REDUCED SPACE APPROACH TO THE OPTIMAL ANALYSIS OF HISTORICAL MARINE OBSERVATIONS: ACCOMPLISHMENTS, DIFFICULTIES, AND PROSPECTS

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1. INTRODUCTION

Use of leading empirical orthogonal functions (EOFs) for reconstructing historical data sets has become quite popular in recent years (Shriver and O'Brien (1995), Smith et al. (1996), Rayner et al. (1996), Mann et al. (1998)). Kaplan et al. (1997) combined this approach with the least squares based optimal estimation to formulate reduced space analogues of the traditional technique of optimal analysis (optimal interpolation, Kalman filter, optimal smoother). Applications of this technique to the historical data sets of sea surface temperature and marine sea level pressure resulted near-global monthly analyses of these variables going back to more than 140 years accompanied by the error bars (Kaplan et al. (1998,1999)) which are publicly available. The assumptions underlying the method, namely the stationarity of the mean field and covariance of the signal, have been recently criticized (Hurrell and Trenberth (1999)). Additionally, the current settings of the analysis results in globally incomplete fields of comparatively sparse resolution ($4\div5^o$ grid size) which limits considerably the use of such analyses in GCM studies. In section 2 we bring the reduced space optimal analysis into the context of more traditional objective data analyses and summarize its advantages and existing applications. Section 3 discusses the current difficulties in applications of the method and suggests the ways of resolving them. Section 4 concludes the paper by emphasizing the prospects of the method and directions for the further applications.

2. ACCOMPLISHMENTS

2.1. Theoretical background

Least-squares-based popular methods of data analysis, such as optimal interpolation (OI), Kalman filter (KF), or optimal smoother (OS), are supposed to give optimal solutions if certain requirements are satisfied, among which is that covariance matrices of all errors involved are known. However, in actual applications to the problems of climate research the realistic dimensions of data are often large enough to warrant two outcomes:

1. error covariance matrices are not known in all their details since there are not enough data to resolve them completely, so some crude parameterizations are used instead,
2. if no simplifications are done, optimal data analysis procedures are very expensive (OI), extremely expensive (KF), or prohibitively expensive (fixed-interval OS).

Both these difficulties, however, can be dealt with at once if certain features of optimal solutions of realistic climate fields are taken into account.

Consider as an example a standard OI problem whose solution is a minimizer $\mathcal{T}$ of the cost function

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

Here $\mathcal{T}^o$ is a (column-) vector of observations, $\mathcal{T}^b$ is a first guess (background) solution, H is a transfer matrix from a complete field to the set of observed points, R and C are covariances of observational and first guess errors respectively (for a detailed explanation of notation, terminology and basic facts of optimal estimation a reader is referred to Kaplan et al. (1997)). The two terms of the cost function $\mathbf{S}$ "punish" the solution $\mathcal{T}$ for deviation from observations and from the background values.

Solution to this OI problem is

$$\mathcal{T} = P\left(H^T R^{-1}\mathcal{T}^o + C^{-1}\mathcal{T}^b\right),$$

where

$$P = \left(H^T R^{-1} H + C^{-1}\right)^{-1}$$

is estimated covariance of its error. According to the Gauss–Markov theorem (e.g., Mardia et al. (1979), Rao (1973)), this solution has minimum error variance among all linear estimates of $\mathcal{T}$, and because of that it is usually referred as the "optimal" solution. In fact, if additional assumptions on the Gaussian distribution of errors or the signal are made, the same solution receives an interpretation as the maximum likelihood estimate, or becomes the best solution among all, even nonlinear estimates, for a wide class of optimality criteria.

Let us subtract the first guess solution from the estimated field, so that the new $\mathcal{T}$ is $\mathcal{T} - \mathcal{T}^b$ and new $\mathcal{T}^o$ is $\mathcal{T}^o - H\mathcal{T}^b$. If the first guess solution is a climatological field, then we have redefined the signal to be a field of anomalies. After such a change in definitions the first guess solution equals zero, so that the signal $\mathcal{T}$ equals the first guess error, and the matrix C becomes the covariance of the signal $\langle \mathcal{T}\mathcal{T}^T \rangle$. It can be expanded into its canonical representation

$$C = E\Lambda E^T, \qquad (2)$$

E being a matrix of eigenvectors (EOFs if C is effectively a sample covariance estimate), and Λ is a diagonal matrix of eigenvalues. We can use eigenvector patterns to rotate an estimated field

$$\mathcal{T} = E\alpha \qquad (3)$$

so that $\alpha = E^T\mathcal{T}$ becomes a new unknown: a vector of projections of a target field on eigenvectors.

