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Eftychios A. Pnevmatikakis, Kamiar Rahnama Rad, Jonathan Huggins & Liam Paninski
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Fast Kalman Filtering and Forward–Backward Smoothing via a Low-Rank Perturbative Approach

Eftychios A. PNEVMATIKAKIS, Kamiar Rahnama RAD, Jonathan HUGGINS, and Liam PANINSKI

Kalman filtering-smoothing is a fundamental tool in statistical time-series analysis. However, standard implementations of the Kalman filter-smoother require \(O(d^3)\) time and \(O(d^2)\) space per time step, where \(d\) is the dimension of the state variable, and are therefore impractical in high-dimensional problems. In this article we note that if a relatively small number of observations are available per time step, the Kalman equations may be approximated in terms of a low-rank perturbation of the prior state covariance matrix in the absence of any observations. In many cases this approximation may be computed and updated very efficiently (often in just \(O(k^2d)\) or \(O(k^2d + kd \log d)\) time and space per time step, where \(k\) is the rank of the perturbation and in general \(k \ll d\)), using fast methods from numerical linear algebra. We justify our approach and give bounds on the rank of the perturbation as a function of the desired accuracy. For the case of smoothing, we also quantify the error of our algorithm because of the low-rank approximation and show that it can be made arbitrarily low at the expense of a moderate computational cost. We describe applications involving smoothing of spatiotemporal neuroscience data. This article has online supplementary material.

Key Words: Covariance approximation; Fast algorithm; Low-rank methods; Numerical analysis; Tracking.

1. INTRODUCTION

Understanding the dynamics of large systems for which limited, noisy observations are available is a fundamental and recurring scientific problem. A key step in any such analysis involves data assimilation: we must incorporate incoming observations and update our beliefs about the dynamical state of the system accordingly. The Kalman filter may be considered the canonical method for data assimilation; this method provides a conceptually simple recursive framework for online Bayesian inference in the context of linear and
Gaussian dynamics and observation processes. Furthermore, the Kalman filter serves as the underlying computational engine in a wide variety of more complicated non-Gaussian and nonlinear statistical models.

However, these methods face a major limitation: standard implementations of the Kalman filter require $O(d^3)$ time and $O(d^2)$ space per time step, where $d$ denotes the dimension of the system state variable, and are therefore impractical for applications involving very high-dimensional systems. The bottleneck is in the representation and computation of the forward covariance matrix $C_t = \text{cov}(x_t | Y_{1:t})$: this is the posterior covariance of the $d$-dimensional state vector $x_t$, given the sequence of observations $Y_{1:t}$ up to the current time $t$. Two natural ideas for reducing the computational burden of storing and computing this $d \times d$ matrix have been explored. First, if $C_t$ is sparse (i.e., consists of mostly zeros), then we can clearly store and perform matrix-vector computations with $C_t$ with $O(d^2)$ complexity. In many examples $C_t$ has a nearly banded, or strongly tapered, structure (i.e., most of the large components of $C_t$ are near the diagonal), and sparse approximate matrix updates can be exploited. This approach has been shown to be extremely effective in some cases (Furrer and Bengtsson 2007; Bickel and Levina 2008; El Karoui 2008; Kaufman, Schervish, and Nychka 2008; Khan and Moura 2008), but in many settings there is no a priori reason to expect $C_t$ to have any useful sparse structure, and therefore this idea can not be applied generally.

Second, we could replace $C_t$ with a low-rank approximation. For example, a major theme in the recent literature on numerical weather prediction (where the system of interest is the atmosphere discretized in a spatial grid, leading in many cases to a state dimension in the tens or hundreds of millions) has been the development of the theory of the “ensemble Kalman filter” (Verlaan 1998; Treebushny and Madsen 2005; Chandrasekar et al. 2008; Evensen 2009), which implements a Monte Carlo-based, low-rank approximation of the full Kalman filter. Low-rank approximations for $C_t$ are typically justified on computational grounds but may also be justified statistically in the case that many high signal-to-noise ratio (SNR) observations are available: in this setting, we can argue that our posterior uncertainty $C_t$ will be approximately restricted to a subspace of dimension significantly less than $d$, as discussed, for example, by Solo (2004). Alternatively, we may impose a low-rank structure on the posterior covariance $C_t$ directly by choosing our prior covariance matrix to be of low rank (Wikle and Cressie 1999; Wood 2006; Banerjee et al. 2008; Cressie and Johannesson 2008; Cressie, Shi, and Kang 2010); however, our focus in this work is on approximating $C_t$ given a prior covariance matrix which is of full rank.

The low-SNR setting, where a relatively small number of noisy observations are available per time step, has been explored less thoroughly. One exception is the neuronal dendritic application discussed by Paninski (2010), where we noted that $C_t$ could be approximated very accurately in terms of a low-rank perturbation of $C_0$, the prior equilibrium covariance of the state variable $x_t$ in the absence of any observations $Y$. (Note that this approximation is very different from the high-SNR case, where we approximate $C_t$ as a low-rank perturbation of the zero matrix, not of $C_0$.) To efficiently update this low-SNR approximation to $C_t$, Paninski (2010) exploited the special structure of the dynamics in this application: dendritic voltage dynamics are governed by a cable equation on a tree (Koch 1999), which may be solved using symmetric sparse matrix methods in $O(d)$ time (Hines 1984). In turn, this implied that $C_t$ could be updated in $O(k^2d)$ time, where $k$ is the rank of the perturbation of
C_0 used to represent C_t. Because empirically a k \ll d sufficed to accurately approximate C_t in this application, this approach resulted in a much faster implementation of the Kalman filter, with linear instead of cubic complexity in d.

In this article we extend this basic idea in a number of ways. We first develop a methodology that provides upper bounds on the rank of the perturbation on C_0 required to represent C_t. Our analysis shows that the basic idea is applicable to both high- and low-SNR cases, and that the rank of the perturbation is indeed small and thus the algorithm can lead to substantial computational gains. We also develop a similar fast algorithm for full forward–backward smoothing by deriving an efficient low-rank block-Thomas (LRBT) recursive algorithm for the solution of block-tridiagonal systems. For this LRBT algorithm, we also characterize the trade-off between the rank of the approximation (and thus the computational cost) and the induced approximation error. We show that the error can be made arbitrarily small, with a relatively moderate computational cost incurred by the corresponding increase in the rank of the perturbation. We also show that the LRBT algorithm efficiently calculates the steepest descent direction under an appropriate quadratic norm. As a result, it can be used as an iterative steepest-descent algorithm, or as a preconditioner in standard iterative methods (e.g., conjugate gradients), to converge to the exact solution faster than exact forward–backward methods.

We describe a number of examples where special features of the system dynamics allow us to compute and update the low-rank approximation to C_t efficiently (often in just O(k^2d) or O(k^2d + kd log d) time and O(kd) space per time step), using fast methods from numerical linear algebra. One particularly simple setting involves spatiotemporal smoothing applications; as a concrete example, we describe how to apply the proposed methods to efficiently smooth certain kinds of high-dimensional spatiotemporal neuroscience data. Finally, we briefly describe extensions of our methods to nonlinear, non-Gaussian settings.

2. BASIC KALMAN FILTERING SETUP

We begin by briefly reviewing the Kalman filter and establishing notation. Again, let x_t denote our d-dimensional state variable, and y_t the observation at time t. We assume that x_t and y_t satisfy the following linear-Gaussian dynamics and observation equations:

\[
\begin{align*}
x_{t+1} &= A x_t + u_t + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, V), \\
y_t &= B_t x_t + \eta_t, \quad \eta_t \sim \mathcal{N}(\mu_{\eta_t}, W_t),
\end{align*}
\]

with initial conditions x_0 \sim \mathcal{N}(\mu_0, V_0). Here, A represents the system dynamics matrix, u_t is a deterministic input to the system at time t, and \epsilon_t is an iid. Gaussian vector with mean zero and covariance V. B_t denotes the observation gain matrix, W_t the observation noise covariance, and \mu_{\eta_t} an offset mean in the observation. Our methods are sufficiently general that the dimension of y_t can vary with time. From now on, without loss of generality we assume that \mu_0 = 0, and u_t = 0, \mu_{\eta_t} = 0 for all t. Nonlinear and non-Gaussian observations may also be incorporated in some cases, as we will discuss further below. Moreover, extensions to nonstationary models, where A and/or V in the dynamics equation vary with time, are also possible in some cases (Pnevmatikakis and Paninski 2012), but will not be discussed here.
Now the focus of this article is the efficient implementation of the Kalman filter recursion for computing the forward mean $\mu_t = \mathbb{E}(x_t | Y_{1:t})$, and covariance $C_t = \text{cov}(x_t | Y_{1:t})$, where $Y_{1:t}$ denotes the observed data $\{y_i\}$ up to time $t$. The Kalman recursions may be written as (Anderson and Moore 1979):

$$C_t = \left( P_{t-1}^{-1} + B_t^T W_t^{-1} B_t \right)^{-1},$$

$$\mu_t = A \mu_{t-1} + P_t B_t^T (W_t + B_t P_t B_t^T)^{-1} (y_t - B_t A \mu_{t-1}),$$

with $P_t \triangleq \text{cov}(x_t | Y_{1:t-1}) = A C_{t-1} A^T + V$. (5)

Note that computing the inverses in the recursion for $C_t$ requires $O(d^3)$ time in general, or $O(d^2)$ time via the Woodbury lemma (Golub and Van Loan 1996) if the observation matrix $B_t$ is of low rank (i.e., if rank$(B_t) \ll d$). In either case, $O(d^2)$ space is required to store $C_t$.

