UltimateKalman: Flexible Kalman Filtering and Smoothing Using Orthogonal Transformations

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Abstract

UltimateKalman is a flexible linear Kalman filter and smoother implemented in three popular programming languages: MATLAB, C, and Java. UltimateKalman is a slight simplification and slight generalization of an elegant Kalman filter and smoother that was proposed in 1977 by Paige and Saunders. Their algorithm appears to be numerically superior and more flexible than other Kalman filters and smoothers, but curiously has never been implemented or used before. UltimateKalman is flexible: it can easily handle time-dependent problems, problems with state vectors whose dimensions vary from step to step, problems with varying number of observations in different steps (or no observations at all in some steps), and problems in which the expectation of the initial state is unknown. The programming interface of UltimateKalman is broken into simple building blocks that can be used to construct filters, single or multi-step predictors, multi-step or whole-track smoothers, and combinations. The paper describes the algorithm and its implementation as well as a test suite of examples and tests.

1 Introduction

The invention of the Kalman filter by Rudolf E. Kálmán in 1960 (Kalman, 1960) is considered one of the major inventions of the 20th century. The filter efficiently and incrementally tracks the hidden state of a linear discrete dynamic system; each state estimate uses all the observations of the system up to that point in time. The filter can also predict future states and with suitable adaptations, can handle nonlinear dynamic systems and smooth entire state trajectories. The literature on Kalman filters and their applications is vast and the importance of Kalman filters is beyond doubt. We mention a few relatively recent and relatively comprehensive sources (Brown and Hwang, 1997; Grewal and Andrews, 2015; Humpherys et al., 2012), but there are numerous other authoritative sources on Kalman filtering.

Twelve years later, Duncan and Horn discovered that mathematically, the Kalman filter computes the solution to a generalized linear least squares problem (Duncan and Horn, 1972). Algorithmically and numerically, however, the Kalman filter algorithm is far from state-of-the-art algorithms for linear least squares problems. In particular, it does not use orthogonal factorizations, which were invented and published in the 1950s (Givens, 1954; Householder, 1958).
Numerically, the most stable algorithms for least squares minimization are based on orthogonal transformations, and more specifically on the QR factorization, the singular-value decomposition, or their variants (Björck 1996; Golub and Loan 2013; Higham 2002). Kalman filter algorithms are not, and many of them, including Kalman’s original algorithm, are based on algebraic building blocks, like explicit matrix inversion, that are prone to instability.

In 1977, Paige and Saunders discovered and published an elegant Kalman filter algorithm based on orthogonal transformations (Paige and Saunders 1977). Their algorithm is a specialized QR factorization and it can easily implement filtering, prediction, and smoothing.

Strangely, the Paige-Saunders algorithm appears to have had very limited impact, even though it was about as efficient as other Kalman filters and smoothers and was claimed to be more numerically stable. Their paper was not cited much, nobody approached the authors to discuss it (Saunders 2018), and to the best of our knowledge, it was never implemented (Paige and Saunders’ paper describes the algorithm and analyzes it, but does not mention an implementation).

The present paper and the software that it describes, called UltimateKalman, aim to make the algorithm widely available and to highlight its advantages over other Kalman filtering and smoothing algorithms. Indeed, the Paige and Saunders algorithm is more flexible than other Kalman algorithms in two important senses. First, unlike other Kalman filters, it does not need to know the expectation of the initial state of the system. Second, it can be easily generalized to handle quantities that are added or dropped from the state vector. These features make modeling easier, as we demonstrate with concrete examples in Sections 5.4 and 5.5. The algorithm can also easily handle problems with a varying number of observations and with missing observations, and it can both filter and smooth. Many other Kalman filter algorithms lack these two characteristics, but some do possess them, so they are not completely unique.

UltimateKalman is not completely identical to the Paige-Saunders algorithm, but rather a variant that is simpler and more general at the same time. We explain later in the paper the differences from the original algorithm, but at the same time acknowledge that all the fundamental algorithmic ideas in UltimateKalman come from the Paige-Saunders algorithm and paper.

Our implementation is split into a collection of easy-to-understand building blocks from which a user can compose a variety of Kalman-based computations, including filters, predictors, and smoothers, and combinations of these.

The implementation is available in three popular programming languages: MATLAB, Java, and C.

The rest of the paper is organized as follows. Section 2 provides background material on discrete linear dynamic systems and Kalman filters and smoothers. Section 3 describes the details of UltimateKalman. Section 4 presents our implementations of the algorithm, and Section 5 describes a suite of examples and tests that come with UltimateKalman, demonstrate its correctness, and show how to use it in various cases, some nontrivial. We discuss the algorithm and the software and our conclusions from this project in Section 6.

This paper does not directly compare UltimateKalman to other Kalman filtering algorithms and does not prove its correctness and its numerical properties; the paper by Paige and Saunders addresses these issues thoroughly, and the analyses there are equally applicable to UltimateKalman (Paige and Saunders 1977).
2 Background

The discrete Kalman filter is a method to efficiently estimate the state of a discrete linear dynamic system from indirect observations. UltimateKalman can handle more general cases than Kalman filters, so we describe here the more general version.

2.1 Discrete linear dynamic systems

The instantaneous state of a discrete dynamic system at time $t_i$ is represented by an $n_i$-dimensional state vector $u_i \in \mathbb{R}^{n_i}$. We assume that $u_i$ satisfies a recurrence that we refer to as an evolution equation and possibly another equation that we refer to as an observation equation. Note that we do not require all the states to have the same dimension, although the uniform-dimension case is very common. The evolution equation has the form

$$H_i u_i = F_i u_{i-1} + c_i + \epsilon_i,$$

where $H_i \in \mathbb{R}^{\ell_i \times n_i}$ and $F_i \in \mathbb{R}^{\ell_i \times n_{i-1}}$ are known full-rank matrices, $c_i \in \mathbb{R}^{\ell_i}$ is a known vector, called a control vector, that represents external forces acting on the system, and $\epsilon_i$ is an unknown noise or error vector. The control vector is often assumed to be the product of a known matrix and a known vector, but this is irrelevant for the Kalman filter. The noise or error vector $\epsilon_i$ admits state vectors that do not satisfy the equation $H_i u_i = F_i u_{i-1} + c_i$ exactly. The matrix $H_i$ is often assumed to be the identity matrix, but we do not require this (and do not require it to be square). When $H_i$ and $F_i$ are square and full-rank, $u_i$ is a function of $u_{i-1}$ and $c_i$ up to the error term. Obviously, the first state $u_0$ that we model is not defined by an evolution recurrence.

