# The Power of the Duality in Spatial–Temporal Estimation

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ABSTRACT

Space–time filtering has a long and often confusing history in the geosciences. It is called by different names in different areas of geoscience, where numerous applications have been developed. The variety of notations that have emerged adds to this confusion. A unified treatment of spatial–temporal estimation is presented, which highlights its duality and the associated trade-off in the construction of any optimal estimation algorithm.

The duality in optimal estimation comes from the requirement that the representation of the spatial–temporal statistical structure of the increments between the true field and the system-operator model used by the filter be matched with the true ensemble structure of the increment field. The associated trade-off arises from the following dichotomy: the closer the system-operator model corresponds to the true system operator, the less ensemble structure remains in the increment field. Conversely, the simpler the model of the system operator, the more residual statistical structure remains to be represented.

Several examples of estimation of spatial–temporal systems, in practice, are presented to illustrate the power of the duality. The rationale for determining the placement of effort in modeling the system operator vis-à-vis representing residual statistical structure is discussed.

## 1. Introduction

This paper is about unification of concepts of field estimation for stochastic–dynamic processes and about clarification of some esoteric methodologies. The present level of interest and sophistication in writing time-varying estimates for spatial fields, as demonstrated at the Sixth International Meeting on Statistical Climatology (6IMSC) in Galway, Ireland, invites an overview of nominally different ways of achieving space–time estimation. A single formalism can be written to describe their common purpose. In this one formalism, nominally different variations in approach are seen in relation to one another, their elemental differences are clearly evident, and guidance may be found for increasing resolution and accuracy with their algorithms.

Several examples from climatological research are used to illustrate both the appropriateness of the conceptual unification and the duality of its formalism. These examples are taken from the three invited papers in the session on spatial statistics at the Galway meeting. A final example is based on the U.S. Navy's operational analysis system for nowcasting global sea surface temperatures. The latter provides an excellent illustration of the power and consequences of working with the duality to heighten the resolution of algorithms for the estimation of large-scale geophysical fields.

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## 2. Current approaches to estimation of spatial–temporal processes

Statistically based techniques for the estimation of spatially evolutionary systems have developed in different areas of scientific research. The nomenclatures differ, just as the goals of the underlying scientific inquiries differ. Excellent examples of these differences and of work done in this broad area are provided by the three papers of the Spatial Statistics Session of the 6IMSC meeting: ''Space–Time Covariance Modeling,'' by W. Meiring, P. Guttorp, and P. D. Sampson; ''Linear Models for Spatial or Temporal Multivariate Data,'' by H. Wackernagel and M. Grzebyk; and ''Spatial–Temporal Rainfall Processes: Stochastic Models and Data Analysis,'' by R. Chandler, V. Isham, A. Kakou, and P. Northrop.

The goal of the first paper is to create gridpoint averages of surface ozone from observation-point data for direct comparison with the output of deterministic models. The deterministic models are based on known chemical and physical processes of ozone production and atmospheric transport. However, to provide objective verifications, the estimated gridpoint averages require the use of independent information. The estimator is based upon hourly surface ozone monitoring data, with a detailed model of the diurnally varying covariance structure of the observed field incorporated into the gridpoint interpolation algorithm. Modeling the spatial covariance structure becomes a complex process in accurately representing temporal and spatial inhomogeneities of the observed ozone increment covariances. (An additional reference to this approach is provided by Guttorp et al. 1994.)

The second paper presents a formalism that the authors call ''complex kriging,'' with an associated bilinear model of coregionalization for a multivariate nested covariance function. The scientific goal behind the theoretical work of this paper is the creation of an algorithm for description and estimation of systems for which the cross-covariance functions are not ''even functions.'' As an application example the authors cite analysis of data from the earth observing Landsat satellite. Here, as in the first paper of the session, the detail of the system estimator must be in the representation of the covariance structure. (See Wackernagel 1994 for a more detailed discussion.)

The third paper, on spatial–temporal models for rainfall processes, focuses on derivation of models for description of the complexities of the clustering of rain cells within moving storm events. The result of this work will be a stochastic model that can generate synthetic rainfall data for hydrologic studies. In contrast to the complex nonlinear deterministic models and empirical statistical models of other researchers, the stochastic model developed by V. Isham and colleagues uses a modest number of parameters relating to the underlying physical phenomena, such as rain cells. The stochastic model is then fitted to empirical data. (Cox and Isham 1994 include additional discussion of stochastic models of precipitation.)

