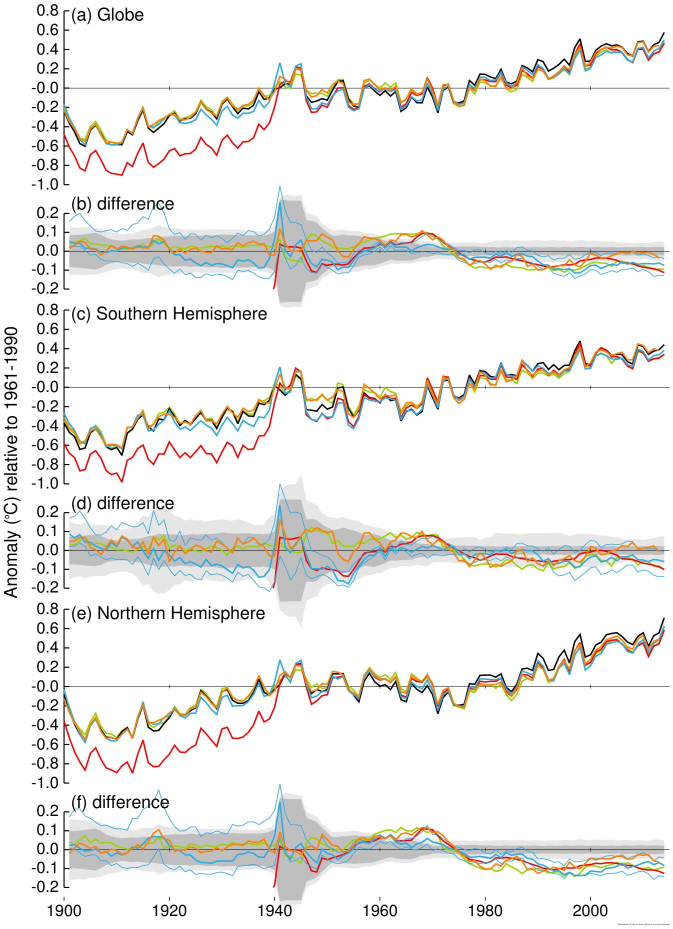

Figure 3: From [10]. (a) (c) and (e) Global and regional average SST anomaly 1850-2012 (°C relative to 1961-1990) series from HadSST.4.0.0.0 (black), ERSSTv5 (blue, thick line is operational version and thin-thick dashed lines are ensemble range from the 1000-member ERSSTv4 ensemble), COBE-SST-2 (orange), HadSST.3.1.1.0 (green) and unadjusted SSTs (red). The green line is HadSST.3.1.1.0. (b) (d) and (f) Differences from the HadSST.4.0.0.0 median. The grey shading indicates the 95% uncertainty range for HadSST.4.0.0.0 including effects from measurement, sampling and bias-adjustment errors. The bias-adjustment uncertainty range is shown in darker grey. Colours for other lines are as in panels (a), (c) and (e).