For simplicity let us consider the case of a completely observed system ($H = I$) with white uniform error ($R = rI$). OI solution for such a system has a closed form for each component of α:

$$\alpha_i = \frac{\lambda_i}{\lambda_i + r}\alpha_i^o$$

($i = 1 \cdots N$ is an index of components, eigenvalues and eigenvectors, $\alpha^o = E^T\mathcal{T}^o$ is a vector of projections of the observed field $\mathcal{T}^o$ on eigenvectors). We assume that eigenvalues are arranged in a descending order. The usual case then is that $\lambda_N \ll r \ll \lambda_1$. This means that $\alpha_1 \approx \alpha_1^o$, and $\alpha_N \approx 0$. In other words, the standard least squares procedure of OI in its search for the optimal solution will damp the observed values of all eigenvector amplitudes whose energy in the signal does not dominate over the observational error. Eigenvector modes which are expected to have energy much below the level of observational error will not be represented in the OI solution.

Consequently, computing the OI solution in all its details (projection to all EOFs) is superfluous: results as good can be achieved by computing only projections on some set of leading eigenvectors. It should be noted that for many physical variables the most energetic modes are those of the largest spatial scale. Details of the solution on small scales (projection to high number eigenvectors) is controlled by the fine details of the covariance matrix C which usually cannot be reliably estimated from the data. Large scale patterns of C (leading eigenvectors), however, can be estimated in a more reliable way. Approximation of C in (2) by only a few leading terms (truncation) results in infinite coefficients in the second term of the cost function (1) which totally disallow projection of the solution on truncated modes. The same result, of course, can be achieved by truncating the eigenvector representation of the solution (3) to begin with. We call such a truncation a reduced space representation of the solution; inserting the truncated form of (3) into cost functions followed by their minimization with regards to the low-dimensional vector α allowed to develop the reduced space analogues of the OI, KF, and OS algorithms (Cane et al. (1996), Kaplan et al. (1997)).

While these solutions are formally suboptimal among full grid solutions, they are optimal among all reduced space solutions, being also far cheaper and much easier to feed by a priori error covariance information. For the settings which allow direct comparison, the solutions in the reduced space prove to be not inferior to the actually existing full grid solutions (Cane et al. (1996)). The reason for that is the poor representation of small scales in full grid error covariance estimates. As a result, full grid data assimilation on small scales does more harm than good. Moreover, the assimilation for those scales represents the major computational expense of the entire procedure. Hence the savings of reduced space analysis occur at the scales which are not really constrained by the data. Estimation on such scales is meaningless, but the traditional schemes cannot selectively cut off computation there. The tunable nature of the dimension of a reduced space allows to put into the solution all scales down to the smallest resolved by available data, and the choice of leading EOFs for a basis guarantees to some extent the minimal dimension of the analysis space.

When the covariance of a climatic variable is dominated by a few large-scale modes, the generic OI analysis with correctly estimated covariance structures will predominantly reconstruct the patterns manifested in the large-scale climate dynamics. When this is not the case, the results of covariance estimation and of the OI analysis applied to the sparsely observed data are likely to be less robust and more error-prone.

2.2. Applications

We applied the reduced space OS to produce the near-global analysis of $5^o \times 5^o$ sea surface temperature (SST) monthly anomaly grids for the period

1856–1991 (Kaplan et al. (1998)). Observational data used in this work is known as MOHSST5 compilation of ship observations produced by the U.K. Meteorological Office (Bottomley et al. (1990), Parker et al. (1994)). The results of this analysis are available at http://ingrid.ldgo.columbia.edu/SOURCES/.KAPLAN/.RSA_MOHSST5.html

We also applied the reduced space OI analysis to the sea level pressure (SLP) data of Comprehensive Ocean–Atmosphere Data Set (COADS, release 1 extended by standard release 1a; Woodruff et al. (1987, 1993)) to produce $4^o \times 4^o$ fields of SLP monthly anomaly for the period 1854–1992 (Kaplan et al. (1999)). The results are accessible at
http://ingrid.ldgo.columbia.edu/SOURCES/.KAPLAN/.RSA_COADS_SLP1.html.

