Data assimilation schemes for non-linear shallow water flow models

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Abstract

In theory Kalman filters can be used to solve many on-line data assimilation problems. However, for models resulting from the discretization of partial differential equations the number of state variables is usually very large, leading to a huge computational burden. Therefore approximation of the Kalman filter equations is in general necessary.

In this paper two new algorithms are proposed, that extend the idea of the Reduced Rank Square Root filter [15] for use with non-linear models. The algorithms are based on a low rank approximation of the error covariance matrix and use a square root representation of the error covariance. For both algorithms the tangent linear model is not needed. The first algorithm proposed is accurate up to first order terms, which is comparable to the extended Kalman filter. The second, at the cost of twice the number of computations, is second order accurate, which may be important for strongly nonlinear models.

Several experiments were performed on a model of the southern part of the North Sea to measure the performance of both algorithms. Both algorithms perform well when the the number of modes, i.e. the rank of the approximation, is set to 30. This corresponds to a computation time of approximately 30 model runs for the first order algorithm and 60 for the second order algorithm.

1 Introduction

Accurate forecasts of storm surges in the North Sea are very important for a timely closure of the storm surge barriers in the 'Eastern Scheldt' and for protection of the many dikes along the Dutch coast. These barriers and dikes are vital for protection of the densely populated western part of the Netherlands against the sea. The storm surge forecasts are also used by large ships entering the Rotterdam harbour, because at some points the depth is not enough at low-tide.

In the current operational system forecasts are based on simulations of a numerical model of the continental shelf of the North Sea. To improve the forecasts waterlevel measurements are assimilated into the model with a steady state Kalman filter. Essential in the steady state approach is that

the model is nearly linear and the use of a fixed measurement network that produces reliable measurements at regular intervals.

In order to further improve the forecasts and extend the applicability of the Kalman filtering program it is desirable to add nonlinearities and time varying parts to the model. Although the general Kalman filter approach can still be used, the number of computations needed for direct use of the Kalman filter equations [13] is not feasible with the available computers and thus clever approximations are needed. After Cohn and Todling [5] we will call these approximate Kalman filters, SubOptimal Schemes or SOS's.

For nonlinear models computation of the minimum variance estimate is only feasible for very small systems. Therefore approximations like the extended Kalman filter and second order filters [11, 10] are often used. For very large systems these second order filters are very time consuming and can not be used.

In the sequel two new algorithms will be described that are approximations to the extended Kalman filter and the truncated second order filter respectively and some experiments will be presented that show that computation times can be reduced dramatically without significant loss in performance.

2 Model and data

In order to obtain forecasts that are consistent with physical laws, like conservation of mass and momentum, the stochastic model was based on the two dimensional shallow water equations with a stochastic disturbance on the forcing. The advection of momentum was neglected since it is not very important for this application. This results in the following set of equations:

$$\frac{\partial h}{\partial t} + \frac{\partial Hu}{\partial x} + \frac{\partial Hv}{\partial y} = 0 \tag{1}$$

$$\frac{\partial u}{\partial t} + g\frac{\partial h}{\partial x} - fv + \frac{gu\sqrt{u^2+v^2}}{C^2 H} - \tau_x = 0 \tag{2}$$

$$\frac{\partial v}{\partial t} + g\frac{\partial h}{\partial x} + fu + \frac{gv\sqrt{u^2+v^2}}{C^2 H} - \tau_y = 0 \tag{3}$$

where (u, v) denotes depth averaged current, h is the waterlevel relative to the reference plane, D is the depth relative to the reference plane, $H = h + D$ is the total water depth, g is the gravity acceleration, f a coefficient for the Corriolis force, C the Chézy coefficient and (τ_x, τ_y) is the wind stress.

At the land-sea boundaries the normal current velocity was set to 0 and at the 'open' boundaries, where the model borders on the northern part of the North Sea, a set of harmonic constituents was given for the waterlevels.

The numerical integration was performed with an ADI type scheme on a staggered grid.

The main sources of error in this model are the waterlevels at the open boundary in case of an external surge and the meteorological forcing (τ_x, τ_y). These errors were modeled using AR(1) processes [3]. For the error at the open boundary independent processes were used in a few points, after which linear interpolation was used for the rest of the boundary. The error in the wind was first modelled on a coarse grid and then interpolated ([9] p140). Exponential correlation in space was used. Kalman filter algorithms can be expressed more easily when a state space formulation of the model is used. Therefore the above model was formulated in a state space form (see for eg. [9]).