A key quantity is the prior covariance $C_{0,t}$, that is, the covariance of $x_t$ in the absence of any observations. From the Kalman filter recursion, $C_{0,t}$ evolves as

$$C_{0,t} = A C_{0,t-1} A^T + V.$$ (6)

This is just the Kalman recursion for $C_t$ above in the special case that $B = 0$ (i.e., no observations are available). Throughout the article we make the assumption that $A$ is stable, that is, $\|A\| < 1$, where $\| \cdot \|$ denotes the spectral norm. In this case $C_{0,t}$ converges to the equilibrium prior covariance $C_0 = \lim_{t \to \infty} C_{0,t}$. To enforce stationarity of the prior, the Kalman recursion is often initialized with $V_0 \triangleq C_{0,0} = C_0$. In this case, we have $C_{0,t} = C_0$ for all $t$, because the equilibrium covariance $C_0$ satisfies the discrete Lyapunov equation

$$A C_0 A^T + V = C_0.$$ (7)

This equation can be solved explicitly in many cases (Anderson and Moore 1979), as we discuss briefly now. If $A$ is normal (i.e., $AA^T = A^T A$), and commutes with the dynamics noise covariance $V$, then $C_0$ can be explicitly computed using the standard moving-average recursion (Brockwell and Davis 1991) for the autoregressive model $x_t$:

$$C_0 = \sum_{i=0}^{\infty} A^i V (A^T)^i = V \sum_{i=0}^{\infty} (AA^T)^i = V (I - AA^T)^{-1}.$$ (8)

More generally, if $V$ and $A$ do not commute then we can employ the (linear) whitening change of variables $\bar{x}_t = V^{-1/2} x_t$ (assuming $V$ is of full rank). Defining the reparameterized covariance matrix $C'_0$ via $C_0 = V^{1/2} C'_0 V^{1/2}$, $A'_V$ through the similarity transformation $A'_V = V^{-1/2} A V^{1/2}$, and assuming $A'_V$ is normal, we rewrite (7) as

$$A'_V C'_0 A'^T_V + C'_0 \Rightarrow C'_0 = (I - A'_V A'^T_v)^{-1} \Rightarrow C_0 = V^{1/2} (I - A'_V A'^T_v)^{-1} V^{1/2}.$$ (9)

The case where $V$ is of reduced rank, or the resulting $A'_V$ is nonnormal, appears to be more difficult, as noted in more detail in the Discussion section. From now on, unless noted otherwise, we make the assumption that $A$ is normal and commutes with $V$. 


3. FAST KALMAN FILTERING

Now the basic idea is that when \( \text{rank}(B_t) \ll d \), \( C_t \) should be close to \( C_{0,t} \); that is, we should be able to represent the time-varying covariance \( C_t \) as a small perturbation about the prior covariance \( C_{0,t} \), in some sense. Thus, more concretely, we will approximate \( C_t \) as

\[
C_t \approx \tilde{C}_t \triangleq C_{0,t} - L_t \Sigma_t L_t^T,
\]

where \( L_t \Sigma_t L_t^T \) is a low-rank matrix we will update directly, and \( C_{0,t} = \text{cov}(x_t) \). We will show that it is straightforward to compute and update the perturbations \( L_t \) and \( \Sigma_t \) efficiently whenever fast methods are available to solve linear equations involving \( A \) and \( C_{0,t} \).

But first, why does the approximation in Equation (10) make sense? It is easy to see, using the Woodbury matrix lemma, that if we make \( b \) observations at time \( t = 1 \), then (10) will hold exactly, for \( L_1 \Sigma_1 L_1^T \) of rank at most \( b \). If we make no further observations, then \( C_t \) follows the simple update rule

\[
C_t = AC_{t-1}A^T + V \Rightarrow C_2 = A \left( C_{0,1} - L_1 \Sigma_1 L_1^T \right) A^T + V = C_{0,2} - A L_1 \Sigma_1 L_1^T A^T;
\]

the last equality follows from (6). Iterating, we see that

\[
C_t = C_{0,t} - A^{t-s} L_s \Sigma_s L_s^T (A^{t-s})^T,
\]

where \( s \) denotes the time of the last available observation. Because \( A \) is assumed to be stable, this implies that the perturbation to \( C_t \) around the equilibrium covariance \( C_{0,t} \), caused by the observations up to time \( s \) will decay exponentially; for \( t - s \) sufficiently large, we can discard some dimensions of the perturbation \( A^{t-s} L_s \Sigma_s L_s^T (A^{t-s})^T \) without experiencing much error in \( C_t \). In the case that additional observations become available with each time step \( t \), a similar phenomenon governs the behavior of \( C_t \); long-ago observations are eventually “forgotten,” because of the exponential decay caused by the double multiplication \( A C_t A^T \). We may exploit this exponential decay by discarding some dimensions of \( C_t - C_{0,t} \) as they become sufficiently small, and if the observations are sufficiently low rank relative to the decay rate imposed by \( A \), then the effective rank of \( C_t - C_{0,t} \) will remain small.

3.1 THE FAST KALMAN FILTERING ALGORITHM

Now we can describe a method for efficiently updating \( L_t \) and \( \Sigma_t \). We will use \( A \) and \( C_{0,t} \) in what follows; it is easy to substitute the transformed matrices \( A_V \) and \( C'_{0,t} \) (defined previously) if necessary. First, as above, for the approximate predictive covariance \( \tilde{P}_t \) write

\[
\tilde{P}_t^{-1} \triangleq (A \tilde{C}_{t-1} A^T + V)^{-1} = (A \left( C_{0,t-1} - L_{t-1} \Sigma_{t-1} L_{t-1}^T \right) A^T + V)^{-1}
= (C_{0,t} - A L_{t-1} \Sigma_{t-1} L_{t-1}^T A^T)^{-1} = C_{0,t}^{-1} + \Phi_t \Delta_t \Phi_t^T,
\]

where we applied (6) and the Woodbury lemma, and abbreviated \( \Phi_t = C_{0,t}^{-1} A L_{t-1} \) and \( \Delta_t = (\Sigma_{t-1} L_{t-1}^T A C_{0,t}^{-1} A L_{t-1})^{-1} \).
Now plug this into the covariance update and apply Woodbury\(^1\) again:

\[
\begin{align*}
\hat{C}_t &= (C_{0,t}^{-1} + \Phi_t \Delta_t \Phi_t^T + B_t^T W_t^{-1} B_t)^{-1} = (C_{0,t}^{-1} + O_t Q_t O_t^T)^{-1} \\
&= C_{0,t} - C_{0,t} O_t (Q_t^{-1} + O_t^T C_{0,t} O_t)^{-1} O_t^T C_{0,t},
\end{align*}
\]

(12)

where \(O_t = [\Phi_t, B_t^T]\), \(Q_t = \text{blkdiag} \{\Delta_t, W_t^{-1}\} \).