Some of the state vectors $u_i$ (but perhaps not all) also satisfy an observation equation of the form

$$o_i = G_i u_i + \delta_i,$$

where $G_i \in \mathbb{R}^{m_i \times n_i}$ is a known full-rank matrix, $o_i \in \mathbb{R}^{m_i}$ is a known vector of observations (measurements), and $\delta_i$ represents unknown measurement errors or noise. The dimension $m_i$ of the observation of $u_i$ can vary; it can be smaller than $n_i$ (including zero, meaning that there are no observations of $u_i$), equal to $n_i$, or greater than $n_i$.

We can write all of the evolution and observation equations up to step $k$ as a single large block-matrix equation,

$$
\begin{bmatrix}
o_0 \\
e_1 \\
o_1 \\
e_2 \\
\vdots \\
o_k
\end{bmatrix} =
\begin{bmatrix}
G_0 & H_1 & \cdots \\
- F_1 & G_1 & \cdots \\
- F_2 & H_2 & \cdots \\
\vdots & \vdots & \ddots \\
- F_k & H_k & \cdots \\
G_k & \cdots & \cdots & G_k
\end{bmatrix}
\begin{bmatrix}
u_0 \\
u_1 \\
u_2 \\
\vdots \\
u_{k-1} \\
u_k
\end{bmatrix} +
\begin{bmatrix}
\delta_0 \\
\epsilon_1 \\
\delta_1 \\
\epsilon_2 \\
\vdots \\
\epsilon_k \\
\delta_k
\end{bmatrix}.
$$

We denote this system by $b = Au + e$. The matrix $A$ and the vector $b$ are known. The noise or error terms $e$ are not known, but we assume that they are small. Our task is to estimate $u$ from $A$ and $b$. 

3
If $e$ is random, has zero expectation $E(e) = 0$, and has a known nonsingular covariance matrix $\text{cov}(e) = E(ee^T)$ with $\text{cov}(e)^{-1} = U^T U$, where $U$ is square then the solution $\hat{u}$ of the generalized least squares problem

$$
\hat{u} = \arg \min_u \| U (Au - b) \|_2^2
= \left( A^T U^T U \right)^{-1} A^T U^T U b
$$

is the so-called best linear unbiased estimator (BLUE) of $u$ [Aitken, 1936]. If we add the assumption that $e$ has a Gaussian (normal) distribution, then the same minimizer is also the maximum-likelihood estimator of $u$. (In this paper, capital letters and small letters denote unrelated objects; in this paragraph, for example, $E$ denotes the expectation and $e$ denotes an error or noise vector.)

If the structure of the $G_i$s, $F_i$s, and $H_i$s guarantees that the rank of $A$ always equals the number of columns, the system is called observable. This guarantees that (4) has a unique solution. We use this term also in a more concrete sense: we say that a matrix or a block of a matrix is observable if its rank equals its column dimension. We also use the terms flat to describe a rectangular matrix or block with more columns than rows (a flat matrix cannot be observable) and tall to describe a rectangular matrix or block with more rows than columns.

Because our goal is to estimate the states of a dynamic system, we also denote the linear system (3) by $b^{(k)} = A^{(k)} u^{(k)} + e^{(k)}$, to provide a notation for the matrix $A$ and for the right-hand $b$ at a particular step $k$. Similarly, we denote $\text{cov}(e^{(k)})^{-1} = (U^{(k)})^T U^{(k)}$.

### 2.2 Kalman filters and smoothers

Kalman filters and smoothers are a large family of efficient algorithms for solving problem (4) for some of the $\hat{u}_k$s when $\text{cov}(e)$ is block diagonal with known blocks,

$$
\text{cov}(e) = \begin{bmatrix}
C_0 & K_1 & & \\
& C_1 & & \\
& & \ddots & \\
& & & C_k
\end{bmatrix}.
$$

That is, we assume that the matrices

$$
K_i = \text{cov} (\epsilon_i) = E (\epsilon_i \epsilon_i^T)
$$

$$
C_i = \text{cov} (\delta_i) = E (\delta_i \delta_i^T)
$$

are known and that the offdiagonal blocks of $\text{cov}(e)$ are all zero:

$$
E (\epsilon_i \delta_j^T) = 0 \text{ for all } i \text{ and } j
$$

$$
E (\epsilon_i \epsilon_j^T) = 0 \text{ for } i \neq j
$$

$$
E (\delta_i \delta_j^T) = 0 \text{ for } i \neq j.
$$

Most Kalman filtering and smoothing algorithms make additional assumptions. For example, many Kalman filters assume that $G_0 = I$, which is equivalent to assuming that
the expectation of \( u_0 \) is known. UltimateKalman also makes an additional assumption: that all the \( C_i \)s and all the \( K_i \)s are nonsingular.

The generalized least-squares solution of Equation (3) estimates all the state vectors \( u_1, \ldots, u_k \) using all the observations up to and including step \( k \). We denote the vectors that make up this solution by

\[
\begin{bmatrix}
\hat{u}_{0|k} \\
\hat{u}_{1|k} \\
\vdots \\
\hat{u}_{k|k}
\end{bmatrix}
\]

(5)

The vector \( \hat{u}_{k|k} \) is called the filtered estimate at step \( k \). This estimate uses all the available observations of present and past states, but not of any future state. Vectors \( \hat{u}_{0|k}, \ldots, \hat{u}_{k-1|k} \) are step-\( k \) smoothed estimates; they use observations of past, present, and future states. We can hope to compute filtered estimates almost in real time, whereas smoothed estimates can only be computed after a time lag. If we extend system (3) with one or more block rows and columns that represent only evolution equations, the new vector components of the solutions are predicted estimates. For example, if we add a block row and a block column that contain \( -F_{k+1}, H_{k+1}, \text{ and } c_{k+1} \), but not \( G_{k+1} \) and not \( o_{k+1} \), the last vector in the solution, denoted \( \hat{u}_{k+1|k} \), is a prediction of \( u_{k+1} \) from the information we have up to step \( k \). We can obviously continue to predict into the future by adding more evolution equations.