Note that both analyses utilize only ship observations presented in the form of monthly "superobservations" (Smith et al. (1996)) – mean values for $5^o \times 5^o$ (MOHSST5) or $2^o \times 2^o$ (COADS) bins. The U.K. Met Office applies so called "winsorization" (Bottomley et al. (1990)) to the content of their bins which makes the bin average more similar to a median. The COADS maintains variety of statistical characteristics of the bin contents in their "monthly summaries": in addition to the mean they provide number of observations, their standard deviation, median, sextiles, etc. Pre-war SST data of the U.K. Met Office has Folland and Parker (1995) "bucket corrections" applied to it.

Figure 1 shows the monthly values of the analyzed NINO3 (mean SST for the eastern equatorial Pacific 5^oS–5^oN, 150^o–90^oW), a familiar El Niño – Southern Oscillation index, with 3σ error bars supplied by the analysis. Obviously, the analysis eliminates a great deal of noise present in direct NINO3 estimates from the observed data, and agrees well with the Quinn (1992) list of El Niño events, which is based on a variety of land-based, historical factors known to be associated with El Niño. The summary comparison of annual mean NINO3 with Quinn's data is shown in Figure 2. The relation is strong but not perfect: six El Niño events, rated as "moderate" or weaker by Quinn have in fact negative (as large as -1^{o}C for 1874) annual NINO3 from our analysis. The latest of them has happened in 1943, others in the 19th century. However, the analysis of the Southern Oscillation (SO) and associated coastal phenomena for the period 1926-1986 by Deser and Wallace (1987) suggests that the coastal SST index (like NINO12: average of 10^oS–0^oN, 90^o–80^oW), might show stronger connection to Quinn's index of El Niño events. Indeed, the comparison presented in Figure 2 qualitatively supports this suggestions: only

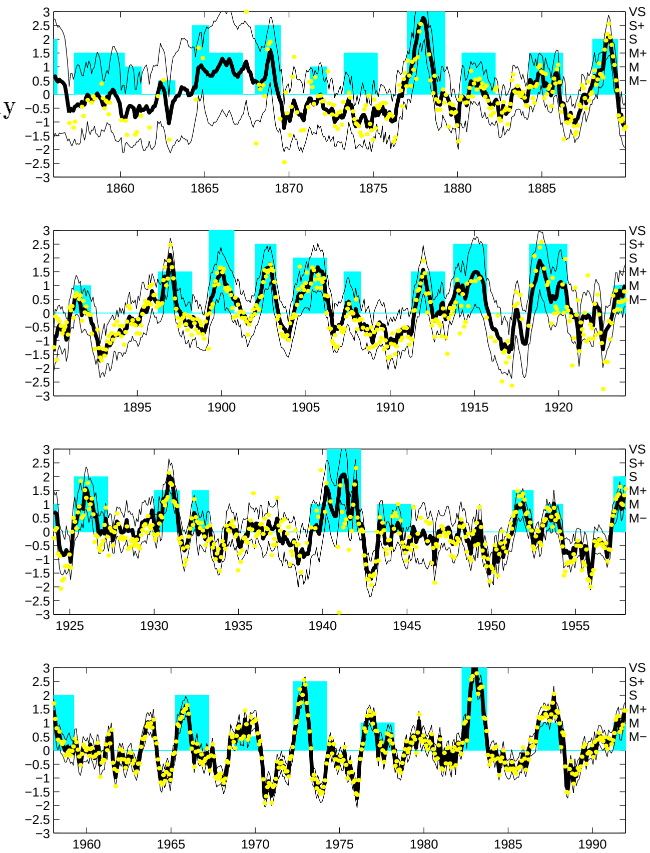

Figure 1: The reduced space optimal smoother reconstruction of the NINO3 index based on ship observations of SST (thick solid line) (Kaplan et al. (1998)). Also shown are 3σ error bars on the analysis values (thin lines), the straight estimates of NINO3 from raw data (dots), and the ENSO event ratings of Quinn et al. (1992) (histogram bars). Histogram bars are scaled to the Quinn et al. (1992) ratings: M-, M (moderate), M+, S (strong), S+, and VS (very strong).

