Abstract

We examine stochastic dynamical systems where the transition matrix, $\Phi$, and the system noise, $\Gamma Q \Gamma^T$, covariance are nearly block diagonal. When $H^T R^{-1} H$ is also nearly block diagonal, where $R$ is the observation noise covariance and $H$ is the observation matrix, our suboptimal filter/smoothers are always positive semidefinite, and have improved numerical properties. Applications for distributed dynamical systems with time dependent pixel imaging are discussed.
I. INTRODUCTION

In this article, we examine suboptimal filters and smoothers of stochastic systems when the dynamics and the measurements are nearly block diagonal (N.B.D.). We assume that the transition matrix, \( \Phi(i+1,i) \), the system noise covariance, \( \Gamma Q \Gamma^T \), the initial state covariance, \( P(0|0) \), and the measurement information matrix, \( J_i \equiv H_i^T R_i^{-1} H_i \), are all N.B.D. We then derive estimation equations for the state vector, \( \hat{x}_i \), and the covariance, \( P(i|i) \), which approximate the optimal estimates to second order in \( \epsilon \).

Our stochastic systems are similar to the widely studied weakly coupled system (Kokotovic et al. (1969), Sezer and Siljak (1986), Gajic et al. (1990), Shen and Gajic (1990)). Our N.B.D. systems are not limited to two block systems, but apply to an arbitrary number of blocks. Furthermore, we require only that \( H_i^T R_i^{-1} H_i \) is N.B.D. This contrasts to the stronger hypothesis of weakly coupled systems that \( H_i \) and \( R_i \) are separately weakly coupled.

The existing theory of weakly coupled systems concentrates on the convergence of approximations to the complete system as \( \epsilon \) tends to zero. Thus the existing analysis considers only the case where \( \epsilon \) is sufficiently small as to preclude the loss of positive definiteness in the approximate equations. Therefore previous analyses have not explicitly required positive definiteness.

Our emphasis is on well-conditioned approximation of \( \hat{x}_i \) and \( P(i|i) \) for finite, but small values of the coupling parameter, \( \epsilon \). Formally, our expansions require that the zeroth order N.B.D. matrices are all uniformly much larger than the remaining offdiagonal terms. In practice, the coupling parameter, \( \epsilon \), is not vanishingly small, and there may be component directions where the first order terms almost cancel the zeroth order terms. To prevent the approximate covariance matrix, \( P^{(e)}(i|i) \), from losing positive definiteness, we add second order terms to the approximate covariance. These additional terms not only guarantee positive semidefiniteness, but also provide a matrix factorization.

Our motivation for the study of N.B.D. systems is the analysis of distributed systems of partial differential equations for fluid flow. We estimate the fluid flow as a
function of time and space, \( \vec{u}(\vec{r}, t) \), where \( \vec{u}(\vec{r}, t) \) satisfies the Navier-Stokes equations:

\[
\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = \nabla p + \nu \Delta \vec{u}, \quad \nabla \cdot \vec{u} = 0.
\]

We are given continuous time measurements of velocity field on a coarse grid in space. We expand the Navier-Stokes equation in the set of eigenfunctions of the laminar flow linear stability problem (Canuto et al. (1988)). We truncate the eigenfunction expansion in the middle of the inertial range, and model the effects of the discarded modes through an anomalously large diffusion coefficient.

When spatial inhomogeneities and nonlinearities are weak, the transition matrix, \( \Phi(i + 1, i) \), for the zeroth order eigenfunction basis often will be N.B.D. To decouple the estimation equations to leading order, we assume both \([\Gamma \Psi \Gamma^T]_i\) and \(P(0|0)\) are nearly block diagonal.

In our prototypical system, the elements of the measurement evaluation matrix, \( \mathbf{H}_i \), are evaluations of basis functions, \( \Psi_k \), at the spatial locations, \( y_\ell \). When the \( y_\ell \) are distributed more or less uniformly in space, and the \( \Psi_k \) are orthogonal, and \( R_i \) is a multiple, \( \sigma_i^2 \), of the identity, then

\[
(\mathbf{H}_i^T R_i^{-1} \mathbf{H}_i)_{k,k'} = \frac{1}{\sigma_i^2} \sum_{\ell=1}^m \Psi_k(y_\ell)\Psi_{k'}(y_\ell) \sim \frac{m}{\sigma_i^2} \int \Psi_k(z)\Psi_{k'}(z)dz \sim c_k \delta_{k,k'}.
\]

Thus for distributed systems of partial differential equations with leading order to eigenfunctions as the basis functions, the requirement that \( \mathbf{H}_i^T R_i^{-1} \mathbf{H}_i \) is nearly block diagonal corresponds to the measurement locations being nearly uniformly distributed and approximating spatial integration on the scalelength of the shortest wavelength basis function.

For such pixel type measurements, the number of pixels needs to exceed the number of different diagonal blocks of eigenfunctions. If the measurements are spatially uniform, but of insufficient number to distinguish the various eigenfunctions, the evolution equations will be partially coupled due to spatial aliasing.

Section II defines N.B.D. matrices, and presents several stabilizing transformations and approximate factorizations. In Section III, we review the standard discrete Kalman filter and derive a positive definite suboptimal approximation to the Kalman filter. Section IV and Appendix B derive similar suboptimal positive definite ap-
proximations to the discrete Kalman smoothers for fixed intervals and for fixed lags respectively. Section V discusses our N.B.D. formulation. Appendix A examines the numerical advantages of computing the basic matrix operations only to first order.