We obtain \(L_t\) and \(\Sigma_t\) by truncating the partial singular value decomposition (SVD) of the right-hand side of (12):

\[
\begin{bmatrix}
\hat{L}_t, \hat{\Sigma}_t^{1/2}
\end{bmatrix} = \text{svd}(C_{0,t} O_t (Q_t^{-1} + O_t^T C_{0,t} O_t)^{-1/2}),
\]

(14)

then choose \(L_t\) as the first \(k_t\) columns of \(\hat{L}_t\) and \(\Sigma_t\) as the first \(k_t\) diagonal elements \(\hat{\Sigma}_t\), where \(k_t\) is chosen to be large enough (for accuracy) and small enough (for computational tractability). A reasonable choice of \(k_t\) is as the least solution of the inequality:

\[
\sum_{i \leq k_t} [\hat{\Sigma}_t]_{ii} \geq \theta \sum_{i} [\hat{\Sigma}_t]_{ii} ;
\]

(15)

that is, choose \(k_t\) to capture at least a large fraction \(\theta\) of the term \(\hat{L}_t \hat{\Sigma}_t^{1/2}\) (i.e., the square root of the term perturbing \(C_{0,t}\) in (12)). Now for the update of the approximate Kalman mean \(\hat{\mu}_t\) we can use the exact formula (4) but replace \(P_t\) with the approximate predictive covariance \(\hat{P}_t\) (11). Note that we update the mean \(\hat{\mu}_t\) first, then truncate \(L_t\) and \(\Sigma_t\).

To review, we have introduced simple low-rank recursions for \(L_t\), \(\Sigma_t\), and \(\hat{\mu}_t\) in terms of \(C_{0,t}\) and \(A\). The key point is that \(C_{0,t}\) or \(C_{0,t}^{-1}\) need never be computed explicitly; instead, all we need is to multiply by \(A\) and multiply and divide by \(C_{0,t}\) or \(C_{0,t}^{-1}\), whichever is easiest (by “divide,” we mean to solve equations of the form \(C_{0,t} v = r\) for the unknown vector \(v\) and known vector \(r\)). The SVD step requires \(O((k_{t-1} + b_t)^2 d)\) time, where \(k_{t-1}\) is the order of the perturbation (effective rank) at time step \(t - 1\), and \(b_t\) is the number of measurements taken at time step \(b_t\). All the other steps involve \(O(k_t)\) matrix-vector multiplications or divisions by \(C_{0,t}\) or \(A\). Thus, if \(K(d)\) denotes the cost of such a single matrix-vector operation, the computational complexity of each low-rank update is approximately \(O(k_t^2 d + k_t K(d))\). In many cases of interest (see below) \(K(d) = o(d^2)\), and therefore the low-rank method is significantly faster than the standard Kalman recursion for large \(d\). The algorithm is summarized below (Algorithm 1).

We close this section by noting that the posterior marginal variance difference \([\hat{C}_t - C_{0,t}]_{ii}\) can be computed in \(O(k_t d)\) time, because computing the diagonal of \(\hat{C}_t - C_{0,t}\) just requires us to sum the squared elements of \(\Sigma_t^{1/2} L_t\). This quantity is useful in a number of contexts (Huggins and Paninski 2012). In addition, the method can be sped up significantly in the special case that \(B\) and \(W\) are time-invariant (or vary in a periodic manner): in this

---

\(^1\)It is well known that the Woodbury formula can be numerically unstable when the observation covariance \(W\) is small (i.e., the high-SNR case). It should be possible to derive a low-rank square-root filter (Treebush and Madsen 2005; Chandrasekhar et al. 2008) to improve the numerical stability here, though we have not yet pursued this direction. Meanwhile, a crude but effective method to guarantee that \(C_t\) remains positive definite is to simply shrink \(\Sigma_t\) slightly if any negative eigenvalues are detected. This can be done easily in \(O(d)\) time by restricting attention to the subspace spanned by \(L_t\).
Algorithm 1 Fast Kalman filtering algorithm

\[ L_1 = C_{0,1} B_1^T, \quad \Sigma_1 = (W_1 + B_1 C_{0,1} B_1^T)^{-1} \]  
\[ \tilde{C}_1 = C_{0,1} - L_1 \Sigma_1 L_1^T \]  
\[ \tilde{\mu}_1 = L_1 \Sigma_1^{-1} y_1 \]

for \( t = 2 \) to \( T \)

\[ C_{0,t} = A C_{0,t-1} A^T + V \]  
\[ \Phi_t = C_{0,t}^{-1} A L_{t-1}, \quad \Delta_t = (\Sigma_{t-1}^{-1} - L_{t-1}^T A^T C_{0,t}^{-1} A L_{t-1})^{-1} \]  
\[ O_t = [\Phi_t, B_t], \quad \tilde{Q}_t = \text{blkdiag}\{\Delta_t, W_t^{-1}\} \]  
\[ \tilde{L}_t, \tilde{\Sigma}_t^{1/2} = \text{svd}(C_{0,t} O_t (Q_t^{-1} + O_t^T C_{0,t} O_t)^{-1/2}) \]  
\[ \text{Truncate } \tilde{L}_t \text{ and } \tilde{\Sigma}_t \text{ to } L_t \text{ and } \Sigma_t. \]  
\[ \bar{C}_t = C_{0,t} - L_t \Sigma_t L_t^T \]  
\[ \bar{P}_t = C_{0,t} - A L_{t-1} \Sigma_{t-1} L_{t-1}^T A^T \]  
\[ \tilde{\mu}_t = A \tilde{\mu}_{t-1} + \bar{P}_t B_1^T (W_1 + B_1 \bar{P}_t B_1^T)^{-1} (y_t - B_1 A \tilde{\mu}_{t-1}) \]

\( \text{(cost } O(b_1^3 + b_1 K(d))) \)

case, \( \bar{C}_t \) will converge to a limit as an approximate solution of the corresponding Riccati equation, (or \( \tilde{C}_t \) will also be periodic) and we can stop recomputing \( L_t \) and \( \Sigma_t \) on every time step.

3.2 Examples for which the proposed fast methods are applicable

There are many examples where the required manipulations with \( A, V, \) and \( C_0 \) are relatively easy. The following list is certainly nonexhaustive. First, if \( A \) or its inverse is banded (or tree-banded, in the sense that \( A_{ij} \neq 0 \) only if \( i \) and \( j \) are neighbors on a tree) then so is \( C_0^{-1} \), and multiplying and dividing by \( C_0 \) costs just \( O(d) \) time and space per time step (Rue and Held 2005; Davis 2006).

Second, in many cases \( A \) is defined in terms of a partial differential operator. (The example discussed in Paninski (2010) falls in this category; the voltage evolution on the dendritic tree is governed by a cable equation.) \( A \) in these cases is typically sparse and has a specialized local structure; multiplication by \( A \) and \( C_0^{-1} \) requires just \( O(d) \) time and space. In many of these cases multigrid methods or other specialized partial differential equation (PDE) solvers can be used to divide by \( C_0^{-1} \) in \( O(d) \) time and space (Briggs, Henson, and McCormick 2000). As one specific example, multigrid methods are well established in electroencephalographic and magnetoencephalographic analysis (Wolters 2007; Lew et al. 2009), and therefore could potentially be used to significantly speed up the Kalman-based analyses described in Long et al. (2006), Galka et al. (2008), and Freestone et al. (2011).

Third, \( A \) will have a Toeplitz (or block-Toeplitz) structure in many physical settings, for example, whenever the state variable \( x_t \) has a spatial structure and the dynamics are spatially invariant in some sense. Multiplication by \( A \) and \( C_0^{-1} \) via the fast Fourier transform (FFT) requires just \( O(d \log d) \) time and space in these cases (Press et al. 1992). Similarly, division by \( C_0^{-1} \) can be performed via preconditioned conjugate gradient (PCG) descent, which in many cases again requires \( O(d \log d) \) time and space (Chan and Ng 1996). Of course, if \( A \) is circulant then FFT methods may be employed directly to multiply and divide by \( C_0 \) with cost \( O(d \log d) \).
Finally, in all of these cases, block or Kronecker structure in $A$ may be exploited easily, because the transpose and product involved in the construction of $C_0$ will preserve this structure.

### 3.3 Analysis of the Effective Rank

As discussed above, the complexity of each iteration is $O(k_t^2 d + k_t K(d))$, where $k_t$ is the effective rank of the perturbation to $C_{0,t}$ at time $t$. In this section, we formalize the notion of the effective rank and present some simple bounds that provide some insight into the efficiency of our algorithm. A more detailed treatment can be found in online Appendix B.

**Definition 1.** Let $U$ be a matrix and $\theta$ a constant with $0 \leq \theta \leq 1$. The effective rank of $U$ at threshold $\theta$, $z_\theta(U)$, is defined as the minimum integer $k$ such that there exists a matrix $X$ with rank($X$) = $k$ and
\[
\|X - U\|_F^2 \leq (1 - \theta)\|U\|_F^2,
\]
where $\|\cdot\|_F$ denotes the Frobenius norm.