3 Suboptimal Kalman filters

3.1 Introduction

The Kalman filter, as derived by Kalman [13], gives a recursive procedure for computation of the optimal estimate, in the minimum variance sense, in case of a linear system with Gaussian noise. Consider the linear system

$$x(k+1) = A(k)x(k) + B(k)u(k) + F(k)w(k) \quad (4)$$

$$y(k) = C(k)x(k) + v(k) \quad (5)$$

where $x(k) \in R^n$, $w(k) \in R^m$ and $v(k), y(k) \in R^p$, $u(k) \in R^l$. The system noise w and the measurement noise v are are zero mean white and Gaussian and. The covariances are given by $E[w(k)w(k)'] = \Sigma_s(k)$, $E[v(k)v(k)'] = \Sigma_o(k)$ and $E[w(k)v(l)'] = 0$ for all k, l. The initial condition is given by

$$E[x(0)] = x_0 \quad (6)$$

$$E[(x(0) - x_0)^2] = P_0 \quad (7)$$

Using this notation the Kalman filter equations can be denoted as

$$\hat{x}(k+1|k) = A(k)\hat{x}(k|k) + B(k)u(k) \quad (8)$$

$$P(k+1|k) = A(k)P(k|k)A(k)' + F(k)\Sigma_s(k)F(k)' \quad (9)$$

$$\hat{x}(k+1|k+1) = \hat{x}(k+1|k) + K(k+1)(y(k+1) - C(k+1)\hat{x}(k+1|k)) \quad (10)$$

$$K(k+1) = P(k+1|k)C(k+1)' (C(k+1)P(k+1|k)C(k+1)' + \Sigma_o(k+1))^{-1} \quad (11)$$

$$P(k+1|k+1) = P(k+1|k) - K(k+1)C(k+1)P(k+1|k) \quad (12)$$

$$\hat{x}(0|-1) = x_0 \quad (13)$$

$$P(0|-1) = P_0 \quad (14)$$

where $\hat{x}(k|l)$ denotes the estimate at time k using the measurements $y(0), \ldots, y(l)$ and $P(k|l)$ denotes the covariance matrix of the error of this estimate. Although these equations can in principle be used for many on-line data assim -ilation applications, there are in practice three major problems that hamper their use.

The first problem is that the number of computations needed for equation 9 becomes infeasible for large systems, as well as the storage needed for the error covariance matrix. For some applications the steady state approach can be used, where the Kalman gains $K(k)$ are replaced by $K = \lim_{k\to\infty} K(k)$. For this the limit should of course exist, which is not true in most applications. In order to reduce the number of computations also for these applications several approximations of the Kalman filter equations (SOS's) have been proposed (see eg. [7, 6, 1]).

One approach to reduce of the number of computations is the approximation of the matrices $A(.)$ or the matrices $P(.|.)$ by matrices of a lower rank. By means of a factorization the lower rank can be exploited to reduce the number of computations as well as the storage. Both the eigen decomposition and the singular value decomposition are very suited for the factorization, because they can easily be used to approximate a matrix by one of a lower rank. The Partial Singular value Kalman Filter (PSKF) [5] is based on a truncated singular value decomposition of the state transition matrices $A(.)$. The largest singular values and the singular vectors are computed using a Lanczos [8] algorithm, which requires the tangent linear model as well as the adjoint. The PSKF is most efficient if $A(.)$ is constant in time, so that the decomposition has to be computed only once. Two other algorithms, the Partial Eigen decomposition Kalman Filter (PEKF) [5] and the Reduced Rank SQuare RooT algorithm (RRSQRT) [15] use a truncated eigen decomposition of the matrices $P(.|.)$. The PEKF computes the truncated eigen decomposition with a Lanczos type algorithm, while the RRSQRT algorithm uses a square root approach [14] to maintain the factorized form of the error covariances.

