Sampling and Measurement Error Models for ICOADS Ship SST, Based on the ESA CCI SST Analysis

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GHRSST
Group for High Resolution Sea Surface Temperature

Overview

1. Collection of *in situ* SST observations in ICOADS
   - Data sparsity
   - Binned means and their error
   - Earlier error model validation efforts
   - Importance of ESA CCI SST Anaslysis data set
2. Rigorous estimation of random error in ship SST binned means
   - Approach to the estimation
   - Model performance
3. Separation of sampling and measurement errors & their seasonality
4. Measurement error estimates for different SST observation methods on ships
5. Conclusions

ICOADS R3.0: Historical in situ observations

ICOADS

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https://icoads.noaa.gov/

International Comprehensive Ocean-Atmosphere Data Set (ICOADS)

ICOADS Figure 2

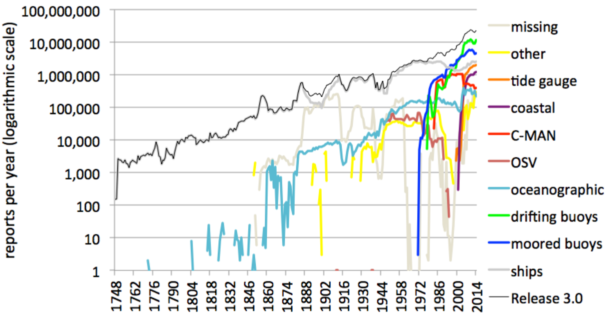

Figure 2. Annual distribution (1748-2014) of major platform types in Release 3.0 (and total) shown as reports per year (logarithmic scale). Ships (mainly VOS plus some R/Vs; and prior to ~1888 hidden by the R3.0 curve), buoys, oceanographic, coastal, and tide gauge are self explanatory, Ocean (permanent) Station Vessel = OSV, Coastal-Marine Automated Network = C-MAN, ocean drilling rigs/platforms and other small entities = other, and unidentified platform types = missing (note: most are probably early ship reports).

ICOADS R3.0: Space/time coverage

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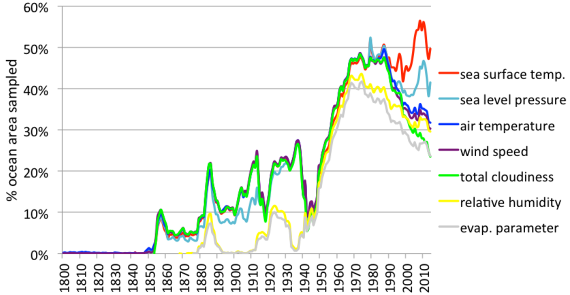
ICOADS Figure 3



Global ocean coverage for SST since 1880s: 10–60%

Figure 3. Percentage global ocean and coastal area (1800-2014) sampled in Release 3.0 based on area-weighted 2° boxes (smoothed) for sea surface temperature (*S*), requiring at least five observations per month in each box, and determined from the "enhanced" (4.5σ trimming) product that includes ship and buoy records. Other curves compare the *S* coverage, at five observations per month, with that for sea level pressure (*P*), air temperature (*A*), wind speed (*W*), total cloudiness (*C*), and relative humidity (*R*). Also plotted is the evaporation parameter (*G*), which is computed from *S*, *P*, *A*, *W*, and dew point temperature, and thus illustrates the extent to which surface fluxes can be computed from the individual observations.

Let bin $\mathcal{B}$ = a grid box of a regular monthly $1^\circ \times 1^\circ$ grid. Let it contain a sample $\mathcal{B}_o$ of $\mathcal{N}_o$ SST observations that passed ICOADS QC:

$$\mathcal{B}_o \stackrel{\text{def}}{=} \{o_1, o_2, \cdots, o_{\mathcal{N}_o}\},$$

characterized by its mean $\mathcal{M}_o$ and $\mathcal{N}_o$.

Monthly $1^\circ \times 1^\circ$ bins for January 2005

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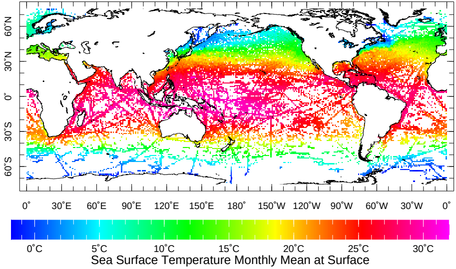

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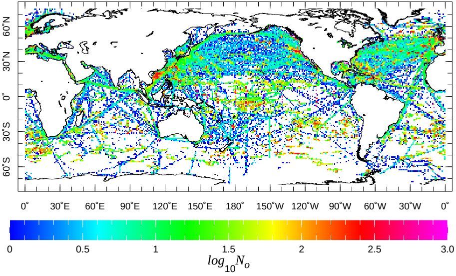

ICOADS Binned Summaries: Means and Nobs

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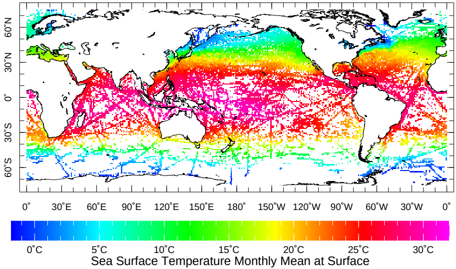

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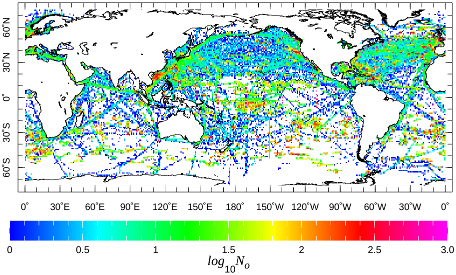

What is the error in $\mathcal{M}_o$?