Kalman filters are efficient incremental algorithms that produce filtered and predicted estimates. Given \( H_k, F_k, G_k, c_k, o_k, C_k, K_k \), and the compact data structure that was used to estimate \( \hat{u}_{k-1|k-1} \), Kalman filters quickly compute \( \hat{u}_{k|k} \) and update the data structure (Brown and Hwang 1997; Grewal and Andrews 2015; Humpherys et al. 2012; Kalman 1960). The data structure itself is of size \( \Theta((n_{k-1} + n_k)^2) \) and the number of operations required is \( O((n_{k-1} + m_k + n_k)^3) \).

3 UltimateKalman and its heritage

This section describes the UltimateKalman algorithm. The algorithm is a slight simplification of the algorithm of Paige and Saunders (Paige and Saunders 1977) in that UltimateKalman uses block orthogonal transformations whereas the algorithm of Paige and Saunders uses Givens rotations. The algorithm is also a generalization of the algorithm of Paige and Saunders in that we allow the user to specify \( H_i \) and we allow the dimension of the state vector to change from step to step.

3.1 A specialized QR factorization

UltimateKalman computes estimates of the state vectors using a thin QR factorization of the weighted matrix
\[ U^{(k)}A^{(k)} = \begin{bmatrix}
W_0G_0 & V_1H_1 & & & \\
-V_1F_1 & W_1G_1 & V_2H_2 & & \\
& -V_2F_2 & & & \\
& & & \ddots & \\
& & & & -V_kF_k & V_kH_k & W_kG_k
\end{bmatrix}, \tag{6}\]

where \( W_i^TW_i = C_i^{-1} \) and \( V_i^TV_i = K_i^{-1} \). The factorization is computed using a series of orthonormal transformations that are applied to block rows to reduce \( U^{(k)}A^{(k)} \) to a block upper triangular form:

\[ R^{(k)} = (Q^{(k)})^T (U^{(k)}A^{(k)}) , \]

where

\[ R^{(k)} = \begin{bmatrix}
R_{0,0} & R_{0,1} & & & \\
R_{1,1} & R_{1,2} & R_{1,3} & & \\
& \ddots & \ddots & \ddots & \\
& & R_{k-1,k-1} & R_{k-1,k} & \\
& & & & \tilde{R}_{k,k}
\end{bmatrix}. \tag{7}\]

The diagonal blocks \( R_{i,i} \) are normally square and upper triangular, but are also allowed to be rectangular with more columns than rows. The superdiagonal blocks \( R_{i-1,i} \) are not identically zero. The same series of transformations is applied to the weighted right-hand side vector

\[ U^{(k)}b^{(k)} = \begin{bmatrix}
W_0o_0 \\
V_1c_1 \\
W_1o_1 \\
V_2c_2 \\
\vdots \\
\vdots \\
V_kc_k \\
W_ko_k
\end{bmatrix}. \tag{8}\]

We denote the transformed right-hand side by \( y^{(k)} = (Q^{(k)})^T (U^{(k)}b^{(k)}) \).

The transformations are discarded immediately after they are applied to the matrix and vector; no representation of \( Q^{(k)} \) is stored.

### 3.2 Observability

Many Kalman algorithms rely on the assumption that \( A \) is observable, which guarantees that all the diagonal blocks \( R_{i,i} \), as well as \( \tilde{R}_{k,k} \), are square and upper triangular. For example, assuming that \( G_0 \) is square or tall (or is the identity) and that the \( F_i \)s and \( H_i \)s are square, along with the standard assumption that all of them have full rank, guarantees that \( A \) is observable. When all the diagonal blocks are square and triangular, we can compute the estimates using back substitution, starting from \( \hat{u}_{k|k} \) and ending with \( \hat{u}_{0|k} \).
However, UltimateKalman works and can provide useful estimates even when \( A \) is not always observable, and even when it is never observable. We explain the different cases in terms of the structure of the \( R \) factor and their meaning to the user.

If \( \tilde{R}_{k,k} \) is flat but all the other \( R_{i,i} \) blocks are square and triangular, the system is not yet observable, but it may become observable in a future state. We currently do not have enough observations to estimate any of the states. As the system evolves and additional observations are made, the system may become observable, allowing us to estimate the states that are currently unobservable.

If for some \( i < k \) the diagonal block \( R_{i,i} \) is flat, then states \( u_0, \ldots, u_i \) are not observable and will never become observable. For any assignment of states \( u_{i+1} \) and up, there is a nontrivial space of equally good (in the sense of (4)) estimates for \( u_0, \ldots, u_i \). UltimateKalman tolerates this situation because even in this case, the observations of \( u_0, \ldots, u_i \) do provide useful information on future states.

If a state is not observable (or not yet observable), the method in UltimateKalman that returns an estimate of the state vector return a vector consisting of NaN values (not-a-number, a floating point value that indicates that a value is not available). This informs client code that the state is not observable.

3.3 The Paige-Saunders factorization algorithm

UltimateKalman uses the technique of the Paige-Saunders algorithm to produce \( R^{(k)} \) incrementally.