Based on the above definition, the number of singular values $k_t$ (15) in the fast Kalman recursion can be expressed as $k_t = z_\theta(G_{t/2}^{1/2})$, with $G_t$ defined as
\[
G_t = C_{0,t} O_t \left( Q_t^{-1} + O_t^T C_{0,t} O_t \right)^{-1} O_t^T C_{0,t}.
\]
(16)
To estimate the complexity of the algorithm, we need to characterize $z_\theta(G_{t/2}^{1/2})$. However, this is challenging because $G_t$ is obtained from a series of successive low-rank approximations. From (12), $G_t$ corresponds to the perturbing term of the approximate covariance $\tilde{C}_t$. We instead analyze the effective rank of the perturbing term of the exact covariance $C_t$ as given in the following proposition (proven in online Appendix B).

**Proposition 1.** The covariance matrices $C_t$ can be written recursively as
\[
C_t = C_{0,t} - C_{0,t} U_t^T Z_t^{-1} U_t C_{0,t},
\]
(17)
where
\[
Z_t = F_t^{-1} + U_t C_{0,t} U_t^T,
\]
(18)
and the matrices $U_t$ and $F_t$ are defined recursively as
\[
U_t = \begin{bmatrix} B_t \\ U_{t-1} C_{0,t-1} A^T C_{0,t}^{-1} \end{bmatrix}, \quad U_1 = B_1
\]
\[
F_t^{-1} = \begin{bmatrix} W \\ 0 \ F_t^{-1} + U_{t-1} (C_{0,t-1} + C_{0,t-1} A^T C_{0,t}^{-1} A C_{0,t-1}) U_t^T \end{bmatrix}, \quad F_1 = W^{-1}.
\]
(19)

Because $\tilde{C}_t$ is an approximation of $C_t$ we expect that for at least high threshold $\theta$ we have
\[
z_\theta(G_{t/2}^{1/2}) \approx z_\theta(Z_t^{-1/2} U_t C_{0,t}).
\]
(20)
Here we analyze the effective rank of the matrices $U_t C_{0,t}$. In the appendix, we analyze the effective rank of $Z_{t}^{-1/2} U_t C_{0,t}$ and also provide a heuristic method for estimating the actual effective rank of $G_{t}^{-1/2}$. Our analysis and simulations show that $z_\theta(G_{t}^{-1/2}) \leq z_\theta(Z_{t}^{-1/2} U_t C_{0,t})$, with equality when $\theta \uparrow 1$; this is unsurprising, because $Z_{t}^{-1/2} U_t C_{0,t}$ corresponds to the full perturbation in $C_{t}$ away from $C_{0,t}$, although $G_{t}^{-1/2}$ is an approximation of this perturbation.

For large $t$, the prior covariance $C_{0,t}$ converges to the equilibrium covariance $C_0$. Therefore, under the assumption that $A$ is normal and commutes with $V$, we can make the approximation $C_{0,t} \approx C_0 = V(I - AA^T)^{-1}$ and the recursion of (19) can be rewritten as

$$U_t \approx [B_t^T, A U_{t-1}^T]^T, \quad F_t^{-1} \approx \text{blkdiag} \{ W, F_{t-1}^{-1} + U_{t-1} V U_{t-1}^T \}. \quad (21)$$

If $b_t$ is the number of measurements taken at time $t$, then the matrices $U_t, F_t$ have dimensions $[\sum_{i=1}^t b_i, d]$ and $[\sum_{i=1}^t b_i, \sum_{i=1}^t b_i]$, respectively. However, we see that at each time step $t$, all the blocks of $U_t$ that correspond to times $1, \ldots, t - 1$ are multiplied with $A^T$. Therefore at time $t$, the effect of the measurements from time $t - s$ will be limited and thus past measurements are eventually “forgotten,” as discussed above.

To characterize the effective rank in a specific tractable setting, suppose that each $B_t$ is a $b \times d$ iid random matrix where each entry has zero mean and variance $1/d$. Let $[U_{t}]_{1:t}$ be the matrix that consists of the first $l$ blocks of $U_t$, and define $k_U$ as the minimum number of blocks required to capture a $\theta$ fraction of the expected energy,

$$k_U = \arg \min_{l \in \mathbb{N}} \left\{ l : \mathbb{E}[\| U_{1:t} C_{0,t} \|_F^2 \geq \theta \mathbb{E}[\| U_t C_{0,t} \|_F^2] \right\}. \quad (22)$$

Using (21), the $(m+1)$th block of $U_t C_{0,t}$ is approximately $B_{t-m}(A^T)^m C_0$. Using the identity $\| X \|_F^2 = \text{Tr}(X^T X)$, we have that the expected energy of the $(m+1)$th block is equal to

$$\mathbb{E}[\| [U_t]_{m+1} C_{0,t} \|_F^2] \approx \mathbb{E}[\| B_{t-m}(A^T)^m C_0 \|_F^2] = \mathbb{E} \left( \text{Tr} \left[ (A^T)^m C_0^2 A^m B_{t-m}^T \right] \right) \approx \frac{b}{d} \text{Tr} \left[ (A^T)^m C_0^2 A^m \right] = \frac{b}{d} \sum_{i=1}^d c_i^2 \alpha_i^{2m}, \quad (23)$$

where $\alpha_1 \geq \cdots \geq \alpha_d$ are the singular values of $A$ and $c_1, \ldots, c_d$ are the corresponding singular values of $C_0$. Plugging into (22) and summing over the blocks, assuming $t \rightarrow \infty$, we get

$$k_U = \arg \min_{l \in \mathbb{N}} \left\{ \sum_{i=1}^d c_i^2 \frac{1 - \alpha_i^{2l}}{1 - \alpha_i^2} \geq \theta \sum_{i=1}^d c_i^2 \frac{1}{1 - \alpha_i^2} \right\} \overset{(*)}{=} \arg \min_{l \in \mathbb{N}} \left\{ 1 - \alpha_i^{2l} \geq \theta \right\} \overset{(*)}{=} \left\lceil \log(1 - \theta) \right\rceil, \quad (24)$$

where $(*)$ follows because $1 - \alpha_i^{2l} \geq \theta \Rightarrow 1 - \alpha_i^{2l} \geq \theta$ for all the other singular values $\alpha_i$ and $[x]$ denotes the least integer greater or equal than $x$. The bound of (24) becomes tight if $c_1 \gg c_2, \ldots, c_d$ or if all the singular values of $A$ are approximately equal, that is, $A$ becomes proportional to the identity matrix. Note that the bound of (24) covers only the expected case and is probabilistic. It is possible to derive concentration inequalities on the probability that the bound does not hold, but for our purposes it suffices to state that the
bound is expected to hold with high probability. Therefore, with high probability the first \( bkU \) rows of \( U_tC_{0,t} \) capture a \( \theta \) fraction of its energy and

\[
z_\theta(U_tC_{0,t}) \leq bkU. \tag{25}
\]

In other words, we expect that the algorithm will lead to high computational gains if \( d \gg bkU \). Note that the derived bound grows only mildly with \( \theta \) and is also independent of \( d \). Therefore, for large \( d \) we see that the total cost of the fast Kalman filtering algorithm becomes at most \( O((k^2 U d + kU K(d))T) \). In online Appendix B we argue that a tighter bound for \( z_\theta(G^{1/2}) \) can be derived by taking into account the recursive nature of the thresholding procedure. More specifically, we argue that

\[
z_\theta\left(G^{1/2}t\right) \leq \arg \min_{l \in \mathbb{N}} \left\{ \mathbb{E} \left[ \|U_t\|_1: lC_{0,t}\|_F^2 \geq \theta \mathbb{E} \left[ \|U_t\|_1: l+1C_{0,t}\|_F^2 \right] \right\} \leq b \left[ \frac{\log(1 - \theta) - \log(1 - \|A\|^2\theta)}{2 \log(\|A\|)} \right],
\]

which provides a significantly tighter bound. Moreover, we examine the effective rank of \( Z_t^{-1/2}U_tC_{0,t} \) and show that \( z_\theta(Z_t^{-1/2}U_tC_{0,t}) \leq z_\theta(U_tC_{0,t}) \) with equality holding in the limiting case where the noise power becomes infinite, that is, in the low-SNR regime. Finally, we derive another heuristic bound on \( z_\theta(G^{1/2}t) \), based on \( z_\theta(Z_t^{-1/2}U_tC_{0,t}) \) and present a simulation example that supports the several bounds.

4. FULL FORWARD–BACKWARD SMOOTHING

So far we have focused on the forward problem of computing estimates of \( x_t \) given the data available up to time \( t \). To incorporate all of the available information \( Y_{1:T} \) (not just \( Y_{1:t} \)), we need to perform a backward recursion. Two methods are available: we can use the Kalman backward smoother (Shumway and Stoffer 2006), which provides both \( \mathbb{E}(x_t|Y_{1:T}) \) and \( \text{cov}(x_t|Y_{1:T}) \), or a version of the Thomas recursion for solving block-tridiagonal systems.