Monthly 1°×1° bins for January 2005, unbiased variance est: $\sigma^2_{\mathcal{B}o} = \mathbb{E}\mathcal{S}^2_o$

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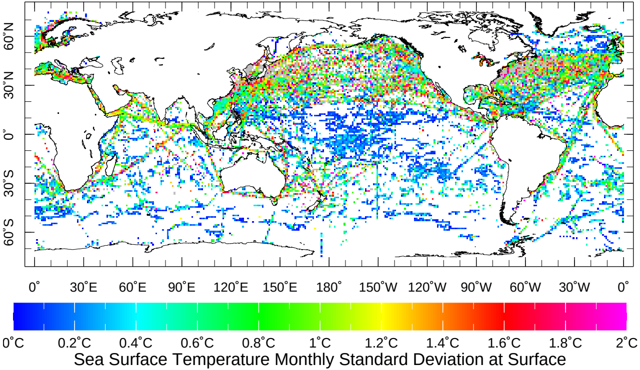

ICOADS Binned Summaries: Standard Deviations

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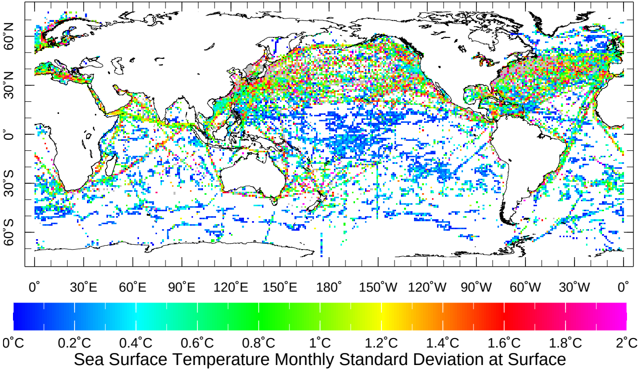

For the purposes of statistical analysis, bins with $\mathcal{N}_o = 1$ are principally different ($\exists\mathcal{M}_o$, but no $\mathcal{S}_o$) from bins with $\mathcal{N}_o \geq 2$

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the time-averaged error in $\mathcal{M}_o$ would have estimated SD

$$\overline{e}_{\mathcal{M}o} = \left\langle \frac{\hat{\sigma}^2_{\mathcal{B}o}}{\mathcal{N}_o} \right\rangle^{1/2} = \hat{\sigma}_{\mathcal{B}o} \left\langle 1/\mathcal{N}_o \right\rangle^{1/2} = \frac{\hat{\sigma}_{\mathcal{B}o}}{\sqrt{\overline{\mathcal{N}}_o^h}} \; ,$$

where $\overline{\mathcal{N}}_o^h = \langle 1/\mathcal{N}_o \rangle^{-1}$ is the harmonic mean of $\mathcal{N}_o$ values.

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Because of systematic **biases** in ship SST data, to get the actual effects of the **random error**, we should subtract from $d_{\mathcal{M}}$ its temporal mean $\overline{d}_{\mathcal{M}}$, i.e., use the SD (not RMS) of the actual error:

$$\mathcal{D}' \stackrel{\text{def}}{=} \left[\frac{1}{N_t - 1} \sum_{t=1}^{N_t} d'_{\mathcal{M}}(t)^2 \right]^{1/2}, \text{ where } d'_{\mathcal{M}}(t) = d_{\mathcal{M}}(t) - \overline{d}_{\mathcal{M}} \; .$$

Back to 2009: *OceanObs '09* [*Rayner et al.*, 2010]

EVALUATING CLIMATE VARIABILITY AND CHANGE FROM MODERN AND HISTORICAL SST OBSERVATIONS

Nick A. Rayner [(1)], Alexey Kaplan [(2)], Elizabeth C. Kent [(3)], Richard W. Reynolds [(4)], Philip Brohan [(1)], Kenneth S. Casey [(5)], John J. Kennedy [(1)], Scott D. Woodruff [(6)], Thomas M. Smith [(7)], Craig Donlon [(8)], Lars-Anders Breivik [(9)], Steinar Eastwood [(9)], Masayoshi Ishii [(10)] and Tess Brandon [(5)]

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1. ABSTRACT

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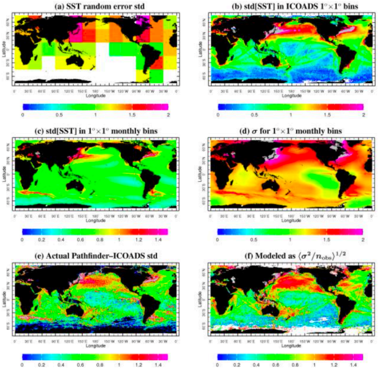