The motivating scientific objective for each of the above studies is the estimation of a time-varying spatial field. The common objective of these estimation programs is the use of models and observations together to estimate the present states of various physical processes that evolve in time and space, with statistically optimal, computationally practical algorithms.

## 3. A unifying representation

A unifying representation for these and many other estimation programs may be written by generalizing Sorenson's (1970) notation for Kalman's time filter, as done by Thiébaux (1991). We will refer to the generalized version as the GKF. In defining the GKF we require a formal representation for whatever spatially and temporally coherent system is under study. For this purpose we may write the present-location, current-time state of the system as the output of a system operator, which carries the process from its spatial and temporal history to the present:

$$X_{\mathbf{s}+\mathbf{\Delta}} = \phi^*_{\mathbf{s}} \mathrm{o} X_{\mathbf{s}}, \text{ where o is the operator.} \qquad (1)$$

This notation can represent highly complex, nonlinear, inhomogeneous, nonstationary systems, as well as far less complex systems. Whatever the nature of the system, (1) represents the present, true state as output of nature's system operator, including such ''unpredictable innovations'' as Lorenz's butterflies. Here, $\phi^*$ denotes the system operator, or ''nature's game plan,'' which will be incompletely known. The star superscript distinguishes it from the representation denoted by $\phi$, which is used in its place in the estimator. System state variables are assumed to be multivariate, and, further, it is assumed that in its greatest generality the GKF formulation admits space- and time-varying system operation, with vector-valued subscripts that index space–time points and increments.

Observations, past and present, are denoted as composites of the true state vectors and observation error vectors:

$$Z_{\mathbf{s}} = X_{\mathbf{s}} + \xi_{\mathbf{s}} \quad \text{and} \quad Z_{\mathbf{s}+\mathbf{\Delta}} = X_{\mathbf{s}+\mathbf{\Delta}} + \xi_{\mathbf{s}+\mathbf{\Delta}}. \qquad (2)$$

We specifically include the possibility that the observation errors $\xi$ will have more stochastic structure than white noise. This is a further generalization of Kalman's theory, with observations of planetary processes made from spatial observing systems. All observation reports from the same instrument and data transmission systems are subject to the effects of consistent instrument bias or correlated errors of measurement and transmission. These factors are particularly significant with respect to data from buoys, ships, aircraft, and satellites. Further, we include the possibility that observation error may not be independent of the state of the system at observation times and locations.

One qualification is appropriate regarding this notation for observed quantities. In the case of satellite reports, for example, data obtained from an instrument may not be measurements of the specific characteristic of the environment in which we are interested. For satellite radiance measurements, the corresponding characteristic of interest is temperature. It is possible to convert from values of one to values of the other by known transformation or transfer functions; for many years such transformations were applied to satellite radiance reports to prepare them for assimilation in numerical weather prediction models. However, more sophisticated models and data assimilation software now use radiances directly. To accommodate such situations, in an inclusive GKF notation, we note that the $X$s in the observed state vectors of (2) may be more generally represented as $H\mathrm{o}X$s—that is, as prognostic quantities whose values are measured by the instruments. We could refine the notation and express it accordingly in (2) to distinguish the sensed variable from the true variable of interest. However, this would seem to add a new level of complexity to the picture, but a complexity that is only apparent. For most state variables, $H$ is the identity transformation. In more complicated cases, it is known nonetheless, and its inverse is built into the algorithm $\phi$. Accordingly, we omit its further, special designation, having made note of it for completeness.