II. NEARLY BLOCK DIAGONAL MATRIX REPRESENTATIONS AND OPERATIONS

A) Matrix Structure

We consider the class of nearly block diagonal (N.B.D.) matrices to be \( N \times N \) matrices of the form:

\[
P(\epsilon) = P(0)(\epsilon) + \epsilon P(1)(\epsilon) + \epsilon^2 P(2)(\epsilon),
\]

where \( P(2)(\epsilon) \) contains second order and higher terms in \( \epsilon \). The weak coupling parameter, \( \epsilon \), is a formal small expansion term parameter. \( P(0)(\epsilon) \) is block diagonal of the form:

\[
P(0)(\epsilon) = \begin{pmatrix}
P_{11}(\epsilon) & 0 & \cdots \\
0 & P_{22}(\epsilon) & 0 \\
0 & \cdots & 0 \\
0 & \cdots & P_{N_b,N_b}(\epsilon)
\end{pmatrix},
\]

where the \( P_{kk}(\epsilon) \) entry is a \( n_k \times n_k \) matrix for \( k = 1, 2, \ldots, N_b \). The block sizes, \( n_1, n_2, \ldots, n_{N_b} \), are fixed in this article, i.e. all matrices have the same block structure. We often suppress the functional dependence on \( \epsilon \) in \( P(i)(\epsilon) \), \( i = 0, 1, 2 \). We denote the truncated approximations of \( P(\epsilon) \) by \( P(\epsilon) \), where \( P(\epsilon) = P(0)(\epsilon) + \epsilon P(1)(\epsilon) \) for first order approximations and \( P(\epsilon) = P(0)(\epsilon) + \epsilon P(1)(\epsilon) + \epsilon^2 P(2)(\epsilon) \) for second order approximations.

The first order block diagonal terms may be included in either \( P(0)(\epsilon) \) or \( \epsilon P(1)(\epsilon) \). Including the block diagonal terms in \( P(0)(\epsilon) \) reduces storage requirements; however, the resulting equations are slightly more complicated. For simplicity, we include the first order block diagonal terms in \( \epsilon P(1)(\epsilon) \). We define \( P_L \) to be the strictly lower triangular part of a matrix \( P \) plus half of the block diagonal part of \( P \).

B) Stabilizing Transformations and the \( LD^{-1}LT \) Factorization

The truncated approximations, \( P(\epsilon) \), to \( P(\epsilon) \) need not be positive semidefinite even when \( P(0) \) and \( P(\epsilon) \) are positive definite. We assume that \( P(0) \) is positive definite and that \( P(0), P(\epsilon) \) and \( P(\epsilon) \) are symmetric, we define the following trans-
formations:

\[ T_1[ P^{(\epsilon)}] \equiv [ P^{(0)} + \epsilon P_L^{(1)}] P^{(0)-1} [ P^{(0)} + \epsilon P_L^{(1)}] T, \]  \hspace{1cm} (2.2) 

for first order approximations, and

\[ T_2[ P^{(\epsilon)}] \equiv [ P^{(0)} + \epsilon P_L^{(1)} + \epsilon^2 ( P_L^{(2)} - G^{(2)} ) ] P^{(0)-1} [ P^{(0)} + \epsilon P_L^{(1)} + \epsilon^2 ( P_L^{(2)} - G^{(2)} ) ]^T, \]  \hspace{1cm} (2.3) 

for second order approximations where \( G^{(2)} \equiv P_L^{(1)} P^{(0)-1} P_L^{(1)T} \). Both transformations produce positive semidefinite matrices with \( LD^{-1}L^T \) block factorizations. \( T_1[ P^{(\epsilon)}] \) differs from \( P^{(0)} + \epsilon P_L^{(1)} \) by the second order term \( \epsilon^2 P_L^{(1)} P^{(0)-1} P_L^{(1)T} \), and is thus strictly larger than \( P^{(0)} + \epsilon P_L^{(1)} \). \( T_2[ P^{(\epsilon)}] \) differs from \( P^{(0)} + \epsilon P_L^{(1)} + \epsilon^2 P^{(2)} \) by third order terms, however these third order terms need not be positive semidefinite. An alternative transformation is \( T_b[ P^{(\epsilon)}] \equiv [ P^{(0)} + \epsilon P_L^{(1)} + \epsilon^2 P_L^{(2)} ] P^{(0)-1} [ P^{(0)} + \epsilon P_L^{(1)} + \epsilon^2 P_L^{(2)} ]^T \). \( T_b[ P^{(\epsilon)}] \) approximates \( P^{(\epsilon)} \) only to second order, but adds only positive terms. Therefore \( T_b[ P^{(\epsilon)}] \) can be used to provide second order upper bounds.

A number of other stabilizing transformations may be defined. \( \epsilon P_L^{(1)} \) can be replaced by \( \frac{1}{2} P^{(1)} \) at the cost of losing the \( LD^{-1}L^T \) block factorization. A more useful transformation is to decompose \( P^{(\epsilon)} \) into its spectral representation, and then to set any negative eigenvalues of \( P^{(\epsilon)} \) to zero. This spectral transformation has the advantage that it uses the smallest possible correction which makes the transformed matrix positive semidefinite. In Appendix A, we describe a first order approximation to the spectral decomposition. Instead of actually performing the singular value decomposition, we may simply test \( P^{(\epsilon)} \) for negative eigenvalues using Eq. (A3). Only the eigenvalues with small \( \lambda_k^{(0)} \) need be tested and/or replaced. Thus the eigendecomposition approach is especially attractive when only a small number of eigenvalues are questionable.