Both recursions can be adapted to our low-rank setting. In the Kalman backward smoother we can approximate \( \text{cov}(x_t|Y_{1:T}) \approx C_0 - L_t^T \Sigma_t(L_t^T)^T \), for an appropriately chosen low-rank matrix \( L_t^T \Sigma_t(L_t^T)^T \), which can be updated efficiently using methods similar to those we have described here for the forward low-rank approximation \( C_0 - L_t^T \Sigma_t(L_t^T)^T \); see Huggins and Paninski (2012) for full details. Here, we focus on deriving an efficient LRBT approach, and examining its convergence characteristics.

4.1 THE LRBT ALGORITHM

First we recall that the output of Kalman filter-smoother, \( s_t = \mathbb{E}(x_t|Y_{1:T}) \), may be written as the solution to a block-tridiagonal linear system (Fahrmeir and Kaufmann 1991; Paninski et al. 2010), that is

\[
Hs = -\nabla|_{x=0}, \tag{26}
\]

where \( \nabla|_{x=0} \), \( H \) denote the gradient evaluated at zero and the Hessian of the negative log-posterior \( f = -\log p(X|Y_{1:T}) \) with respect to \( X \), because \( f \) is simply a quadratic function
in this linear-Gaussian setting. We have
\[
   f \propto \frac{1}{2} \sum_{t=1}^{T} (y_t - B_t x_t)^T W_t^{-1} (y_t - B_t x_t) + \frac{1}{2} \sum_{t=1}^{T-1} (x_{t+1} - A x_t)^T V_t^{-1} (x_{t+1} - A x_t)
\]
\[
   + \frac{1}{2} x_1^T V_0^{-1} x_1
\]
\[
   \nabla_t \triangleq \frac{\partial f}{\partial x_t} = -B_t^T W_t^{-1} (y_t - B_t x_t) - A^T V_t^{-1} (x_{t+1} - A x_t) + V_t^{-1} (x_t - A x_{t-1}),
\]
\[
   H = \begin{bmatrix}
   D_1 + B_1^T W_1^{-1} B_1 & -E_1 & 0 & \ldots & 0 \\
   -E_1^T & D_2 + B_2^T W_2^{-1} B_2 & -E_2 & \ldots & 0 \\
   \vdots & \ddots & \ddots & \ddots & \vdots \\
   0 & 0 & \ldots & -E_{T-1}^T & D_T + B_T^T W_T^{-1} B_T
\end{bmatrix}
\]

with
\[
   D_t = \begin{cases}
   V_0^{-1} + A^T V_1 A, & t = 1 \\
   V_t^{-1} + A^T V_1 A, & 1 < t < T \\
   V_{T-1}^{-1}, & t = T
\end{cases}
\]
and
\[
   E_t = A^T V_1, \quad 1 \leq t \leq T.
\]

The solution of (26), which corresponds to the full forward–backward smoothing can be given by the classic block-Thomas (BT) algorithm (Isaacson and Keller 1994), which we repeat here for completeness (Algorithm 2).

**Algorithm 2** Classic Block-Thomas Algorithm (computes \(s = -H^{-1} \nabla\))

\[
   M_1 = D_1 + B_1^T W_1^{-1} B_1, \quad \Gamma_1 = M_1^{-1} E_1 \quad \text{(cost } O(d^3))
\]
\[
   q_1 = -M_1^{-1} \nabla_1 \quad \text{(cost } O(d^2))
\]
\[
   \text{for } i = 2 \text{ to } T \quad \text{do}
\]
\[
   M_t = D_t + B_t^T W_t^{-1} B_t - E_{t-1} M_{t-1}^{-1} E_{t-1}^T, \quad \Gamma_t = M_t^{-1} E_t \quad \text{(cost } O(d^3))
\]
\[
   q_t = -M_t^{-1} (\nabla_t - E_{t-1}^T q_{t-1}) \quad \text{(cost } O(d^2))
\]
\[
   s_T = q_T
\]
\[
   \text{for } t = T - 1 \text{ to } 1 \quad \text{do}
\]
\[
   s_t = q_t + \Gamma_t s_{t+1} \quad \text{(cost } O(d^2))
\]

The expensive part in the BT algorithm is the multiplication and division with the matrices \(M_t\), which correspond to a modified version of the inverse covariance matrices \(C_{t}^{-1}\). In the case where \(B_s = 0\) for all \(s \leq t\), we have that \(M_t = \tilde{D}_t\) where the matrices \(\tilde{D}_t\) correspond to a modified version of the inverse equilibrium covariance \(C_{0,t}^{-1}\) (in fact for \(t = T\) we have that \(\tilde{D}_T = C_{0,T}^{-1}\) and \(M_T = C_T^{-1}\)) and are defined recursively as
\[
   \tilde{D}_t = D_t - E_{t-1} \tilde{D}_{t-1} E_{t-1}^T, \quad \text{with } \tilde{D}_1 = D_1.
\]

Using a similar argument as in the fast Kalman filtering case (see (3.1)), to derive a similar fast algorithm in the case where \(B_s \neq 0\), we want to approximate the matrices \(M_t^{-1}\) as
\[
   M_t^{-1} \approx \tilde{M}_t^{-1} = \tilde{D}_t^{-1} - L_t \Sigma_t L_t^T,
\]

where \(L_t, \Sigma_t L_t^T\) is a suitable low-rank matrix. To gain some insight into this approximation, suppose that (29) holds at time \(t - 1\). Then following the BT recursion we can define the
matrices \( \hat{M}_t \) as
\[
\hat{M}_t = D_t + B_t^T W_t^{-1} B_t - E_{t-1} \hat{M}_{t-1}^T E_{t-1}^T
\]
\[
= \tilde{D}_t + B_t^T W_t^{-1} B_t + E_{t-1} L_{t-1} \Sigma_{t-1} L_{t-1}^T E_{t-1}^T
\]
\[
\tilde{D}_t = D_t + O_t Q_t O_t^T \Rightarrow
\]
\[
\hat{M}_t^{-1} = \tilde{D}_t^{-1} - \tilde{D}_t^{-1} Q_t \left( Q_t^{-1} + O_t^T \tilde{D}_t^{-1} O_t \right)^{-1} O_t^T \tilde{D}_t^{-1}, \tag{30}
\]
with
\[
O_t = \left[ B_t^T, E_{t-1} L_{t-1} \right], \quad Q_t = \text{blkdiag} \{ W_t^{-1}, \Sigma_{t-1} \}. \tag{31}
\]

The forward–backward procedure allows us to analyze the error of our LRBT algorithm. In online Appendix C we prove that although the algorithm involves an approximation at every step the error does not accumulate, and thus remains of the order \( O(1 - \theta) \).

\textbf{Theorem 1.} The solution \( \hat{s} \) of the LRBT algorithm can be written as
\[
\hat{s} = -\hat{H}^{-1} \nabla|x=0, \tag{32}
\]
with \( \hat{H} = \)
\[
\begin{bmatrix}
\hat{M}_1 & -E_1 & \ldots & 0 \\
-E_1^T & \hat{M}_2 & \ldots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \ldots & -E_{T-1}^T & \hat{M}_T + E_{T-1} \hat{M}_{T-1}^T E_{T-1}
\end{bmatrix}. \tag{33}
\]