The GKF algorithm for estimating $X$ is written in a notation that will serve regardless of whether $\phi$ in the "first-guess" representation $\phi \mathrm{o} \hat{X}$ uses everthing we know about $\phi^*$ from our scientific knowledge base or is simply an ensemble average of available information. Specifically,

$$\hat{X}_{\mathbf{s}+\boldsymbol{\Delta}} = \phi_{\mathbf{s}} \cdot \hat{X}_{\mathbf{s}} + K_{\mathbf{s}+\boldsymbol{\Delta}}(Z_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} X_{\mathbf{s}}). \tag{3}$$

Compare this to expression (1) above for the actual evolution of system states. The algorithm $\phi$ has been substituted for the system operator $\phi^*$. The output of the algorithm is corrected by applying a filter, or gain function $K$, to the collective discrepancies between values of the state variable contained in the observation record and first-guess values for those locations and times. For the present discussion, the only requirement we place on the algorithm $\phi$ that will generate first-guess values is that it be computationally practical. The term $\phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}}$, which appears in two places in (3), is the output of the prediction algorithm applied to the most recent estimated array as input. This first-guess pertains to location and time indexed by $\mathbf{s} + \boldsymbol{\Delta}$; $Z_{\mathbf{s}+\boldsymbol{\Delta}}$ is the coincident vector of observed values.

The mechanism for combining the information in the discrepancies between first-guess and observed values, represented by gain function $K$, is determined from the criterion for optimality of the estimated field. Just as with Kalman's filter, the optimality criterion of the GKF is *minimization of the ensemble squared difference between the true field and the estimated field,* and this criterion determines the gain function as a function of the space–time covariance structure of the increment field. Specifically, the requirement that the structure of the filter minimize

$$\langle\langle (X_{\mathbf{s}+\boldsymbol{\Delta}} - \hat{X}_{\mathbf{s}+\boldsymbol{\Delta}})^T (X_{\mathbf{s}+\boldsymbol{\Delta}} - \hat{X}_{\mathbf{s}+\boldsymbol{\Delta}}) \rangle\rangle$$

leads to the determination that

$$K_{\mathbf{s}+\boldsymbol{\Delta}} = Q_{\mathbf{s}+\boldsymbol{\Delta}} P^{-1}_{\mathbf{s}+\boldsymbol{\Delta}}, \tag{4}$$

where the $Q_{\mathbf{s}+\boldsymbol{\Delta}}$ and $P_{\mathbf{s}+\boldsymbol{\Delta}}$ components of the filter are the following covariance matrices (Thiébaux 1991):

$$\begin{aligned} Q_{\mathbf{s}+\boldsymbol{\Delta}} &= \langle\langle (X_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}})(Z_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}})^T \rangle\rangle \\ &= \langle\langle (X_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}})[(X_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}}) + \xi_{\mathbf{s}+\boldsymbol{\Delta}}]^T \rangle\rangle. \end{aligned} \tag{5}$$

and

$$\begin{aligned} P_{\mathbf{s}+\boldsymbol{\Delta}} &= \langle\langle (Z_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}})(Z_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}})^T \rangle\rangle \\ &= \langle\langle [(X_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}}) + \xi_{\mathbf{s}+\boldsymbol{\Delta}}] \\ &\qquad \times [(X_{\mathbf{s}+\boldsymbol{\Delta}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}}) + \xi_{\mathbf{s}+\boldsymbol{\Delta}}]^T \rangle\rangle. \end{aligned} \tag{6}$$

Note that the difference in the composition of the elements of $Q$ and $P$ is that the covariances of the former have observation error in only one of the increment variables. The covariances of $P$ are the covariances of increments that include observation error at each point.

By replacing the state vector $X_{\mathbf{s}+\boldsymbol{\Delta}}$ in (5) and (6) with its system-operator representation from (1), these may be rewritten as:

$$\begin{aligned} Q_{\mathbf{s}+\boldsymbol{\Delta}} &= \langle\langle (\phi^*_{\mathbf{s}} \mathrm{o} X_{\mathbf{s}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}}) \\ &\qquad \times [(\phi^*_{\mathbf{s}} \mathrm{o} X_{\mathbf{s}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}}) + \xi_{\mathbf{s}+\boldsymbol{\Delta}}]^T \rangle\rangle \end{aligned} \tag{7}$$

and

$$\begin{aligned} P_{\mathbf{s}+\boldsymbol{\Delta}} &= \langle\langle [(\phi^*_{\mathbf{s}} \mathrm{o} X_{\mathbf{s}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}}) + \xi_{\mathbf{s}+\boldsymbol{\Delta}}] \\ &\qquad \times [(\phi^*_{\mathbf{s}} \mathrm{o} X_{\mathbf{s}} - \phi_{\mathbf{s}} \mathrm{o} \hat{X}_{\mathbf{s}}) + \xi_{\mathbf{s}+\boldsymbol{\Delta}}]^T \rangle\rangle. \end{aligned} \tag{8}$$