Figure 2. Effective observational error in in situ SST and its components: (a) random error estimate for one ship observation [21]; (b) actual standard deviation in ICOADS 1° x 1° monthly bins, 1960-2005; (c) SST variability within 1° x 1° monthly bins, 4 km Pathfinder v5 daily SST [20], 1985-2004; (d) standard error for a single observation in 1° x 1° monthly bins, estimated by combining (a) and (c); (e) standard deviation of SST difference between 1° x 1° monthly Pathfinder (night) and ICOADS, 2000-2004; (f) average ICOADS SST error in 1° x 1° monthly grid boxes during 2000-2004, estimated from a single observation error estimate and

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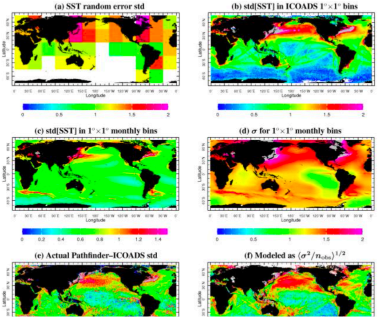
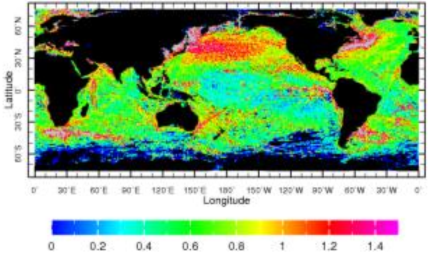


(e) Actual Pathfinder–ICOADS std



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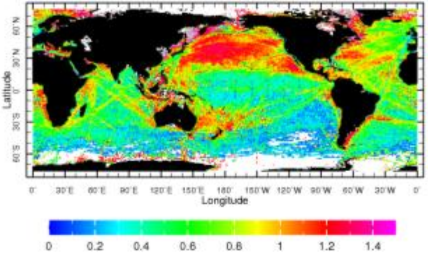

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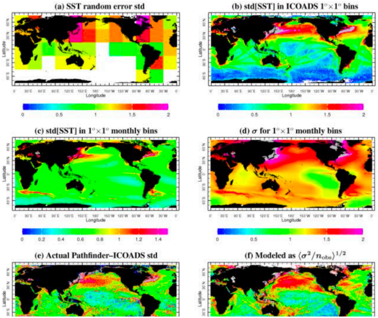

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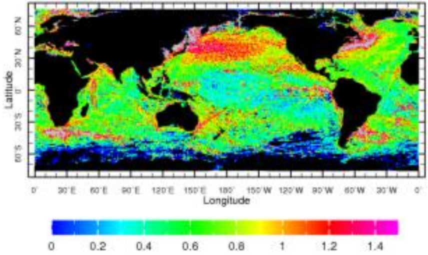

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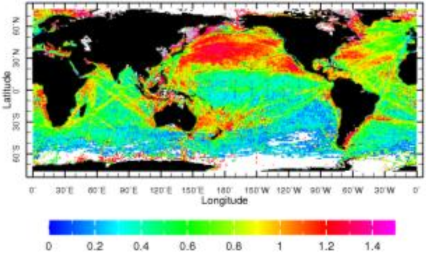

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ESA CCI SST Analysis [v1.0: *Merchant et al.*, 2014]

RMetS Royal Meteorological Society

Geoscience Data Journal

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Sea surface temperature datasets for climate applications from Phase 1 of the European Space Agency Climate Change Initiative (SST CCI)

Christopher J. Merchant[1,*], Owen Embury[1], Jonah Roberts-Jones[2], Emma Fiedler[2], Claire E. Bulgin[1], Gary K. Corlett[3], Simon Good[2], Alison McLaren[2], Nick Rayner[2], Simone Morak-Bozzo[1] and Craig Donlon[4]

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ESA CCI SST Analysis

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- Call a^o values of CCI SST analysis daily 0.05°×0.05° matchups to ship SST opsevations o, included into binning above. Bin a^o to produce data sets $\mathcal{M}_{ao}$ and $\mathcal{S}_{ao}$.
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- For CCI SST analysis uncertainty values e^a and their matchups e^{ao} to ship SST observations o, produce binned data sets $\mathcal{M}_{ea}$ and $\mathcal{S}_{ea}$ as well as $\mathcal{M}_{eao}$ and $\mathcal{S}_{eao}$.

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CCI SST analysis values are estimates of t^a, daily $0.05^\circ \times 0.05^\circ$ averages of true 20 cm temperature t:

$$t^a = a + \varepsilon^a,$$
$$\mathbb{E}\varepsilon^a = 0\,,\;\; \mathbb{E}\,(\varepsilon^a)^2 = (e^a)^2.$$

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To simplify derivations, **ship observations** are related to the "matched-up" version t^{ao} of same "truth" t^a as the CCI analysis:

$$o = t^{ao} + b + \varepsilon^o$$

Here bias b is assumed climatologically-varying and constant within each 1°×1° monthly bin; measurement errors ε^o are assumed independent of true temperature variations t^{ao} and i.i.d. within each bin with mean 0 and variance σ_o^2.

