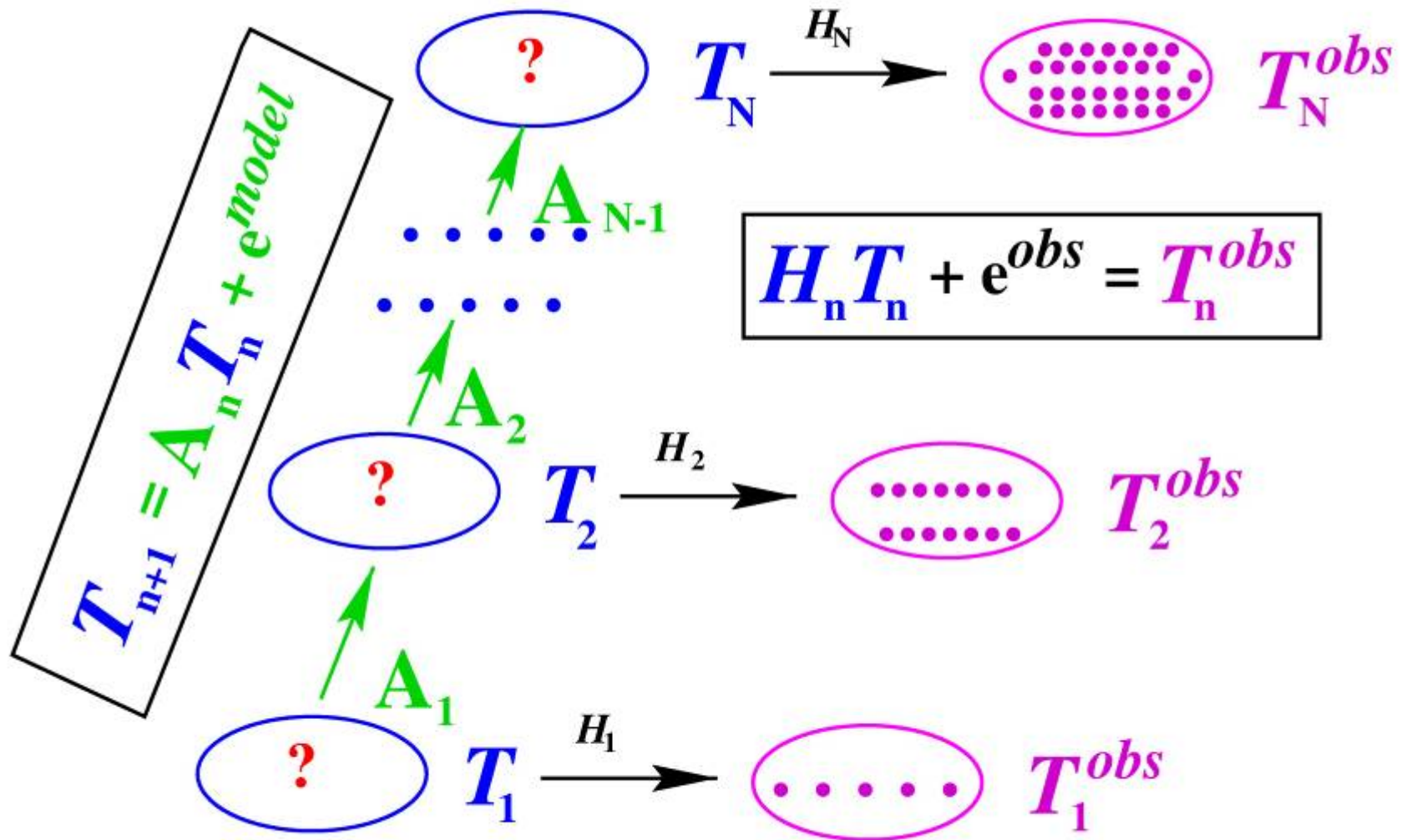


Reduced Space Data Assimilation and Historical Sea Surface Temperature Analyses

Alexey Kaplan

Lamont-Doherty Earth Observatory (LDEO) of Columbia University

Generic problem of the analysis of time-evolving fields



GENERAL PROBLEM OF ANALYSIS OF A HISTORICAL DATASET

$$\mathcal{T}_n^o = H_n \mathcal{T}_n + \varepsilon_n^o, \quad n = 1, \dots, N.$$

$$\mathcal{T}_{n+1} = A_n \mathcal{T}_n + \varepsilon_n^m, \quad n = 1, \dots, N - 1$$

$$\langle \varepsilon_n^o \rangle = 0, \quad \langle \varepsilon_n^o \varepsilon_n^{oT} \rangle = R_n, \quad n = 1, \dots, N$$

$$\langle \varepsilon_{n_1}^o \varepsilon_{n_2}^{oT} \rangle = 0, \quad n_1 \neq n_2, \quad \langle \varepsilon_{n_1}^o \mathcal{T}_{n_2}^T \rangle = 0, \quad n_1, n_2 = 1, \dots, N,$$

$$\langle \varepsilon_n^m \rangle = 0, \quad \langle \varepsilon_n^m \varepsilon_n^{mT} \rangle = Q_n, \quad n = 1, \dots, N - 1$$

$$\langle \varepsilon_{n_1}^m \varepsilon_{n_2}^{mT} \rangle = 0, \quad n_1 \neq n_2, \quad \langle \varepsilon_{n_1}^m \mathcal{T}_{n_2}^T \rangle = 0, \quad n_1, n_2 = 1, \dots, N - 1$$

$$\langle \varepsilon_{n_1}^o \varepsilon_{n_2}^{mT} \rangle = 0, \quad n_1 = 1, \dots, N, \quad n_2 = 1, \dots, N - 1$$

Gauss–Markov Theorem

If $\mathcal{T}^o = H\mathcal{T} + \varepsilon$,

$$\langle \varepsilon \rangle = 0, \quad \langle \varepsilon \varepsilon^T \rangle = R, \quad \langle \varepsilon \mathcal{T}^T \rangle = 0,$$

then the Least Squares Estimate (LSE)

$$\hat{\mathcal{T}} = (H^T R^{-1} H)^{-1} H^T R^{-1} \mathcal{T}^o$$

minimizes

$$S[\mathcal{T}] = (H\mathcal{T} - \mathcal{T}^o)^T R^{-1} (H\mathcal{T} - \mathcal{T}^o)$$

and is the **Best¹ Linear Unbiased Estimate (BLUE)** with error covariance

$$P \stackrel{\text{def}}{=} \langle (\mathcal{T} - \hat{\mathcal{T}})(\mathcal{T} - \hat{\mathcal{T}})^T \rangle = (H^T R^{-1} H)^{-1}.$$

ε is normal $\implies \mathcal{T}$ is a **Maximum Likelihood Estimate (MLE)**

ε and \mathcal{T} are normal $\implies \mathcal{T}$ is the best among **all** (not necessarily linear) estimates.

¹ $\|\mathcal{T} - \hat{\mathcal{T}}\|_S^2 = \langle (\mathcal{T} - \hat{\mathcal{T}})^T S (\mathcal{T} - \hat{\mathcal{T}}) \rangle \longrightarrow \min \quad \forall S \implies$ minimal variance

**MINIMIZATION OF THE FULL COST FUNCTION:
OPTIMAL SMOOTHER (OS) and KALMAN FILTER (KF)**

Cost function:

$$\mathbf{S}[\mathcal{T}_1, \mathcal{T}_2, \dots, \mathcal{T}_N] = \sum_{n=1}^N (H_n \mathcal{T}_n - \mathcal{T}_n^o)^T R_n^{-1} (H_n \mathcal{T}_n - \mathcal{T}_n^o) + \sum_{n=1}^{N-1} (\mathcal{T}_{n+1} - A_n \mathcal{T}_n)^T Q_n^{-1} (\mathcal{T}_{n+1} - A_n \mathcal{T}_n)$$

“Sweep up” – **KF**:

$$\begin{aligned}\hat{\mathcal{T}}_n^a &= \hat{\mathcal{T}}_n^f + K_n \left(\hat{\mathcal{T}}_n^o - H_n \hat{\mathcal{T}}_n^f \right), \\ \hat{\mathcal{T}}_n^f &= A_n \hat{\mathcal{T}}_{n-1}^a, \\ K_n &= P_n^f H_n^T \left(H_n P_n^f H_n^T + R_n \right)^{-1} \\ P_n^a &= (I_M - K_n H_n) P_n^f \\ P_n^f &= A_{n-1} P_{n-1}^a A_{n-1}^T + Q_{n-1}, \quad n = 2, 3, \dots, N\end{aligned}$$

“Sweep down” – **OS**:

$$\begin{aligned}\hat{\mathcal{T}}_n^s &= \hat{\mathcal{T}}_n^a + G_n \left(\hat{\mathcal{T}}_{n+1}^s - A_n \hat{\mathcal{T}}_n^a \right), \quad G_n = P_n^a A_n^T (P_{n+1}^f)^{-1}, \\ P_n^s &= P_n^a + G_n \left(P_{n+1}^s - P_{n+1}^f \right) G_n^T, \quad n = N - 1, \dots, 2, 1\end{aligned}$$

SIMPLIFIED CASE: OPTIMAL INTERPOLATION (OI)

Cost functions:

$$\mathbf{S}_n[\mathcal{T}_n] = (H_n \mathcal{T}_n - \mathcal{T}_n^o)^T R_n^{-1} (H_n \mathcal{T}_n - \mathcal{T}_n^o) + \mathcal{T}_n^T C_n^{-1} \mathcal{T}_n, \quad n > 1.$$

OI solution:

$$\mathcal{T}_n^{\text{OI}} = P_n^{\text{OI}} H_n^T R_n^{-1} \mathcal{T}_n^o, \quad P_n^{\text{OI}} = (H_n^T R_n^{-1} H_n + C_n^{-1})^{-1}.$$

Example of Optimal Interpolation

$$T = T_B + e_B$$

$$HT = T_0 + e_0$$

$$\langle e_B \rangle = \langle e_0 \rangle = \langle e_B e_0^T \rangle = 0$$

$$\langle e_B e_B^T \rangle = C \leftarrow \text{Hard to know in detail!}$$

$$\langle e_0 e_0^T \rangle = R$$

Solution minimizes the cost function

$$S[T] = (HT - T_0)^T R^{-1} (HT - T_0) + (T - T_B)^T C^{-1} (T - T_B)$$

$$T = (H^T R^{-1} H + C^{-1})^{-1} (H^T R^{-1} T_0 + C^{-1} T_B)$$

Projection of OI solution on eigenvectors of C (EOFs)

$$C = EDE^T$$

$$T = Ea$$

For simplicity: $H = I$, $R = rI$, $T := T - T_B$

Then $a = \underline{D(D+R)^{-1}}E^T T_0$

$$D(D+R)^{-1} = \text{diag}[d_i/(d_i+r)], \quad a_0 = E^T T_0$$

Therefore $a_i/a_0 = d_i/(d_i+r)$

In many applications (for spectrally red signals) diagonal elements of this matrix decrease from ~ 1 to ~ 0 . In effect, the solution is constrained to the subspace spanned by the patterns with $d_i \gg r$.

SPACE REDUCTION

$$C = E\Lambda E^T + E'\Lambda'E'^T$$

$$\mathcal{T}_n = E\alpha_n + \varepsilon_n^r, \quad n = 1, \dots, N$$

ESTIMATION PROBLEM IN THE REDUCED SPACE

$$\mathcal{T}_n^o = H_n E \alpha_n + (H_n \varepsilon_n^r + \varepsilon_n^o) \stackrel{\text{def}}{=} \mathcal{H}_n \alpha_n + \check{\varepsilon}_n^o, \quad n = 1, \dots, N,$$

$$\alpha_{n+1} = \mathcal{A}_n \alpha_n + E^T \varepsilon_n^m \stackrel{\text{def}}{=} \mathcal{A}_n \alpha_n + \check{\varepsilon}_n^m, \quad n = 1, \dots, N-1.$$

$$Q_n = \langle \check{\varepsilon}_n^m \check{\varepsilon}_n^{mT} \rangle = E^T \langle \varepsilon_n^m \varepsilon_n^{mT} \rangle E = E^T Q_n E$$

$$\begin{aligned} \mathcal{R}_n &= \langle \check{\varepsilon}_n^o \check{\varepsilon}_n^{oT} \rangle = \langle (H_n \varepsilon_n^r + \varepsilon_n^o)(H_n \varepsilon_n^r + \varepsilon_n^o)^T \rangle = \\ &\langle \varepsilon_n^o \varepsilon_n^{oT} \rangle + H_n \langle \varepsilon_n^r \varepsilon_n^{rT} \rangle H_n^T \stackrel{\text{def}}{=} R_n + H_n Q^r H_n^T \stackrel{\text{def}}{=} R_n + R'_n. \end{aligned}$$

REDUCED SPACE OPTIMAL ANALYSIS

Cost function:

$$\mathcal{S}[\alpha_1, \alpha_2, \dots, \alpha_N] = \sum_{n=1}^N (\mathcal{H}\alpha_n - \mathcal{T}_n^o)^T \mathcal{R}_n^{-1} (\mathcal{H}\alpha_n - \mathcal{T}_n^o) + \sum_{n=1}^{N-1} (\alpha_{n+1} - \mathcal{A}_n \alpha_n)^T \mathcal{Q}_n^{-1} (\alpha_{n+1} - \mathcal{A}_n \alpha_n).$$

KF:

$$\alpha_n^a = \alpha_n^f + \mathcal{K}_n (\mathcal{I}_n^o - \mathcal{H}_n \alpha_n^f),$$

$$\alpha_n^f = \mathcal{A}_n \alpha_{n-1}^a,$$

$$\mathcal{K}_n = (\mathcal{H}_n^T \mathcal{R}_n^{-1} \mathcal{H}_n + \mathcal{P}_n^{f-1})^{-1} \mathcal{H}_n^T \mathcal{R}_n^{-1}$$

$$\mathcal{P}_n^a = (I_L - \mathcal{K}_n \mathcal{H}_n) \mathcal{P}_n^f$$

$$\mathcal{P}_n^f = \mathcal{A}_{n-1} \mathcal{P}_{n-1}^a \mathcal{A}_{n-1}^T + \mathcal{Q}_{n-1}, \quad n = 2, 3, \dots, N$$

OS:

$$\alpha_n^s = \alpha_n^a + G_n (\alpha_{n+1}^s - \mathcal{A}_n \alpha_n^a),$$

$$G_n = \mathcal{P}_n^a \mathcal{A}_n^T (\mathcal{P}_{n+1}^f)^{-1},$$

$$\mathcal{P}_n^s = \mathcal{P}_n^a + G_n (\mathcal{P}_{n+1}^s - \mathcal{P}_{n+1}^f) G_n^T, \quad n = N - 1, \dots, 2, 1$$

OI:

$$\mathcal{S}_n^{\text{OI}}[\alpha_n] = (\mathcal{H}_n \alpha_n - \mathcal{T}_n^o)^T \mathcal{R}_n^{-1} (\mathcal{H}_n \alpha_n - \mathcal{T}_n^o) + \alpha_n^T \mathcal{C}_n^{-1} \alpha_n, \quad n > 1$$

$$\alpha_n^{\text{OI}} = \mathcal{P}_n^{\text{OI}} \mathcal{H}_n^T \mathcal{R}_n^{-1} \mathcal{T}_n^o, \quad \mathcal{P}_n^{\text{OI}} = (\mathcal{H}_n^T \mathcal{R}_n^{-1} \mathcal{H}_n + \mathcal{C}_n^{-1})^{-1}.$$

Projection:

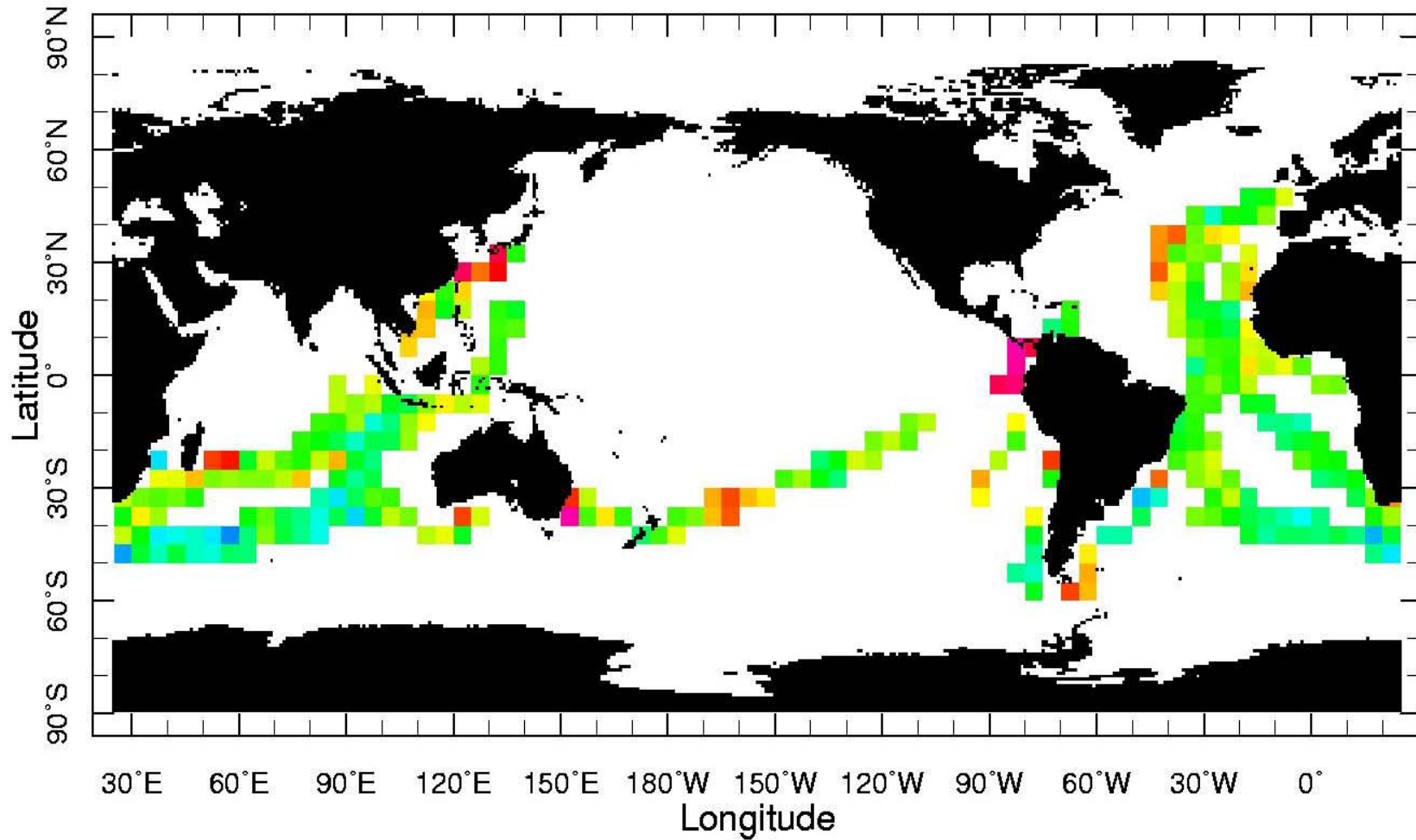
$$\alpha_n^p = \mathcal{P}_n^p \mathcal{H}_n^T \mathcal{R}_n^{-1} \mathcal{T}_n^o, \quad \mathcal{P}_n^p = (\mathcal{H}_n^T \mathcal{R}_n^{-1} \mathcal{H}_n)^{-1}$$

Spagetti-western properties of least-squares estimates of spectrally red signals: **(good)** can be approximated by a few modes, **(bad)** have less variance than the true signal, and **(ugly)** redder than the true signal.

It helps to remember that

$$C = \langle TT^T \rangle + P$$

Dec 1868: Available observations



Dec 1868



Vol. 345

ABSTRACT LOG

RECOMMENDED BY THE

MARITIME CONFERENCE OF BRUSSELS,

Kept on board the U. S. Steamer Commodore
James H. Blake, Commander, during the years 1854 & 1855.

Indexed,

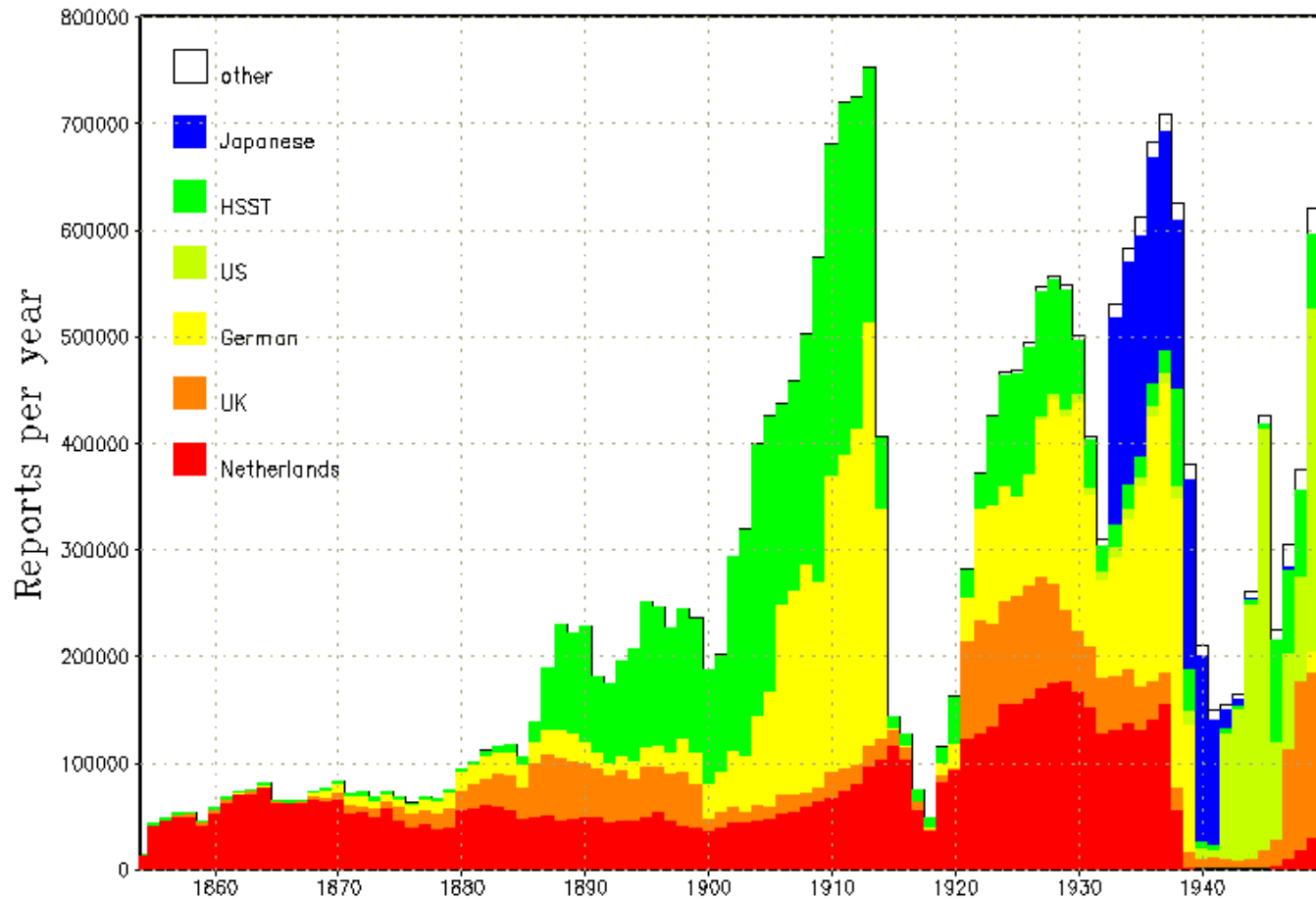
GENERAL ORDER.

NAVY DEPARTMENT,
November 2, 1855.

The form of the "Abstract Log" recommended by the late Maritime Conference at Brussels is hereby approved and set out in the Navy of the United States.
It is recommended to Navigators generally, to — all to faithfully keep on board of all vessels in the Naval Service, according to forms herewith annexed, — changed with the exception of this Order, and they will transmit the Abstracts kept on board, by the Chief of the Bureau of Ordnance and Hydrography, at the end of the year, or at such other times as he may direct.

Signed, J. C. DOJON,
Secretary of the Navy.

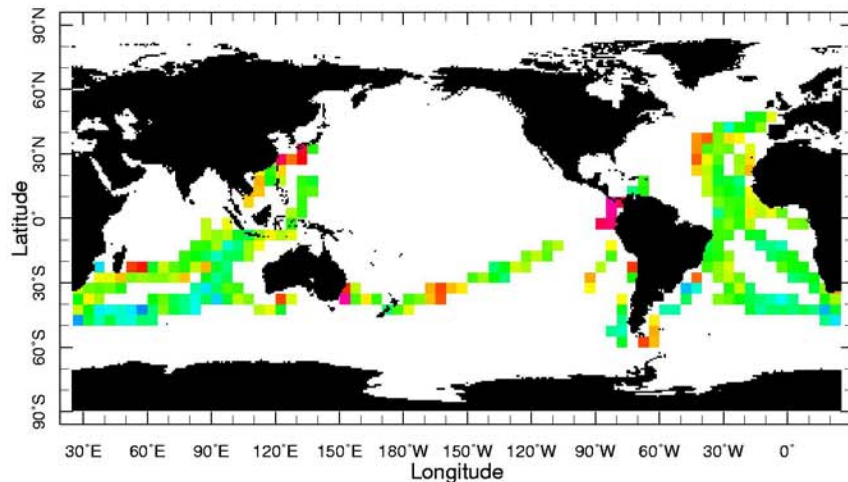
Number of observations in ICOADS



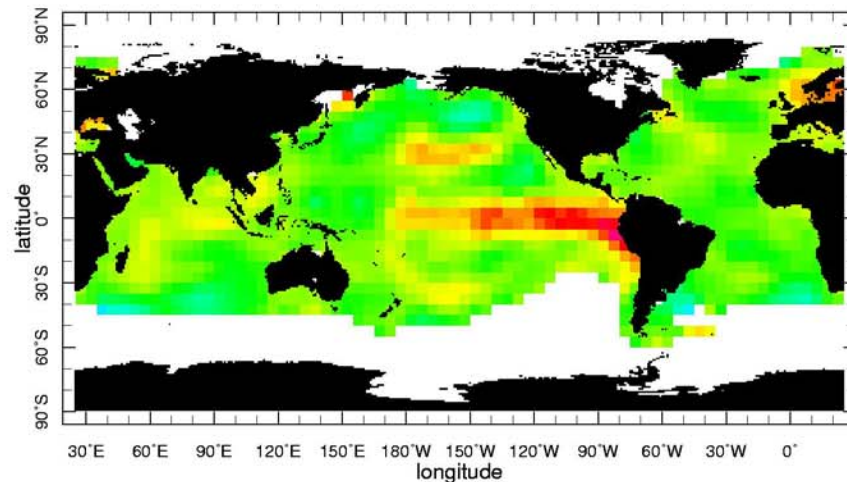
<http://icoads.noaa.gov/>

Given a choice, climatologists in general would rather use the righthand panel below than the lefthand one

Dec 1868: Available observations

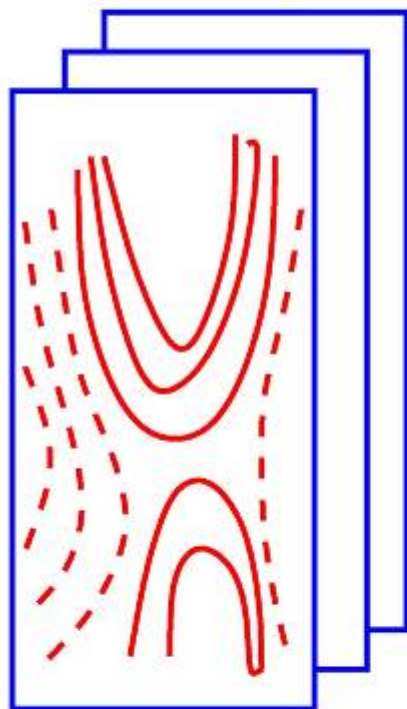


Dec 1868: Reconstruction

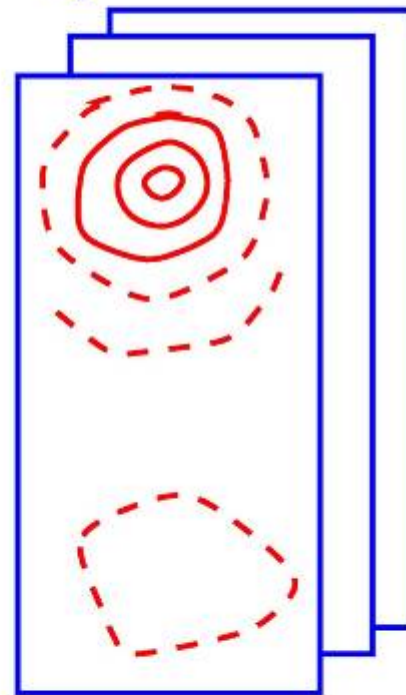


APPROXIMATING COVARIANCE

$$C = E\Lambda E^T + E'\Lambda'E'^T$$



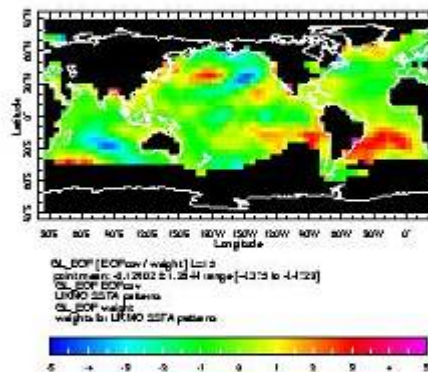
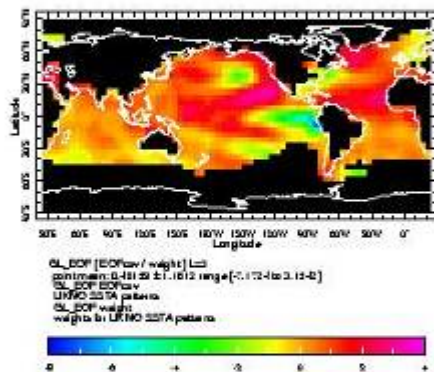
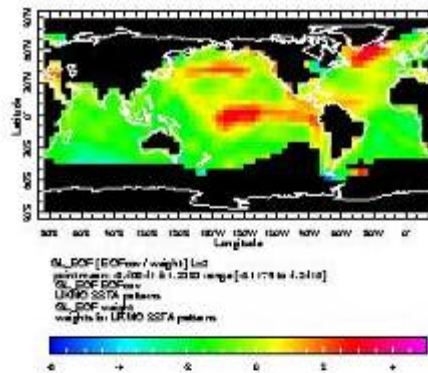
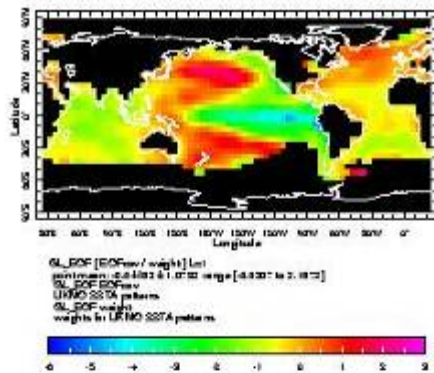
Reduced space
optimal analysis