\( T_1[ P^{(\epsilon)}] \) also has a block \( LDL^T \) representation: \( [ I_N + \epsilon P_L^{(1)} P^{(0)-1} ] P^{(0)} [ I_N + \epsilon P_L^{(1)} P^{(0)-1} ]^T \). This factorization is less numerically efficient than the \( LD^{-1}L^T \) representation.

In our filtering applications, we use the transformation, \( P^{(\epsilon)} = T[ P^{(\epsilon)}] \), to stabilize
the data assimilation and variance evaluations. We note that \(T[T[P(\cdot)]] = T[P(\cdot)]\). This property is important when the covariance matrix, \(P(\cdot)\), is modified many times with small updates. We let \(T[\cdot]\) denote the appropriate stabilizing transformation.

### III. Diagonally Dominant Discrete Kalman Filters

We consider the discrete linear state space model:

\[
\vec{x}_{i+1} = \Phi(i+1, i)\vec{x}_i + \Gamma_i\vec{w}_i, 
\]

\[
\vec{y}_i = H_i\vec{x}_i + \vec{v}_i, 
\]

where \(\vec{x}_i\) is the state vector of dimension \(N\), \(\vec{y}_i\) is the measurement vector of dimension \(m\), and \(\Phi(j, i)\) is the \(N \times N\) nonsingular deterministic part of the map from time \(i\) to time \(j\). The system noise, \(\vec{w}_k\), is assumed to be an \(r\)-dimensional white Gaussian with covariance \(Q_i\). The measurement noise is an \(m\)-dimensional white Gaussian sequence with nondegenerate covariance \(R_i\). The \(m \times N\) measurement evaluation matrix, \(H_i\), maps the state vector, \(\vec{x}_i\), onto the deterministic part of the measurements. We define the \(N \times N\) matrices, \(Q_{\Gamma,i} \equiv \Gamma_i Q_i \Gamma_i^T\) and \(J_i \equiv H_i^T R_i^{-1} H_i\).

The standard Kalman filter estimates the state vector, \(\hat{x}(i|j)\), at time \(i\) given the measurements, \(\vec{y}_1, \ldots, \vec{y}_j\) up to time \(j\) by the time evolution update:

\[
\hat{x}(i+1|i) = \Phi(i+1, i)\hat{x}(i|i). 
\]

The covariance, \(P(i|j)\), of the estimate, \(\hat{x}(i|j)\), evolves as

\[
P(i+1|i) = \Phi(i+1, i)P(i|i)\Phi^T(i+1, i) + Q_{\Gamma,i}. 
\]

We assume that \(\hat{x}(0|0)\) and \(P(0|0)\) are given. The measurement update is

\[
\hat{x}(i|i) = \hat{x}(i|i-1) + K_i(\vec{y}_i - H_i\hat{x}(i|i-1)), 
\]

\[
P(i|i)^{-1} = P(i|i-1)^{-1} + H_i^T R_i^{-1} H_i, 
\]

where \(K_i\) is the \(N \times m\) Kalman gain:

\[
K_i = [P(i|i-1)^{-1} + H_i^T R_i^{-1} H_i]^{-1} H_i^T R_i^{-1} = P(i|i)H_i^T R_i^{-1}. 
\]
We now assume that \( \Phi(i + 1, i), Q_{\mathbf{r}, i}, P(0|0) \) and \( J_i \equiv H_i^T R_i^{-1} H_i^T \) are N.B.D. We assume that the leading order operator, \( \Phi(i + 1, i) \), is normal, so that its eigenvectors are orthogonal. For clarity, we denote \( \Phi^{(0)}(i + 1, i) \) by \( \Lambda_i \). We denote the \( k, \ell \)-th subblocks of \( P(i|j) \) by \( P(i|j)_{(k, \ell)} \), and use similar subscripts for the subblocks of \( J_i, Q_{\mathbf{r}, i} \) etc. We present the expansion of the Kalman filter only to first order. Higher order expressions are similar, but longer.

The time evolution update for \( \tilde{x} \), Eq. (3.3), may be computed to arbitrary order if desired. The time evolution of the covariance for the standard N.B.D. representation satisfies

\[
P^{(0)}(i + 1|i)_{(k,k)} = \Lambda(i)_k P^{(0)}(i|i)_{(k,k)} \Lambda(i)_k^T + [\Gamma Q \Gamma^T]^{(0)}_{i(k,k)},
\]

for the zeroth order block diagonal covariance and

\[
P^{(1)}(i + 1|i)_{(k,k)} = \Lambda(i)_k P^{(1)}(i|i)_{(k,k)} \Lambda(i)_k^T + \Phi^{(1)}(i + 1, i)_{(k,k)} P^{(0)}(i|i)_{(k,k)} \Lambda(i)_k^T + \Lambda(i)_k P^{(0)}(i|i)_{(k,k)} \Phi^{(1)}(i + 1, i)_{(k,k)} P^{(0)}(i|i)_{(k,k)} \Lambda(i)_k^T + [\Gamma r_i]^{(1)}_{(k,k)},
\]

for the first order covariance. The measurement update of \( \tilde{x}(i|i) \) and \( P(i|i) \) is separated into four steps. First, the zeroth order, block diagonal approximation to \( P(i|i) \) is determined by solving the block system

\[
P^{(0)}(i|i) = [P^{(0)}(i|i) - 1]^{-1} + J_i^{(0)}^{-1}
\]

exactly. Second, the first order corrections to \( P(i|i) \) are

\[
P^{(1)}(i|i) = P^{(0)}(i|i)^{-1} [P^{(0)}(i|i) - 1]^{-1} P^{(1)}(i|i) - 1 P^{(0)}(i|i) - 1 - J^{(1)}] P^{(0)}(i|i)^{-1}.
\]