## 4. The trade-off in optimal estimation with the GKF

The key, generic relationship in the estimation algorithm emerges more clearly if we omit the subscripts and use standard notation for covariance arrays, rewriting (7), (8) and (4) as

$$\Sigma_0 = \mathrm{Cov}\{(\phi^* \mathrm{o} X - \phi \mathrm{o} \hat{X}),\ [(\phi^* \mathrm{o} X - \phi \mathrm{o} X) + \xi]\}, \tag{9}$$

$$\Sigma = \mathrm{Cov}\{[(\phi^* \mathrm{o} X - \phi \mathrm{o} X) + \xi],\ [(\phi^* \mathrm{o} X - \phi \mathrm{o} \hat{X}) + \xi]\}, \tag{10}$$

and

$$K = \Sigma_0 \Sigma^{-1}. \tag{11}$$

Here, $\Sigma_0$ and $\Sigma$ embody the covariance structures of the fields of differences between the true–observed system states and the researchers' first-guess states. In (9)–(11) we can see the trade-off in optimal estimation between detail in the first-guess representation, relative to the system operator, and complexity of the covariances of the increments: $\phi$ vis-à-vis $\Sigma_0$ and $\Sigma$. Generically, the elements of $\Sigma_0$ and $\Sigma$ are the covariances of the increments between true–observed and first-guess values, regardless of how complex or simple the first-guess model of the system operator is relative to the true system operator. The structures of $\Sigma_0$ and $\Sigma$ are principally determined by the relationship between $\phi$ and $\phi^*$. This implies that the closer $\phi$ is to $\phi^*$, the less structure there will be in the increment field and, conversely, the simpler $\phi$ is relative to $\phi^*$, the more true field structure will be present in the increment field. This is the trade-off in optimal estimation with the GKF and the basis of the power of its duality.

Elements of the system operator that are not included in the representation that substitutes for it will be embedded in the stochastic structure of the increment field and reflected in ensemble, temporal, and spatial covariations of the increment variables. The statistical optimality criterion of minimization of the ensemble squared error of the estimator has its parallel in the requirement that the residual statistical structure in the algorithm used for constructing the filter be captured. The degree to which the final result achieves statistical optimality will be determined by the degree to which the stochastic structure of the increment field is accurately represented in the filter. If much of the detail in the system operator is missed by the first guess, as it will be with a climatological average, for example, approaching the limit of statistical optimality will require including significant detail in the representation of the covariance structure. This is the primary motivation for the work of Meiring et al. (1995) and of Wackernagel and Grzebyk (1995).

In contrast with the examples just cited, Chandler et al. (1995) and Cox and Isham (1994) work at making the first guess more detailed, which is itself a stochastic model of the state variable. Their work focuses on matching the system state model as closely as possible to the system state operator. Although the resulting system model will not completely remove nontrivial statistical structure from the residual fields, there will be much less structure remaining to be estimated and represented in the construction of the corresponding $\boldsymbol{\Sigma}_0$ and $\boldsymbol{\Sigma}$.

## 5. An application to operational analyses

Recent ocean thermal analyses provide a powerful illustration of the trade-off in the duality. Phoebus and Cummings (1995) and Cummings (1995) compare two global sea surface temperature analysis systems: OTIS 1.1 and OTIS 4.0. These are, respectively, the past and present operational global SST analysis algorithms used by the U.S. Navy at Fleet Numerical Meteorology and Oceanography Center (FNMOC) in Monterey, California, for nowcasting surface temperatures of the global oceans and for updating atmospheric forecast models. Both OTIS algorithms are optimal statistical objective analysis (OSOA) systems. In each case, the regression coefficients of the OSOA estimator for corrections to the first guesses are derived from mathematical approximations to the covariances of the increments between observed and first-guess fields.