Successive corrections;
Kriging

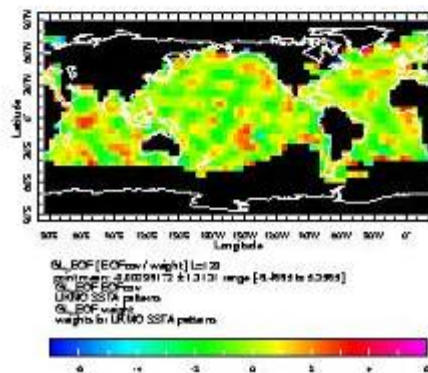
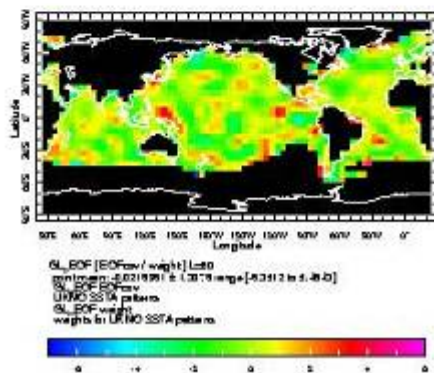
EOFs of SST (#1, 2, 3, 15, 80, 120)

EOF 1
14%



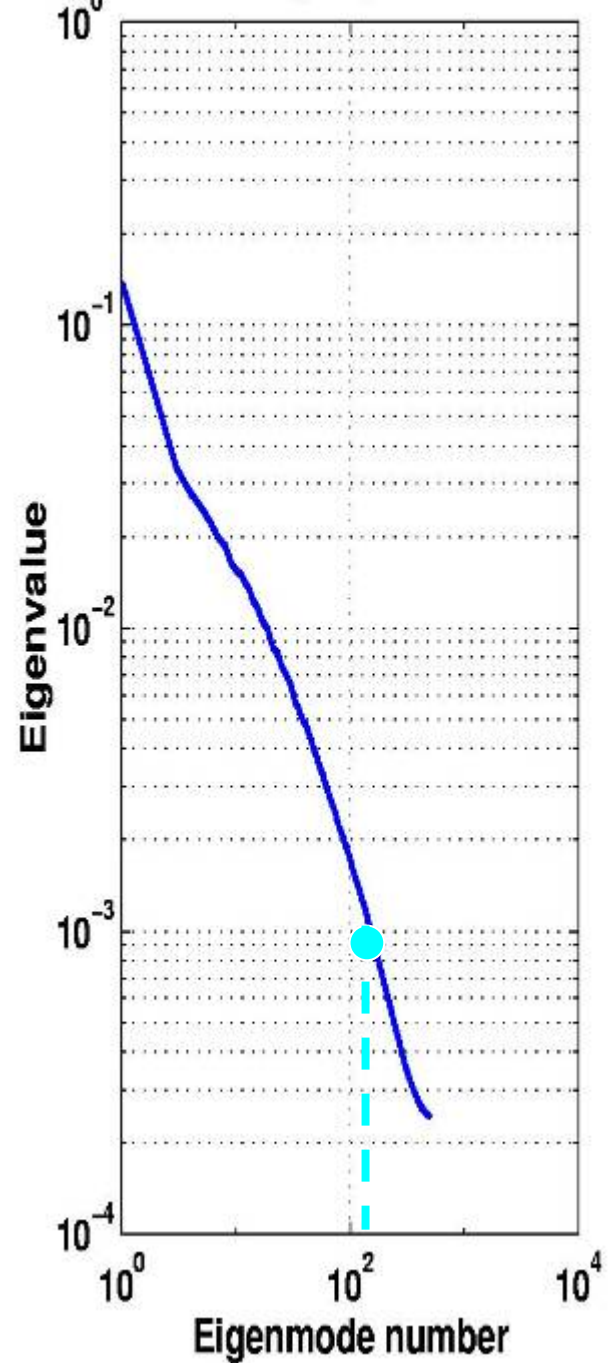
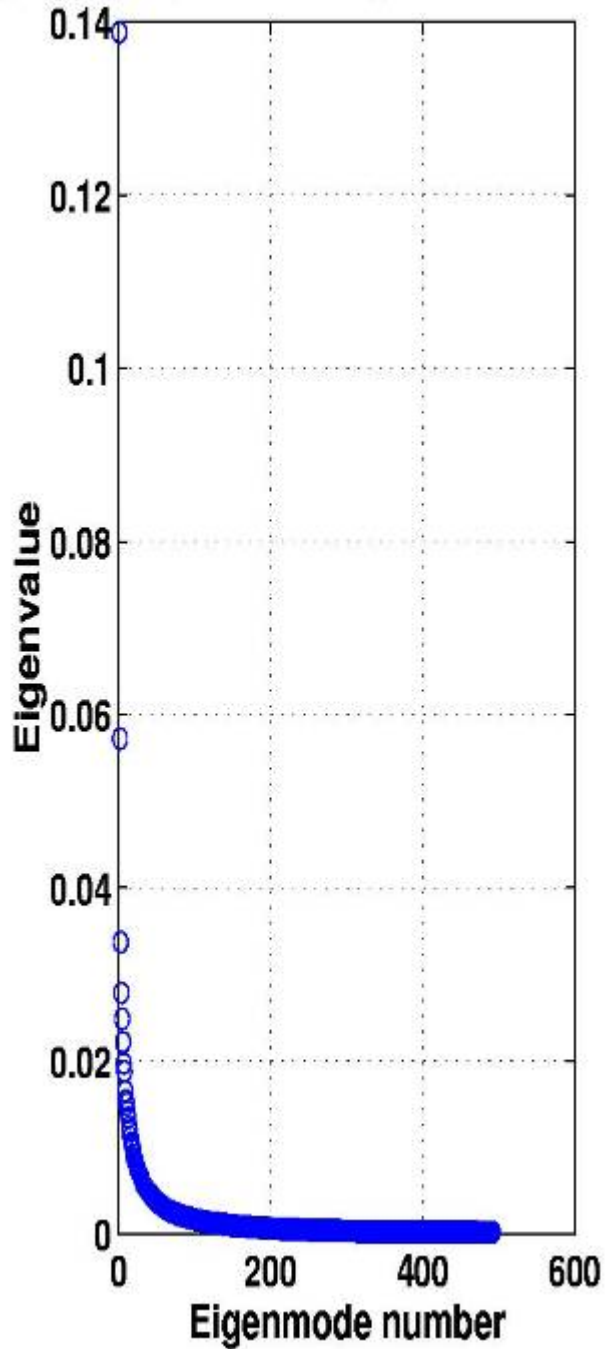
EOF 15
1%

EOF 80
0.1%



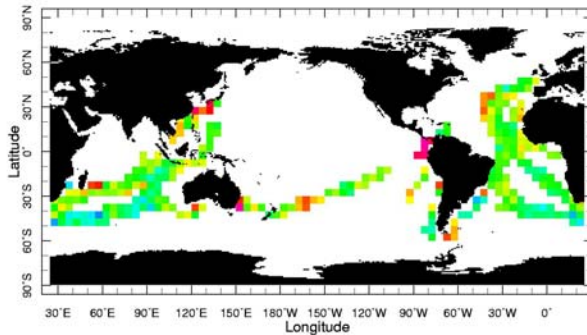
EOF 120
0.02%

Eigenvalue spectrum for global SST: 1951–1991 Same in log–log coordinates



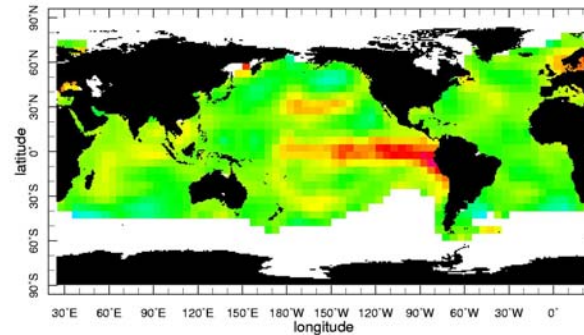
VERIFICATION OF REDUCED SPACE SST ANALYSES

Dec 1868: Available observations



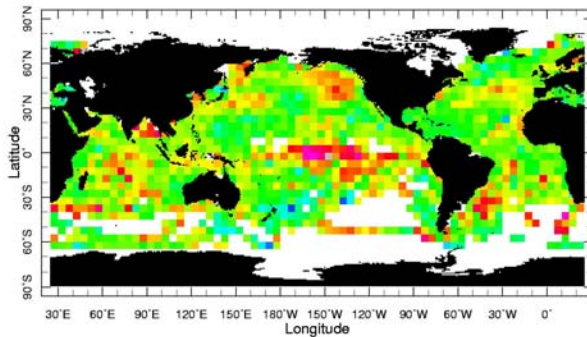
Dec 1868

Dec 1868: Reconstruction



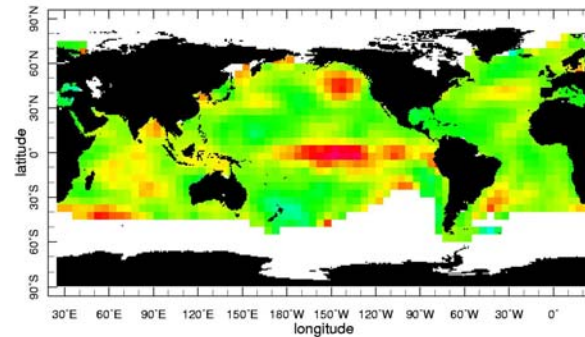
Dec 1868

Dec 1991: Available observations



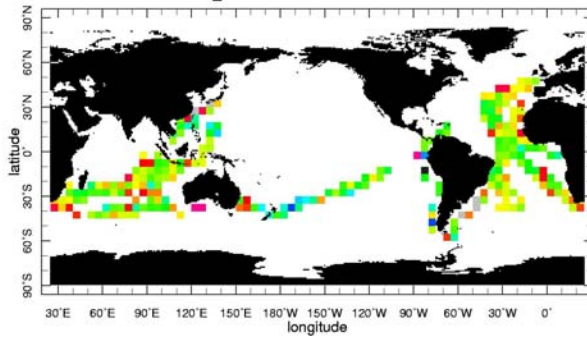
Dec 1991

Dec 1991: Reconstruction



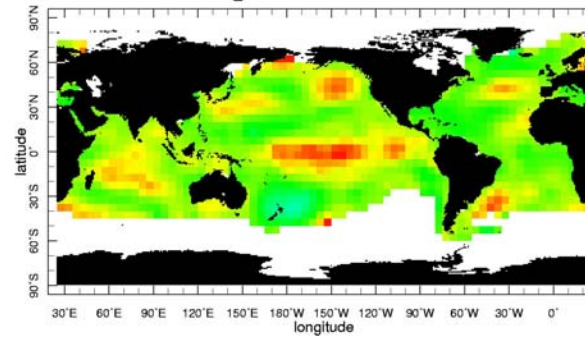
Dec 1991

Dec 1991: observations resampled as in Dec 1868

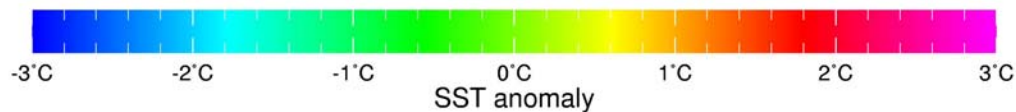


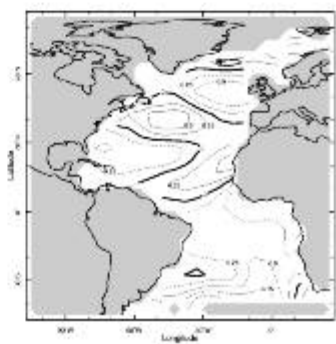
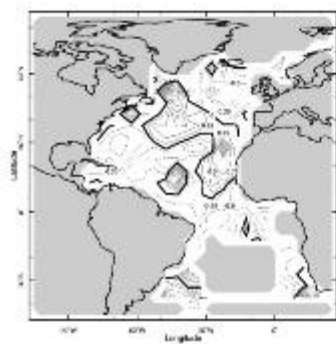
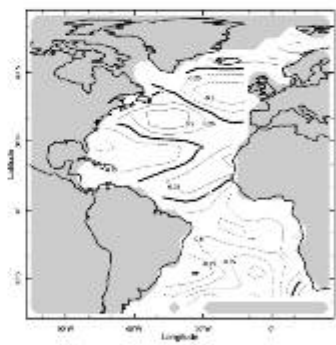
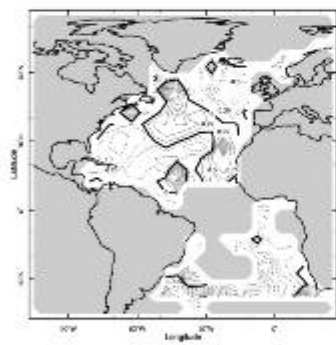
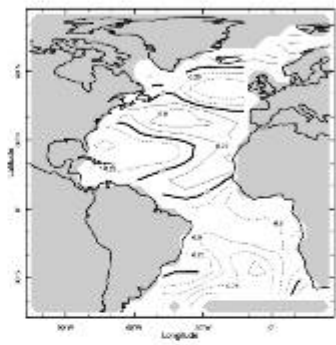
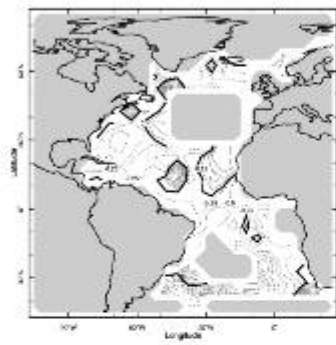
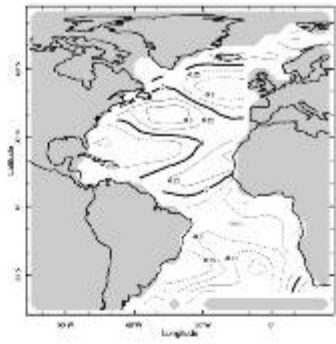
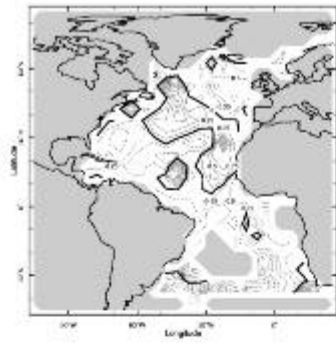
Dec 1991