Bias removal and computing the actual differences RMS

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For a given bin location with data available for M climatological months, with Y_m years available for each month m, the bias estimate is obtained by climatological averaging of d_M differences:

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With the estimated bias removed, there are only

$$\sum_{m=1}^{M} (Y_m - 1) = N - M$$

degrees of freedom (DOF) remaining for the RMS calculation:

$$\mathcal{D}'' = \left[\frac{1}{N-M} \sum_{m=1}^{M} \sum_{y=1}^{Y_m} \left(d_{\mathcal{M}}(y, m) - \hat{b}(m) \right)^2 \right]^{1/2} .$$

Estimating $\mathbb{E}\mathcal{D}''^2$ as the joint effect of random errors

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$$\mathbb{E}\mathcal{D}''^2 = \frac{1}{N-M}\sum_{m=1}^{M}(Y_m - 1)\left(\frac{\sigma_{\mathcal{B}o}(m)^2}{\overline{\mathcal{N}}_o^h(m)} + \overline{\mathcal{M}}_{ea}^q(m)^2\right),$$

where

$$\overline{\mathcal{M}}_{ea}^q(m) = \left[\frac{1}{Y_m}\sum_{y=1}^{Y_m}\mathcal{M}_{ea}(y,m)^2\right]^{1/2}$$

is the climatological quadratic mean of the temporal $\mathcal{M}_{ea}$ sample for the given $1^\circ\times1^\circ$ bin location and, similarly, $\overline{\mathcal{N}}_o^h(m)$ is the climatological harmonic mean of available $\mathcal{N}_o$ values for the same location.

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Substituting to the intrabin variance $\sigma_{\mathcal{B}o}(m)^2$ in the expression for $\mathbb{E}\mathcal{D}''^2$ above its "pooled estimate"

$$\hat{\sigma}_{\mathcal{B}o}(m)^2 \stackrel{\text{def}}{=} \frac{\sum_{y=1}^{Y_m}(\mathcal{N}_o(y,m)-1)\,\mathcal{S}_o(y,m)^2}{\sum_{y=1}^{Y_m}(\mathcal{N}_o(y,m)-1)}, \quad m = 1,\cdots,M,$$

obtain the unbiased estimate $\mathcal{E}^2$ of $\mathbb{E}\mathcal{D}''^2$.

How good/bad is the agreement now between $\mathcal{E}$ and $\mathcal{D}''$?

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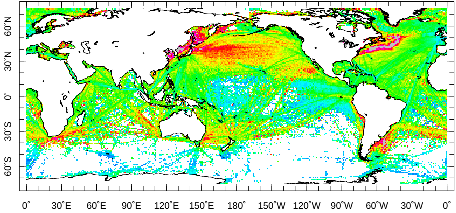
$\mathcal{E}$, est. $d_{\mathcal{M}}$ SD, 0.74°C



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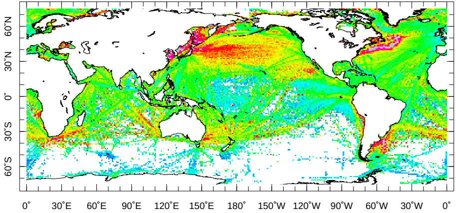
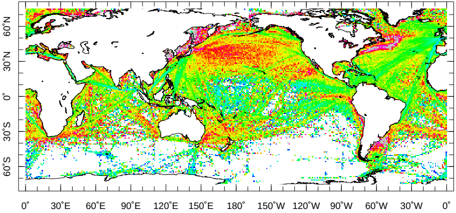


$\mathcal{D}''$, act. $d_{\mathcal{M}}$ anom. SD, 0.91°C



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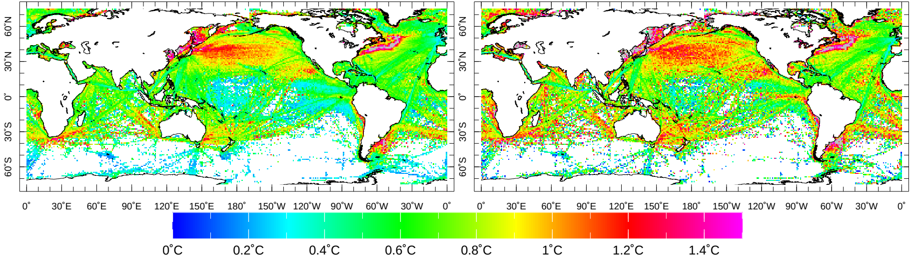

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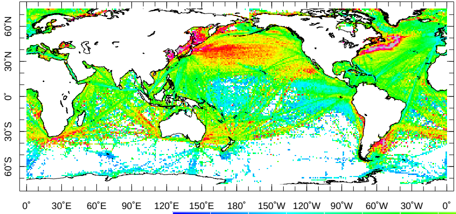