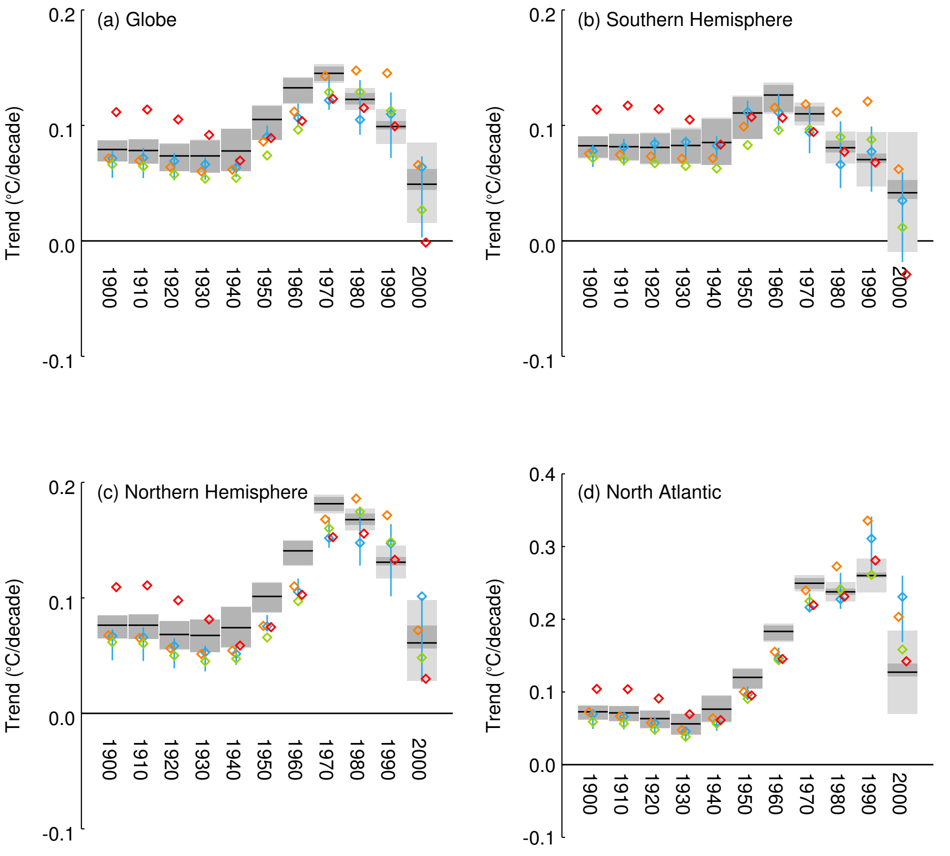

Figure 4: From [10]. Global and regional average SST anomaly trends to 2012. Median trends from HadSST.4.0.0.0 are indicated by a black horizontal line and the grey shading indicates median and 95% uncertainty range including effects from measurement, sampling and bias-adjustment errors. The bias-adjustment uncertainty range is shown in darker grey; ERSSTv5 (blue), the lozenge is the operational version and the vertical line is the 95% ensemble range from the 1000-member ERSSTv4 ensemble); COBE-SST-2 (orange); HadSST.3.1.1.0 (green); and unadjusted SSTs (red).

Except for a period in the late 1940s and early 1950s, differences between HadNMAT.2.0.1.0 and HadSST.4.0.0.0 anomalies (Figure 13b) on a decadal time scale are constant between 1920 and 1990. Outside this period, the differences exceed the estimated uncertainties in the HadSST.4.0.0.0 data set. One notable difference occurs around 1991-1993, when HadNMAT.2.0.1.0 apparently cools relative to HadSST.4.0.0.0 (or HadSST.4.0.0.0 warms). Further investigation shows that the cooling occurs in the tropics, partly offset by warming in the northern extratropical Pacific.

5.3 Instrumentally homogeneous series

Instrumentally homogeneous data sets [3] are data sets which comprise measurements from a single instrument, or standardised collection of instruments, chosen to be stable and accurate.

5.3.1 Argo

Argo floats are autonomous floating devices that make temperature profile measurements usually in the upper 2000m of the water column. Argo floats float with the prevailing currents at a depth of 1000m. Every ten days, the float descends to 2000m then rises to the surface measuring water temperatures along the way. An estimate of SST can be had by taking the measurement nearest to the surface and above a specified depth, in this case 10m. The measurements made by Argo floats are considered to be accurate, with estimated uncertainties of hundredths of a degree or better. However, sampling is relatively sparse with each of the floats sampling the SST only once every 10 days. Nonetheless, the excellent coverage and low noise of the measurements means that a reasonably global average can be calculated from the observations from the mid 2000s. Due to the careful calibration of the sensors, the series (aside from shifts in coverage) is expected to be reasonably stable.

Figure 6 shows a comparison between HadSST.4.0.0.0 and gridded Argo observations. The gridding was the same as was used for HadSST.4.0.0.0. The adjustments applied to HadSST.4.0.0.0 bring the SST series into closer agreement with the Argo data.

5.3.2 ARC ATSR Reprocessing for Climate

Figure 6 also shows a comparison with the ARC ATSR Reprocessing for Climate[15] data set. The ATSR series of instruments were designed to take climate quality measurements. The excellent coverage of the dataset means that it is possible to assess HadSST.4.0.0.0 at a wide range of locations. Here we show the global average. The ARC v1.1 data were gridded using the same method as for HadSST.4.0.0.0 to minimize inconsistencies that might arise from processing. Agreement between the two data sets is good for most of the ATSR2 and AATSR records - roughly from 1995 to 2012. The short segment of data in 1991 was recorded by the ATSR1 instrument before the failure of one of the infra-red channels. The assessed quality of the ATSR1 SST retrievals is lower than for the ATSR2 and AATSR instruments. Note that there are regional biases between ARC and HadSST.4.0.0.0 which are likely due to biases in the ARC retrievals, or subtle differences in the precise measurand. Similar differences are seen between ARC and drifting buoy data.