OTIS 1.1 uses a daily climatology as its first guess and a 60-h window for taking in observations for analyses at 24-h intervals. The ''daily climatology'' is a gridded field of values, time interpolated to the analysis day from monthly climatologies, where the latter have been constructed from historical records. SST values predicted by a mixed layer, thermodynamic model of the oceans, are also incorporated in the OTIS 1.1 analysis, but with the status of special observations.

The new analysis scheme, OTIS 4.0, uses the previous analysis as the primary component of its first guess, with a 12-h analysis cycle and a 12-h data window. Specifically, the first guess for OTIS 4.0 is a 12-h-old analysis based on very recent observations, with occasional assistance from climatology to update grid points in data sparse regions for which there have been long intervals since fresh observations were available. OTIS 4.0 uses new quality control procedures and a multivariate volume analysis technique (Lorenc 1981). However, in the context of the present discussion, the most critical difference between OTIS 1.1 and 4.0 is the difference between the definitions of the first-guess field. The first guess of 4.0 generally has much more of the detail on the current, true state of the SST field than does the first guess of 1.1 because it is the most recent analysis using observations from the prior day, as compared to an average accumulated over many years.

Phoebus and Cummings (1995) report that the analysis increments of OTIS 1.1 have generally produced a very inhomogeneous field, particularly in areas where the SST gradients in the observed field were sharp. Statistical inhomogeneity was reflected in strong variations in the correlation length scales of the increment fields over the grid and marked anisotropy in some regions. This is the structure that should be incorporated in the filter when the first-guess algorithm creates an ensemble average of available information, such as a climatological field. If the filter cannot be designed to supplement the first guess through its own statistical detail, the output of the GKF algorithm will not achieve its potential optimality.

Replacement of a model of the system operator with a different first-guess algorithm will change the statistical structure of the increment field and, thus, the requirement for construction of the optimal filter. Phoebus and Cummings (1995) provide an excellent example of this. The authors note that OTIS 4.0, using the previous analysis as first guess, generally has smaller, more homogeneous analysis increments, with correlation length scales that can be applied uniformly across the analysis grid. This is the trade-off of the GKF duality: a representation for the system operator that conveys more time-specific detail of the true field places a more manageable requirement on filter construction because of the simpler statistical structure of the increment fields.

In the foregoing example, the geographic and computational scales of the nowcasting procedure placed practical constraints on the options for increasing the accuracy of the analysis product from the OTIS 1.1 baseline. In principle, there was a choice of greatly increasing the statistical complexity of a new filter or of including more timely detail in the GKF model substituting for the system operator. Ultimately, the first-guess algorithm was replaced, with consequent simplification of the filter's required statistical representation. This choice and the assignment and parameterization of an appropriately chosen spatial correlation function for the new analysis increments, together with other modifications in the analysis scheme, form the basis for OTIS 4.0. The output produced by this version of the ocean thermal interpolation system shows considerably more detail in the estimated fields than does the baseline analysis. In Figs. 1 and 2, reproduced here from Phoebus and Cummings (1995), we can see, for example, the tighter gradients in the OTIS 4.0 nowcast of the Gulf Stream (Fig. 1b compared with Fig. 1a) and the Kuroshio currents (Fig. 2b compared with Fig.