In algorithms where the error covariance is approximated a major difficulty is the ill conditioning of these matrices (eg. [2, 5, 15]). Small changes, because of the approximations and finite precision computations, easily cause negative eigenvalues to appear in the computed error covariance, and subsequent instability of the filter. The approximation in terms of the square root of the error covariance is more robust since the the condition number of the square root factor is much lower than that of the error covariance matrix and also this formulation guarantees that the matrices $P(.|.)$ remain positive semi-definite at all times.

A third difficulty encountered in application of the Kalman filter is that in reality most systems exhibit some kind of nonlinearity. Although a recursive formulation of the minimum variance estimate for nonlinear systems exists [11] numerical computation of the solution does not seem to be pos-

sible for all but some very small systems in the near future. If the solution is expanded in terms of the central moments and subsequently truncated, several several approximate algorithms can be obtained (see [11, 10] for a derivation), of which the Extended Kalman Filter (EKF) is the most popular (eg.[9, 4]). No applications of higher order truncated filters to large systems are known to the authors, which is probably due to the dramatic increase of the computation time needed compared to the (extended) Kalman filter.

3.2 The RRSQRT filter

The RRSQRT algorithm is based on the fact that for the application in this paper the error covariance matrices $P(k+1|k)$ and $P(k|k)$ tend to have only a few large eigenvalues and many small ones. Boggs [2] and Cohn and Todling [5] also observed this property for meteorological models. The RRSQRT algorithm exploits this property using an eigendecomposition. Let $u_1, \ldots u_n \in R^n$ be the eigenvectors of a covariance matrix $P \in R^{n \times n}$ with the corresponding eigenvalues $d_1 \geq d_2 \geq \ldots \geq d_n \geq 0$, i.e. $P = UDU'$ with $U = [u_1, \ldots u_n]$ and D is diagonal with the eigenvalues on the diagonal. It is well known [8] that the error introduced by truncating the decomposition after the q'th eigenvalue introduces an error of d_{q+1} for the 2-norm. If there are only a few large eigenvalues, then P can be approximated accurately with only a few eigenvectors.

In order to preserve the positive semi definiteness of the error covariance matrices a square root approach is used for the RRSQRT filter. Also square root algorithms have better numerical properties than algorithms based on the covariance form [14]. It is easily seen that the matrix

$$L := \left[\sqrt{d_1}l_1, \ldots \sqrt{d_q}l_q\right] \tag{15}$$

is an approximate square root factor of the matrix P. If $q << n$ then this matrix is much smaller than the matrix P.

If the RRSQRT algorithm [15] is combined with the finite difference approximation of equation

$$\frac{\partial f}{\partial x} l \approx \frac{f(\hat{x}(k|k) + \varepsilon l, u(k)) - f(\hat{x}(k|k), u(k))}{\varepsilon} \tag{16}$$

and the state transition 4 replaced by

$$x(k+1) = f(x(k), u(k)) + F(k)w(k) \tag{17}$$

the following algorithm is obtained:

time step:

$$\hat{x}(k+1|k) \quad = \quad f(\hat{x}(k|k), u(k)) \tag{18}$$

$$L(k+1|k) = \left[\frac{f(\hat{x}(k|k)+\varepsilon l_1, u(k)) - f(\hat{x}(k|k), u(k))}{\varepsilon}, \ldots, \right.$$
$$\left. \frac{f(\hat{x}(k|k)+\varepsilon l_q, u(k)) - f(\hat{x}(k|k), u(k))}{\varepsilon}, FQ^{1/2}\right] \quad (19)$$

where l_i is the i'th column of $L(k|k)$ and $[.,.,.]$ denotes building a block matrix from the arguments.

reduction step:

$$\tilde{L}(k+1|k) = L(k+1|k)\tilde{U}(k+1|k) \quad (20)$$
$$\tilde{U}(k+1|k) = [U(k+1|k)]_{1:q+m,1:q} \quad (21)$$
$$U(k+1|1)D(k+1|k)U(k+1|k)' = L(k+1|k)'L(k+1|k) \quad (22)$$

where $[U(k+1|k)]_{1:q+m,1:q}$ means that all the rows 1 through $q+m$ are used, but only the columns 1 through q. Equation 22 denotes the eigen-decomposition of the matrix $L(k+1|k)'L(k+1|k)$, which is a $q+m$ by $q+m$ matrix. This step of the RRSQRT algorithm reduces the number of columns, while the covariance remains approximately the same, i.e. $\tilde{L}(k+1|k)\tilde{L}(k+1|k)' \approx L(k+1|k)L(k+1|k)'$.