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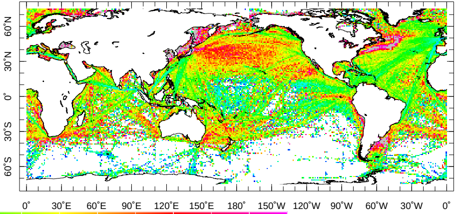
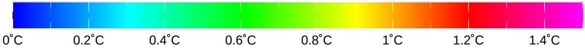
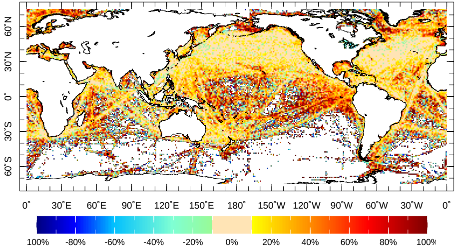




$$\rho \stackrel{\text{def}}{=} \frac{\mathcal{D}''-\mathcal{E}}{\mathcal{E}} 100\%,\ 81\%$$



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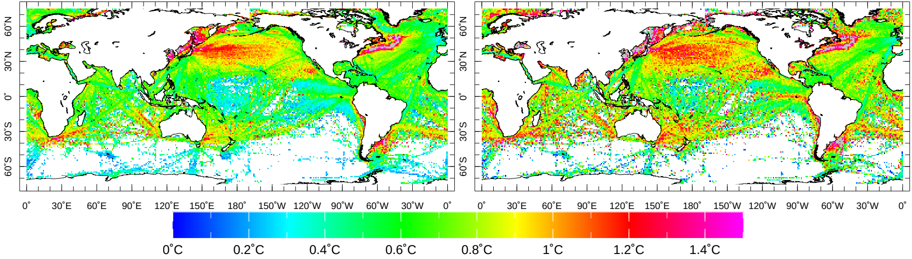

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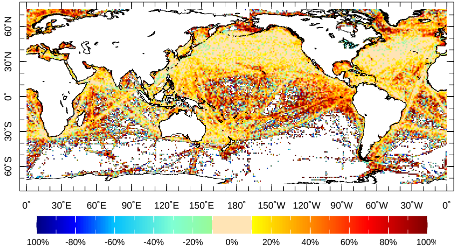
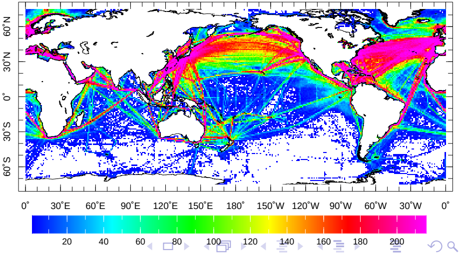
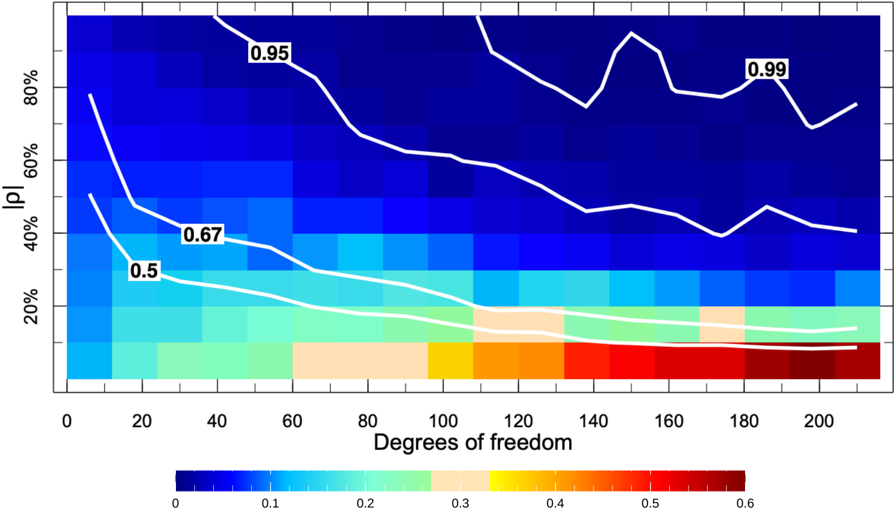


DOF in $\mathcal{D}''$ calculation, 71.3 (mos)



Impact of DOF on the empirical distribution of $|\rho|$



Separation of sampling and measurement error parts in $\sigma_{\mathcal{B}\,o}$ (or $e_{\mathcal{M}\,o} = \sigma_{\mathcal{B}\,o}/\sqrt{\mathcal{N}_o}$) estimates

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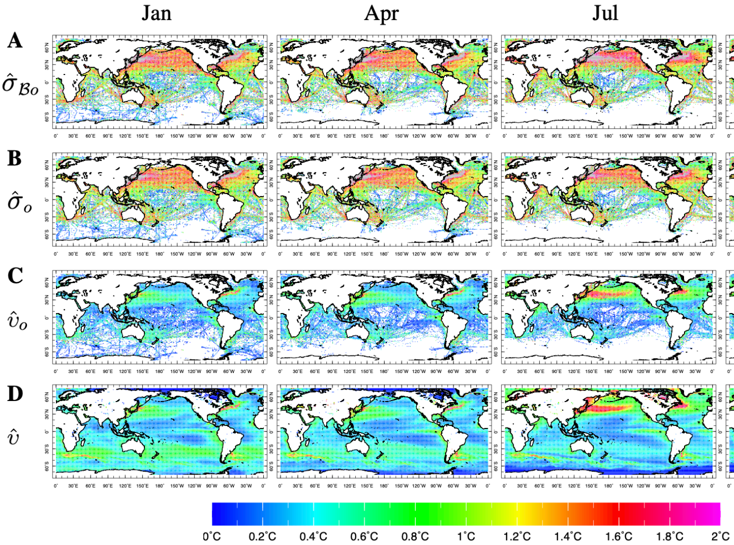
- $\hat{\upsilon}^2_o$ is a part of an approximate split-off $\hat{\sigma}^2_{\mathcal{B}o} \approx \hat{\upsilon}^2_o + \hat{\sigma}^2_o$, but $\hat{\upsilon}^2$ is a better estimate, being based on much more data than what $\hat{\upsilon}^2_o$ is using.