3 events have negative (none below -0.5^{o}C) NINO12, the latest of them happening in 1907. The ability of the analysis to distinguish between geographically close but functionally different area averages (like NINO3 and NINO12 above) is encouraging, because the small-scale differences between close areas could be lost in the sampling and observational noise which our technique is filtering out in the attempt to reconstruct the large-scale dominant structures.

Kaplan et al. (1999) present the comparison of SLP time series measured at a few island or coastal stations (Darwin, Tahiti, Reykjavik, and Gibraltar) affected by large-scale atmospheric phenomena (SO and North Atlantic Oscillations) with their "marine-based proxies" – averages of analyzed COADS SLP over a few analysis grids surrounding a station. The proxies compared favorably with the land-based measurements, despite being produced from the much inferior quality ship report data. Significant portion of this success should be attributed to the fact that the major part of the SLP signal on the stations we considered comes from the large-scale atmospheric oscillations which are being predominantly reconstructed by the global analysis of marine data.

Figure 3 compares correlation coefficients between Darwin and Tahiti station data (Können et al (1998), Ropelewski and Jones (1987)) with the same for these station's marine-based proxies (Kaplan et al. (1999)). Both coefficients are computed in different width time windows and presented as functions of time. The correlation coefficients are close for the modern period, but the land station values are lower during earlier times. We suggest that the correlation between the land-based data weakens for the early part of the record because of degraded data quality. At the same time, the sparser and more erratic marine data forces the analysis to reproduce less of smaller scale (and thus more error-prone) phenomena, and to leave mostly the large-scale SO-associated pressure changes in the reconstruction. That strengthens the correlation between the analysis proxies for Darwin and Tahiti which are located near antinodes of the SO.

In fact, correlation between Darwin and Tahiti SLP records has traditionally been interpreted (Trenberth (1984)) as an indicator of the signal-to-noise ratio when these station records are used as the indices of the SO (in this case the SO is the "signal", everything else is the "noise"). Note that the most of the weakening episodes in 6-year window correlations exhibited by the land stations in the early part of the record are mimicked by the marine proxy correlations. Those episodes are most likely the realistic changes in the strength of SO relative to the back-

