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Estimates of ocean forecast error covariance derived from Hessian Singular Vectors

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ABSTRACT

Experience in numerical weather prediction suggests that singular value decomposition (SVD) of a forecast can yield useful *a priori* information about the growth of forecast errors. It has been shown formally that SVD using the inverse of the expected analysis error covariance matrix to define the norm at initial time yields the Empirical Orthogonal Functions (EOFs) of the forecast error covariance matrix at the final time. Because of their connection to the 2nd derivative of the cost function in 4-dimensional variational (4D-Var) data assimilation, the initial time singular vectors defined in this way are often referred to as the Hessian Singular Vectors (HSVs). In the present study, estimates of ocean forecast errors and forecast error covariance were computed using SVD applied to a baroclinically unstable temperature front in a re-entrant channel using the Regional Ocean Modeling System (ROMS). An identical twin approach was used in which a truth run of the model was sampled to generate synthetic hydrographic observations that were then assimilated into the same model started from an incorrect initial condition using 4D-Var. The 4D-Var system was run sequentially, and forecasts were initialized from each ocean analysis. SVD was performed on the resulting forecasts to compute the HSVs and corresponding EOFs of the expected forecast error covariance matrix. In this study, a reduced rank approximation of the inverse expected analysis error covariance matrix was used to compute the HSVs and EOFs based on the Lanczos vectors computed during the 4D-Var minimization of the cost function. This has the advantage that the entire spectrum of HSVs and EOFs in the reduced space can be computed. The associated singular value spectrum is found to yield consistent and reliable estimates of forecast error variance in the space spanned by the EOFs. In addition, at long forecast lead times the resulting HSVs and companion EOFs are able to capture many features of the actual realized forecast error at the largest scales. Forecast error growth via the HSVs was found to be significantly influenced by the non-normal character of the underlying forecast circulation, and is accompanied by a forward energy cascade, suggesting that forecast errors could be effectively controlled by reducing the error at the largest scales in the forecast initial conditions. A predictive relation for the amplitude of the basin integrated forecast error in terms of the mean aspect ratio of the forecast error hyperellipse (quantified in terms of the mean eccentricity) was also identified which could prove useful for predicting the level of forecast error *a priori*. All of these findings were found to be insensitive to the configuration of the 4D-Var data assimilation system and the resolution of the observing network.

1. Introduction

An important part of ocean forecasting is providing estimates of forecast errors. A common approach is to use ensemble prediction methods (*i.e.* where an ensemble of forecasts is generated by perturbing and rerunning the forecast model many times for a given forecast interval) which have become an important component of atmosphere, ocean and climate prediction at most operational centers, and provide information about the most likely state of the system (the ensemble mean) and uncertainty in the forecast state (the ensemble spread). Nonetheless, several important technical issues surround ensemble prediction methods which can hamper their application. First, because of the computational cost of running a large forecast model, the number of ensemble members is necessarily resource-limited. This leads to questions about the minimum required ensemble size and how each ensemble member should be generated given that the dimension of the forecast

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model will typically be several orders of magnitude larger than the affordable number of ensemble members. Related to these issues is the need for covariance localization in order to eliminate potentially spurious correlations that arise from the limited size ensemble. Finally, experience shows that the forecast error covariance of the resulting ensemble tends to underestimate the true forecast error, so some form of covariance inflation is typically required.

An alternative approach to the problem of predicting forecast errors is using singular value decomposition (SVD; Ehrendorfer and Tribbia, 1997) which we believe is more elegant than traditional ensemble methods, has a solid theoretical basis, and potentially avoids many of the aforementioned issues that surround ensemble methods. During the last three decades, analysis of singular vectors has advanced generalized stability theory (Farrell and Ioannou, 1999), and non-normal perturbations in non-autonomous flow fields in both the atmosphere (Farrell, 1982, 1990) and the oceans (Farrell and Moore, 1992), have been shown to disrupt the predictability in the short- and medium-range (Lorenz, 1965; Farrell, 1990; Betti and Navarra, 1995; Houtekamer, 1995; Houtekamer and Derome, 1995). These so-called "optimal perturbations" are identified with respect to norms chosen *a priori* at the initial and final times of perturbation growth, and differences arising from different choices of norm yield a variety of singular vector archetypes that have been explored in the literature.

As a prelude to the important ideas that follow in later sections, let $\delta\mathbf{x}$ denote a perturbation to the time evolving state-vector $\mathbf{x}$ of the atmosphere or ocean, where $\mathbf{x}$ and $\delta\mathbf{x}$ are column vectors. SVD in geophysical problems of very large dimension is usually approached in terms of the Rayleigh quotient:

$$\lambda = \delta\mathbf{x}^T(0)\mathbf{M}^T\mathbf{D}\mathbf{M}\delta\mathbf{x}(0)/\delta\mathbf{x}^T(0)\mathbf{G}\delta\mathbf{x}(0) \qquad (1)$$

where $\mathbf{M}$ denotes the tangent linear propagator that evolves the perturbation $\delta\mathbf{x}$ over the interval $[0,t]$, while $\mathbf{D}$ and $\mathbf{G}$ define the norms at final time and initial time respectively. Therefore λ represents the ratio of the final time norm to the initial time norm. The perturbation $\delta\hat{\mathbf{x}}$ that maximizes (1) with unit initial norm $\delta\hat{\mathbf{x}}^T\mathbf{G}\delta\hat{\mathbf{x}}$ is, by definition, the leading eigenvector of the generalized eigenvalue equation:

$$\mathbf{M}^T\mathbf{D}\mathbf{M}\delta\hat{\mathbf{x}} = \lambda\mathbf{G}\delta\hat{\mathbf{x}} \qquad (2)$$

The vector $\delta\hat{\mathbf{x}}$ is a right singular vector of $\mathbf{D}^{\frac{1}{2}}\mathbf{M}$ and $\lambda^{\frac{1}{2}}$ is the corresponding singular value.