Seasonality of errors' magnitudes



Hypotheses on seasonality of variance estimates for error

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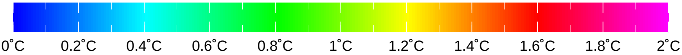
  (3) Recombining the estimate for $\sigma_{\mathcal{B}o}$ using the full analysis version $\hat{\upsilon}(m)$, will result in a superior estimate

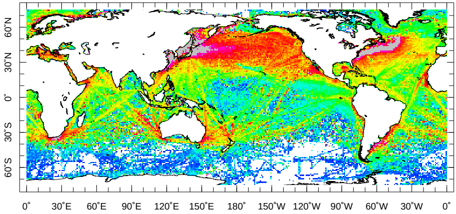
$$\hat{\sigma}_{\mathcal{B}o}(m)^2 = \hat{\sigma}_o^2 + \hat{\upsilon}(m)^2 \,.$$

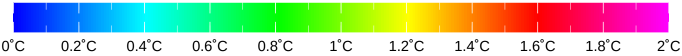
Ship SST measurement error $\hat{\sigma}_o$, by method



Ship SST measurement error $\hat{\sigma}_o$, by method

All methods, 1.05°C





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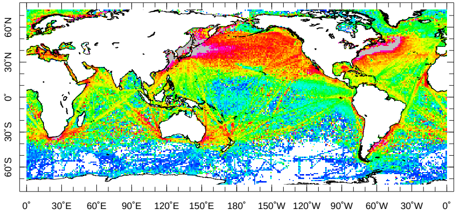
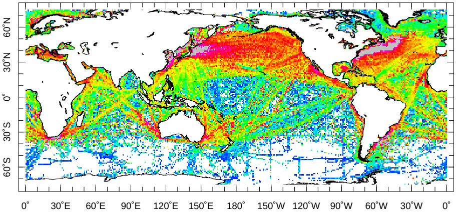
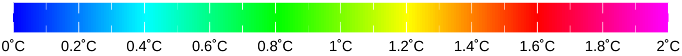


Engine Room Intake (ERI), 45.0%, 1.13°C





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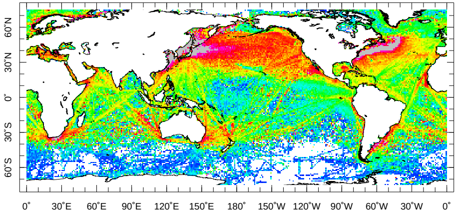

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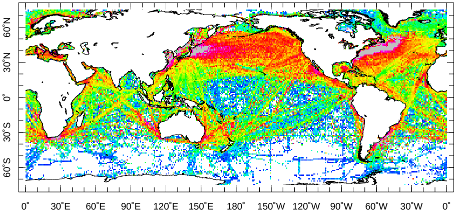
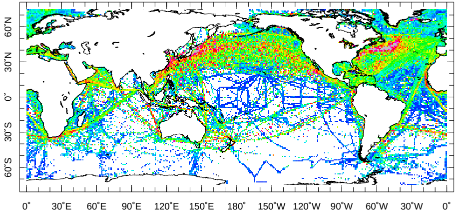
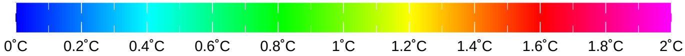


Hull Contact Sensor, 13.0%, 0.89°C





Ship SST measurement error $\hat{\sigma}_o$, by method

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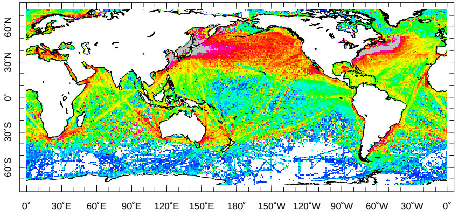

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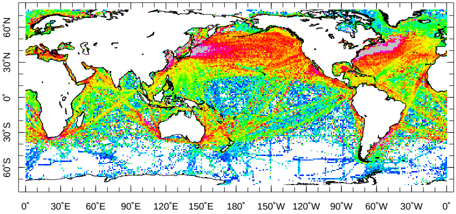
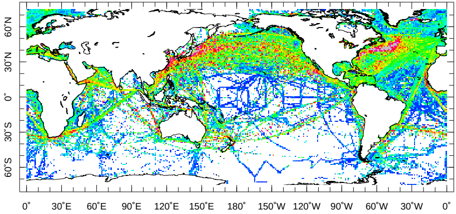
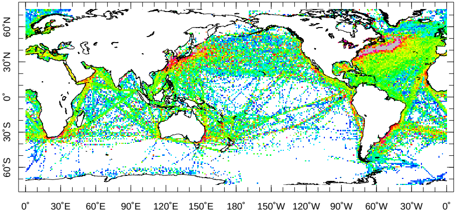
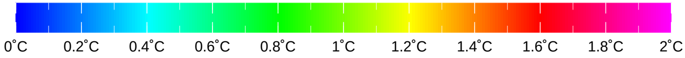