Dec 1991: Reconstruction from the resampled set

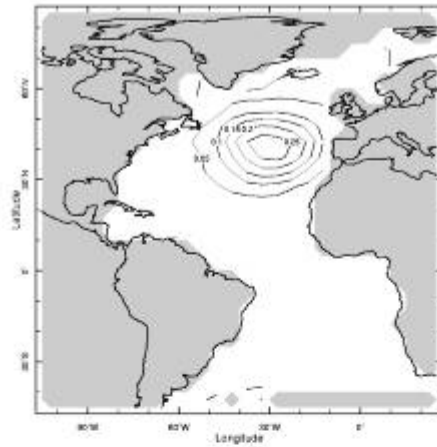


Dec 1991

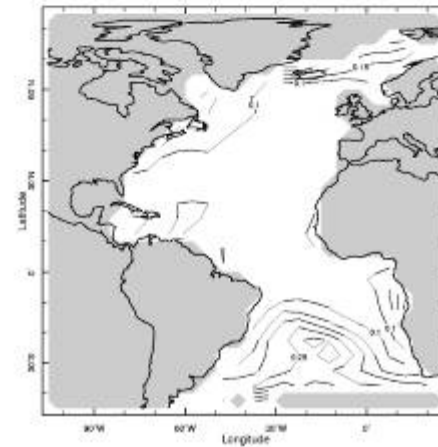
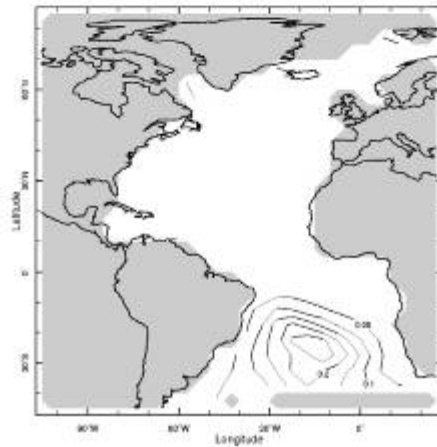
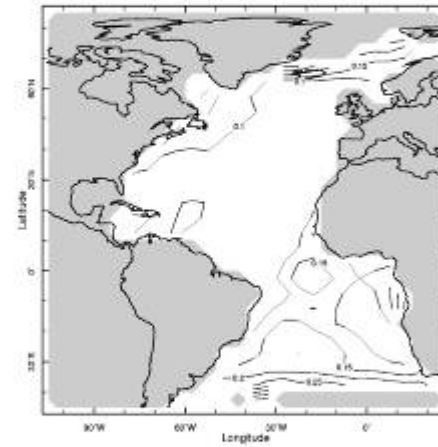
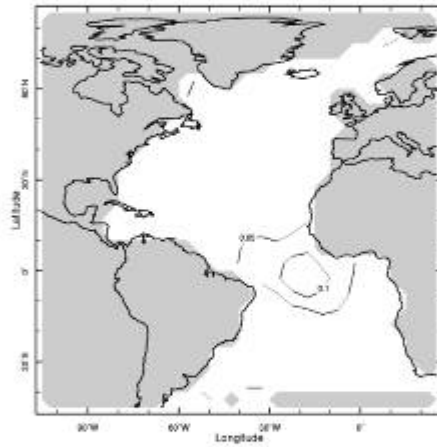
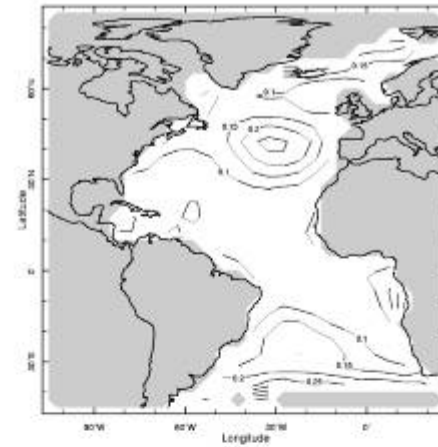




Actual rms difference



Theoretical error



El Niño of 1877-1878 in analyzed anomalies

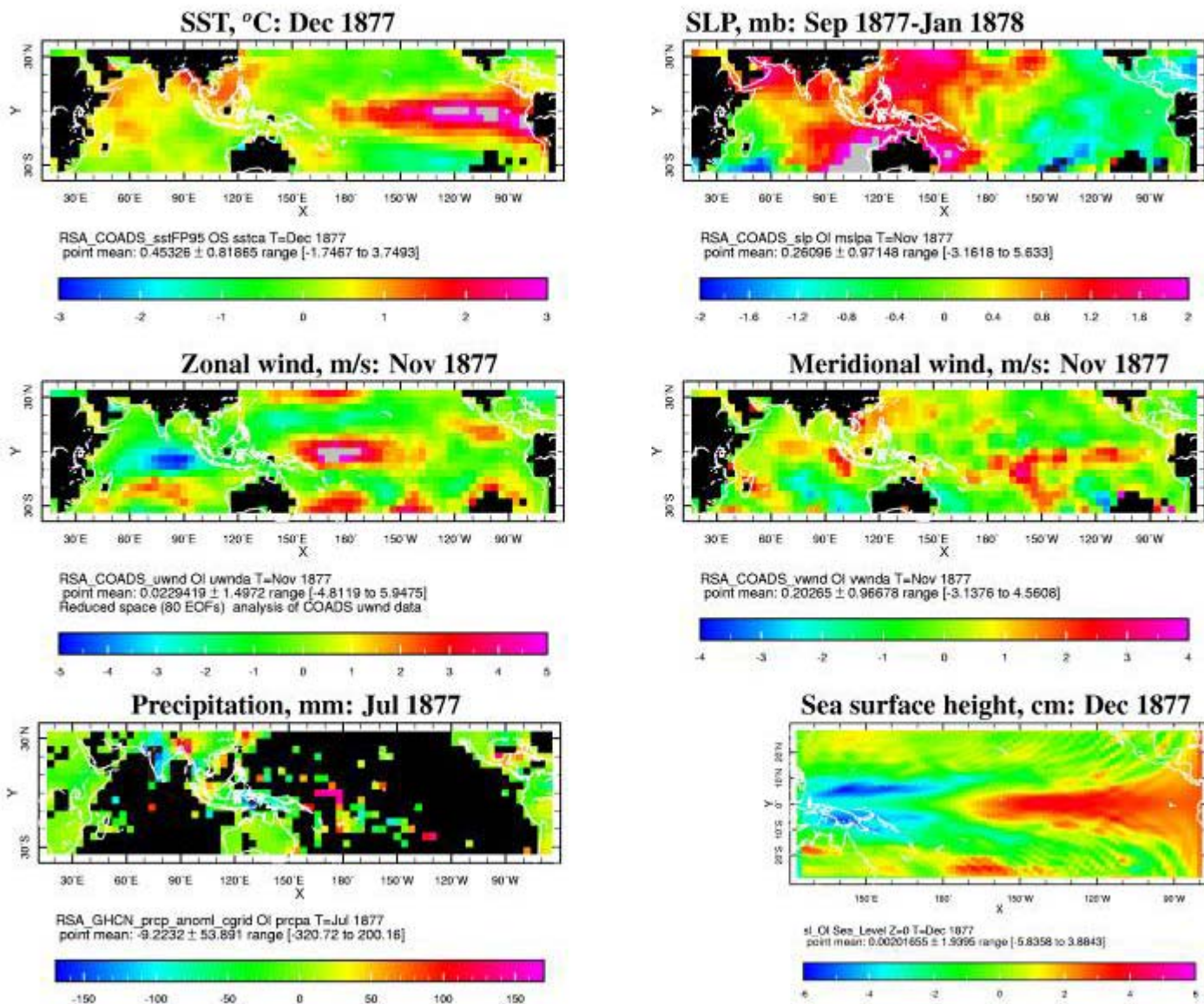
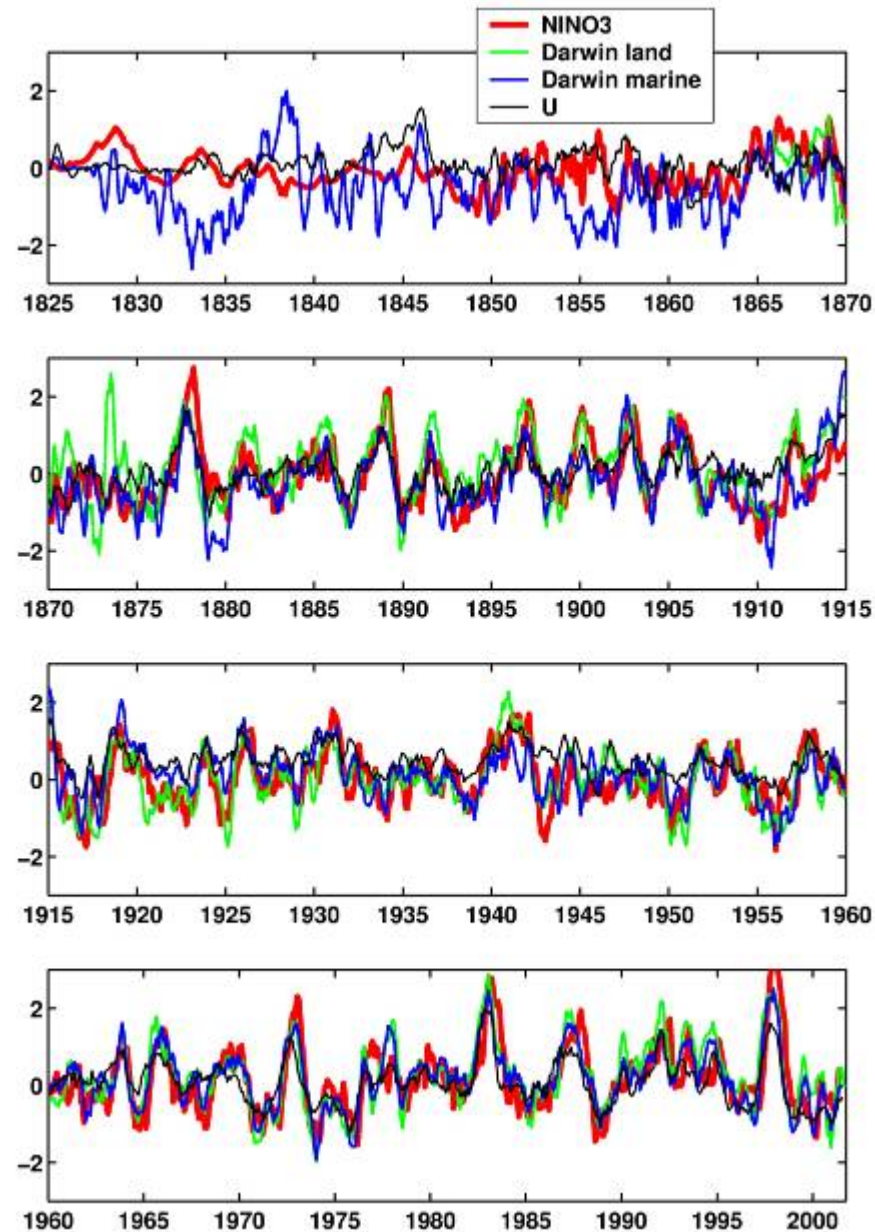


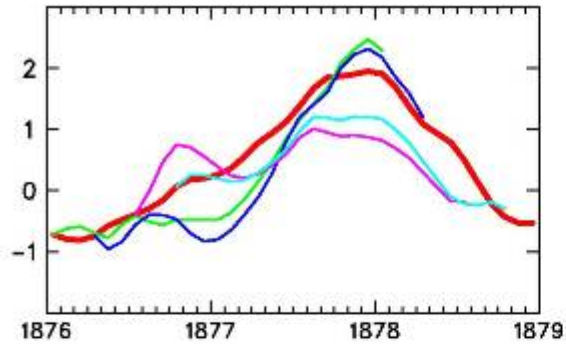
Figure 4: Anomalies of 1877-1878 El Niño illustrated by univariate reduced analyses by *Kaplan et al.* [2001b]

Independent ENSO indices

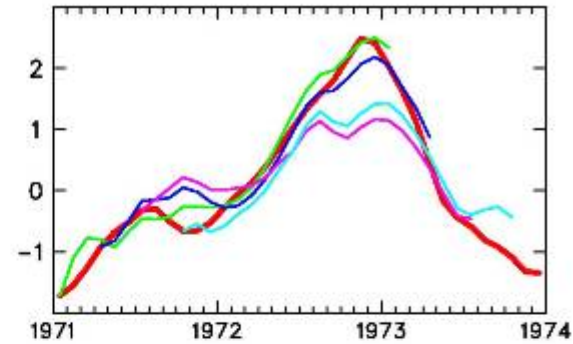


NINO3 (SST 5S-5N, 150W-90W)