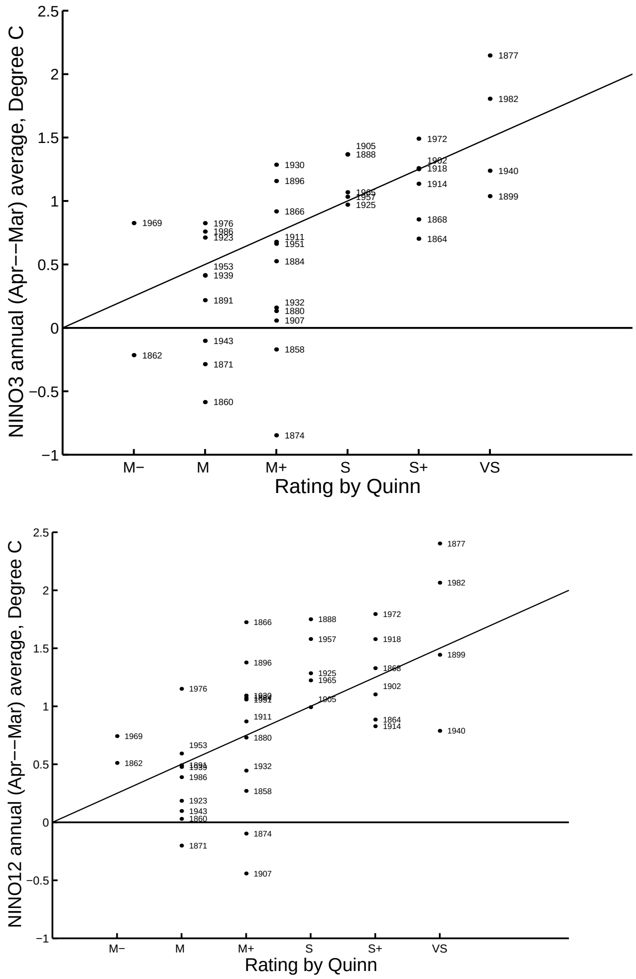

Figure 2: (top) Summary of shown in Figure 1 comparison of reconstructed NINO3 with the Quinn et al. (1992) ratings of El Niño events: events are represented by points on a (Quinn's rating, annual NINO3) plane; (bottom) same for NINO12.

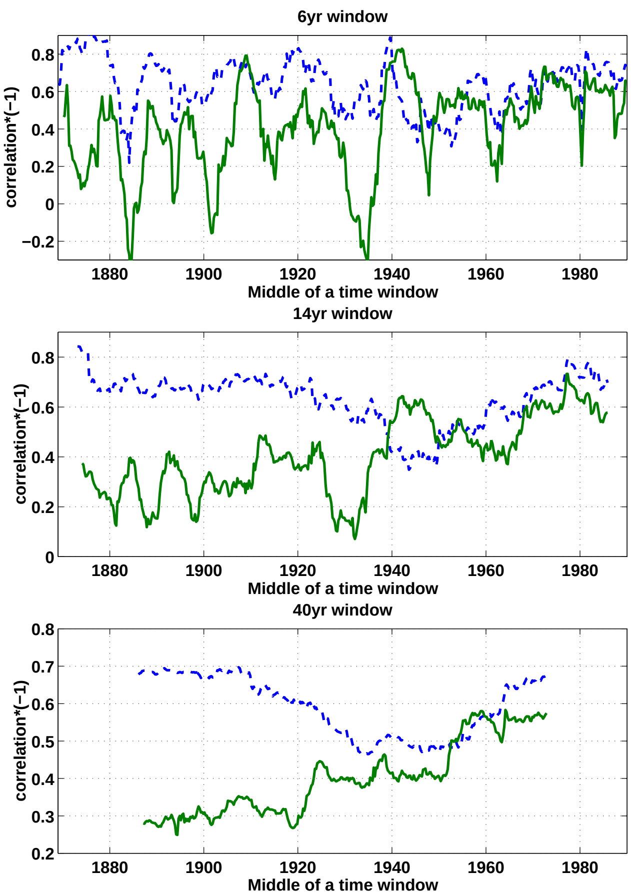

Figure 3: Correlation coefficient between Darwin and Tahiti land station records (solid lines) and their marine-based proxies (dashed lines) shown as a function of time for time windows of 6, 14, and 40 years

ground atmospheric noise. Those which are present in the land records only might be either spurious or missed in the marine records because of the sparsity of COADS coverage at those particular times. The level of certainty of the latter possibility may change significantly when the SLP from the “Dutch” deck, a major COADS component prior to World War II, is included in the monthly summaries in further COADS releases (Woodruff et al. (1998)). Even at the present level of coverage the indices based on ship observations may provide cleaner indication of the large-scale phenomena than the local land-based records.

3. DIFFICULTIES AND WAYS TO RESOLVE THEM

3.1. Specification of observational uncertainty

Advantages of the reduced space optimal analysis do not come for free: they are based on our knowledge of a priori estimates, namely covariances of observational error R and of the first two statistical moments of the solution: its mean field $\mathcal{T}_m$ and its covariance C. All these necessary values can be computed only approximately from the observations.

In computing R (which allows the analysis to distinguish between poor and high quality superobservations) we use intrabox variability and number of observations for the superobservational bins. When we analyze the U.K. Met Office SST data, we have to estimate their intrabox standard deviations from the COADS monthly summaries because the U.K. Met Office does not maintain any intrabox statistics but winsorized means in its official data format. Our estimates of observational error are far from being perfect: Figure 4 shows the map of our estimated single ship observational error compared to $5^o\times5^o$ superobservations (these values were used in the analysis of Kaplan et al. (1998)). Comparison of this map with the map of random error estimates by Kent et al. (1999) brings uneven conclusions. The latter map does not include any kind of sampling error. This explains the much larger values of Figure 4 in the regions of Gulf Stream and Kuroshio Current. However, outside of these areas the map of Figure 4 should still be giving larger values everywhere. This does not seem to be the case, but the rough correspondence between the maps' values is still encouraging. For the SLP the contribution of sampling variability into our estimates of a single ship error (not shown) is so large, that our COADS-based estimates (used by Kaplan et al. (1999)) exceed those of Kent et al. (1999) by the factor of 3 in the midlatitudes