Third, our estimate of \( P(i|i) \) is forced to be positive semidefinite using the transformation: \( P^{(c)}(i|i) = T[P^{(c)}(i|i)] \). Finally, we update our estimate of \( \tilde{x}(i|i) \) using

\[
\tilde{x}(i|i) = \tilde{x}(i|i) - 1 + P^{(c)}(i|i) H_i^T R_i^{-1} [\tilde{y}_i - H_i \tilde{x}(i|i) - 1],
\]

where the data assimilation is evaluated exactly. In our stabilized filter, the stabilizing terms, \( T[P^{(c)}(i|i)] - P^{(c)}(i|i) \), are not propagated in the filter. Instead, new stabilizing terms are calculated at every data assimilation step. If \( P(i + 1|i) \) or \( P(i|i) \) needs to be
evaluated to assess the uncertainty in the state space estimate, we use the stabilized approximations.

Comments:

1) Our covariance matrices, $P^{(e)}(i|i)$, are approximations of the covariance matrices of the optimal estimate, $\hat{x}(i|i)$, and not the actual covariance of the approximate estimate, $\hat{x}^{(e)}(i|i)$.

2) Computational savings occurs only for the first order approximation to the state vector covariance matrix, $P$, and not for the state estimate. The computational requirements of second order calculations are approximately equal to the costs of the original Kalman filter. Our approximate filter does not require successive matrix inversions, and is therefore more numerically stable.

3) The zeroth order block matrices, $P^{(0)}(i|i)$ and $P^{(0)}(i|i-1)$, are positive definite since the matrix operations are performed exactly on the each separate block of the zeroth order matrix.

4) Positive definite reformulations of the Kalman filter such as Potter’s algorithm, square root filtering and UD filtering (Bierman (1977)) are not often unnecessary since the transformations, $P \rightarrow T[P]$, guarantee positive semidefiniteness.

5) In general, the block diagonal structure is incompatible with sequential processing of the measurements since each $H_{i,k}R_{k,k}^{-1}H_{i,k}$ separately is usually not block diagonal.

6) Suboptimal versions of the information filter reformulation may be constructed using duality. A second order upper bound on $P^{-1}$, constructed using an information filter and the stabilizing transformation, $T_b$, and thereby producing a lower bound on $P$.

7) Different suboptimal filters with positive definite covariance may be constructed by expanding other formulations of the Kalman filter order by order and inserting the transformation $P \rightarrow T[P]$ whenever necessary. To guarantee that the N.B.D. structure is fully utilized, each matrix in the reformulation should be N.B.D. For example, replacing Eq. (3.6) by $P (i|i) = P (i|i-1) - K_iH_iP (i|i-1)$, or $P (i|i) = [I_N - K_iH_i]P (i|i-1)[I_N - K_iH_i]^T + K_iR_iK_i^T$ yields a system of equations where
each term in the evaluations is not explicitly N.B.D. Similarly, replacing the Kalman gain matrix, $K_i$, of Eq. (3.7) with the representation,

$$K_i ≡ P (i|i−1)H_i^T[H_iP (i|i−1)H_i^T + R_i]^{-1},$$

which is not in N.B.D. form, results in a system which is not explicitly N.B.D.

**IV. N.B.D. FIXED INTERVAL SMOOTHERS**

In this section, we derive suboptimal, second order approximations to the various formulations of the fixed interval Kalman smoother. We denote the final measurement time by $N_f$. We begin with the Rauch-Tung-Striebel (R.T.S.) formulation of the smoother. We then present a new information formulation of the R.T.S. smoother as well as the Bryson-Frazier formulation. The R.T.S. smoother consists of a forward Kalman filter followed by a backward smoother correction. This structure arises because the estimation equations for $\hat{x}(i|N_f)$ have a block tribanded structure. The forward-backward sweeps correspond to the standard algorithm for solving block tribanded matrices. In our notation, the R.T.S. smoother (Rauch et al. (1965), Bryson and Ho, Ch. 13.2 (1969)) is

$$\hat{x}(i|N_f) = \hat{x}(i|i) + P (i|i)Φ(i + 1|i)^T P^{-1}(i + 1|i) \left(\hat{x}(i + 1|N_f) - \hat{x}(i + 1|i)\right), \quad (4.1)$$

$$P (i|N_f) = P (i|i) +$$

$$P (i|i)Φ(i + 1|i)^T P^{-1}(i + 1|i) \left[P (i + 1|N_f) - P (i + 1|i)\right] P^{-1}(i + 1|i)Φ(i + 1|i) P (i|i), \quad (4.2)$$

We assume that $P (i,i)$ and $P (i + 1,i)$ have been computed using the N.B.D. approximations and stabilizing transformations of Sec. II. We stabilize both $P (i|i)$ and $P^{-1}(i + 1|i)$ before evaluating Eq. (4.1) to all orders. The R.T.S. fixed interval smoother is explicitly in N.B.D. form, and the N.B.D. expansion of Secs. II and III is used to evaluate $P (i|N_f)$ to second order. To ensure positive definiteness, we stabilize our estimate of $P (i|N_f)$: $P^+(i|N_f) = T[P^-(i|N_f)]$.