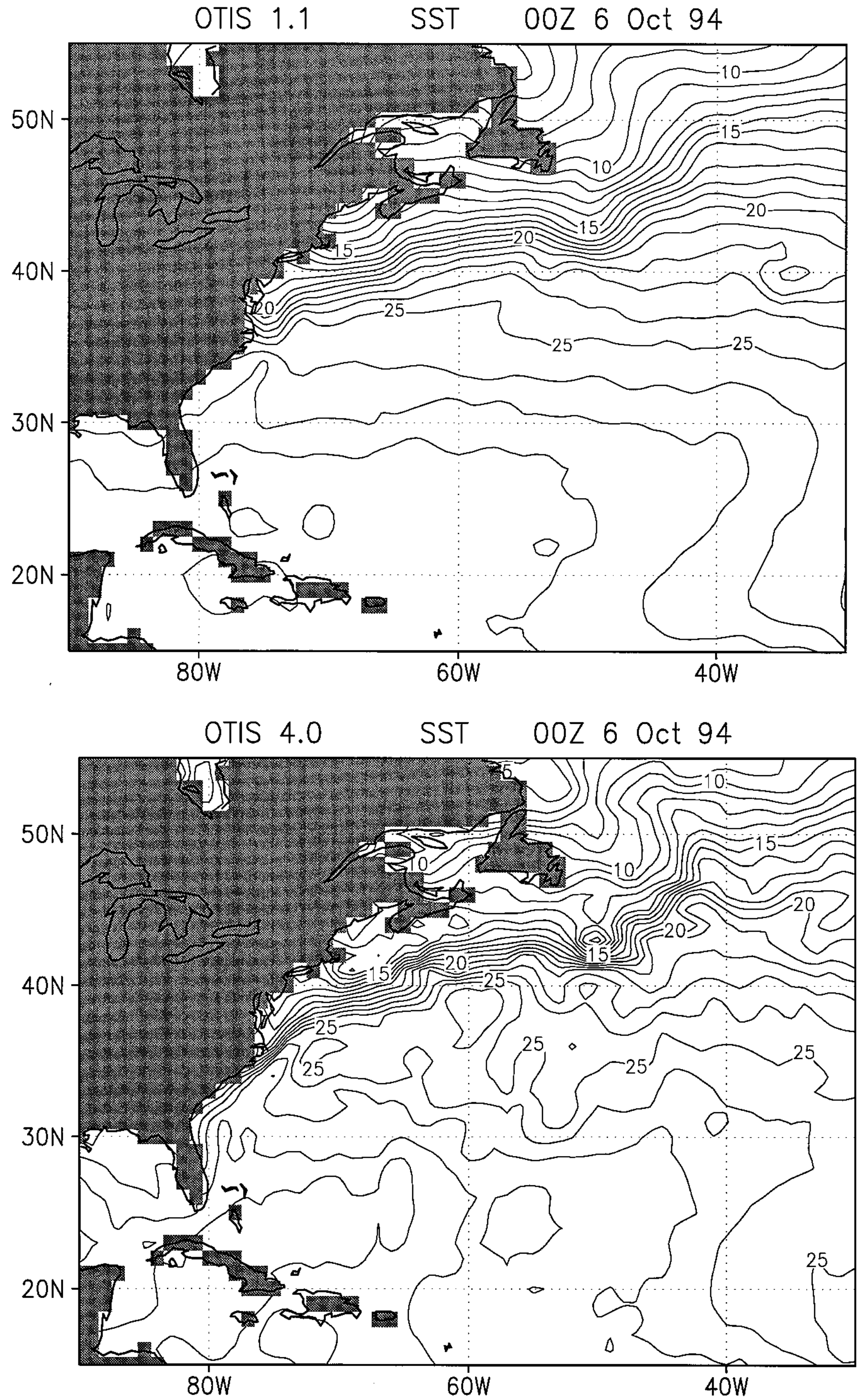


FIG. 1. SST analyses with temperatures in degrees Celsius for the western Atlantic at 0000 UTC, 6 October 1994, (a) using OTIS 1.1 and (b) using OTIS 4.0 (Figs. 1a,b. of Phoebus and Cummings 1995).