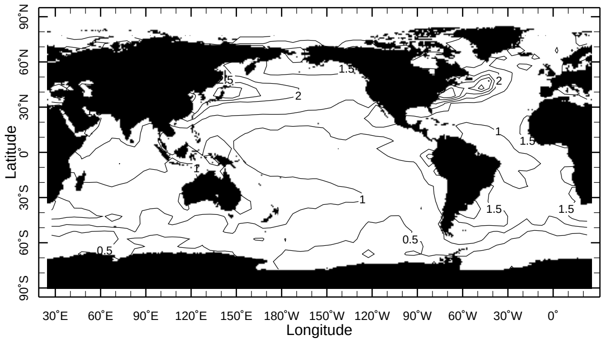

Figure 4: Intrabox SST variability, ^oC, inside $5^o \times 5^o$ bins, estimated from COADS, and used as a single ship error by Kaplan et al. (1998)

and marginally in the tropics.

Clearly a lot more work should be done in this direction till really reliable observational error estimates will enter gridded analyses of climate variables. Important step on this way would be to bring to the attention of all data centers the necessity to include the statistics of intrabox distributions into their standard data formats, rather than just provide box mean values. This seems to be particularly crucial in the planned blending project of the COADS and UKMO data banks (Woodruff et al. (1998)).

3.2. Characterization of the signal

The problems with the reliable estimation of $\mathcal{T}_m$ and C are even more fundamental. Ideally, these statistical characteristics of the signal are supposed to be applicable to the entire period of the analysis. In fact, poor data quality and sparse coverage in the early part of the record forces us to use only the modern data period for the derivation of $\mathcal{T}_m$ and C. In the applications described above we used climatological means for the period 1951-1980 and estimated the covariance for the period from 1950 to the end of the record. Analysis is then done using these values for as far back as the middle of the 19th century.

Problems with the mean. It is been observed by Hurrell and Trenberth (1999) that a linear trend for the 20th century computed from our SST analysis shows somewhat less of the warming than other estimates. They suggested that it happens due to our “stationarity” assumption: the hypothesis that the modern-period mean and covariance are applicable for the entire record. If in fact the long-term variability of SST (e.g. trend) resulted in a much different mean SST state for the first half of the century, and the pattern of this change is not well-represented by the modern-period covariance, the analysis might underestimate this change.

At present we are addressing this issue via the analysis of data residuals, the difference between the observed data and our analysis. These residuals presumably consist of two major components: observational and sampling error and part of long-term variability unresolved by the analysis. Because of very different characteristics of these components, it should be relatively easy to isolate the latter. Prospective methods of isolation include application of the reduced space OI and OS technique to the residuals and covariance reestimation (Kaplan et al. (1997, 1999)) and polynomial spline smoothing of the residuals (Wahba (1990)). Note that bestfitting a straight line or other slowly changing function of time to the residuals can be brought into the prospect of optimal estimation and provide error bars for the trend estimates, because all other variability in the residuals is expected to be temporally uncorrelated errors. The same approach does not work for fitting a slowly changing functions of time to the actual temperature changes, as the latter contains complete spectrum of temporally correlated variability, from secular to intermonthly. If those are not removed, one should not assume the “whiteness” (mutual statistical independence) of errors, for such an assumption will result in unrealistically low theoretical estimates for the uncertainty of the fit.

Our preliminary analysis indeed shows some long-term variability left in the residuals. Once we are done with its complete estimation, we will be able to estimate the total long-term variability in the SST record and measure its uncertainty. Then we will either separate it from the raw observations before applying the analysis procedure, or make sure that it is properly represented in the covariance structure.