Step \( k \) starts by adding to \( R^{(k-1)} \) a block row and a block column that express an evolution equation,

\[
\begin{bmatrix}
\vdots & \vdots \\
R_{k-2,k-2} & R_{k-2,k-1} \\
\tilde{R}_{k-1,k-1} & -V_k F_k & V_k H_k \\
\vdots & \vdots 
\end{bmatrix}
\]

We now examine the block

\[
\begin{bmatrix}
\tilde{R}_{k-1,k-1} \\
-V_k F_k 
\end{bmatrix}
\] (9)

If this block is flat (or more generally, if its rank is smaller than \( n_k \), which implies that it can be orthogonally reduced to a flat block), the algorithm leaves the bottom 2-by-2 block as is, but treats it as a 1-by-2 block matrix \( \begin{bmatrix} R_{k-1,k-1} & R_{k-1,k-1} \end{bmatrix} \), with the same column partitioning. This allows the algorithm to handle all shapes of (9) in a uniform way. That is, we rename the blocks as

\[
\begin{bmatrix}
R_{k-1,k-1} & R_{k-1,k-1} \\
\tilde{R}_{k-1,k} & -V_k F_k & V_k H_k 
\end{bmatrix}
\]

Otherwise, the algorithm computes a QR factorization of (9), uses the resulting \( R \) factor as \( R_{k-1,k-1} \), and applies the orthonormal transformation to the last block column and to the right-hand side \( y \). This transforms the \( R \) factor into

\[
\begin{bmatrix}
\vdots & \vdots \\
R_{k-2,k-2} & R_{k-2,k-1} \\
R_{k-1,k-1} & R_{k-1,k} \\
\tilde{R}_{k,k} 
\end{bmatrix}
\]

7
Block row \( k - 1 \) is now sealed; it will not change any more. If \( \bar{R}_{k-1, k-1} \) was square, then so is \( R_{k-1, k-1} \). If \( \bar{R}_{k-1, k-1} \) was flat, then \( R_{k-1, k-1} \) might be either square or flat, depending on \( V_k F_k \).

The bottom right block \( \bar{R}_{k,k} \) is not upper triangular, and it might be completely missing if \( \bar{R}_{k-1, k-1} \) is flat, or square if \( \bar{R}_{k-1, k-1} \) is square. If \( \bar{R}_{k,k} \) is flat, then \( R_{k,k} \) might be square or flat, depending on \( V_k F_k \).

The bottom right block \( \bar{R}_{k,k} \) is not upper triangular, and it might be completely missing if \( \bar{R}_{k-1, k-1} \) is square or flat. If \( \bar{R}_{k,k} \) is square or tall and we now need to predict \( \hat{u}_{k|k-1} \) (and perhaps additional future states), we compute the QR factorization of \( \bar{R}_{k,k} \) and apply the transformation to \( y \).

If \( \bar{R}_{k,k} \) is square or tall and we now need to predict \( \hat{u}_{k|k-1} \) (and perhaps additional future states), we compute the QR factorization of \( \bar{R}_{k,k} \) and apply the transformation to \( y \). We denote the \( R \) factor of \( \bar{R}_{k,k} \) by \( \tilde{R}_{k,k} \).

If there are no observations of \( u_k \), then \( \tilde{R}_{k,k} = \bar{R}_{k,k} \) (or \( \tilde{R}_{k,k} = \bar{R}_{k,k} \) if \( \bar{R}_{k,k} \) is flat or missing) and we are done with step \( k \).

If there are observations in step \( k \), we add another block row to the \( R \) factor:

\[
\begin{pmatrix}
  \ddots & & \\
  & R_{k-2, k-2} & R_{k-2, k-1} \\
  & R_{k-1, k-1} & R_{k-1, k} \\
  & \bar{R}_{k,k} \& W_k G_k
\end{pmatrix}
\]

If we computed \( \tilde{R}_{k,k} \), in principle we can use it instead of \( \bar{R}_{k,k} \), but there is usually no significant benefit to this. If the block

\[
\begin{pmatrix}
  \bar{R}_{k,k} \\
  W_k G_k
\end{pmatrix}
\]

is flat, it becomes \( \tilde{R}_{k,k} \) and we are done. Otherwise we compute the QR factorization of this block, use the \( R \) factor as \( \tilde{R}_{k,k} \), and apply the transformation to \( y \).

We now have \( R^{(k)} \) and \( y^{(k)} \). Note that we have not used in this step block rows \( 1, \ldots, k - 2 \) of \( R^{(k-1)} \) and \( y^{(k-1)} \).

### 3.4 Forgetting and rolling back

Given \( R^{(k)} \) and \( y^{(k)} \), the estimates \( \hat{u}_{ijk} \) are computed by back substitution, from the bottom up.

Therefore, if we need only filtered estimates \( \hat{u}_{ijk} \), we only need the last sealed block row, row \( k - 1 \), and the incomplete block rows of step \( k \). If we also need smoothed estimates but only for time step \( i + 1 \) and higher, we need to store block rows \( i + 1 \) and higher, but not earlier rows.

Dropping old rows that would not be used for smoothing in the future saves memory. UltimateKalman allows the user to forget the rows of steps \( \leq i \) from \( R^{(k)} \) and \( y^{(k)} \).

Smoothing uses \( R^{(k)} \) but does not modify it. UltimateKalman also retains \( y^{(k)} \) when smoothing. This allows the algorithm to smooth again later if more observations are obtained, enabling easy implementation of strategies such as fixed-lag smoothing (Grewal and Andrews, 2015), in which each state is estimated once from past observations and from observations of the next \( n \) steps for some fixed lag \( n \).

In many cases it is useful to predict future states before any observations of them are available. In particular, by comparing the expectation of the observations of a predicted state \( \hat{G}_k \hat{u}_{k|k-1} \) with the actual observation vector \( o_k \) it is sometimes possible to detect and discard outlier observations.

UltimateKalman allows the user to predict future states while retaining the ability to provide observations later. To do so, UltimateKalman stores with sealed rows the
incomplete diagonal block $R_{k,k}$ and the associated right-hand side $\bar{y}_i$. If the user later asks UltimateKalman to roll back to step $k$, the algorithm discards from memory sealed rows $k$ and higher and restores $R_{k,k}$ and $\bar{y}_i$ as the bottommost incomplete row. Obviously, it is not possible to roll back to a forgotten step.

3.5 Computing the covariance matrices of estimates

UltimateKalman computes representations of the covariance matrices $\text{cov}(\hat{u}_{i|k})$ of estimates using orthogonal transformations of $R^{(k)}$. We assume here that $\bar{R}_{k,k}$ is square and triangular (otherwise existing steps are not yet observable).