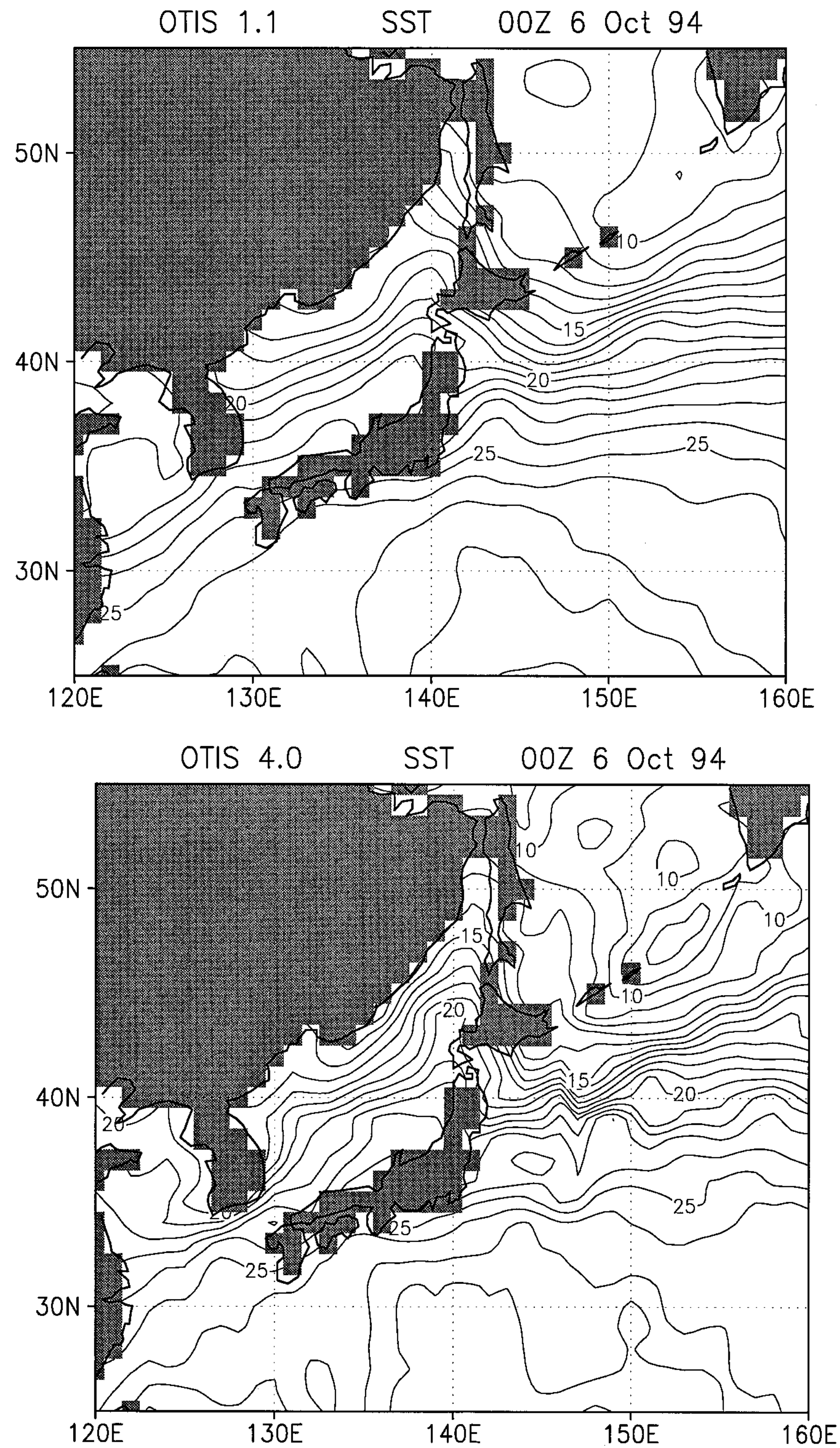


FIG. 2. SST analyses with temperatures in degrees Celsius for the western Pacific at 0000 UTC, 6 October 1994, (a) using OTIS 1.1 and (b) using OTIS 4.0 (Figs. 2a,b. of Phoebus and Cummings 1995).

2a). Furthermore, according to Phoebus and Cummings, ''OTIS 4.0 analyses will even depict cold and warm core eddies that are almost never observed in the OTIS 1.1 fields.''

## 6. Summary

Examples that illustrate the power of the duality in spatial–temporal estimation have been drawn from papers presented at a recent meeting on statistical climatology. Their underlying objectives are placed in a common context, and a generic generalized Kalman filter notation is proposed to include them. The common representation for nominally different approaches to the estimation of systems that evolve in time and space highlights the origins of differences in algorithms, as well as the avenues for increasing resolution and accuracy. The trade-off in constructing an estimator is shown to be between incorporating detail into the first guess of the system operator and the detail remaining to be included in the statistical structure of the gain function that incorporates corrections to the first guess. This trade-off is further related to the initial examples where the choices are clearly dictated by research objectives.

The output of a GKF will be optimal in a statistical sense only to the degree that the covariance representation of the filter matches the covariance structure of the true-minus-guess increments. Ocean sea surface temperature analyses further illustrate the power of working with the duality within practical constraints of existing computational and statistical technologies.

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