Problems with the covariance: stationarity. Assumption of covariance stationarity and possibility of its negative consequences comes up quite often in discussions, but has not been, to the best of our knowledge, systematically researched. As the first attempt at it, we compared covariance matrices estimated in different 40 year time windows for our SST analysis. Since the current SST analysis was performed under a conservative assumption of stationary covariance, this comparison probably underestimate the actual covariance variability. As a measure of distance between two covariance matrices we use the Frobenius norm: the square root of the sum of squares of all elements in the matrix difference (Golub and Van Loan (1996)). Even the norm of covariance matrix itself seem to change over time dramatically, with the minimum in 1930-1970, and the maximum in 1890-

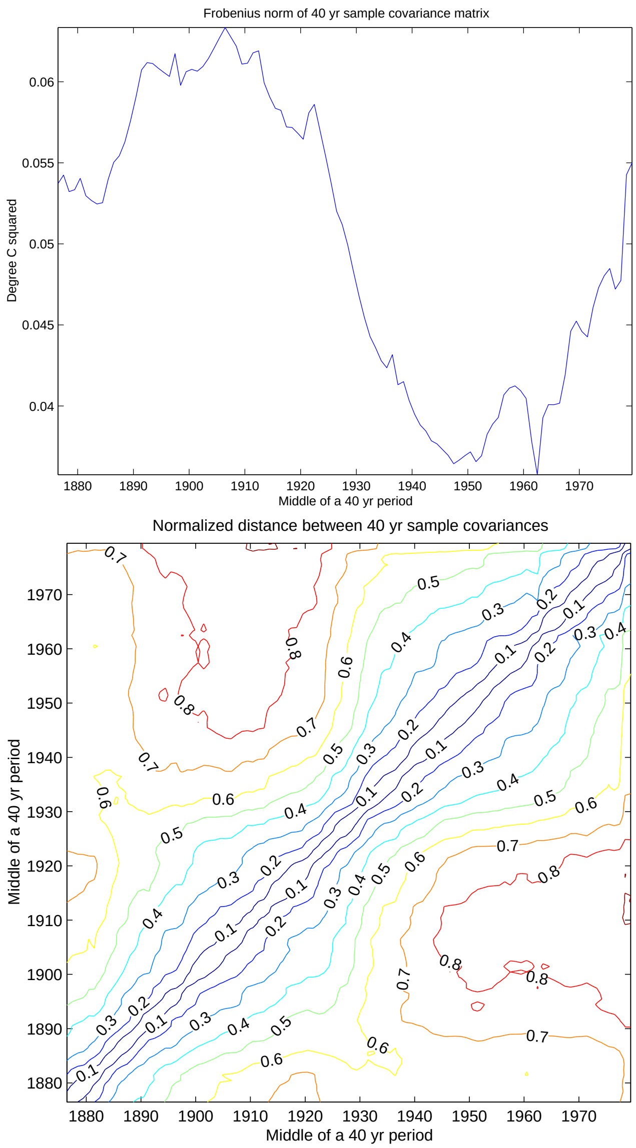

Figure 5: (top) The Frobenius norm of SST covariance estimated in 40 year time windows, (bottom) normalized distance between sample covariance matrices estimated for different 40 year windows

1920 (Figure 5, top). The diagram of normalized distances (norm of a difference divided by the norm of the covariance matrix computed for the recent 40 years) suggests that every period in the last 1.5 centuries was in some sense unique: the farther from each other middles of a sample periods get, the larger is the normalized distance between matrices (Figure 5, bottom). In some periods (like the one centered on 1930) this change happens very fast, in others (1910 and 1950) more slowly.

Successful validation of many aspects of our SST analysis so far shows that the exhibited instability of the covariance matrix does not render the analysis completely wrong or useless: the inherent robustness of the least squares estimates can absorb some level of inadequacy of a priori estimates. Moreover, all the different covariance matrices compared in the Figure 5 were produced by the analysis of Kaplan et al. (1998) under the assumption that the covariance of the SST field is constant and equal to the sample covariance of 1951–1991! It seems reasonable, however, to involve data of all time periods in the computation of the covariance and either use the estimate which would be applicable to the entire analysis period, or account for slow changes in time of the covariance structure in our analysis methodology.