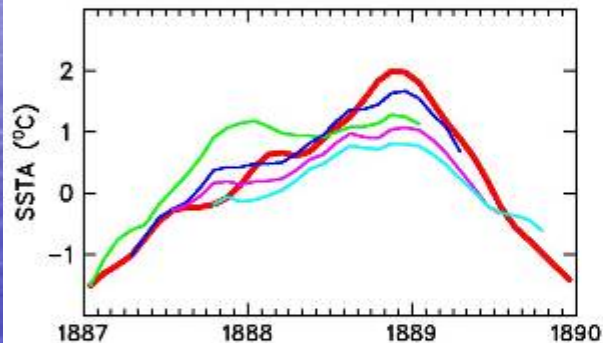
1877-1878



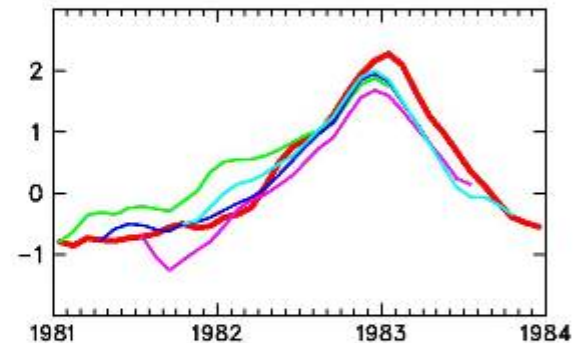
1972-1973



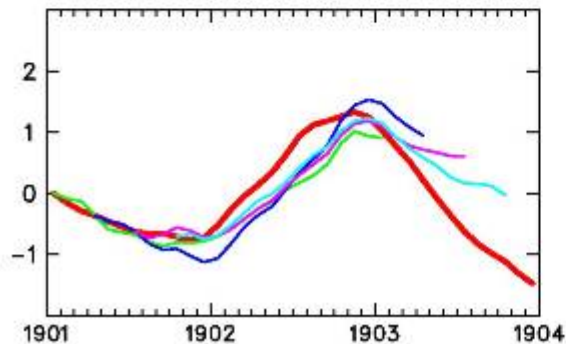
1888-1889



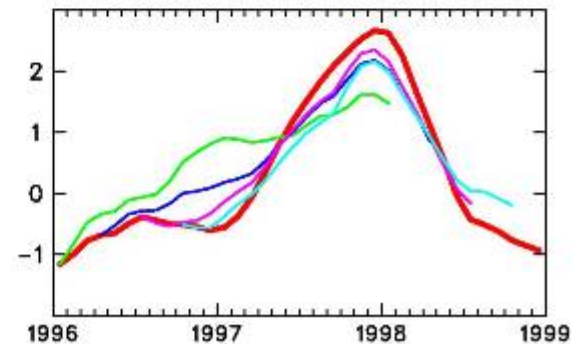
1982-1983



1902-1903

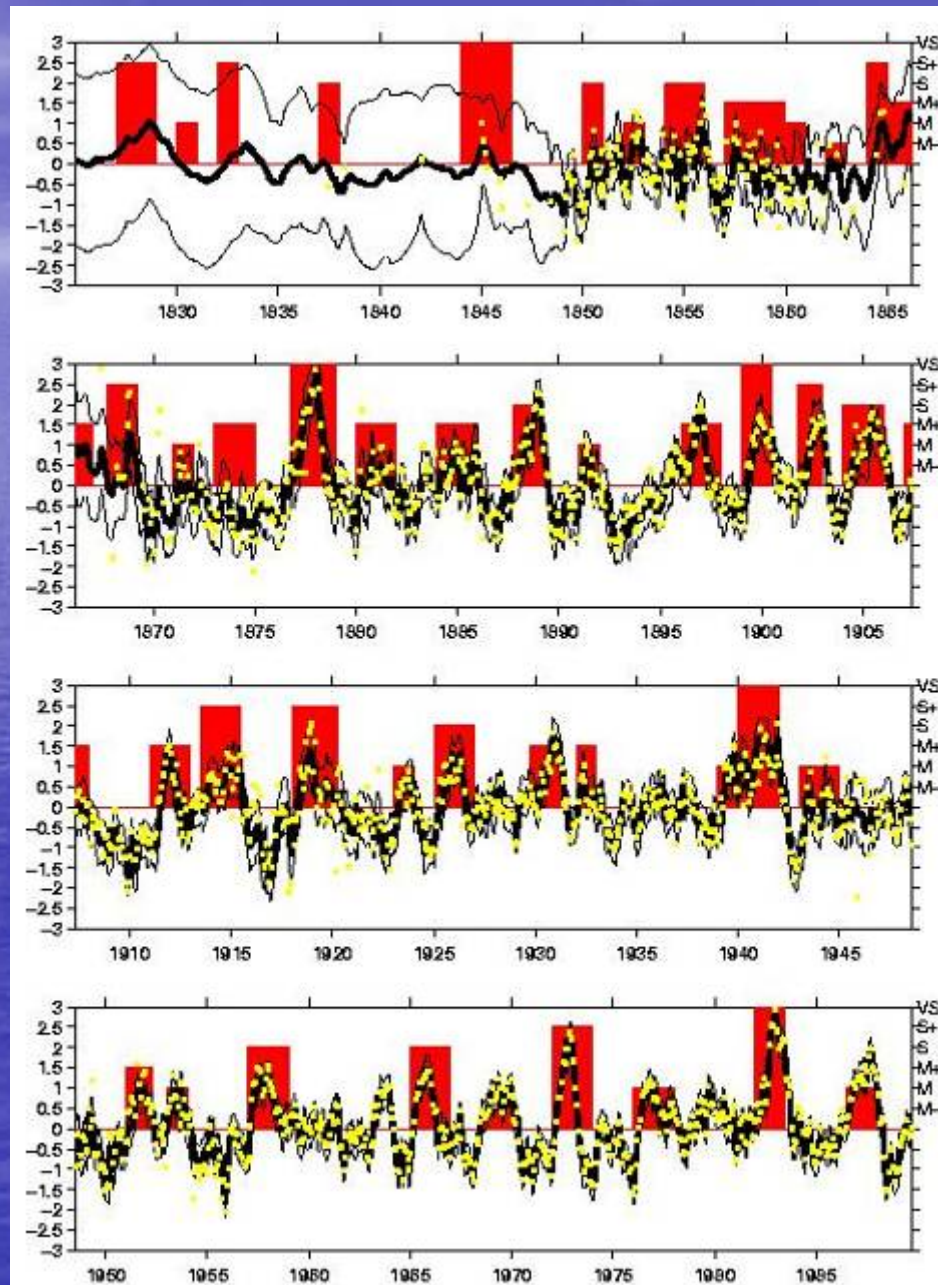


1997-1978



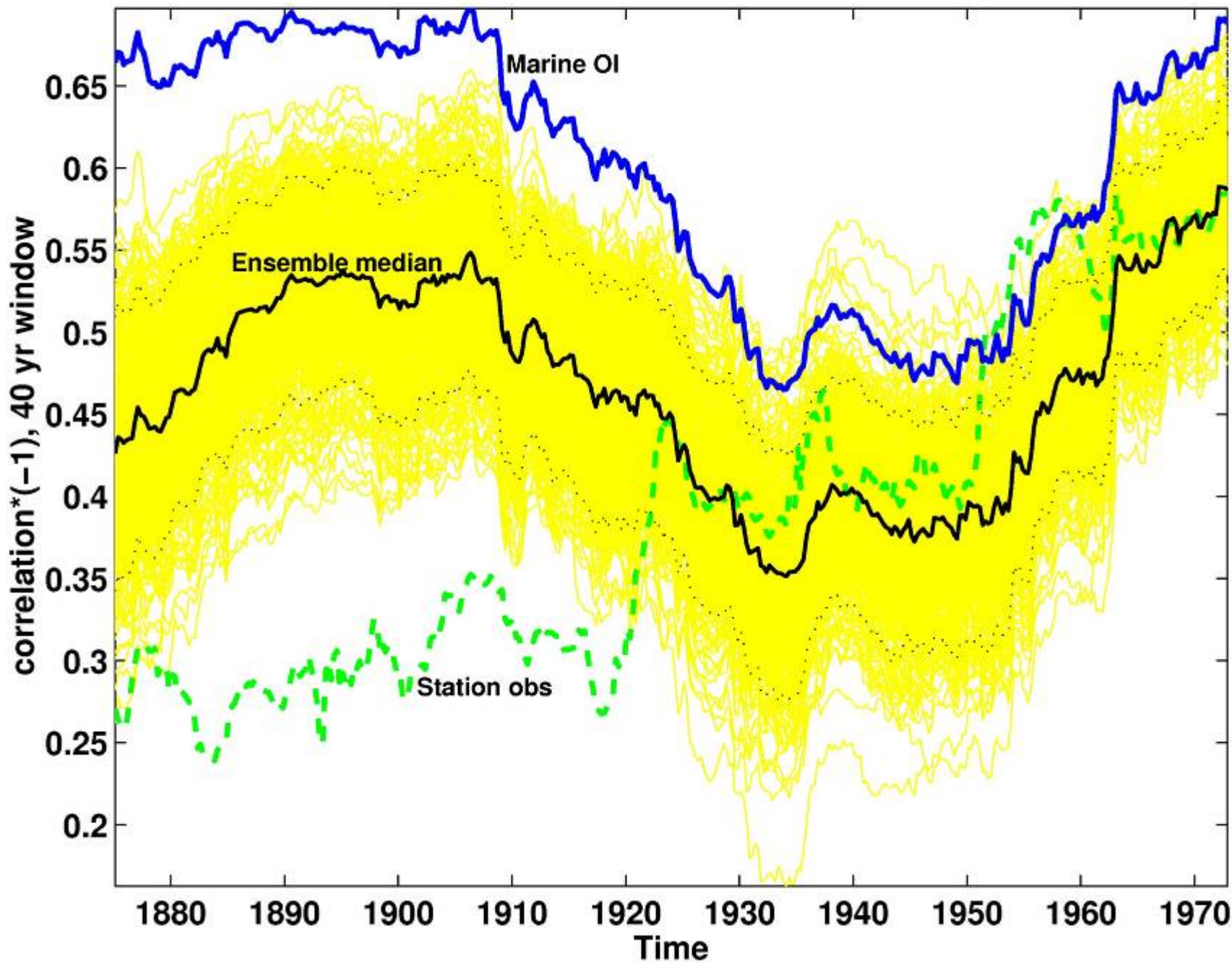
YEAR

SST El Nino indices vs Quinn's historical rankings

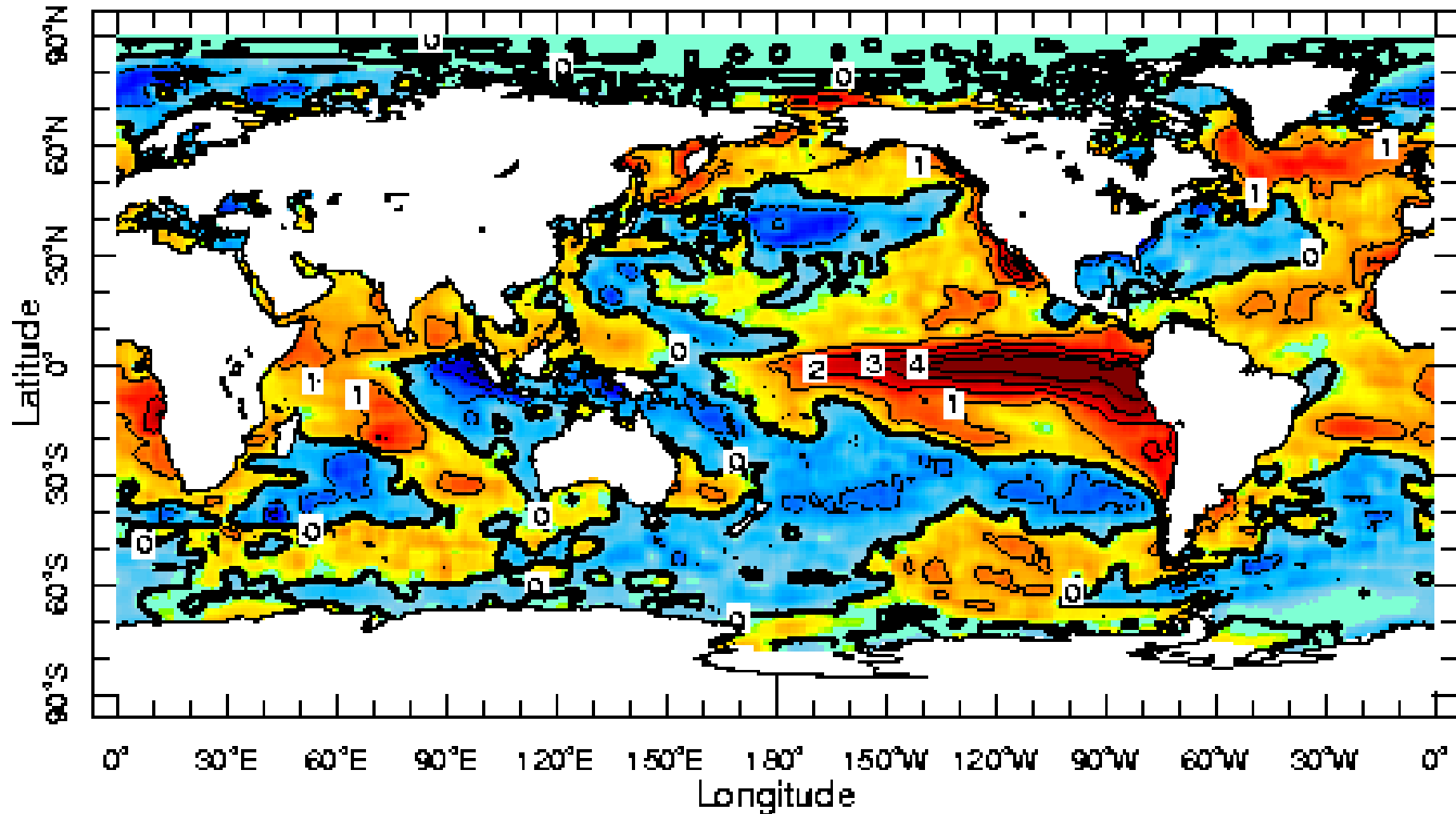


OUTSTANDING PROBLEMS

Correlations between Darwin and Tahiti seasonal atmospheric pressure



Sea Surface Temperature Anomaly (Reynolds and Smith's NCEP OI v.2)