A desirable property of a smoother is that $P^-(i|i) ≥ P^-(i|N_f) ≥ 0$, and unfortunately our suboptimal approximation of the R.T.S. smoother does not explicitly insure this property for moderate values of $\epsilon$. In contrast, we now show the information formulation of the R.T.S. smoother covariance equation possesses the property...
that $P^{-1}(i|N_f) \geq P^{-1}(i|i) \geq 0$. We apply the Sherman-Morrison matrix inverse
identity to Eq. (4.2) twice and simplify to yield

$$P^{-1}(i|N_f) = P^{-1}(i|i) + \Phi(i+1|i)^T \left[ \left( P^{-1}(i+1|N_f) - P^{-1}(i+1|i) \right)^{-1} + Q_{\mathbf{r},i} \right]^{-1} \Phi(i+1|i).$$

We construct a suboptimal smoother by expanding the estimation equations in powers
of $\epsilon$ and applying the stabilizing transformation, $P^{-1(\epsilon)}(i|N_f) \rightarrow T[P^{-1(\epsilon)}(i|N_f)]$.

The original R.T.S. formulation requires that the evolution equations be integrated
backward in time during the backward sweep. Since we are interested in distributed
dynamical systems with dissipation and diffusion, such a backward integration is ill-
conditioned. The Bryson-Frazier formulation of the fixed interval smoother reduces
this problem by making the following change of variables for the smoother correction:

$$\hat{x}(i|N_f) = \hat{x}(i|i) - P(i|i)\Phi(i+1|i)\lambda(i), \quad (4.4)$$

$$P(i|N_f) = P(i|i) - P(i|i)\Phi(i+1|i)\Lambda(i)\Phi(i+1|i)^T P(i|i). \quad (4.5)$$

In terms of the auxiliary $N$ vector $\tilde{\lambda}(i)$ and $N \times N$ positive definite symmetric matrix
$\Lambda(i)$, equations (4.1)-(4.2) transform to

$$\tilde{\lambda}(i-1) = (I_n - P(i|i)J_i)\hat{x}(i|i) - H_i^T R_i^{-1} (\hat{y}_i - H_i \hat{x}(i|i-1)), \quad (4.6)$$

$$\Lambda(i-1) = (I_n - P(i|i)J_i)\Phi(i+1,i)\Lambda(i)\Phi(i+1,i)(I_n - P(i|i)J_i) + J_i - J_i P(i|i)J_i, \quad (4.7)$$

subject to the final conditions: $\tilde{\lambda}(N_f) = 0$, $\Lambda(N_f) = 0$. $\Lambda(i)$ is positive semidefinite,
but its approximation, $\Lambda^{(\epsilon)}(i)$, need not be. We do not stabilize our estimate of $\Lambda^{(\epsilon)}(i)$
or any term in Eq. (4.7), since adding positive definite terms to $\Lambda(i)$ will tend to
underestimate $P(i|N_f)$. Instead, we again apply the stabilizing transformation only
to $P(i|N_f)$: $P(i|N_f) \rightarrow T[P(i|N_f)]$.

**V. CONCLUSION**

In this article, we have given first and second order approximations for the Kalman
filter and a number of smoothers by expanding the estimation equations in powers of
the coupling parameter. We have described the formulations the estimation equations which explicit preserve the N.B.D. structure. We apply stabilizing transformations to ensure the approximate covariance is positive semidefinite. We do not propagate these stabilizing terms in the Kalman filter in order to minimize the perturbation.

Other N.B.D. formulations are possible where stabilizing terms are added to the covariance and propagated in the filter. To minimize the effect of the terms the approximate spectral representation of Eq. (A5) may be used. Only the small or negative eigenvalues need be modified. The stabilizing transformation need not be applied at every time step. Instead, the values of $P_{i|i}$ may be examined occasionally or regularly, and stabilized if they have eigenvalues near zero.

The computational advantage in reducing the operations count by using first order approximations is apparent and scales as $O(1/N_b)$. If the stochastic system has a special structure like nearest neighbors block structure, computational savings may also be present for second order approximations.

For general N.B.D. structure, second order approximation actually increases the computational work over straightforward, nonexpansion calculations. In spite of the additional complication and computational cost, higher order calculations are sometimes necessary and valuable. Higher order calculations for weakly coupled systems have been given in Shen and Gajic (1990). To motivate second order approximations, we consider a case where $P^{(0)}$ is the identity matrix and that $P^{(1)}(\epsilon)$ has a large negative eigenvalue, $\lambda_1^{(1)}$, such that $\epsilon^*\lambda_1^{(1)} = -1 + \delta^*$ for the value of $\epsilon^*$ of interest. $P^{(0)} + \epsilon^*P^{(1)}(\epsilon^*)$ will have at least one small eigenvalue, $\lambda_1 \sim \delta^*$, and a corresponding large eigenvalue, $O(1/\delta^*)$, for its inverse. Our approximate filter effectively replaces this large matrix component by terms of order $O(1/4)$. Thus we have increased the stability at the cost of accuracy and slightly longer computational time. The enhancement in numerical stability will be greatest when $P^{(0)}$ is bounded from below and $P^{(0)} + \epsilon^*P^{(1)}(\epsilon^*)$ is close to singular.