In the study of forecast predictability and sensitivity, $\mathbf{D}$ is chosen such that the final time norm is a useful metric of the forecast error. Following Houtekamer (1995), Ehrendorfer and Tribbia (1997) showed that identifying $\mathbf{G}$ as the inverse of the analysis error covariance matrix yields singular vectors that evolve over the forecast time interval into the leading eigenvectors of forecast-error covariance matrix at final time (*i.e.* the forecast error Empirical Orthogonal Functions (EOFs)). Unfortunately, the inverse analysis-error covariance matrix can be difficult to obtain operationally, although several approximations have proven useful. In 3D- and 4D-Var data assimilation, the Hessian of the cost function yields the inverse analysis-error covariance matrix, derived implicitly from the background error and observation error covariance matrices used in the assimilation system. Identifying $\mathbf{G}$ with the Hessian yields the so-called Hessian Singular Vectors (HSVs) which have been used to initialize forecast ensembles at the European Centre for Medium-range Weather Forecasts (ECMWF; Barkmeijer et al., 1999). However, despite the practical utility of HSVs, they can be costly to compute (Houtekamer, 1995; Barkmeijer et al., 1998). As a first-order proxy for the analysis-error covariance, a frequent choice of norm at both initial- and final-time is total perturbation energy, in which case $\mathbf{D} = \mathbf{G}$ in (1) and (2). The resulting Energy Singular Vectors (ESVs) are generally more straightforward to compute and in the atmosphere have been shown to share properties in common with analysis error statistics, unlike other proxies such as the enstrophy or squared-streamfunction norms (Palmer et al., 1998). While the skill of ESVs in operational numerical weather prediction (NWP) has made them a standard measure of success when compared to other norms, ESVs do not directly use any information from the data assimilation system. Gelaro et al. (2002) and Reynolds et al. (2005) investigated the utility of the inverse analysis error variance (the diagonal of the analysis error covariance matrix) from a 3D-Var system for $\mathbf{G}$ to define the initial norm. Although different in structure, the resulting SVs explain similar fractions of the forecast error variance as ESVs.

While most applications of SVD have been in meteorology and NWP, similar methods have also been successfully applied in oceanography (e.g. Moore and Farrell, 1993; Moore and Mariano, 1999; Moore et al., 2002; Chhak et al., 2006a,b, 2007, 2009) and climate (e.g. Blumenthal, 1991; Penland and Sardeshmukh, 1995; Moore and Kleeman, 1996).

The current work investigates the potential for using a reduced-rank formulation of HSVs for quantifying ocean forecast errors. This is explored in a model of a baroclinically unstable temperature front in a re-entrant channel. Because the dimension of any state-of-the-art model is generally very large, computation of the HSVs in the full dimension of the system may be prohibitive in a real-time forecast environment. The main objective here is to reduce the dimension of the problem by searching only the model subspace explored by data assimilation, as opposed to the entire state-space of the model. In this approach, the search directions employed in a 4D-Var system are used as basis functions for a reduced-rank SVD calculation. An important caveat of the method proposed is that it has only been applied here to an idealized situation in an identical twin environment. While this may yield overly optimistic results, it is nevertheless demonstrated that the proposed method may also prove useful in realistic operational environments. The computational cost of the reduced-rank approximation described here is significantly less than that for methods based on the full rank approach. This provides motivation for pursuing the reduced-rank approach further.

The paper proceeds as follows: We first formalize the calculation of HSVs in a reduced space in Section 2, starting with the framework of SVD as well as the reduced rank approximation of the inverse analysis-error covariance matrix via the Hessian of the 4D-Var cost function. The configuration of the model is described in Section 3, while the properties of the 4D-Var data assimilation system, validation of the tangent linear assumption, and the efficacy of the HSVs and EOFs in various configurations are examined in Section 4. The potential practical utility of using the properties of the HSV singular value spectrum as a predictor of forecast error is addressed in Section 5. The energetics of the HSVs and the role of non-normality in controlling HSV growth is considered in Section 6. We conclude with a summary and discussion of the results and their implications in Section 7.

2. Hessian Singular Vectors and EOFs

2.1. Forecast error EOFs and SVD

Following the notation introduced in Section 1, consider the situation shown in Fig. 1 in which an ocean forecast is initialized at time $t = 0$ from an initial state $\mathbf{x_a}(0)$ that is derived from an ocean analysis using observations from the time interval $t = [-\tau, 0]$. In the specific case considered here, the analysis is computed using 4D-Var. The time evolution of $\mathbf{x_a}(0)$ by the forecast model will be denoted by $\mathbf{x_r}(t) = \mathcal{M}(\mathbf{x_a}(0))$ where $\mathcal{M}$ describes the model which