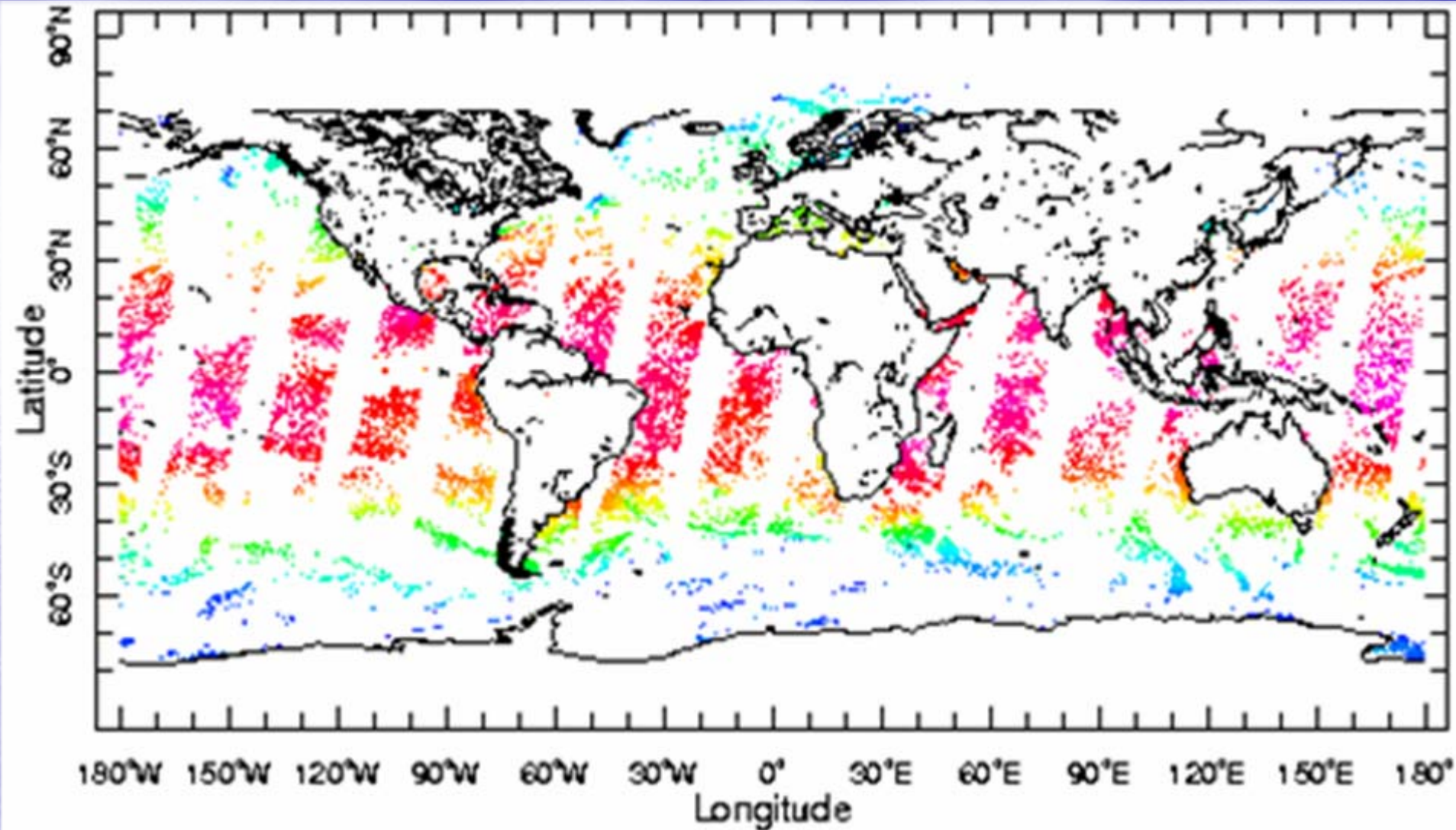


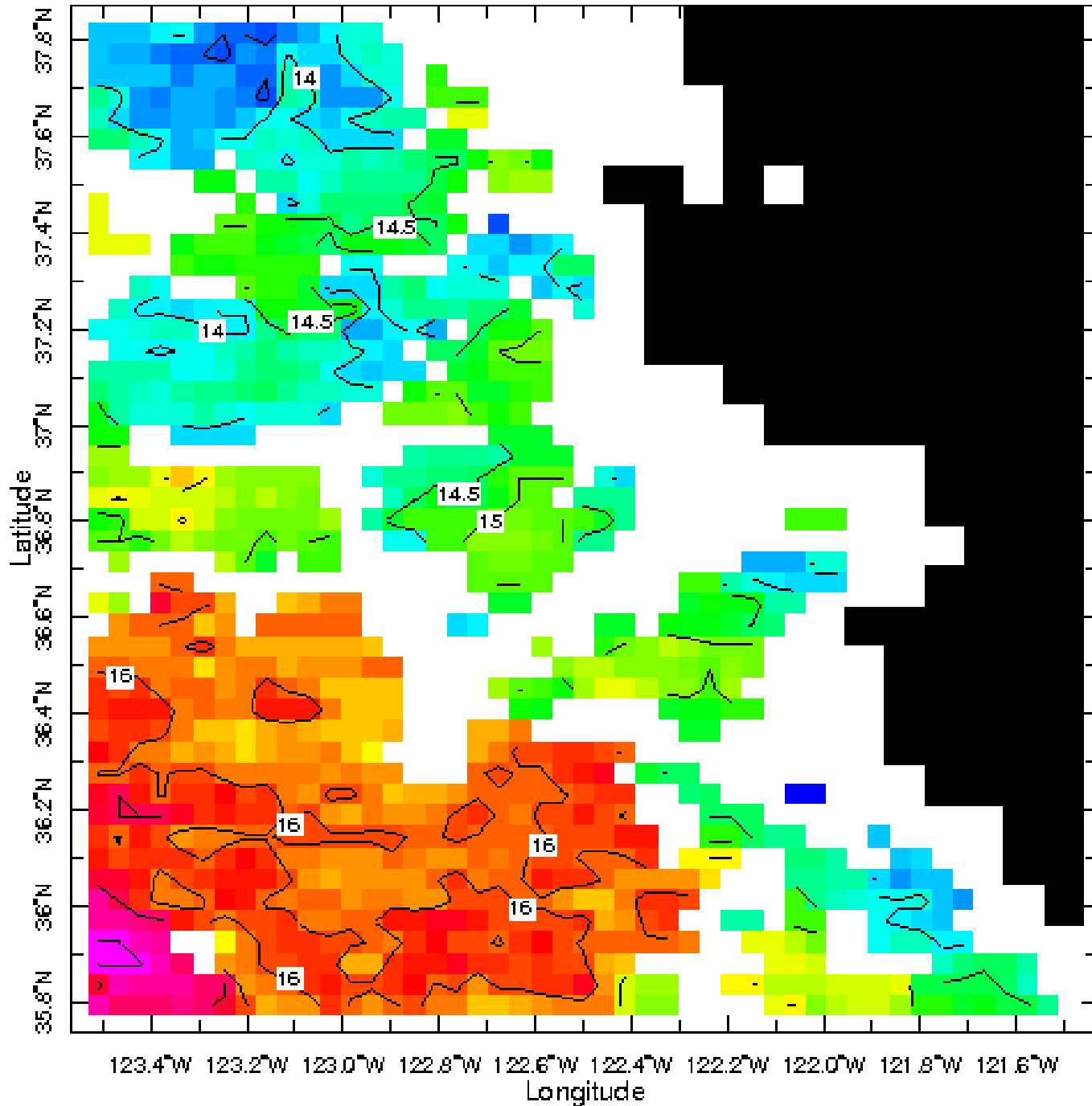
9-15 Nov 1997

MODIS Scanning Swath



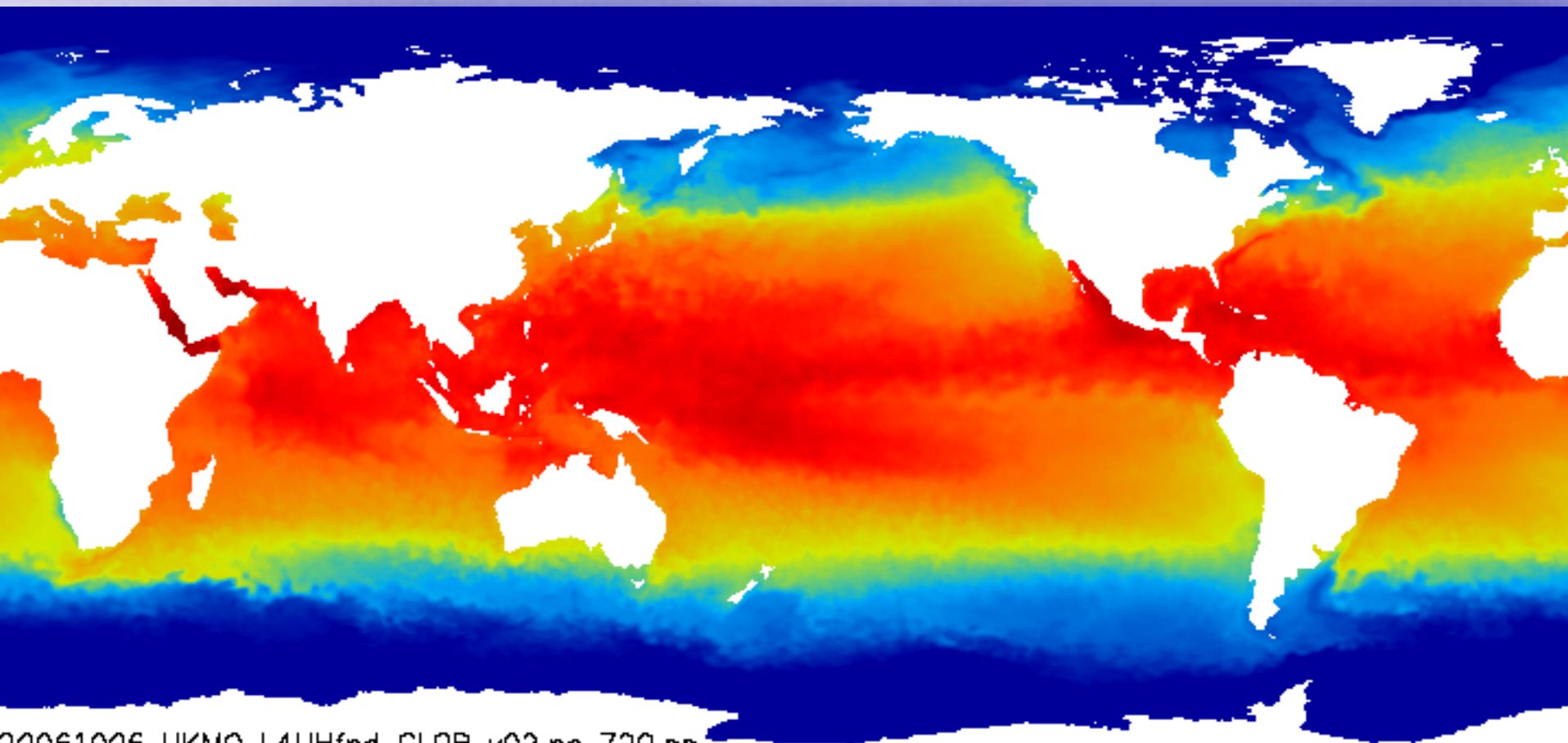
Satellite Sea Surface Temperature Measurements for one day





Pathfinder SST:
Monterey Bay,
Oct 8, 1996
4km resolution

Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA), from U.K. Met Office and GHRSSST, blend of many satellite data streams

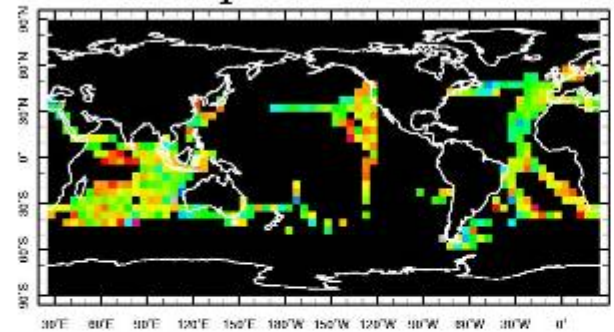


20061006_UKMO_L4UHfnd_GLOB_v02.nc_720.pp
Copyright Met Office 2006

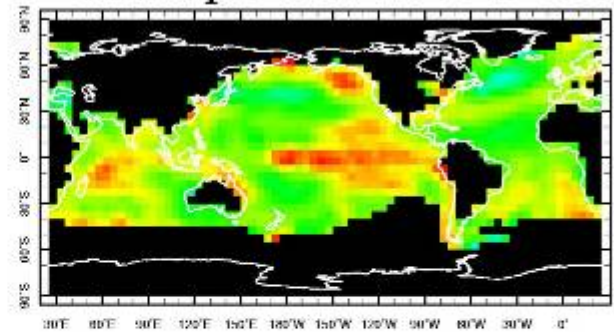
INVESTIGATION OF WHAT IS "LOST":

ERROR OF TRUNCATION

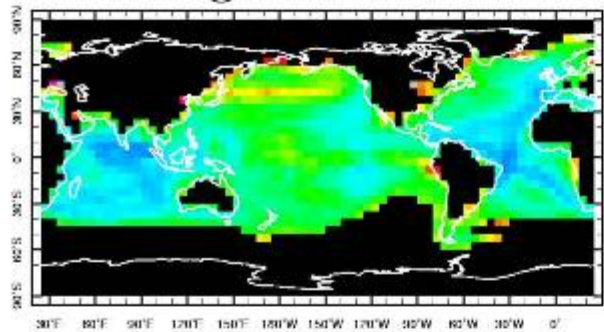
(e) Observations of Dec 1986 resampled as in Dec 1877



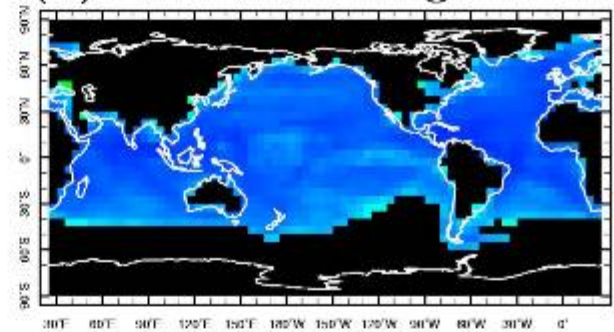
(f) Analysis of Dec 1986 for obs resampled as in Dec 1877



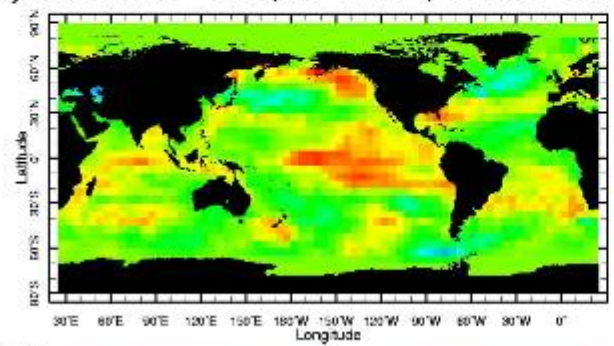
(g) Estimated large scale error for 1877



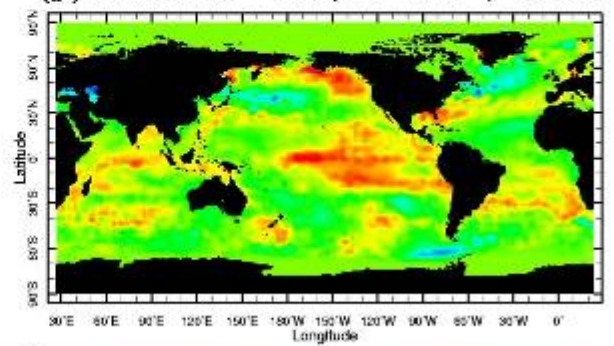
(h) Estimated large scale error for 1986



(i) NCEP OI, $5^\circ \times 5^\circ$; Dec 1986

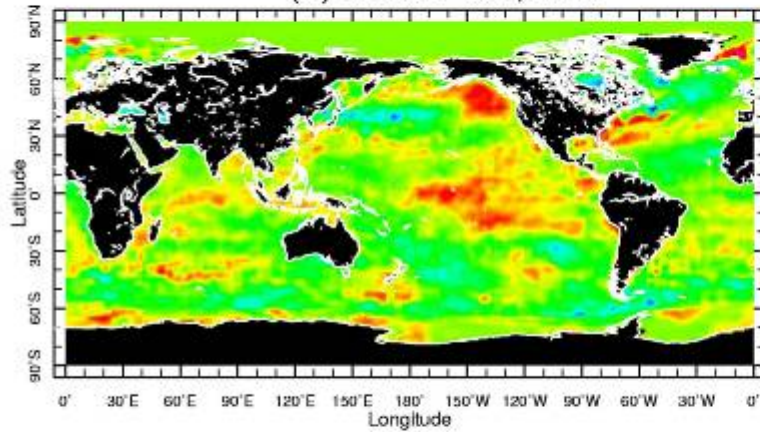


(j) NCEP OI, $1^\circ \times 1^\circ$; Dec 1986



December 1986

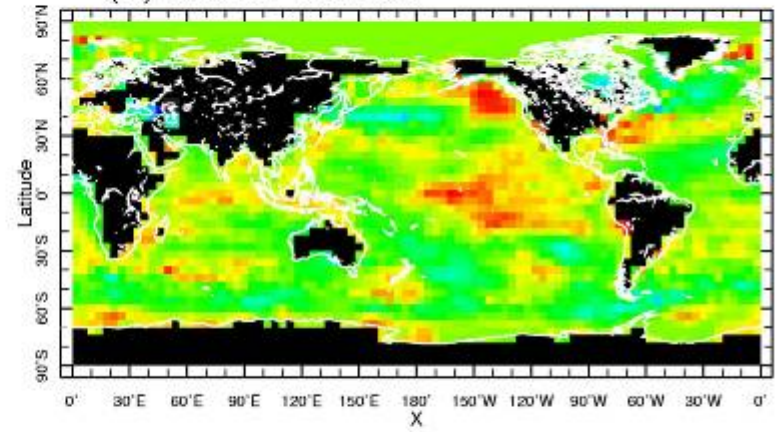
(a) NCEP OI, 1x1



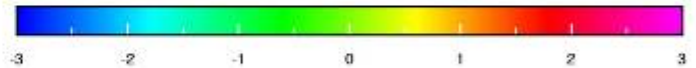
Olv2 ssta T=Dec 1986
point mean: 0.00872406 ± 0.64682 range [-5.5607 to 3.9531]



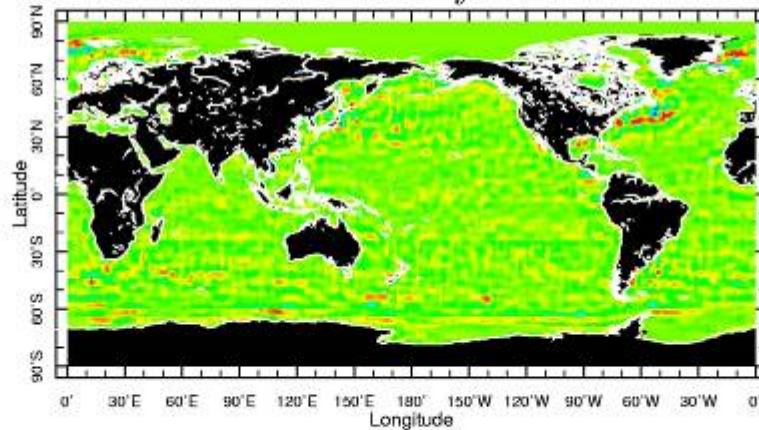
(b) NCEP OI: 4x4



Olv2 ssta T=Dec 1986
point mean: 0.00392506 ± 0.62818 range [-5.1969 to 3.3084]



Small-scale variability: 1x1-4x4

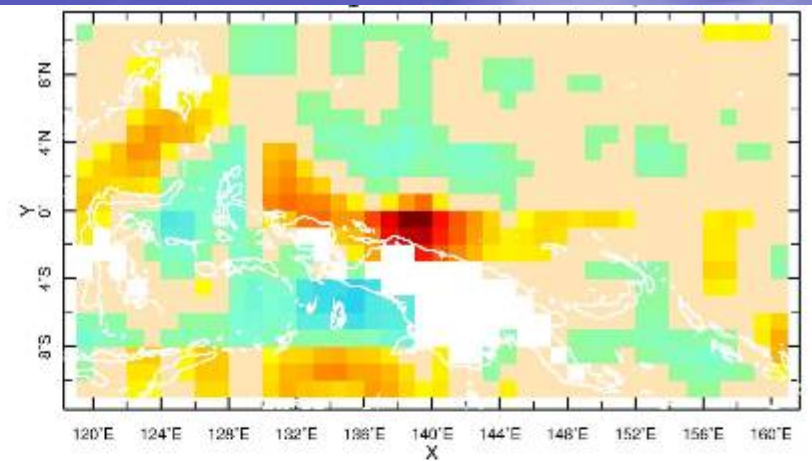
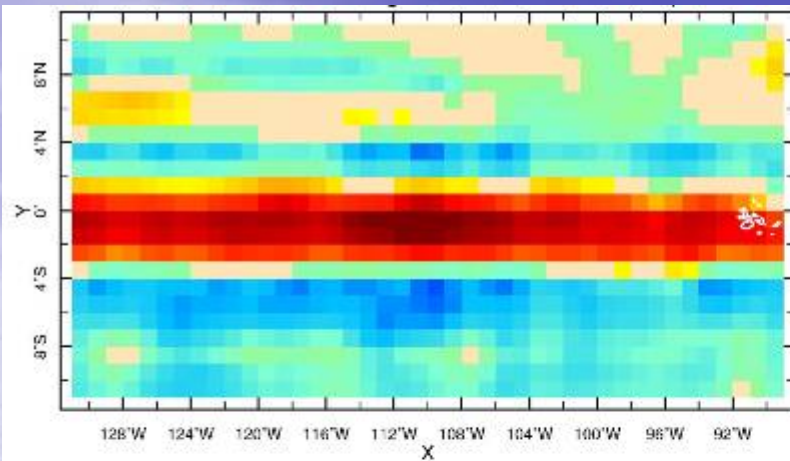