Hull Contact Sensor, 13.0%, 0.89°C



Buckets, 11.1%, 0.96°C



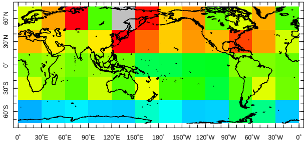


Ship SST error: Comparison with Kent&Challenor (2006)

All

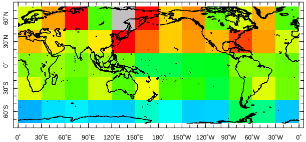
Ship SST error: Comparison with Kent&Challenor (2006)

All $\hat{\sigma}_o$ **by 30°×30° , 1.07°C**

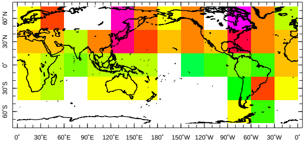


Ship SST error: Comparison with Kent&Challenor (2006)

All $\hat{\sigma}_o$ **by 30°×30° , 1.07°C**

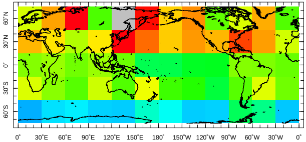


KC2006 error, 1.26°C

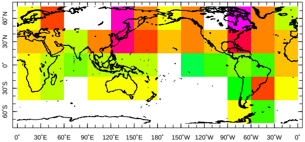


Ship SST error: Comparison with Kent&Challenor (2006)

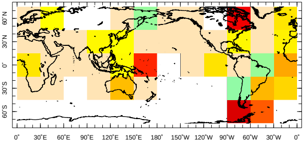
All $\hat{\sigma}_o$ **by 30°×30° , 1.07°C**



KC2006 error, 1.26°C

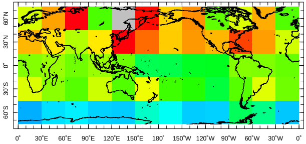


Relative error ρ, 22%

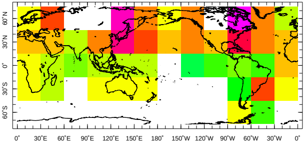


Ship SST error: Comparison with Kent&Challenor (2006)

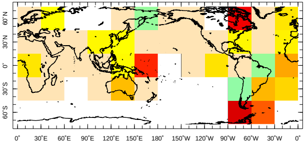
All $\hat{\sigma}_o$ **by 30°×30° , 1.07°C**



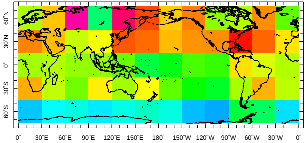
KC2006 error, 1.26°C



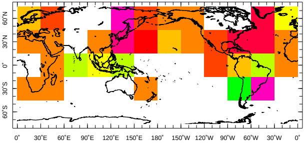
Relative error ρ, 22%



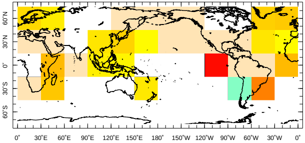
ERI $\hat{\sigma}_o$ **by 30°×30° , 1.11°C**



KC2006 error, 1.43°C

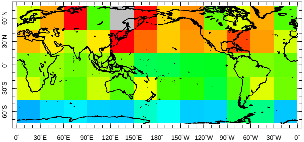


Relative error ρ, 22%

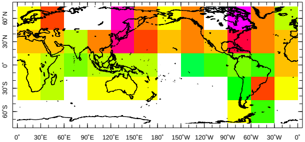


Ship SST error: Comparison with Kent&Challenor (2006)

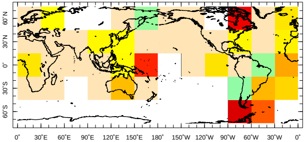
All $\hat{\sigma}_o$ **by 30°×30° , 1.07°C**



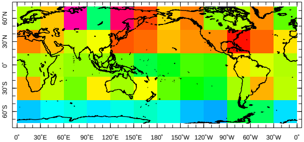
KC2006 error, 1.26°C



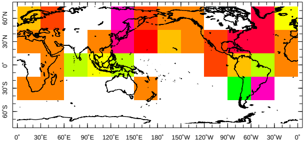
Relative error ρ, 22%



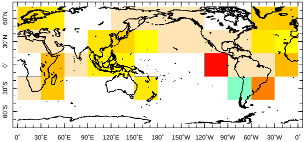
ERI $\hat{\sigma}_o$ **by 30°×30° , 1.11°C**