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APPENDIX A: FIRST ORDER N.B.D. MATRIX OPERATIONS

A) Storage and Operations Count

We examine the computational savings which occur when the matrix opera-
tions are performed only to first order in \( \epsilon \). We define the following moments 

\[
N_2 \equiv \left( N_b \sum_{k=1}^{N_b} n_k^2 \right)^{1/2}
\]

and 

\[
N_3 \equiv \left( N_b^2 \sum_{k=1}^{N_b} n_k^3 \right)^{1/3}.
\]

Thus if all blocks are the same size, \( n_1 = n_2 = n_b \), \( N_2 = N_3 = N \). Our operation count is for the number of scalar multiplications. In contrast to the other sections, we store the first order block diagonal terms, \( \epsilon P_{(k,k)}^{(1)} \), in \( P^{(0)}(\epsilon) \), and assume \( P_{(k,k)}^{(0)}(\epsilon) = P_{(k,k)}^{(0)} + \epsilon P_{(k,k)}^{(1)} \) is positive definite. This representation slightly reduces the operation count.

We consider two subclasses of N.B.D. matrices: general and nearest neighbor. General block diagonal matrices have no particular structure in \( P^{(1)} \) and \( P^{(2)} \). We say a matrix \( P^{(\epsilon)} \) has nearest neighbor structure if and only if \( P^{(1)} \) has nonzero elements only on the diagonal, \( P_{(k,k)}^{(1)} \) and the adjacent bands, \( P_{(k,k\pm1)}^{(1)} \). We say a matrix \( P^{(\epsilon)} \) has a strongly nearest neighbor structure if and only if \( P^{(2)} \) has nonzero elements only on the diagonal and two adjacent bands, \( P_{(k,k\pm1)}^{(2)} \) and \( P_{(k,k\pm2)}^{(2)} \) as well.

For the N.B.D. matrices with a general structure on \( P^{(1)} \), the storage requirement is \( N^2 \) for an arbitrary matrix and \( N(N+1)/2 \) for a symmetric matrix. When the matrix is weakly coupled, the storage is \( \sum_{k=1}^{N_b} n_k^2 + 2n_k n_{k+1} \) for arbitrary matrices and \( \sum_{k=1}^{N_b} \frac{n_k(n_k+1)}{2} + n_k n_{k+1} \) for symmetric matrices, where \( n_{N_b+1} \equiv 0 \). When all the \( n_k \) are equal, \( n_1 = n_2 = n_b \), the sums storage requirements for nearest neighbor matrices are \( (3N_b - 2)n_1^2 \) for no symmetry, and \( (\frac{3}{2}N_b - 1)n_1^2 + \frac{N_b n_1}{2} \) for symmetric matrices.

B) \( LD^{-1}L^T \) Factorization

The transformation \( T[P^{(\epsilon)}] \equiv [P^{(0)} + \epsilon P_L^{(1)}]P^{(0)}[P^{(0)} + \epsilon P_L^{(1)}]^T \) need not be explicitly computed by multiplying \( P_L^{(1)}P^{(0)}[P^{(0)} + \epsilon P_L^{(1)}]^T \). Instead, the implicit \( LD^{-1}L^T \) representation is usually sufficient. The \( LD^{-1}L^T \) factorization requires just \( \frac{1}{2} \sum_{k=1}^{N_b} n_k^3 \) multiplications to compute \( P^{-1}_\delta \). The \( LD^{-1}L^T \) representation of \( T[P^{(\epsilon)}] \) does require that both \( P^{(0)} \) and \( P^{(0)}^{-1} \) be stored. Since both matrices are symmetric, this requires an additional storage allocation of \( N_b n_1 n_1^2 \).

C) First Order Matrix Multiplication

The N.B.D. structure is preserved under matrix multiplication. Let \( R = PQ \), then \( R^{(0)} = P^{(0)}Q^{(0)} \) and \( R^{(1)} = P^{(0)}Q^{(1)} + P^{(1)}Q^{(0)} \). Calculating \( R^{(0)} \) requires \( \sum_{k=1}^{N_b} n_k^3 \) operations and calculating \( R^{(1)} \) requires \( 2 \sum_{k=1}^{N_b} n_k^2(N - n_k) \) for a total of \( 2\frac{N N^2}{N_b} - \frac{N^3}{N_b} \) operations. If both \( P \) and \( Q \) have nearest neighbor symmetry, calculating
\( \mathbf{R}^{(1)} \) requires only \( 2 \sum_{k=1}^{N_b} n_k^2(n_k+1+n_{k-1}) \) operations where \( n_0 \equiv 0, \) and \( n_{N_b+1} \equiv 0. \) For equal size blocks, the total operation count is \( \frac{5N^3}{N_b^2} - \frac{4N^3}{N_b^2} \).