The covariance matrix of the filtered estimate satisfies

$$\text{cov}(\hat{u}_{k|k})^{-1} = \bar{R}_{k,k}^T \bar{R}_{k,k},$$

so UltimateKalman simply returns $\bar{R}_{k,k}$ as a representation of $\text{cov}(\hat{u}_{k|k})$. We refer to this as an inverse-factor representation.

Producing inverse-factor representations of smoothed estimates requires a series of orthogonal transformations. The algorithm first computes the QR factorization of the bottom-right 2-by-1 block of

$$R^{(k)} = \begin{bmatrix} \cdots & \cdots & R_{k-2,k-2} & R_{k-2,k-1} \\ & & R_{k-1,k-1} & R_{k-1,k} \\ & & & R_{k,k} \end{bmatrix}$$

and applies the transformation to the entire two bottom block rows, to produce

$$\begin{bmatrix} \cdots & \cdots & R_{k-2,k-2} & R_{k-2,k-1} \\ & & S_{k,k-1} & S_{k,k} \\ & & & S_{k,k} \end{bmatrix}$$

with $S_{k,k-1}$ square. This block satisfies

$$\text{cov}(\hat{u}_{k-1|k})^{-1} = S_{k,k-1}^T S_{k,k-1},$$

so it is returned as a representation of the covariance matrix. The algorithm now permutes the last two block rows to obtain

$$\begin{bmatrix} \cdots & \cdots & R_{k-2,k-2} & R_{k-2,k-1} \\ & & S_{k,k-1} & 0 \\ & & & S_{k,k} \end{bmatrix}$$

and continues in the same way. The process continues with the QR factorization of

$$\begin{bmatrix} R_{k-2,k-1} \\ S_{k,k-1} \end{bmatrix},$$

repeating the same procedure. The correctness of this algorithm is shown in [Paige and Saunders, 1977] and in a perhaps slightly clearer way, in [Toledo, 2020].

The computation proceeds upwards in $R^{(k)}$ and can produce the covariance matrices of all the steps that have not been forgotten.
4 Implementation

UltimateKalman is currently available in MATLAB, C, and Java. This section describes the main features of the implementations, but not their details. A user guide that is distributed together with the source code of the library explains the programming interfaces of the library and how to build it, how to build test programs, and how to run these tests.

Each implementation is separate and does not rely on the others. The implementation includes MATLAB adapter classes that allow invocation of the C and Java implementations from MATLAB and from GNU Octave, a free open-source MATLAB-like environment. This allows a single set of test functions to test all three implementations. The code also includes standalone demonstration programs in Java and C, to show users how to use the library without MATLAB.

The MATLAB implementation does not rely on any MATLAB toolbox, only on functionality that is part of the core product. The implementation also works under GNU Octave. The C implementation relies on basic matrix and vector operations from the BLAS (Dongarra et al., 1990b,a) and on the QR and Cholesky factorizations from LAPACK (Anderson et al., 1999). The Java implementation uses the Apache Commons Math library for both basic matrix-vector operations and for the QR and Cholesky factorizations.

4.1 Programming interface

All three versions implement a data type that encapsulates the state of a Kalman filter or smoother. The operations on the data type are evolve, which describes an evolution equation (Equation (1) together with the associated covariance matrix $K_i$), observe, which describes an observation equation (Equation (2) and $C_i$), estimate, which returns an estimated state vector $\hat{u}_i$ and its covariance matrix, smooth, which performs back substitution to compute smoothed estimates, and forget and rollback, described in Section 3.4.

The MATLAB and Java implementations use overloading (using the same method name more than once, with different argument lists) to express variants of these operations, while the C implementation uses NULL to express missing or default values. The estimate method returns two values in the MATLAB implementation, the estimated vector and its covariance matrix, but only the estimated vector in the Java and C implementations. The covariance matrix is returned in these implementations by a separate method, covariance. These design decisions reflect good programming practices in each programming language.

4.2 The representation of vectors and matrices

The MATLAB implementation uses native MATLAB matrices and vectors. The Java implementation uses the types RealMatrix and RealVector from the Apache Commons Math library (both are interface types with multiple implementations).

The C implementation defines a type called matrix_t to represent matrices and vectors. The implementation defines functions that implement basic operations of matrices and vectors of this type. The type is implemented using a structure that contains a pointer to an array of double-precision elements, which are stored columnwise as in the BLAS and LAPACK, and integers that describe the number of rows and columns in the matrix and the stride along rows (the so-called leading dimension in the BLAS and
LAPACK interfaces). To avoid name-space pollution, in client code this type is called `kalman_matrix_t`.

State vectors are not always observable. This topic is explained in Section 3.2 in the companion article. This situation usually arises when there are not enough observations to estimate the state. The function calls and methods that return estimates of state vectors and the covariance matrices of the estimates return in such cases a vector of NaNs (not-a-number, a floating point value that indicates that the value is not available) and a diagonal matrix whose diagonal elements are NaN.

### 4.3 The representation of covariance matrices

Like all Kalman filters, UltimateKalman consumes covariance matrices that describe the distribution of the error terms and produces covariance matrices that describe the uncertainty in the state estimates $\hat{u}_i$. The input covariance matrices are not used explicitly; instead, the inverse factor $W$ of a covariance matrix $C = (W^TW)^{-1}$ is multiplied, not necessarily explicitly, by matrices or by a vector.

The programming interface of UltimateKalman expects input covariance matrices $C_i$ and $K_i$ to be represented as objects belonging to a type with a method `weigh` that multiplies the factor $W_i$ such that $C_i = (W_i^TW_i)^{-1}$ by a matrix $A$ or a vector $v$. In the MATLAB and Java implementations, this type is called `CovarianceMatrix`. The constructors of these classes accept many representations of a covariance matrix:

- An explicit covariance matrix $C$; the constructor computes an upper triangular Cholesky factor $U$ of $C = U^TU$ and implements $X = C_.\text{weigh}(A)$ by solving $UX = A$.
- An inverse factor $W$ such that $W^TW = C^{-1}$; this factor is stored and multiplied by the argument of `weigh`.
- An inverse covariance matrix $C^{-1}$; the constructor computes its Cholesky factorization and stores the lower-triangular factor as $W$.
- A diagonal covariance matrix represented by a vector $w$ such that $W = \text{diag}(w)$ (the elements of $w$ are inverses of standard deviations).
- A few other, less important, variants.