Note that in a slight abuse of notation, we will recycle the names of some matrices (e.g., \( O_t \) and \( Q_t \)) that play a similar role in the LRBT approach as in the fast Kalman method described in the previous sections.
Algorithm 3 Low-Rank Block-Thomas Algorithm

\[
\begin{align*}
\tilde{D}_1 &= D_1, L_1 = D_1^{-1}B_1^T \quad \text{(cost } O(b_1 K(d)), k_1 = b_1) \\
\Sigma_1 &= (W_1 + B_1 D_1^{-1}B_1^T)^{-1} \quad \text{(cost } O(b_1^2)) \\
\tilde{q}_1 &= (-D_1^{-1} + L_1 \Sigma_1 L_1^T)\nabla_1 \quad ( = -\tilde{M}_1^{-1}\nabla_1) \quad \text{(cost } O(b_1 K(d))) \\
\text{for } t = 2 \text{ to } T \text{ do} \\
\tilde{D}_t &= D_t - E_{t-1}\tilde{D}_{t-1}^{-1}E_{t-1}^T \\
O_t &= \{B_t^T, E_{t-1}L_{t-1}\}, \quad Q_t = \text{blkdiag}\{W_t^{-1}, \Sigma_{t-1}\} \\
[\tilde{L}_t, \tilde{\Sigma}_t] &= \text{svd}(\tilde{D}_t^{-1}O_t(Q_t^{-1} + O_t^T\tilde{D}_t^{-1}O_t)^{-1/2}) \quad \text{(cost } O((b_t + k_{t-1})^2 K(d))) \\
\text{Truncate } \tilde{L}_t \text{ and } \tilde{\Sigma}_t \text{ to } L_t \text{ and } \Sigma_t. & \quad \text{(effective rank } k_t \leq b_t + k_{t-1} \ll d) \\
\tilde{q}_t &= (-\tilde{D}_t^{-1} - L_t \Sigma_t L_t^T)(\nabla_t - E_{t-1}^T\tilde{q}_{t-1}) \quad ( = -\tilde{M}_t^{-1}(\nabla_t - E_{t-1}^T\tilde{q}_{t-1})) \quad \text{(cost } O(k_t K(d))) \\
\bar{s}_T &= \tilde{q}_T \\
\text{for } i = T - 1 \text{ to } 1 \text{ do} \\
\bar{s}_i &= \tilde{q}_i + (\tilde{D}_i^{-1}E_i^T - L_i \Sigma_i L_i^T E_i^T)\bar{s}_{i+1} \quad ( = \tilde{q}_i + \tilde{\Gamma}_i\bar{s}_{i+1}) \quad \text{(cost } O(k_i K(d))) 
\end{align*}
\]

Moreover, \( \tilde{H} \) is positive definite and, under the assumption \( \|A\| < 1 \), it approximates the true Hessian \( H \), defined in (27), as

\[
\|\tilde{H} - H\| = O(1 - \theta). \quad (34)
\]

Theorem 1 has several useful implications. First, it establishes that the LRBT smoother approximation error is also of order \( O(1 - \theta) \), because

\[
\|\bar{s} - s\| = \|H^{-1} - H\nabla|_{x=0}\| \leq \|H^{-1} - H^{-1}\|\|\nabla|_{x=0}\|. \quad (35)
\]

Moreover, because \( \tilde{H} \) is positive definite, it follows that the LRBT performs the steepest descent step for the quadratic norm \( \|x\|_Q = (x^T\tilde{H}x)^{1/2} \). Therefore when applied as a search direction in an iterative algorithm, it converges to the solution of (26). The convergence rate is linear, but can be made arbitrarily fast as it is controlled by the threshold \( \theta \). In fact, if \( f^* \) is the minimum value of the negative log-likelihood function \( f \) (27), then we can show that \( f(s_n) - f^* \propto \gamma_n^\theta \), with \( \gamma_0 = O(1 - \theta) \). A short discussion can be found in online Appendix C. \( \tilde{H} \) can also be used as an effective preconditioner for other iterative methods, for example, conjugate gradients that in general lead to faster convergence than plain steepest descent. Note that the condition \( \|A\| < 1 \) is critical for the \( O(1 - \theta) \) approximation error, because it guarantees that the matrix \( M_t \) that we approximate stays finite. This issue is discussed in somewhat more detail in online Appendix C (Remark C.3). Finally, we note that the effective rank of the matrices involved in the LRBT algorithm has exactly the same scaling properties as in the fast Kalman filtering case. The interested reader is referred to online Appendix B for more details.

5. APPLICATION TO HIGH-DIMENSIONAL SMOOTHING

Now for the main statistical examples we have in mind. In many statistical settings, the dynamics matrix \( A \) and noise covariance \( V \) are not directly defined; the analyst has...
some flexibility in choosing these matrices according to criteria including physical realism and computational tractability. Perhaps the simplest approach is to use a separable prior, defined most easily as \( A = aI \), \( 0 < a < 1 \). Now \( C_0 = (1 - a^2)^{-1}V \); thus it is clear that when it is easy to multiply and divide by \( V \), we may apply the fast methods discussed above with no modifications. Note that in this case the prior covariance of the vector \( X \) is separable: \( \text{cov}(X) = C_0 \otimes C_{AR} \), where \( \otimes \) denotes the Kronecker product and \( C_{AR} \) denotes the covariance of the standardized one-dimensional autoregressive AR(1) process, \( x_{t+1} = ax_t + \sqrt{1 - a^2} \epsilon_t, \epsilon_t \sim \mathcal{N}(0, 1) \). However, the posterior covariance \( \text{cov}(X|Y) \) is not separable in general, which complicates exact inference.

It is straightforward to construct more interesting nonseparable examples. For example, in many cases we may choose a basis so that \( V \) and \( A \) are diagonal and the transformation back to the “standard” basis is fast. Examples include the discrete Fourier basis, common spline bases, and wavelet bases. Now the interpretation is that each basis element is endowed with an AR(1) prior: the \((i, i)\)th element of \( A \) defines the temporal autocorrelation width of the \( i \)th process, although the elements of the diagonal matrix \((I - A^2)^{-1}V \) set the processes’ prior variance (and therefore \((I - A^2)^{-1}V \) expressed in the “standard” basis sets the prior covariance \( C_0 \)). The difficulty in applying the standard Kalman recursion in this setting is that if \( B \) is not also diagonal in this representation, then direct implementations of the Kalman filter require \( O(d^3) \) time per time step, because \( C_t \) does not remain diagonal in general. Nonetheless, the fast low-rank smoother may be applied in a straightforward manner in this setting: computing \( \mathbb{E}(x_t|Y) \) and \( \text{cov}(x_t|Y) \) requires \( O(k_d^2d) \) time, to which we add the time necessary to transform back into the standard basis.

A further speedup is possible in this diagonal case, if the observation matrices \( B_t \) are sparse; that is, if each observation \( y_t \) only provides information about a few elements of the state vector \( x_t \). This setting arises frequently in environmental applications, for example, where just a few sampling stations are often available to take spatially localized samples of large spatiotemporal processes of interest (Stroud, Muller, and Sanso 2001). Another example, from neuroscience, will be discussed in the following section. If \( I_t \) denotes the set of indices for which \( B_t \) is nonzero for \( s \leq t \), then it is easy to show that the forward covariance \( C_t \) matrix need only be evaluated on the \(|I_t| \times |I_t| \) submatrix indexed by \( I_t \); if \( i \) or \( j \) are not in \( I_t \), then \( (C_t)_{ij} = (C_0)_{ij} \). Thus, we need only update the low-rank matrix \( L_t \) at the indices \( I_t \), reducing the computational complexity of each update from \( O(k_d^2d) \) to \( O(k_d^2|I_t|) \). Clearly, with each new update at time \( t \), we will add some elements to \( I_t \), but we can also discard some elements as we go because our low-rank updates will effectively “forget” information as time progresses, as discussed above. (In particular, the indices for which the recent observations provide no information will eventually be dropped.) Thus, in practice \(|I_t| \) often remains much smaller than \( d \), leading to a significant speedup.

### 5.1 Two Neuroscience Examples

To make these ideas more concrete, we now examine two examples from neuroscience. For our first example we consider neurons in the rodent hippocampal brain region; many of these neurons respond selectively depending on the animal’s current location. This spatial dependency can be summarized in terms of a “place field” \( f(\vec{x}) \), where \( f(\vec{x}) \) is the expected response of the neuron (quantified by the number of action potentials emitted by the neuron
in a fixed time interval), given that the animal is located at position $\vec{x}$. It is known that these place fields can in some cases change with time; in this case we might replace $f(\vec{x})$ with $f(\vec{x}, t)$. These time-varying place fields $f(\vec{x}, t)$ are often represented as a sum of some fixed spatial basis functions (Brown et al. 2001; Frank et al. 2002; Czanner et al. 2008), weighted by some appropriate weights which are to be inferred:

$$f(\vec{x}, t) = \sum_i q_{it} f_i(\vec{x}).$$

(36)

For example, the basis $\{f_i(\vec{x})\}$ could consist of spline functions defined on the spatial variable $\vec{x}$. Now we place a prior on how the weights $q_{it}$ evolve with time. In the simplest case, $q_{it}$ could evolve according to independent AR(1) processes; as emphasized above, this means that the dynamics matrix $A$ is diagonal. Now the observation model in this setting may be taken to be $y_i = f(\vec{x}_i, t) + \eta_i$, with $\eta_i$ denoting an iid Gaussian noise source, or we can use a slightly more accurate Poisson model, $y_i \sim \text{Poiss}(\exp(f(\vec{x}_i, t)))$, where in either case $\vec{x}_i$ represents the (known) location of the animal as a function of time $t$, and $\text{Poiss}(\lambda_i)$ denotes a Poisson process with rate $\lambda_i$. The observation matrix $B_t$ is just a $d$-dimensional vector, $B_t = f_i(\vec{x}_i)$, if we use $d$ basis vectors to represent the place field $f$. Computing $B_t$ requires at most $O(d)$ time; if the basis functions $f_i$ have compact support, then $B_t$ will be sparse (i.e., computable in $O(1)$ time), and we can employ the speedup based on the sparse index vector $I_t$ described above. More detailed models are possible, of course (Czanner et al. 2008; Rahnama Rad and Paninski 2010), but this basic formulation is sufficient to illustrate the key points here.