A second matrix operation which is often performed in filtering is \( \mathbf{S} = \mathbf{RQR}^T \), where \( \mathbf{Q} \) is symmetric. For ordinary matrices, this symmetric product requires \( \frac{3}{2}N^3 + \frac{1}{2}N^2 \) operations. Computing \( \mathbf{S}^{(0)} = \mathbf{R}^{(0)}Q^{(0)}R^{(0)T} \) and \( \mathbf{R}^{(0)}Q^{(0)}R^{(1)T} \) requires \( \sum_{k=1}^{N_b} n_k^2 + (N + \frac{1}{2})n_k^2 = \frac{(N+1/2)NN^2}{N_b} + \frac{N^3}{2N_b^2} \). Estimating \( \mathbf{R}^{(0)}Q^{(1)}R^{(0)T} \) requires \( \frac{3}{2}(\frac{NN^2}{N_b^2} - \frac{N^3}{N_b^2}) \) multiplications. Thus the symmetric product requires a total of \( \frac{N^3}{2N_b} \) multiplications. For nearest neighbor matrices, a total of \( \frac{1}{2} \sum_{k=1}^{N_b} n_k^2(3n_k + 1 + 5(n_k-1 + n_{k+1})) \) multiplications are required.

D) Matrix Inversion and \( D^{-1}[D - L]D^{-1}[D - L]^TD^{-1} \) Factorization

To stabilize the order by order approximate inversion, we define the \( \text{Inv}[\cdot] \) transformation to be the \( T[\cdot] \) transformation applied to the approximate inverse: \( \text{Inv}[\mathbf{P}^{(e)}] \equiv T[\mathbf{P}^{(e)-1}] \). When the approximation is first order, \( \text{Inv}[\cdot] \) reduces to \( T[\mathbf{P}^{(0)-1} - e\mathbf{P}^{(0)-1}\mathbf{P}^{(1)}\mathbf{P}^{(0)-1}] = \mathbf{P}^{(0)-1}[\mathbf{P}^{(0)} - e\mathbf{P}^{(1)}][\mathbf{P}^{(0)} - e\mathbf{P}^{(1)}]^T\mathbf{P}^{(0)-1} \). We refer to this factorization of the approximate inverse as the \( D^{-1}L'D^{-1}L^TD^{-1} \) factorization where \( L' \equiv \mathbf{P}^{(0)} - e\mathbf{P}^{(1)}. \)

The approximate inverse, \( \text{Inv}[\mathbf{P}] \), usually does not need to be computed explicitly. Instead the \( D^{-1}L'D^{-1}L^TD^{-1} \) representation of \( \text{Inv}[\mathbf{P}^{(e)}] \) is defined implicitly. Given the \( L^TD^{-1}L \) representation of \( T[\mathbf{P}^{(e)}] \), the \( D^{-1}L'D^{-1}L^TD^{-1} \) representation of \( \text{Inv}[T[\mathbf{P}^{(e)}]] \) requires no additional storage and no multiplications. The inverse of \( \text{Inv} \) is \( \text{Inv} : \text{Inv}[\text{Inv}[T[\mathbf{P}^{(e)}]]] = T[\mathbf{P}^{(e)}] \), and the \( \text{Inv}[\cdot] \) operation commutes with the \( T[\cdot] \) operation: \( \text{Inv}[T[\mathbf{P}^{(e)}]] = T[\text{Inv}[\mathbf{P}^{(e)}]] \).

E) Inverse Matrix Updates

In Kalman filtering, we successively update the covariance matrix and then its inverse. We now examine updates of the \( D^{-1}(D - L)D^{-1}(D - L)^TD^{-1} \) representation under matrix addition. We let the matrices, \( \mathbf{M} \) and \( \mathbf{J} \), be block diagonally dominant symmetric matrices with \( LD^{-1}L^T \) representations. We wish to derive an \( LD^{-1}L^T \) representation of \( \mathbf{P} \) where \( \mathbf{P}^{-1} \equiv \mathbf{M}^{-1} + \mathbf{J} \). The zeroth order matrix \( \mathbf{P}^{(0)} \) satisfies \( \mathbf{P}^{(0)-1} = \mathbf{M}^{(0)-1} + \mathbf{J}^{(0)} \). Since \( \mathbf{M}^{(0)-1} \) is given in the \( LD^{-1}L^T \) factorization, the computation of \( \mathbf{P}^{(0)-1} \) requires only additions and no multiplications. However \( \mathbf{P}^{(0)} \)
must then be computed and this requires \( \frac{1}{2} \sum_{k=1}^{N_k} n_k^3 + n_k^2 \) operations. We note that \( P^{(0)-1} = P^{(0)}\) but that \( P^{-(1)} \neq P^{(1)}\). To determine \( P^{(1)} \), we first determine \( P^{-(1)} \), and then solve for \( P^{(1)} \):

\[
P^{(1)} = P^{(0)} M^{(0)} M^{(0)}^{-1} M^{(1)} M^{(0)}^{-1} P^{(0)} - P^{(0)} J^{(1)} P^{(0)},
\]

(A1)

or

\[
P^{(1)} = [I - P^{(0)} J^{(0)}] M^{(1)} [I - J^{(0)}]^{-1} P^{(0)} - P^{(0)} J^{(1)} P^{(0)}.
\]

(A2)

Equation (A2) is better conditioned than Eq. (A1) when \( J^{(0)} \ll M^{(0)}^{-1} \). Either formulation requires \( \left[ \sum_{k=1}^{N_k} n_k^2 (3N - 2n_k) \right] \) operations.