5.3.3 Buoys

The final panel in Figure 6 shows comparisons between buoy data and HadSST.4.0.0.0. The buoy data are used in the creation of HadSST.4.0.0.0, so this does not constitute validation of the dataset. However, it is important to note that the inclusion of ship data has not degraded the analysis. There is a divergence between the series in 1992/1993. This is a period of relatively low buoy coverage. One thing to note is that the bias adjustments applied to HadSST.4.0.0.0 cool the ship data particularly between 1990 and 2010.

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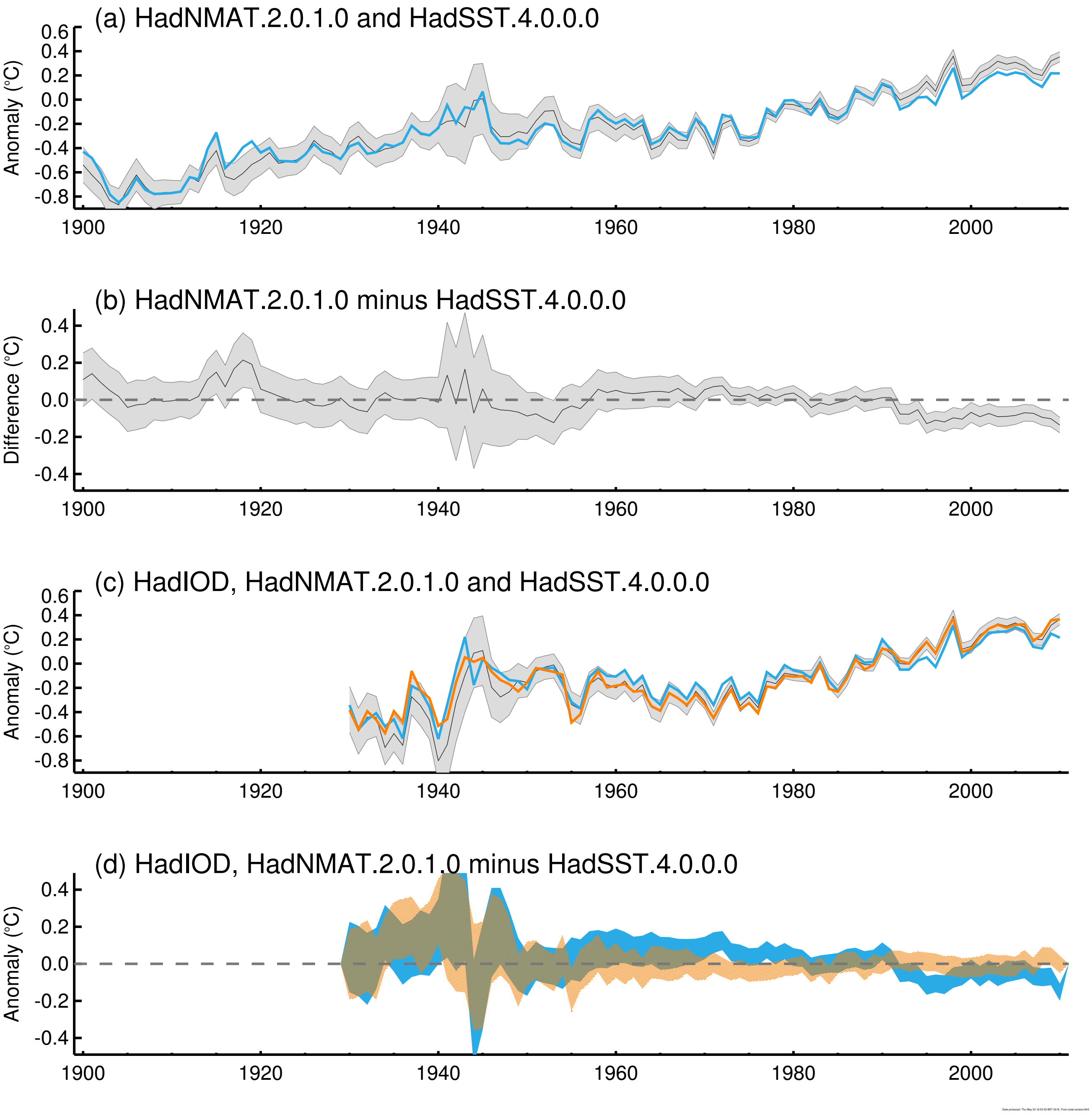

Figure 5: From [10]. (a) Collocated global annual average NMAT anomalies (°C) 1900-2010 offset by 0.15°C (blue, relative to 1961-1990) and global annual average SST anomalies from HadSST.4.0.0.0 (black is central estimate and grey shading indicates 95% uncertainty range). (b) Offset NMAT anomalies minus SST anomalies with combined 95% uncertainty range (taking into account the bias errors from the HadSST.4.0.0.0 ensemble, and measurement and sampling errors in the SST). The dashed line indicates zero difference. (c) Collocated global annual average offset NMAT anomalies (blue), global annual average near-surface water temperature from HadIOD excluding Argo (orange) and SST (black is central estimate and grey shading again indicates 95% uncertainty range). (d) Difference between HadIOD and HadSST.4.0.0.0 (orange) and NMAT and HadSST.4.0.0.0 (blue). The shaded area indicates the 95% uncertainty range..