[Olv2 ssta] - [Olv2 ssta] T=Dec 1986
point mean: 0.000300759 ± 0.19686 range [-2.3099 to 2.2916]

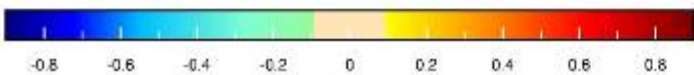
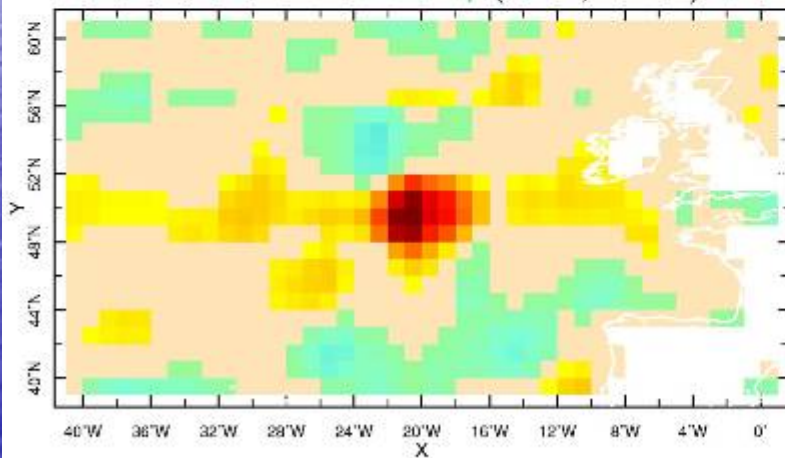


Truncation error autocovariance patterns: Eastern Equatorial Pacific at 110W

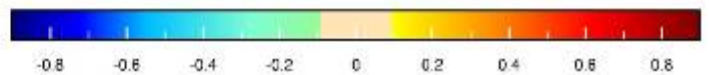
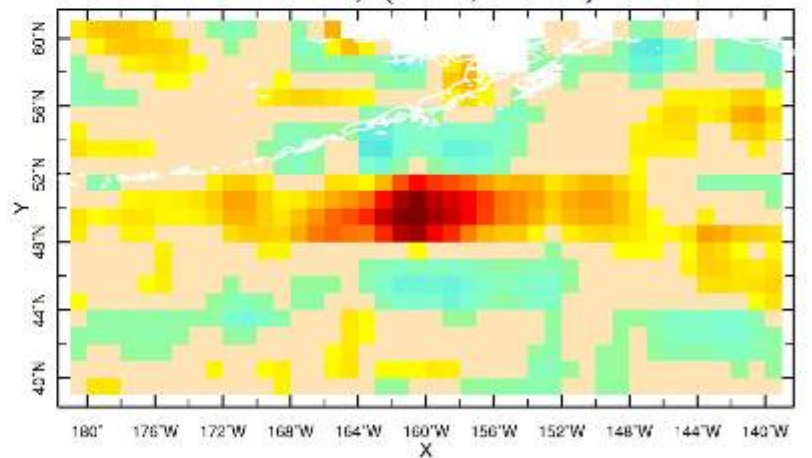
Western Equatorial Pacific at 140E



North Atlantic, (50N, 20W)



North Pacific, (50N, 160W)



Scale separation in a field estimate

OI problem: estimating a field \mathcal{T} from a first-guess (background) solution \mathcal{T}^b and an incomplete set of observations \mathcal{T}^o is given by:

$$\begin{aligned}\mathcal{T}^b &= \mathcal{T} + \varepsilon^b, & \langle \varepsilon^b \rangle &= 0, & \langle \varepsilon^b \varepsilon^{bT} \rangle &= C, \\ \mathcal{T}^o &= H\mathcal{T} + \varepsilon^o, & \langle \varepsilon^o \rangle &= 0, & \langle \varepsilon^o \varepsilon^{oT} \rangle &= R.\end{aligned}$$

The solution to this OI problem is a minimizer $\hat{\mathcal{T}}$ of the cost function

$$\mathbf{S}[\mathcal{T}] = (H\mathcal{T} - \mathcal{T}^o)^T R^{-1} (H\mathcal{T} - \mathcal{T}^o) + (\mathcal{T} - \mathcal{T}^b)^T C^{-1} (\mathcal{T} - \mathcal{T}^b).$$

$$\hat{\mathcal{T}} = CH^T (R + HCH^T)^{-1} \mathcal{T}^o.$$

$$C = E\Lambda E + E'\Lambda'E' = E\Lambda E + C'$$

$$\hat{\mathcal{T}} = E\hat{\alpha} + \Delta\hat{\mathcal{T}}.$$

$$\mathcal{T}^o = HE\alpha + \check{\varepsilon}^o, \quad \langle \alpha\alpha^T \rangle = C', \quad \langle \check{\varepsilon}^o\check{\varepsilon}^{oT} \rangle = HC'H^T + R.$$

$$\hat{\alpha} = \Lambda E^T H^T (HE\Lambda E^T H^T + HC'H^T + R)^{-1} \mathcal{T}^o.$$

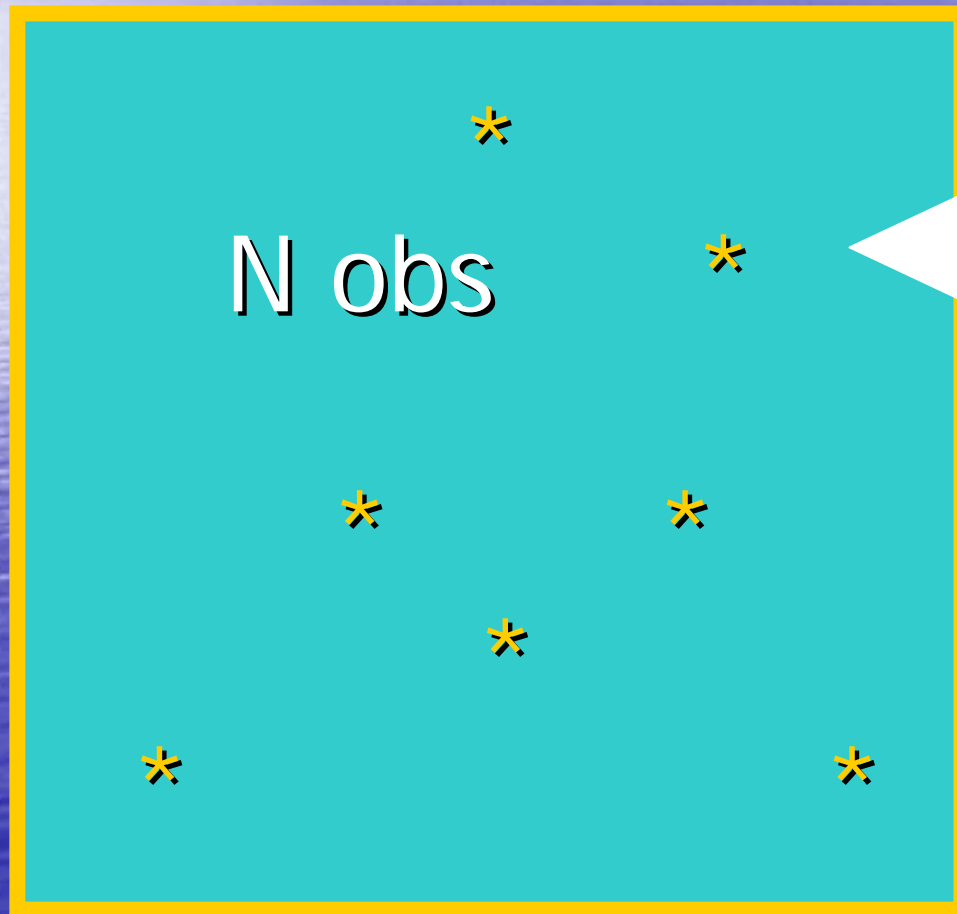
Observational residual: $\Delta\mathcal{T}^o = \mathcal{T}^o - HE\hat{\alpha}$

$$\Delta\mathcal{T}^o = H\Delta\mathcal{T} + \varepsilon^o, \quad \langle \Delta\mathcal{T}\Delta\mathcal{T}^T \rangle = C', \quad \langle \varepsilon^o\varepsilon^{oT} \rangle = R.$$

$$\Delta\mathcal{T} = C'H(HC'H^T + R)^{-1} \Delta\mathcal{T}^o$$

OBSERVATIONAL ERROR OF IN SITU DATA

What is the error in the binned obs mean
(as estimates of the "true" bin area average)?



$F(x,y)$ [or $F(x,y,t)$]



Error variance
for the mean
of N observ is
 σ^2/N

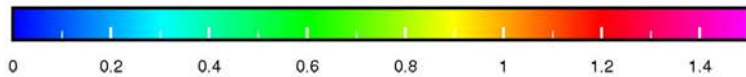
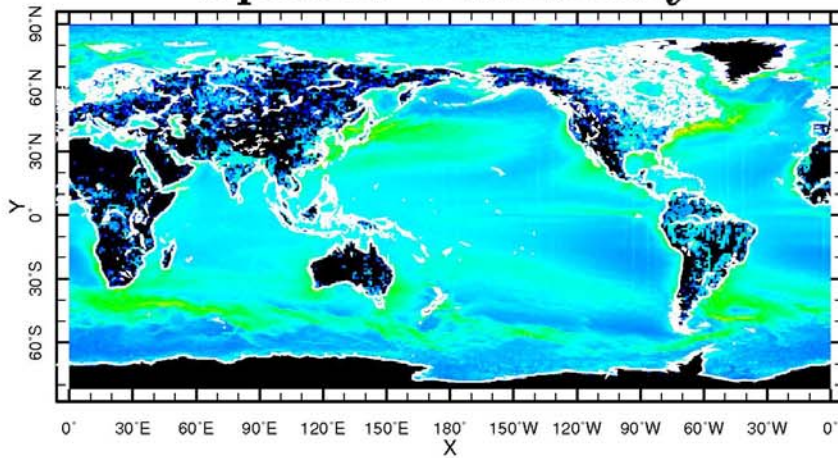
High spatial and temporal resolution of satellite data can help pinpoint natural SST variability on small scales (below 1 deg) and short terms (within 1 month).

A few weeks of background processing of 20 years of daily 4km maps of Pathfinder SST gave us the SST variability inside 1x1 monthly boxes estimated.

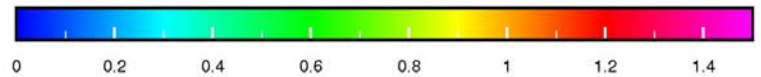
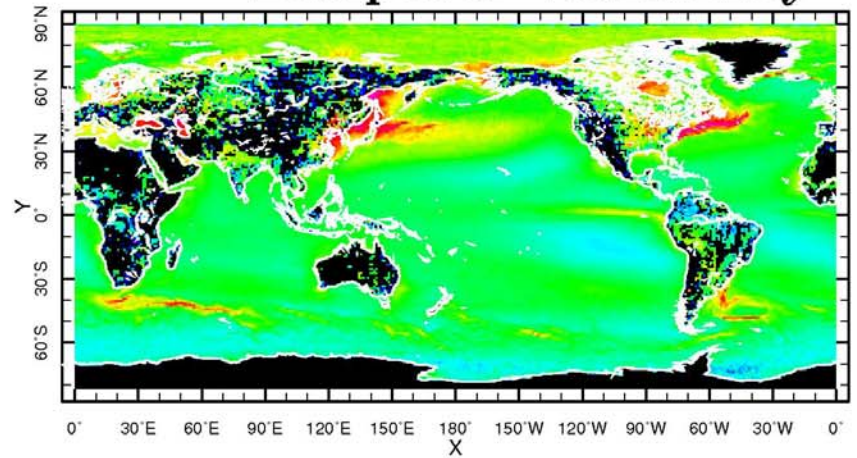
[http://rainbow.ideo.columbia.edu/~alexeyk/Satellite_SST.html]

Small-scale variability in SST, °C

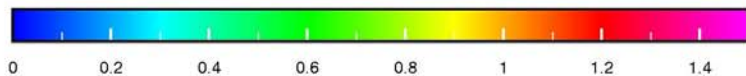
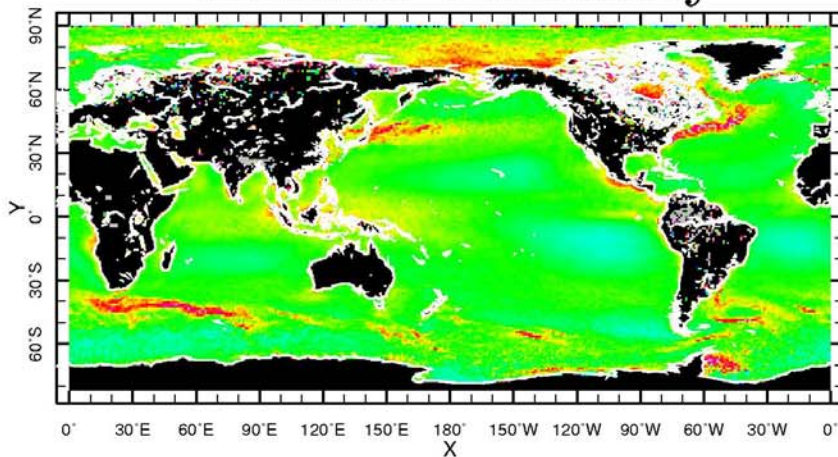
Spatial Variability