UltimateKalman always returns the covariance matrix of an estimated state vector $\hat{u}_i$ as an upper-triangular inverse factor $W_i$. The MATLAB and Java implementations return covariance matrices as objects of the `CovarianceMatrix` type (always with an inverse-factor representation); the C implementation simply returns the inverse factor as a matrix.

### 5 Examples and tests

We implemented an extensive set of tests for UltimateKalman. The individual tests are implemented by several MATLAB functions. Most of the functions receive as a first argument a handle to a function that serves as a factory of UltimateKalman filters. These functions are invoked by a top-level function called `replication` that defines the factory function and performs the tests. The factory function can produce objects of either the MATLAB implementation or objects of adapter classes that invoke the C or Java implementation.
Figure 1: Kalman filtering, prediction, and smoothing of the trajectory of a rotating point in the plane. On the left $G = I$ and observations are indicated by red dots. The yellow curve represents a simulated system; the blue curve represents filtered estimates, the cyan whole-trajectory smoothed estimates, and the green predictions from one observation. On the right $G = [1 \ 0]$; we cannot predict the state from one such observation, and we cannot produce a filtered estimate of the first state.

The function that performs performance testing is a little different: it includes a factory function and it can test multiple implementations, to enable plotting their performance on one graph.

The tests generate graphs similar to the ones presented below. The user can inspect the output visually, to ensure that the results are similar to those presented here. The tests do not produce pass/fail flags.

The tests were run on a laptop with an Intel quad-core 14nm i7-8565U processor running Windows 11 using MATLAB version R2021b. We also verified that the MATLAB implementation works correctly under GNU Octave. The C version is compiled into a MATLAB-callable dynamic link library (a so-called mex file) by MATLAB itself using a script, compile.m. In our tests, MATLAB used the C compiler from Microsoft’s Visual Studio 2019. The Java version is compiled using Eclipse so that it can be used by Java 1.8 and up (this is the version that MATLAB R2021b uses) and is packaged into a jar file by a simple shell script, build.bat.

5.1 Basic tests

We demonstrate and test the basic features of UltimateKalman using a simple model of a point in the plane that rotates around the origin. The initial state is $[1 \ 0]^T$. The evolution matrix is

$$F = \begin{bmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{bmatrix}$$

for $\alpha = 2\pi/16$, the observation matrix $G$ has between 1 and 6 rows, with an identity in the first two rows, $K = 0.001^2I$ and $C = 0.1^2I$. With these parameters, the rotation is very accurate, but the observations are not. The system is simulated for 16 steps, just short of a complete rotation.
Figure 1 shows the results of simulation, predicting, filtering, and smoothing with $G = I$ and with $G = [1 \ 0]$. The code, called rotation, first simulates the system and produces the ground-truth $u_1, \ldots, u_{15}$ and the observations $o_0, \ldots, o_{15}$. Then the code creates an UltimateKalman filter and runs it for 16 steps while providing only the first observation $o_0$. This attempts to predict $u_1, \ldots, u_{15}$. Then the code rolls back to step 1 and runs the filter again, providing all the observations. Finally, the code smooths the trajectory and collects the smoothed observations.

The first observation in the case of $G = I$ is quite inaccurate, so predictions from it are far from the real track, but they do follow nicely the system dynamics of exact rotation. The filtered estimates, on the other hand, improve quickly. The smooth estimates are nearly perfect, at least visually.

When $G = [1 \ 0]$ the block $R_{0,0}$ is flat, so the algorithm fails to produce a filtered estimate of $u_0$, but it does produce filtered estimates of $u_1, \ldots, u_{15}$.

This example is also used to test the code with overdetermined $G$s.

5.2 Variance variations

The next example demonstrates and tests the evaluation of covariance matrices, and it also demonstrates the effectiveness of Kalman filtering even when the model of the system is not perfect.

The code simulates a scalar that evolves either according to $u_i = u_{i-1} + \epsilon_i$ with $\epsilon_1 \sim N(0,1)$ (the errors are distributed normally with expectation 0 and standard deviation 1) or according to $u_i = u_{i-1} + 0.2$. However, even in the latter case, the Kalman filter uses the $u_i = u_{i-1} + \epsilon_i$ evolution equations, which do not reflect the true dynamics of the system. The observations are direct, $o_i = u_i + \delta_i$, with $\delta_i$ having a standard deviation of 10 in almost all cases.

Figure 2 shows results for the case $u_i = u_{i-1} + 0.2$. The graphs show both the estimates and their standard deviations. We see that the variance of the filtered estimates drops quickly in the first few steps and then stabilizes. If the standard deviation of $o_{50}$ is much smaller than the rest, 0.25, the variance of the filtered estimate also drops at that step, but it climbs back up. The variance of the smoothed estimates is impacted in both directions around step 50. It also increases towards iteration 0 and 100, but not dramatically.

All the estimates track the trajectory nicely, even though the Kalman filter and smoother use evolution equations that are different from those of the actual dynamic system. This is an important reason that Kalman filtering is so useful in practice: it often works well even when it models the dynamic system only approximately.

The results for a simulation with $u_i = u_{i-1} + \epsilon_i$ are similar and not shown in the paper.