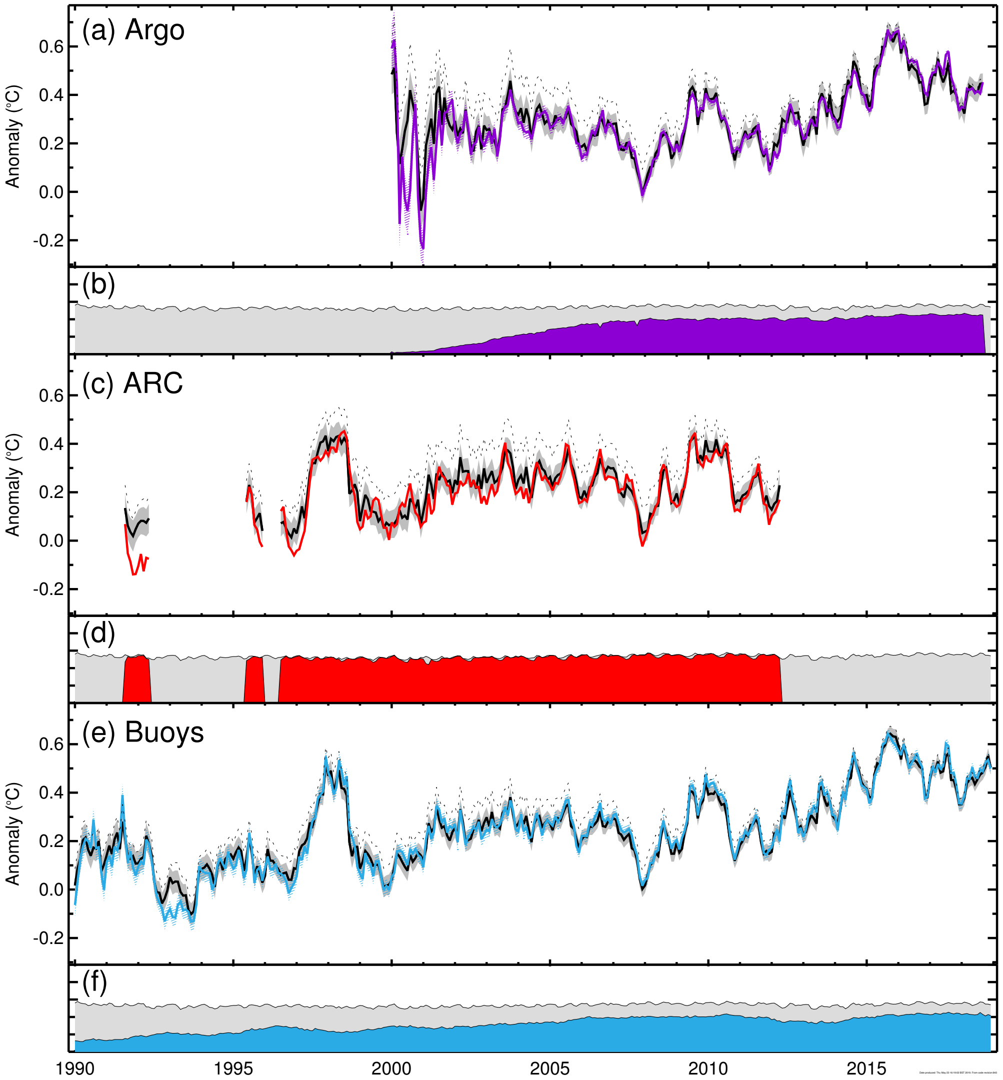

Figure 6: From [10]. Comparison to instrumentally homogeneous data sets. (a) global average SST anomalies from Argo (purple) and HadSST.4.0.0.0 (black and grey shading). The dotted line shows a global average calculated from unadjusted data. All comparisons are colocated. (b) coverage of HadSST.4.0.0.0 (grey) and coverage of the Argo data (purple). (c) and (d) as for (a) and (b) but for ARC data. (e) and (f) as for (a) and (b) but for drifting buoy data.

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