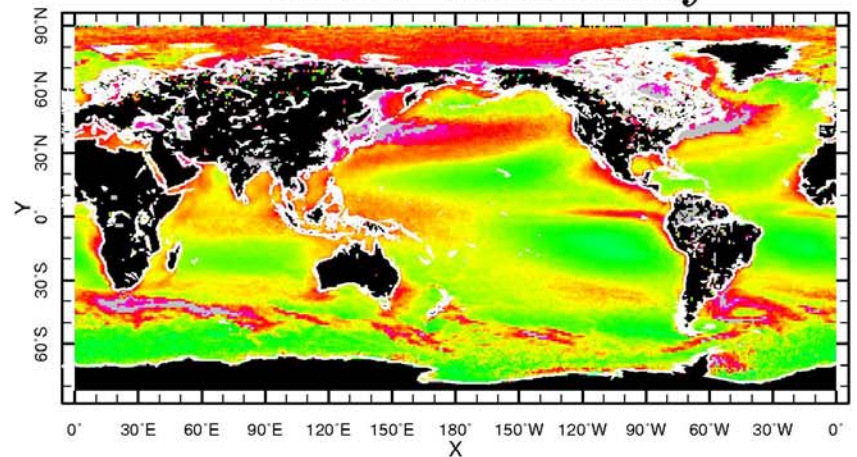
Temporal Variability



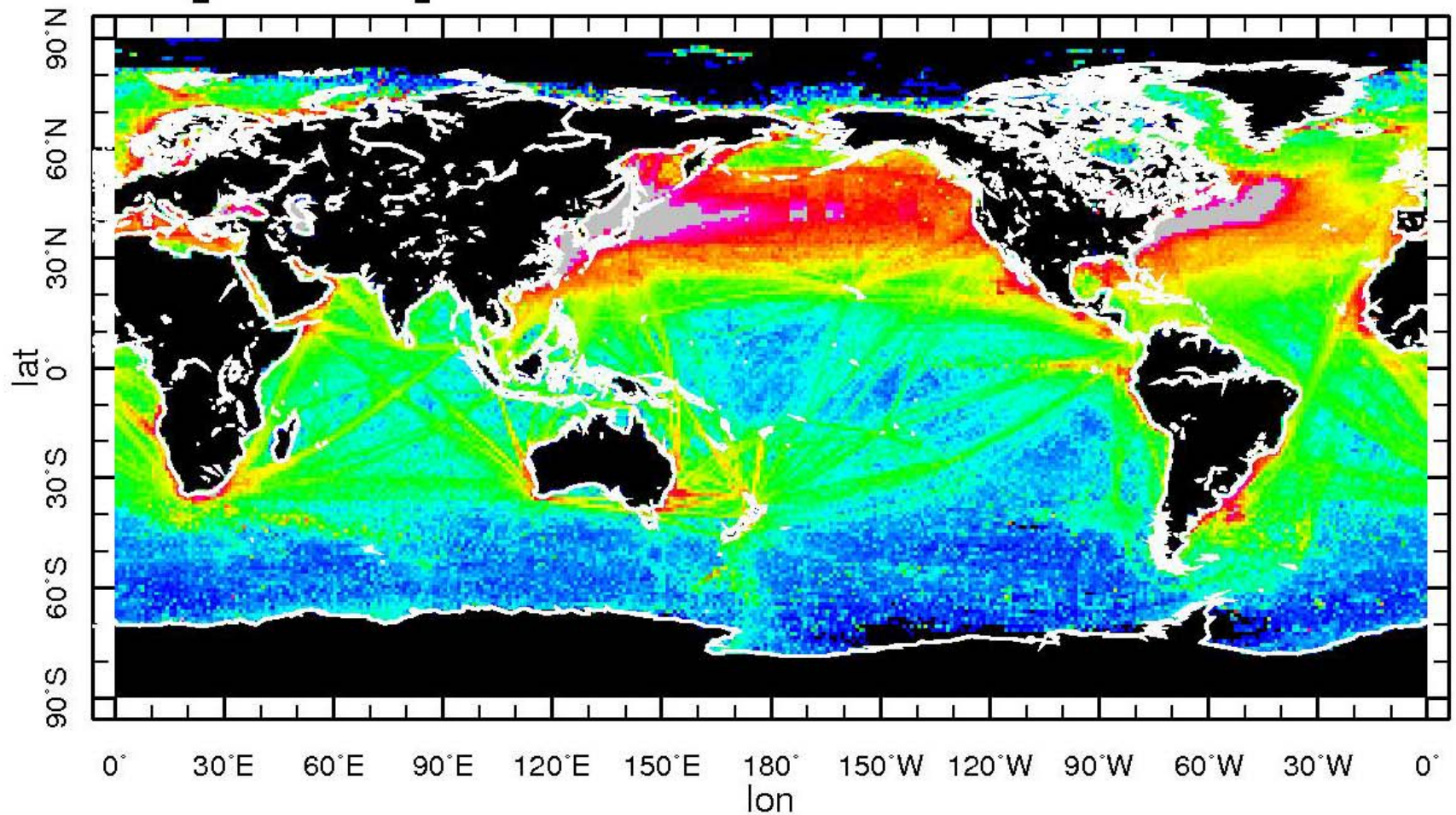
Diurnal Variability



Total Variability



STD[SST] in ICOADS $1^{\circ} \times 1^{\circ}$ bins

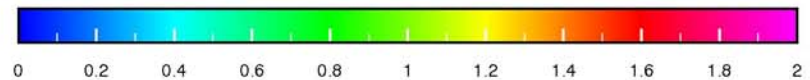
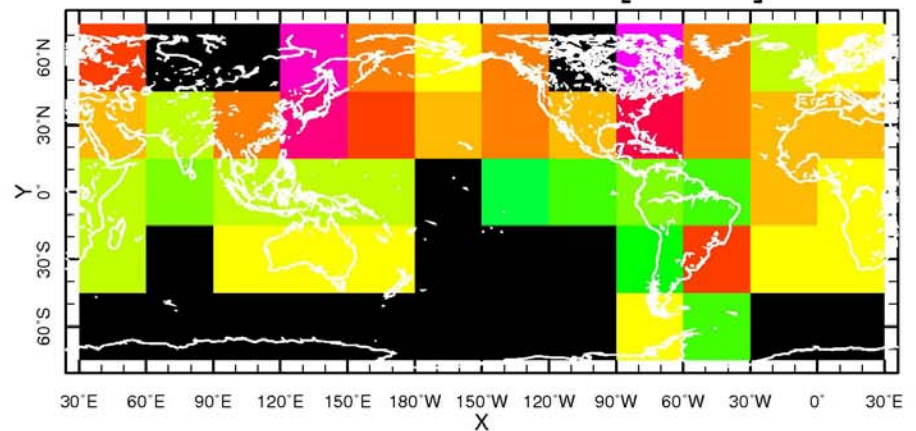
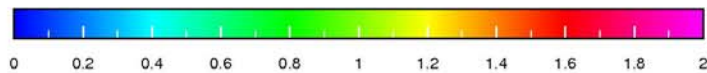
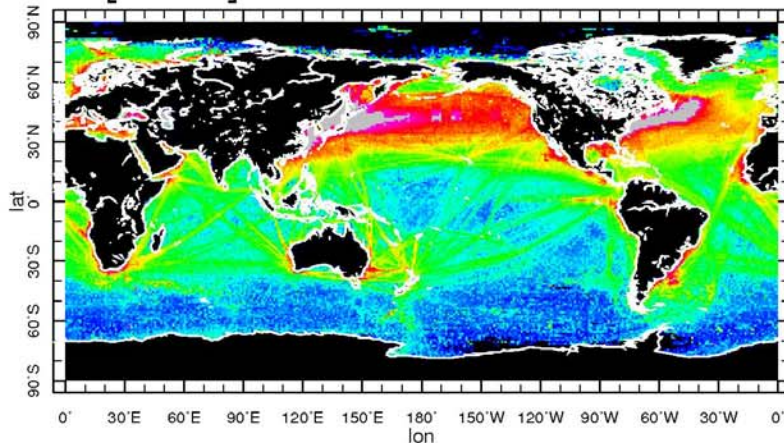


0 0.2 0.4 0.6 0.8 1 1.2 1.4 1.6 1.8 2

Measurement error (or very small-scale variability) has to be taken into account

Effects of measurement error

STD[SST] in ICOADS $1^\circ \times 1^\circ$ bins Kent and Challenor [2006] estimate

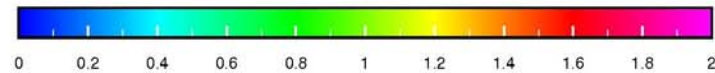
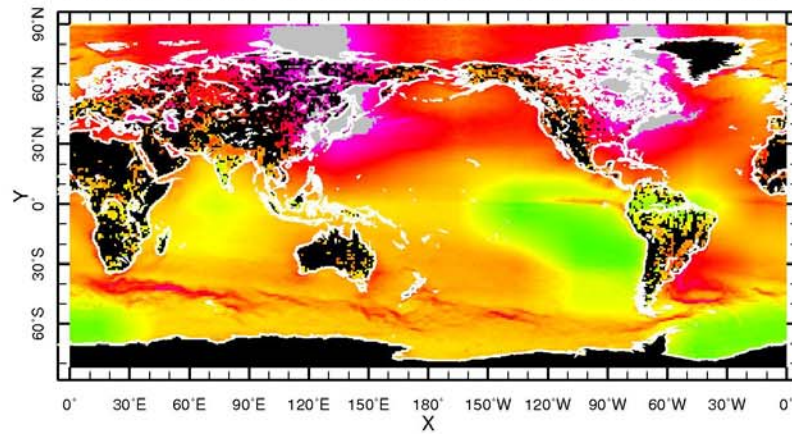
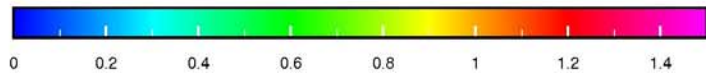
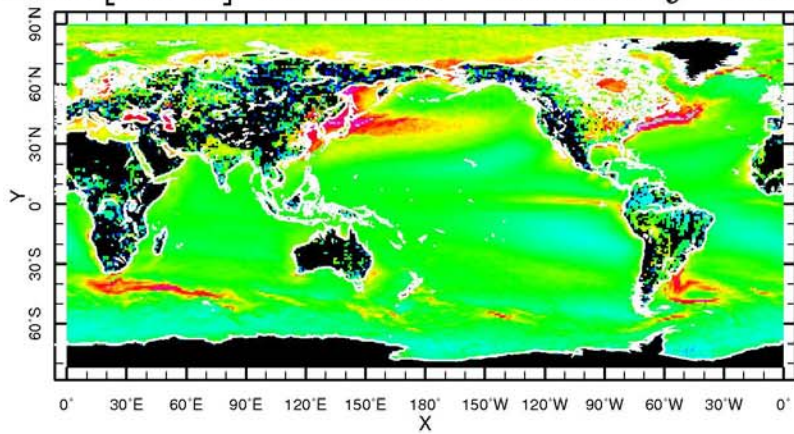


Combining the two estimates to obtain σ :

Sampling error estimates for a single observation

STD[SST] in $1^\circ \times 1^\circ$ monthly bins

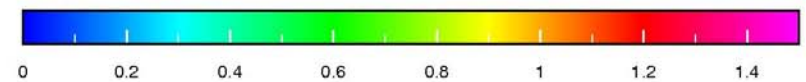
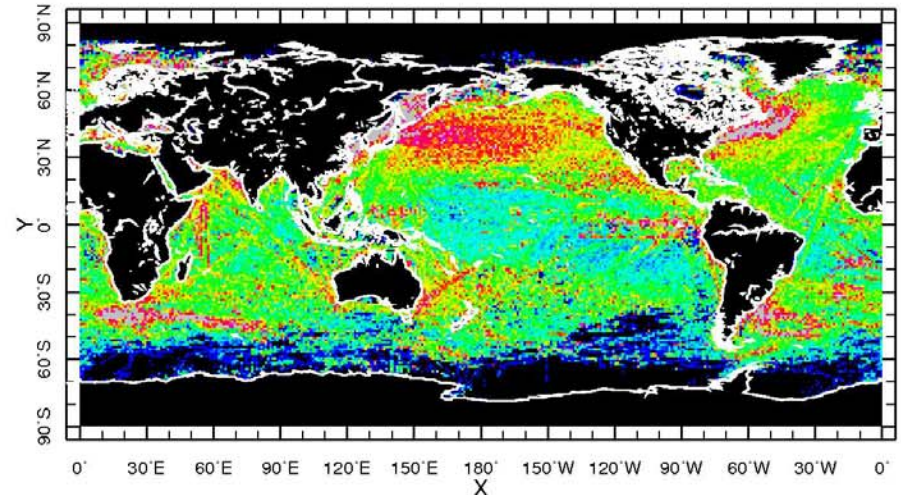
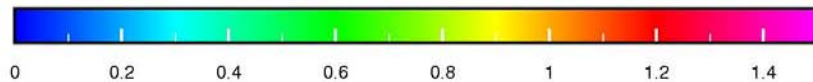
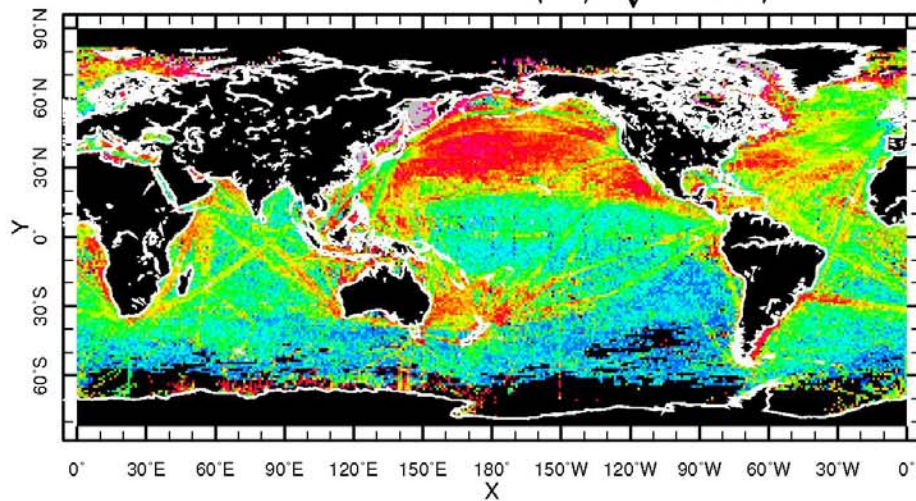
With the addition of KC2006 estimate



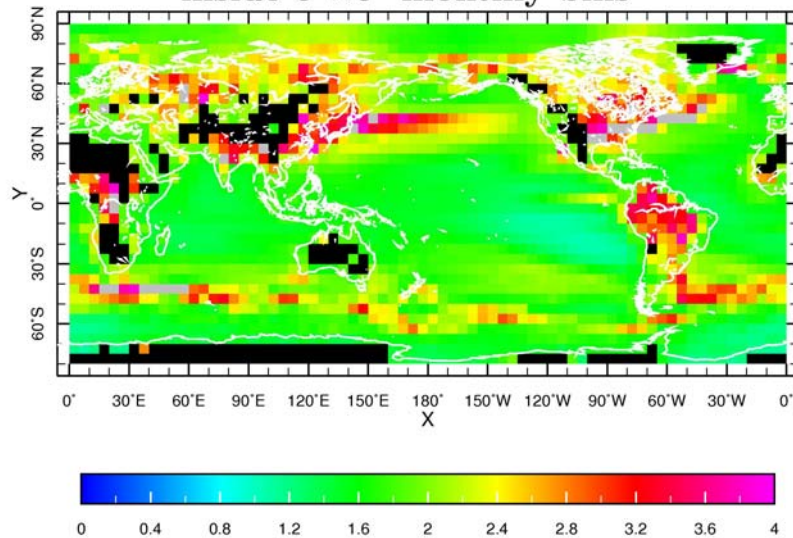
Does left look like right?

Modeling in situ data error for 1° bins
Modeled as $\langle \sigma / \sqrt{n_{\text{obs}}} \rangle$

Actual MODIS-ICOADS STD

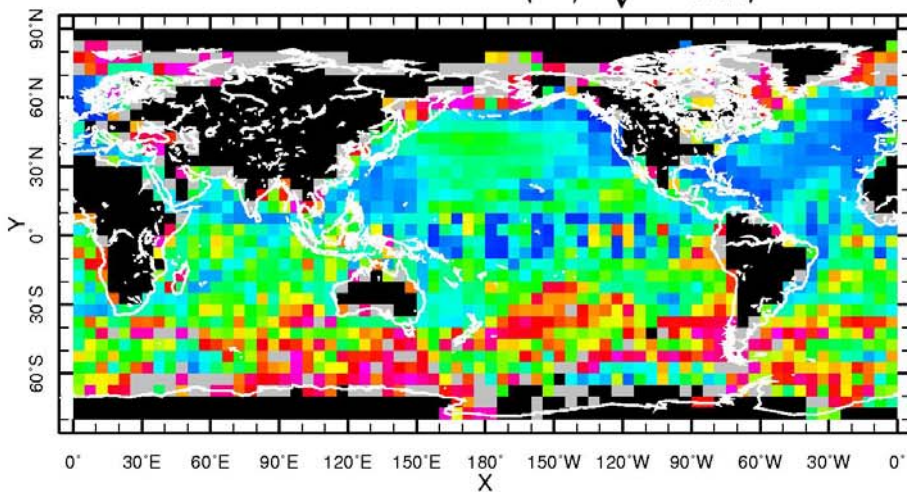


Single observation SST sampling+measurement error, °C,
inside 5°×5° monthly bins



Modeling in situ data error for 5° bins

Modeled as $\langle \sigma / \sqrt{n_{\text{obs}}} \rangle$



Actual MODIS-ICOADS STD