5.3 Adding and removing parameters

The add_remove example shows how to add and remove parameters from the state vector. In the first two steps, the filter tracks the constant 1 using the evolution equation $u_i = u_{i-1} + \epsilon_i$ and observation equation $o_i = u_i + \delta_i$ with both error terms having a standard deviation of 0.1. In the third step, we add a dimension to the state; the first argument to evolve is now 2. This causes UltimateKalman to construct and use a matrix

$$H_i = \begin{bmatrix} 1 & 0 \end{bmatrix},$$

which represents a normal evolution of the first component of the state while not using any historical information about the second, new component. The evolution matrix $F_2$
Figure 2: Kalman filtering and smoothing of a scalar trajectory. The yellow lines show the actual trajectory, the red dots show the observations, the blue lines show the filtered estimates (left column), the cyan lines show smoothed estimates (right column), and the gray areas represent values that are $\pm 3\hat{\sigma}_i$ from the estimate $\hat{u}_i$, where $\hat{\sigma}_i$ is the estimated standard deviation of $\hat{u}_i$. In the top row, the standard deviation of $\delta_i$ is always 10; in the bottom row, it drops down to 0.25 at iteration 50 and then goes back up to 10.
remains a 1-by-1 identity in this step, but $G_2$ is now a 2-by-2 identity; $o_2$ becomes 2-dimensional as well. The actual value of the second parameter is 2 and the observations reflect that. In the next iteration, $F_3$ grows to 2-by-2. After two iterations with a 2-dimensional state vector, we drop the first (original) component of the state vector by calling evolve with a first argument 1 and by providing an explicit matrix

$$H_4 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$  

This matrix causes the filter to retain the second component of the state and to drop the first. In this step $F_4$ remains 2-by-2 but $G_4$ is 1-by-1. In the next iteration $F_5$ shrinks back to a 1-by-1 identity.

This demonstrates how to handle addition and removal of parameters and tests that UltimateKalman handles these cases correctly. The evolution and observation equations are very simple and track the two parameters separately, but this is immaterial for the addition and removal procedures.

### 5.4 A Projectile problem

The next example that we consider is taken almost as is from Humpherys et al. [Humpherys et al. 2012]. The problem uses a linear dynamic system to model a projectile. The states are four-dimensional; they model the horizontal and vertical displacements and the horizontal and vertical velocities. The model accounts for gravity, reducing the vertical velocity by a constant every time step, and for drag, which scales both components of the
velocity by a constant in every step. The matrices and vectors associated with the system are

\[
F_i = F = \begin{bmatrix}
1 & 0 & \Delta t & 0 \\
0 & 1 & 0 & \Delta t \\
0 & 0 & 1 - b & 0 \\
0 & 0 & 0 & 1 - b
\end{bmatrix}
\quad \text{and} \quad
c_i = c = \begin{bmatrix}
0 \\
0 \\
0 \\
-9.8 \Delta t
\end{bmatrix}
\]

\[
G_i = G = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{bmatrix},
\]

where \( \Delta t = 0.1 \) and \( b = 10^{-4} \). The example in (Humpherys et al., 2012) invites the reader to simulate the dynamic system for 1200 steps of 0.1 s each, starting from a known state, to generate noisy observations of the displacements (not the velocities) in steps 400 to 600, and to estimate the trajectory using a Kalman filter. They also ask the reader to use the filter to predict when and where the projectile will fall back to its original altitude, and to estimate the point of departure by reversing the dynamic system.

We have successfully applied UltimateKalman to this problem. The example code, projectile, generated the plots in Figure 3 which are similar to Figures 7.1a and 7.1b in (Humpherys et al., 2012). (It seems that the measurement noise shown in their Figure 7.1b has variance larger than the value 500 specified in (Humpherys et al., 2012).)

UltimateKalman also allows the user to easily extrapolate the trajectory by evolving the filter without providing additional observations, and to estimate the point of departure by smoothing time steps 0 to 600. Reversing the dynamic system is not required (and in particular, it is not necessary to invert the evolution matrix).

### 5.5 Clock offsets in a distributed system

The clock_offsets example highlights the utility of the \( H_i \) matrices. The aim is to estimate the relative offsets of a set of clocks in a distributed system. Each clock is
associated with a receiver and we assume that at time $\tau$, clock $j$ shows $t_j = \tau + f_{ij}$ where $f_{ij}$ is the offset of clock $j$ from real time at the time in which it displays the value $t_j$. The receivers receive radio packets from a beacon transmitter. The locations of the transmitter and receivers are known, so the line-of-sight propagation delays $d_j$ between the transmitter and receiver $j$ are also known. The receivers estimate the time of arrival of the packets using their local imperfect clocks. The observation equation for the time of arrival of packet $i$ at receiver $j$ is

$$t_{ij} = \tau_i + d_j + f_{ij} + \delta_{ij},$$

where $t_{ij}$ is the time-of-arrival estimate, as represented by imperfect clock $j$, $\tau_i$ is the unknown time of departure of the $i$th packet, $f_{ij}$ is the offset of clock $j$ at (local) time $t_{ij}$, $d_j$ is the known delay to receiver $j$, and $\delta_{ij}$ is the time-of-arrival estimation error.

The evolution equations are very simple:

$$f_{ij} = f_{i-1,j} + \epsilon_{ij}.$$  

They express the belief that the offsets change slowly. Note that the number of evolution equations is equal to the number of clocks, so is smaller than the dimension of the state vectors by one. The code uses the following matrices and vectors, including an explicit fixed $H_i$:

$$
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & 1 & 0 \\
\end{bmatrix}
\begin{bmatrix}
\epsilon_{i1} \\
\epsilon_{i2} \\
\vdots \\
\epsilon_{i\ell} \\
\end{bmatrix}
+ 
\begin{bmatrix}
\epsilon_{i1} \\
\epsilon_{i2} \\
\vdots \\
\epsilon_{i\ell} \\
\end{bmatrix}
+ 
\begin{bmatrix}
\tau_{i-1} \\
\tau_{i-1} \\
\vdots \\
\tau_{i-1} \\
\end{bmatrix}
= 
\begin{bmatrix}
1 & 0 & \cdots & 0 & 1 \\
0 & 1 & \cdots & 0 & 1 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
0 & 0 & \cdots & 1 & 1 \\
\end{bmatrix}
\begin{bmatrix}
f_{i-1,1} \\
f_{i-1,2} \\
\vdots \\
f_{i-1,m} \\
\end{bmatrix}
+ 
\begin{bmatrix}
f_{i-1,1} \\
f_{i-1,2} \\
\vdots \\
f_{i-1,m} \\
\end{bmatrix}
+ 
\begin{bmatrix}
\delta_{i1} \\
\delta_{i2} \\
\vdots \\
\delta_{i\ell} \\
\end{bmatrix}
.$$  

The structure of $H_i$ and $F_i$ reflects the removal of $\tau_{i-1}$ and the introduction of $\tau_i$ in every step.