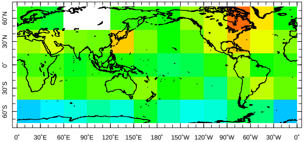
KC2006 error, 1.43°C



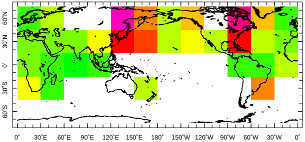
Relative error ρ, 22%



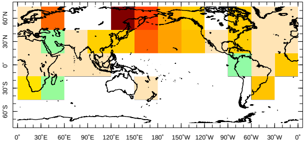
BU $\hat{\sigma}_o$ **by 30°×30° , 0.91°C**

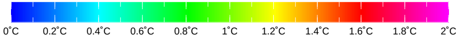


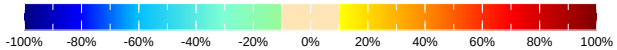
KC2006 error, 1.16°C



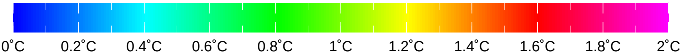
Relative error ρ, 27%





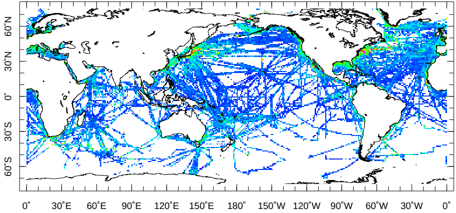


Ship SST measurement error $\hat{\sigma}_o$, more methods

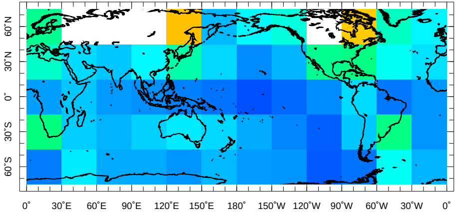


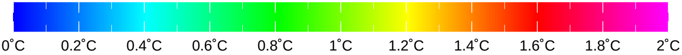
Ship SST measurement error $\hat{\sigma}_o$, more methods

Electronic sensor, 3.7%, 0.35°C

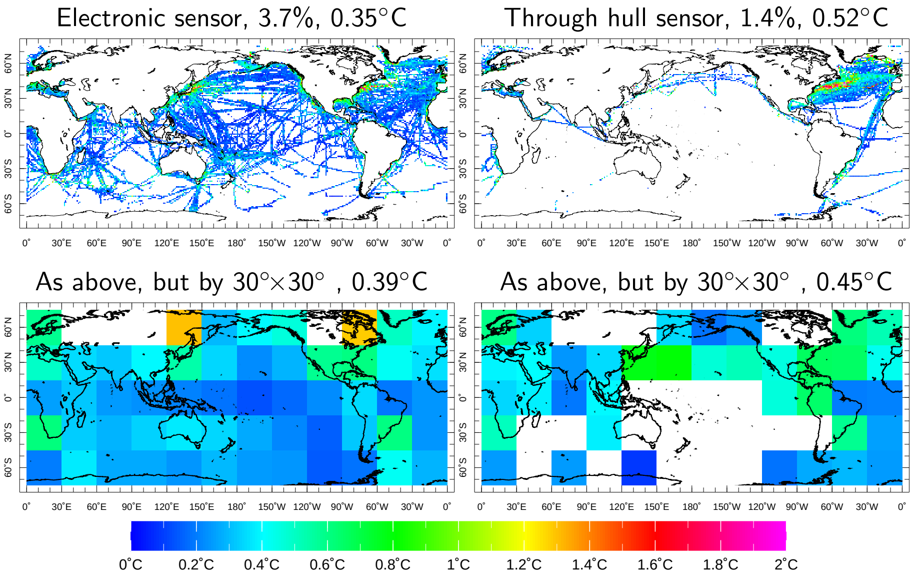


As above, but by 30°×30° , 0.39°C





Ship SST measurement error $\hat{\sigma}_o$, more methods



Global estimates of ship measurement error

Method name	% of observations	$\hat{\sigma}_o$,°C, by 1°×1°	$\hat{\sigma}_o$,°C, by 30°×30°
engine room intake	45.061	1.13	1.11
empty method field	17.277	1.22	**1.17**
hull contact sensor	12.964	0.89	0.85
bucket	11.118	0.96	0.91
"other"	4.902	1.13	1.06
electronic sensor	3.707	**0.35**	**0.39**
"unknown or non-bucket"	2.436	0.60	0.79
through hull sensor	1.444	0.52	0.45
bait tanks thermometer	0.837	**1.32**	1.06
trailing thermistor	0.250	0.69	0.78
radiation thermometer	0.003	0.60	0.46
All	100.000	1.05	1.07

Conclusions

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- Measurement error estimates, including those obtained by ERI and buckets, agree well with those by Kent and Challenor (2006). Estimates for hull measurement types and for electronic sensors (appearing to be the most accurate) were obtained as well.

Publication

Results shown here partly are in a preprint accessible at ESSOAr:
Kaplan, A., Random error in space-time bin averages of sea surface temperature o bservations from ships *Earth and Space Science*, in revision.

Accessible at
https://www.essoar.org/doi/abs/10.1002/essoar.10505940.1

Data sets are accessible at
http://rainbow.ldeo.columbia.edu/~alexeyk/ShipSSTerr/

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