Problems with the covariance: resolution and coverage. Significant volatility of the covariance structure discourages uses of only the modern period of particularly good (helped by satellite coverage) data for covariance estimation. If we are determined to estimate the large-scale covariance structures from the period no shorter than a few decades, that imposes certain restrictions on the spatial resolution with which covariance can be estimated. Before analyzing COADS SLP data we tried to estimate covariance for $2^o \times 2^o$ spatial bins, and found that the analysis domain had large holes (shown in black color in Figure 6) in the tropical Pacific. It took averaging to $4^o \times 4^o$ grid to "close" these holes. As a result the analysis domain we obtain has quite coarse resolution and still is globally incomplete. This severely limits the usage of such analyses in the GCM studies. It seems very important to be able to generalize the technique of the reduced space optimal estimation to the stage at which it can produce high resolution and globally complete analyses.

In fact, the reduced space reconstruction technique can be empowered by the multivariate approach. Principal modification of the reduced space optimal analysis that can produce high- resolution globally complete fields is to separate an estimated field into a few terms which correspond to different scales of resolution (and thus variability). Different terms can be

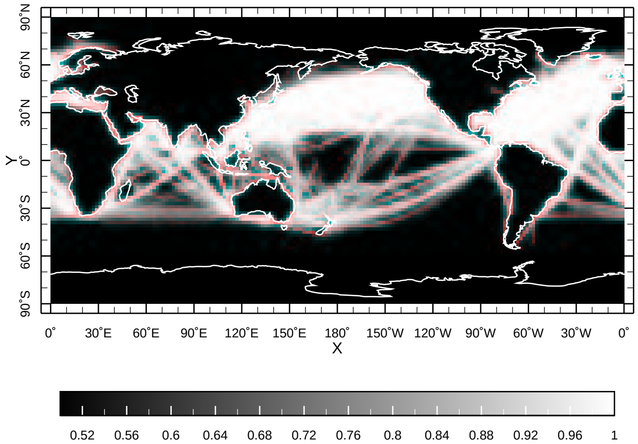

Figure 6: Percentage of months with observed SLP in COADS $2^o \times 2^o$ monthly summaries for the period 1951-1992

observed through different sources. For example, the most of the ocean $5^o \times 5^o$ resolution term is well observed by ships during last 50 years, and $1^o \times 1^o$ variability within $5^o \times 5^o$ boxes plus all variability in the Southern ocean can be estimated from the NCEP OI (Reynolds and Smith 1994) for the last 15 years, etc. The set of all terms can be subjected to multivariate EOF analysis, each piece being a separate variable in this analysis. These multivariate EOFs then used for the reconstruction of all pieces together, and thus for the entire high-resolution globally-complete field. This approach has certain "modular" nature because of which it allows to push further in both directions: very large scale variability can be estimated for very long periods from the paleodata, extending the analysis to very long periods, and certain areas of high gradients and/or good observational networks can be "refined" by adding special high resolution "patches."

4. PROSPECTS

We have shown that the reduced space optimal estimation is a computationally effective restructuring of the process of obtaining the full-grid optimal solution, and that it delivered verifiable analyses of climatic fields in both available applications (for SST and SLP).

The problems of the method are the same as those of any objective analysis technique: difficulty to derive reliable a priori estimates from the sparse and erratic data. Partially these problems might get relieved if new significant volumes of the data for the early periods become available (Woodruff et al. (1999)). It is very important that all data centers involved provide extensive statistics of intrabin distributions (as opposed to providing means only), like e.g. current COADS model of monthly summaries.

Land station data is another powerful information resource which can be combined in the analyses with marine observations to the advantage of the product (cf. recent SLP analysis of the U.K. Met Office by Basnett and Parker (1997))

Further improvement of the analysis technique should include systematic a priori estimation of mean, covariance, or long-term variability and changing covariance structure from the entire period of available data. Separation of the estimated fields into large and small scale varying components allows for the generalization of the technique which can produce high resolution globally complete products.

The technique of reduced space optimal estimation should be used more systematically in application to all climate variables for which historical (COADS) data sets are available, e.g. meridional and zonal winds, marine air temperature, humidity, or (non-COADS) precipitation, and possibly sea surface height.

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