A second example comes from sensory systems neuroscience. The activity of a neuron in a sensory brain region depends on the stimulus which is presented to the animal. The activity of a visual neuron, for example, is typically discussed using the notion of a “receptive field,” which summarizes the expected response of the neuron as a function of the visual stimulus presented to the eye (Dayan and Abbott 2001). We can use a similar model structure to capture these stimulus-dependent responses; for example, we might model $y_i = s_i^T f^i + \eta_i$ in the Gaussian case, or $y_i \sim \text{Poiss}(\exp(s_i^T f^i))$ in the Poisson case, where $s_i$ is the sensory stimulus presented to the neuron at time $t$, $s_i^T f^i = \sum x s(\vec{x}, t) f(\vec{x}, t)$ denotes the linear projection of the stimulus $s_i$ onto the receptive field $f^i$ at time $t$, and $f(\vec{x}, t)$ is proportional to the expectation of $y_i$ given that a light of intensity $s(\vec{x}, t)$ was projected onto the retina at location $\vec{x}$. As indicated by the notation $f^i$, these receptive fields can in many cases themselves vary with time, and to capture this temporal dependence it is common to use a weighted sum of basis functions model, as in Equation (36). This implies that the observation matrix $B_t$ can be written as $B_t = s_t^T F$, where the $i$th column of the basis matrix $F$ is given by $f_i$. If the basis functions $f_i$ are Fourier or wavelet functions, then the matrix-vector multiplications $s_t^T F$ can be performed in $O(d \log d)$ time per time step; if $f_i$ are compactly supported, $F$ will be sparse, and computing $s_t^T F$ requires just $O(d)$ time.

Now in each of these settings the fast Kalman filter is easy to compute. In the case of Gaussian observation noise $\eta_i$ we proceed exactly as described above, once the observation matrices $B_t$ are defined; in the Poisson case we can employ well-known extensions of the Kalman filter described, for example, in Fahrmeir and Kaufmann (1991), Fahrmeir and Tutz (1994), Brown et al. (1998), and Paninski et al. (2010); see online Appendix A for details. In either case, the filtering requires $O(k^2 |I_t|)$ time for time step $t$. When the filtering is complete
Figure 1. Output of the filter-smoother applied to simulated one-dimensional place field data. The superimposed black trace in all but the lower left panel indicates the simulated path $\vec{x}_t$ of the animal; $\vec{x}_t$ begins by sampling a wide range of locations for $t < 200$, but settles down to a small spatial subset for larger values of $t$. Upper left: True simulated place field $f(\vec{x}, t)$ is shown in color; $f(\vec{x}, t)$ has a Gaussian shape as a function of $\vec{x}$, and the center of this Gaussian varies sinusoidally as a function of time $t$. Top middle and right panels: Estimated place fields, forward ($E(f(\vec{x}, t)|Y_{1:t})$) and forward–backward ($E(f(\vec{x}, t)|Y_{1:T})$), respectively. Here (in a slight abuse of notation) we use $E(f_t|Y)$ to denote the projected mean $FE(q_t|Y)$, where $F$ is the basis matrix corresponding to the basis coefficients $q$. Note that the estimated place fields are accurate near the observed positions $\vec{x}_t$, but revert to the prior mean when no information is available. Bottom middle and right panels: Marginal variance of the estimated place fields, forward ($V(f(\vec{x}, t)|Y_{1:t})$) and forward–backward ($V(f(\vec{x}, t)|Y_{1:T})$), respectively. Again, note that the filter output is most confident near $\vec{x}_t$. Lower left panel: Effective rank of $C_0 - C_s$ as a function of $t$ in the forward–backward smoother; the effective rank is largest when $\vec{x}_t$ samples many locations in a short time period.

(i.e., $E(q_t|Y)$ has been computed for each desired $t$), we typically want to transform from the $q_t$ space to represent $E(f|Y)$; again, if the basis functions $f_i$ correspond to wavelet or Fourier functions, this costs $O(d \log d)$ time per time step, or $O(d)$ time if the $f_i$ functions are compactly supported.

Figures 1 and 2 illustrate the output of the fast filter-smoother applied to simulated place field data. The spatial variable $\vec{x}$ is chosen to be one-dimensional here, for clarity. We chose the true place field $f(\vec{x}, t)$ to be a Gaussian bump (as a function of $\vec{x}$) whose mean varied sinusoidally in time but whose height and width were held constant (see the upper left panel of Figure 1). The basis matrix $F$ consisted of 50 equally spaced bump functions with compact support (specifically, spatial Gaussians truncated at $\sigma \approx 4$, with each bump located one standard deviation $\sigma$ apart from the next.) The dynamics coefficient $a$ (in the diagonal dynamics matrix $A = aI$) was about 0.97, which corresponds to a temporal correlation time of $\tau = 30$ time steps; the simulation shown in Figure 1 lasted for $T = 1000$ time steps. To explore the behavior of the filter in two regimes, we let $\vec{x}_t$ begin by sampling a wide range of locations (see Figure 1 for $t < 200$ or so), but then settling down to a small spatial subset for larger values of $t$. We used the Gaussian noise model for $y_i$ in this simulation with standard deviation 0.1.
Figure 2. Justification of our low-rank approximation in the place field example (Section 5.1). Upper row: \(C_t\) is fairly close to \(C_0\). Left: true \(C_t\). Middle: \(C_0\). Both \(C_0\) and \(C_t\) are plotted on the same colorscale, to facilitate direct comparison. Right: Eigenvalue spectrum of \(I - C_0^{-1/2}C_tC_0^{-1/2}\); an approximation of rank about 20 seems to suffice here. Lower row: Comparison of the true versus approximate projected covariance \(FC_tF^T\) and mean \(F\mu_t\) at \(t = 200\). Left panel: True forward projected covariance \(FC_tF^T\). Middle panel: Approximate forward covariance \(F(C_0 - L_t\Sigma_tL_t^T)F^T\). The maximal pointwise error between these two matrices less than 1%. Right panel: True (exact) and approximate means. The traces for the exact and approximate means are barely distinguishable.

We find that, as expected, the filter does a good job of tracking \(f(\tilde{x}, t)\) for locations \(\tilde{x}\) near the observation points \(\tilde{x}_i\), where the observations \(y_i\) carry a good deal of information, but far from \(\tilde{x}_i\), the filter defaults to its prior mean value, significantly underestimating \(f(\tilde{x}, t)\). The posterior uncertainty \(V(f(\tilde{x}, t)|Y) = \text{diag}(Fcov(q_t|Y)F^T)\) remains near the prior uncertainty \(\text{diag}(FC_0F^T)\) in locations far from \(\tilde{x}_i\), as expected. Figure 2 illustrates that the low-rank approximation works well in this setting, despite the fact that (at least for \(t\) sufficiently large) only a few singular values are retained in our low-rank approximation (see Figure 1, lower left panel). We set \(\theta = 0.99\) in (15) for this simulation.

We have also applied the filter to real neuronal data, recorded from single neurons in the mouse hippocampal region by Dr. Pablo Jercog. In these experiments the mouse was exploring a two-dimensional cage, and so we estimated the firing rate surface \(f(\tilde{x}, t)\) as a function of time \(t\) and a two-dimensional spatial variable \(\tilde{x}\). The results are most easily viewed in movie form; see [http://www.stat.columbia.edu/~liam/research/abstracts/fast-Kalman-abs.html](http://www.stat.columbia.edu/~liam/research/abstracts/fast-Kalman-abs.html) for details.