F) Approximate Eigenvalues and Eigenvectors

The eigenvalues and eigenvectors may be estimated from perturbation theory. We use the following basic result from linear algebra. Let \( P \) be a symmetric matrix form \( S_0 + \epsilon S_1 \), let \( \{ \vec{e}_k^{(0)} \} \) and \( \{ \lambda_k^{(0)} \} \) be the eigenvectors and eigenvalues of \( S_0 \), then the eigenvalues of \( S \) are asymptotically

\[
\lambda_k \sim \lambda_k^{(0)} + \epsilon \vec{e}_k^{(0)T} S_1 \vec{e}_k^{(0)},
\]

(A3)

and the eigenvectors are asymptotically

\[
\vec{e}_k \sim \vec{e}_k^{(0)} - \epsilon (S_0 - \lambda_k^{(0)} I) - (S_1 - (\vec{e}_k^{(0)T} S_1 \vec{e}_k^{(0)}) I) \vec{e}_k^{(0)},
\]

(A4)

where “\(-\)” denotes the Moore-Penrose generalized inverse. Equation (A3) can be used to track the small eigenvalues under successive updates. The first order spectral decomposition is given by

\[
P = \sum_{k=1}^{N} \lambda_k \vec{e}_k \vec{e}_k^T \sim \sum_{k=1}^{N} (\lambda_k^{(0)} + \epsilon \lambda_k^{(1)}) (\vec{e}_k^{(0)} + \epsilon \vec{e}_k^{(1)}) (\vec{e}_k^{(0)} + \epsilon \vec{e}_k^{(1)})^T.
\]

(A5)

Equations (A3-5) generalize the first order decoupling transformation used in weakly coupled systems.

APPENDIX B: N.B.D. FIXED LAG DISCRETE SMOOTHERS

We consider suboptimal approximations of fixed lag Kalman smoothers with N.B.D. structure. Moore derived the fixed lag Kalman smoother (Moore (1973);
Ch. 7.3 of Anderson and Moore (1979)) as the Kalman filter for the augmented state space, \( \bar{x}_A(t)^T \equiv (\bar{x}(t)^T, \bar{x}(t-1)^T \ldots \bar{x}(t-n)^T) \), and then simplified the resulting augmented filter. In presenting the fixed lag smoother, we rewrite the equations and reorder the matrix indices of Anderson and Moore to achieve an explicit N.B.D. structure. We define \( e_i^{(1)} = [I_N - J_iP(i|i)]H_i^T R_i^{-1}(\bar{y}_i - H_i \hat{x}(i|i-1)) \) and \( e_i^{(j+1)} = \Phi(i-j+1, i-j)[I_N - P(i-j|i-j)J_{i-j}]e_i^{(j)} \). The fixed lag smoother is
\[
\hat{x}(i|i+n) = \hat{x}(i|i) + P(i|i-1) \sum_{\ell=1}^n e_i^{(\ell+1)}.
\] (B1)

The covariance of \( \hat{x}(i|i+n) \) is
\[
P(i|i+n) = P(i|i) - \sum_{\ell=1}^n P^{(\ell)}(i+\ell|i+\ell-1)(J_{i+\ell} - J_i \ell P(i+\ell|i+\ell)J_{i+\ell})P^{(\ell)}(i+\ell|i+\ell-1),
\] (B2)

where
\[
P^{(\ell)}(i+\ell|i+\ell-1) \equiv P(i|i-1) \prod_{j=0}^{\ell-1} [I_N - J_{i+j}P(i+j|i+j)]\Phi(i+j+1, i+j)^T.
\] (B3)

To achieve an explicit N.B.D. form, we have replaced \([I_N - H_i^T K_i^T]\) with \([I_N - J_iP(i|i)]\), and replaced \(H_i[H_iP(i|i-1)H_i^T + R_i]^{-1}\) with \([I_N - J_iP(i|i)]H_i^T R_i^{-1}\). Alternatively, we could replace \([I_N - J_iP(i|i)]\) with \(P(i|i-1)^{-1}P(i|i)\) and/or replace \(H_i^T R_i^{-1} - J_iP(i|i)H_i^T R_i^{-1}\) by \(P^{-1}(i|i-1)P(i|i)H_i^T R_i^{-1}\). The alternative formulations have the advantages that they involve fewer matrix multiplications. Our present formulation has the advantage that \(P(i|i-1)\) appears only once in the expression, and that all the other terms are input quantities, usually known to all orders. In the limit that \(J_i \ll P(i|i-1)^{-1}\), our formulation approximates small terms while the alternative formulation approximates large terms. For these reasons, we generally prefer our formulation in Eqs. (B1-3).

We stabilize the data assimilation by using \(P_+^{(e)}(i-j|i-j) = T[P^{(e)}(i-j|i-j)]\) in evaluating \(e_i^{(j+1)}\) and using \(P_+^{(e)}(i|i-1)\) in Eq. (B1). If \(P(i|i+n)\) is of interest, we also stabilize our approximation of it.

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Our work is motivated by and generalises the results of Cohn and Parrish. In Appendix B of Cohn and Parrish (1991), the authors show that if $H_i^T R_i^{-1} H_i$ is diagonal and the evolution equations are diagonal, then the estimation covariance will be diagonal. In this article, we extend their results to include block diagonal systems and Kalman smoothers. More importantly, we relax the requirement of exact diagonality and consider small offdiagonal terms. We expand the estimation equations in powers of the offdiagonal terms and develop numerically wellconditioned algorithms to compute these approximate estimation.

In applying Kalman filtering to global circulation models, Cohn and Parrish (Cohn and Parrish (1991)) noted that the evolution equations are simplest in an eigenfunction basis while the data assimilation is simplest in a finite difference or finite element representation. By requiring that the measurement locations be distributed such that $H_i^T R_i^{-1} H_i$ is nearly block diagonal, we are able to simplify the data assimilation equation in the eigenfunction domain.