The problem as presented up to now is clearly rank-deficient, because the residual is invariant under an addition of a constant $T$ to all the offsets and a subtraction of $T$ from all the departure times. Nothing anchors the solution relative to absolute time; indeed, we only want to estimate the relative offsets. To address this issue, we add a pseudo-observation of one offset in the first step. This removes the rank-deficiency.

This model can be easily extended to allow for packets that are not received by all receivers, for multiple transmitters, for slowly-changing rate-errors instead of slowly-changing offsets, and so on. The model can also allow receivers to join and leave the system without restarting the estimation process, as we have done in Section 5.3.

The results are shown in Figure 4.

5.6 Performance testing

Figure 5 shows the result of testing the performance of the three implementations using their perftest method. The experiments were carried out on a laptop with an Intel i7
Figure 5: Performance testing of the three UltimateKalman implementations. The graphs show the time per step (window averages of nonoverlapping groups of steps) when the algorithm filtered systems with random square unitary matrices $F_i$ and $G_i$.

The graphs in Figure 5 show the average runtimes per step, averaged over groups of 1000 steps.

The results show that on small problems ($n_i = 6$), the C implementation is the fastest, filtering taking about $8 \mu s$ per step. The Java implementation is about a factor of two slower, with periodic jumps that are most likely caused by the garbage collector. The MATLAB implementation is much slower, taking about $140 \mu s$ per step. Both the Java and MATLAB implementations are initially even slower, probably due to just-in-time compilation of the code.

On larger problems ($n_i = 48$), the C implementation is still the fastest. The MATLAB implementation is now only about two times slower than the C implementation. The improved ratio is most likely the result of $\Theta(n^3)$ dense-matrix operations (matrix multiplications and QR factorizations) taking a significant fraction of the running times. The data structure and method invocation overheads in C are much smaller than in MATLAB, but dense-matrix operations are performed at the same rate. On these larger problems, the Java implementation is the slowest, most likely because of the relative poor performance of the Apache Commons Math library relative to the BLAS and LAPACK implementations that come with MATLAB.

Some of the changes in the runtimes that are visible in some of the plots are likely due to the computer, a laptop, slowing down to avoid overheating.

Smoothing takes more time per step, due to the back substitution phase, and perhaps more importantly, a lot more memory, because the code retains the blocks of $R$ and the transformed $b$. Still, the library can smooth very long sequences. On the same computer we were able to smooth 5 million steps with $n_i = m_i = 6$ in about 96 s and 100,000 steps with $n_i = m_i = 48$ in 84 s. Both runs required less than 16GB of memory.
6 Discussion

Orthogonal transformations are the bedrock of numerical linear algebra. The numerical stability of algorithms that rely solely or mostly on orthogonal transformations is often both superior and easier to analyze than the stability of algorithms that use non-orthogonal transformations or explicit matrix inversion. From this standpoint, the fact that the Paige-Saunders algorithm did not become the standard linear Kalman filter and smoother is both puzzling and unfortunate. There is no good reason not to use it.

UltimateKalman aims to rectify this defect. It is a simplified version of the Paige-Saunders algorithm that is easier to implement, hopefully also easier to understand, and is probably just as efficient. UltimateKalman also generalizes the Paige-Saunders algorithm, making it more flexible. While there are certainly many high-quality and well-documented Kalman filter implementations, for example ([Torres] 2010 [Tusell] 2011), we are not aware of any other linear Kalman filter algorithm that is as flexible and that can handle problems with varying state-vector dimensions, does not require the expectation of the initial state, can handle missing observations, and can easily filter, predict, and smooth.

The Paige-Saunders algorithm does have two limitations that UltimateKalman inherits. First, it assumes that the covariance matrices $C_i$ and $K_i$ are all nonsingular. Traditional Kalman filters can cope with singular covariance matrices. However, this is not a significant limitation, since physical observations are always associated with some level of uncertainty, and physical evolution equations usually are too. Continuous evolution equations can be exact, with no uncertainty (e.g., equations of motion), but discrete evolution equations have at least discretization (truncation) error terms. Even continuous evolution equations sometimes suffer from uncertainty due to incomplete physical modeling (e.g., a missing or simplified drag term). Second, the algorithm is almost completely sequential, except for parallelism within the matrix operations that are carried out in each step. In real-time filtering applications, this limitation is meaningless, as the application is inherently sequential. However, in post-processing applications the ability to use many cores to reduce runtimes could be beneficial; the Paige-Saunders algorithm and UltimateKalman lack this ability.

The MATLAB implementation has been optimized for clarity and conciseness, not for computational efficiency. In particular, the sequence of steps in memory is represented by a dynamically-resized cell array. We made this design choice in order to make UltimateKalman easy to port to other languages and easy to specialize.

The C implementation was optimized for computational and memory efficiency while retaining full generality (e.g., it can handle changes in the dimension of the state vector, and it can smooth, like the other implementations) and without a specialized memory manager. The main cost of these design decisions is the dynamic allocation and deallocation of several matrices in every step. Specializing the algorithm to simple special cases, say only filtering and no changes in the state-vector dimension, would have allowed the algorithm to avoid dynamic memory allocation, making it faster and perhaps better suited to tiny embedded systems.

We hope that the numerical robustness afforded by the use of orthogonal transformations, the flexibility, the convenient programming interfaces, and the availability of the algorithm in multiple languages will make UltimateKalman the standard linear Kalman filter and smoother in new software. We also hope that authors and maintainers of statistical software packages of wider scope ([Peng and Aston] 2011 [Villegas and Pedregal] 2018), which often include nonlinear Kalman filters and other state-space models, will
incorporate UltimateKalman into their packages, ideally exposing some of the unique features through their own programming and user interfaces. Finally, we hope that authors of code generators that automatically generate Kalman filter code optimized for specific cases (Whittle and Schumann [2004]) will also incorporate the algorithm into their generators. The code clarity that we strived to achieve should simplify such efforts, as well as efforts to implement the algorithm in additional programming languages that are widely used for numerical computing like Python and Julia.

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