Figure 3 illustrates an application of the fast filter-smoother to the second context described above. We simulated neuronal responses of the form \(y_t = s_t^T f_t + \eta_t\), where the sensory stimulus \(s_t\) was taken to be a spatiotemporal Gaussian white noise process normalized to unit energy and the response noise \(\eta_t\) was also modeled as Gaussian and white, for simplicity with variance 0.1. As discussed above, we represented \(f_t\) as a time-varying weighted sum of fixed basis functions \(f_i\). In this case the basis \(F\) consisted of real-valued Fourier
Figure 3. Tracking a time-varying one-dimensional receptive field (Section 5.1). Top panel: The true receptive field $f^t$ was chosen to be a spatial Gaussian bump whose center varied sinusoidally as a function of time $t$. Second panel: The stimulus $s_t$ was chosen to be spatiotemporal white Gaussian noise. Third panel: Simulated output observed according to the Gaussian model $y_t = s_t^T f^t + \eta_t$ with $\eta_t \sim N(0, 0.1)$. Lower four panels: The forward filter mean $E(f^t | Y_{1:t})$ and marginal variance $\text{var}(f^t | Y_{1:t})$ and the full forward–backward smoother mean $E(f^t | Y_{1:T})$ and marginal variance $\text{var}(f^t | Y_{1:T})$. The dimension of the state variable $f^t$ here was $2^{10}$; inference required seconds on a standard laptop. Time units are arbitrary here; the assumed prior autocorrelation time was $\tau = 50$ time steps, leading to $A = \alpha I$ with $\alpha \approx 0.98$, although the total length of the experiment was $T = 200$ time steps.
functions (sines and cosines), and multiplication by this basis matrix was implemented via the FFT. As in the previous example, we chose the dynamics matrix $A$ to be proportional to the identity; the effective autocorrelation time was $\tau = 50$ time steps here. The dynamics noise covariance $V$ was diagonal (and therefore so was the prior covariance $C_0$), with the diagonal elements chosen so that the prior variance of the $\omega$th frequency basis coefficient falls off proportionally to $\omega^{-2}$; this led to an effective smoothing prior. The dimensionality of this basis was chosen equal to $d = 2^9$. Figure 3 provides a one-dimensional example, where the full spatiotemporal output of the filter-smoother can be visualized directly. We have also applied the filter to higher-dimensional examples; a two-dimensional example movie is available at http://www.stat.columbia.edu/~liam/research/abstracts/fast-Kalman-abs.html.

As discussed in Section 4, both the LRBT approach and the fast Kalman filter-smoother can be used to approximate the Newton direction for maximizing the posterior. Apart from approximating the exact solution, the LRBT algorithm can also be used as a preconditioner for solving for the exact direction $s = -H^{-1}v$. We investigated this in Figure 4, where we examine the convergence rates of the PCG method using the LRBT method as a preconditioner, for the example presented in Figure 3. As expected, the number of iterations required for convergence drops as the threshold $\theta$ approaches 1 (see Figure 4 left). Trivially, when $\theta = 1$, the exact BT algorithm is performed and we achieve convergence within one iteration. The cost per iteration increases slowly with the threshold (because the effective rank scales only as $O(|\log(1 - \theta)|)$), so the overall cost to reach a desired tolerance is always significantly smaller than the cost required for the exact BT algorithm. The total cost for the PCG method reaches a global minimum for an intermediate value of $\theta$. This value depends on the behavior of the effective rank (and therefore on the dynamics $A$ and the size of the observation matrices $B_i$), as well as the desired relative tolerance level (set to $10^{-6}$ here).
6. DISCUSSION

We have presented methods for efficiently computing the Kalman filter and the BT smoother recursions in the few-observation setting. For the Kalman filter, the basic idea is that, when fast methods are available for multiplying and dividing by the prior equilibrium state covariance $C_0$, then the posterior state covariance $C_t$ can be well-approximated by forming a low-rank perturbation of the prior $C_0$. A similar argument holds for the BT smoother. These low-rank perturbations, in turn, can be updated in an efficient recursive manner. We provided a theoretical analysis that characterizes the trade-off between the computational cost of the algorithm (via the effective rank), and the accuracy of the low-rank approximation. We also showed that our methods can be applied in an iterative fashion to reach any level of accuracy, at a reduced cost compared to standard exact methods.

There are a number of clear opportunities for application of this basic idea. Some exciting examples involve optimal control and online experimental design in high-dimensional settings; for instance, optimal online experimental design requires us to choose the observation matrix $B_t$ adaptively, in real time, to minimize some objective function that expresses the posterior uncertainty in some sense (Fedorov 1972; Lewi, Butera, and Paninski 2009; Seeger and Nickisch 2011). Our fast methods can be adapted to compute many of these objective functions, including those based on the posterior state entropy, or weighted sums of the marginal posterior state variance. See Huggins and Paninski (2012) for an application of these ideas to the neuronal dendritic setting.

The fast low-rank methods can also greatly facilitate the selection of hyperparameters in the smoothing setting: typically the data analyst will need to set the scale over which the data are smoothed, both temporally and spatially, and we would often like to do this in a data-dependent manner. There are a number of standard approaches for choosing hyperparameters (Hastie, Tibshirani, and Friedman 2001), including cross-validation, generalized cross-validation, expectation-maximization, and maximum marginal likelihood or empirical Bayes methods. In all of these cases, it is clearly beneficial to be able to compute the estimate more rapidly for a variety of hyperparameter settings. In addition, the output of the filter-smoother is often a necessary ingredient in hyperparameter selection. For example, the standard expectation-maximization method of Shumway and Stoffer (2006) can be easily adapted to the low-rank setting: we have already discussed the computation of the sufficient statistics $E(x_t|Y)$ and cov$(x_t|Y)$, and the remaining needed sufficient statistics $E(x_t x_{t+1}^T|Y)$ follow easily. Similarly, a straightforward application of the low-rank determinant lemma allows us to efficiently compute the marginal log-likelihood $\log p(Y)$, via a simple adaptation of the standard forward recursion for the log-likelihood in the Kalman filter model (Rabiner 1989).

We have seen that the prior covariance is especially easy to compute in the case that the dynamics matrix $A$ is normal: here $C_0$ may be computed analytically, assuming the dynamics noise covariance $V$ can be transformed via a convenient whitening transformation. A key direction for future work will be to extend these methods to the case that $A$ is a nonnormal matrix, a situation that arises quite frequently in practice. For example, weather prediction applications involve dynamics with strong drift (not just diffusion) terms, making $A$ nonsymmetric and perhaps nonnormal in many cases. Standard direct methods for solving
the Lyapunov equation given a nonnormal dynamics matrix $A$ (e.g., the Bartels-Stewart algorithm (Antoulas 2005)) require an orthogonalization step that takes $O(d^3)$ time in general. There is a large applied mathematics literature on the approximate solution of Lyapunov equations with sparse dynamics (see, e.g., Sabino (2007) for a nice review), but the focus of this literature is on the case that the noise covariance matrix is of low rank, which may be less relevant in some statistical applications. Further research is needed into how to adapt modern methods for solving the Lyapunov equation to the fast Kalman filter setting.

Another important direction for future research involves generalizations beyond the simple Kalman setting explored here. The smoothers we have discussed are all based on a simple AR(1) framework. It is natural to ask if similar methods can be employed to efficiently handle the general autoregressive-moving average case, or other temporal smoothing methodologies (e.g., penalized spline methods—Green and Silverman 1994; DiMatteo, Genovese, and Kass 2001; Wood 2006), because all of these techniques rely heavily on solving linear equations for which the corresponding matrices are block banded in the temporal domain.

Finally, for the methods discussed here, we assumed that the underlying dynamics model $(A, V)$ does not change with time, to compute the equilibrium state covariance $C_0$. However, as noted in the presentation of our methods $C_0$ can be interpreted as the limit of a time varying prior covariance $C_{0,t}$. In this case, our methods can be applied when $C_{0,t}$ can be updated efficiently and used for fast matrix-vector operations. This is possible in a number of setups (Pnevmatikakis and Paninski 2012), and opens up some interesting applications involving the incorporation of non-Gaussian priors (Park and Casella 2008) and efficient sampling of the full posterior $p(X|Y)$ using the perturbation technique of Papandreou and Yuille (2010). We are currently pursuing these directions further.

SUPPLEMENTARY MATERIAL

Appendix.pdf: Appendix including the omitted proofs and further technical results. Section A deals with extensions to non-Gaussian measurements. Section B provides further analysis and tighter bounds for the effective rank. Section C provides the proof for Theorem 4.1 and discusses the convergence properties of the LRBT algorithm when applied in an iterative fashion. Section D discusses how the LRBT can be extended to provide estimates of the smoothed covariance in $O(K(d)T)$ time and $O(dT)$ space.

Matlab code: Matlab code including routines for all the algorithms described in the paper (fast Kalman filter, LRBT, steepest descent LRBT, conjugate gradients with LRBT preconditioner). The wrapper code calls all the algorithms as well the exact Kalman filter and BT algorithms for the receptive field example presented in Section 5.1.

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