measurement step:

The measurements are processed one at a time. If the measurements are correlated, then the measurements should be transformed using Σ_o. In the following equations it is assumed that Σ_o is diagonal.

$$\hat{x}_0(k+1|k) = \hat{x}(k+1|k) \quad (23)$$
$$\tilde{L}_0(k+1|k) = \tilde{L}(k+1|k) \quad (24)$$
$$H_{i+1}(k+1) = \tilde{L}_i(k+1|k)'C_{i+1}(k+1)' \quad (25)$$
$$\gamma_{i+1}(k+1) = (H_{i+1}(k+1)'H_{i+1}(k+1) + [\Sigma_o(k+1)]^{-1}_{i+1,i+1} \quad (26)$$
$$K_{i+1}(k+1) = \tilde{L}_i(k+1|k)H_{i+1}(k+1)\gamma_{i+1}(k+1) \quad (27)$$

$$\hat{x}_{i+1}(k+1|k) = \hat{x}_i(k+1|k) + K_{i+1}(y_i(k+1) - C_{i+1}(k+1)\hat{x}_i(k+1|k)) \quad (28)$$
$$\tilde{L}_{i+1}(k+1|k) = \tilde{L}_i(k+1|k) - K_{i+1}(k+1)H_{i+1}(k+1)' (1 + (\gamma_{i+1}(k+1)[\Sigma_o(k+1)]_{i+1,i+1})^{1/2})^{-1} \quad (29)$$

$$\hat{x}(k+1|k+1) = \hat{x}_m(k+1|k) \quad (30)$$
$$L(k+1|k+1) = \tilde{L}_m(k+1|k) \quad (31)$$

Where $y_i(k)$ is the i'th measurement ($i = 1, \ldots, m$) at time k. The index i denotes that i measurements have been processed.

For large systems most computations are needed for equation 19. This number is reduced considerably if $q << n$. Note that for $q = n$ the filter reduces to a 'full' square root filter, i.e. there are no approximations. The columns of L are called modes since they resemble the modes of the system in some respects.

3.3 A second order accurate RRSQRT filter

The main idea of the second order accurate algorithm by Julier [12] is that a finite sample can represent the mean and covariance of a random variable and that the mean and covariance of a function of this random variable can be approximated by the sample mean and sample covariance of the sample obtained by applying the function to all elements in the sample. This approximation was then shown to be second order accurate.

It is easy to show that the sample

$$S = \{x + \sqrt{q}l_1, x - \sqrt{q}l_1, \ldots, x + \sqrt{q}l_q, x - \sqrt{q}l_q\} \tag{32}$$

where $L = [l_1, \ldots l_q]$, has sample mean x and sample covariance LL'. Using the theorem by Julier [12] the sample

$$S = \{f(x+\sqrt{q}l_1, u), f(x-\sqrt{q}l_1, u), \ldots, f(x+\sqrt{q}l_q, u), f(x-\sqrt{q}l_q, u)\} \tag{33}$$

has approximately sample mean $E[f(x,u)]$ and sample covariance $E[f(x,u) - E[f(x,u)]]$. The errors in this approximation are all fourth order. Therefore this procedure can be used for the time step in a truncated second order filter.

If the columns l_i are orthogonal the factor $\sqrt{q}$ compensates for the fact that there are only two terms that contribute in that direction, contrary to a random sample where all columns contribute approximately the same amount. Because of this factor the points in the sample S are further away from the mean, if $q > 1$. This will amplify the effect of higher order terms which is not desirable. Therefore we will scale the elements in the sample. This scaling has to be compensated for when computing sample mean and sample covariance.

This approach results in the following second order accurate timestep:

$$\begin{aligned}
\hat{x}(k+1|k) &= f(\hat{x}(k|k), u(k)) \\
&+ \sum_{i=1}^{q} \left(\frac{f(\hat{x}(k|k) + \varepsilon l_1, u(k)) - f(\hat{x}(k|k), u(k))}{2\varepsilon^2} \right. \\
&+ \left. \frac{f(\hat{x}(k|k) - \varepsilon l_1, u(k)) - f(\hat{x}(k|k), u(k))}{2\varepsilon^2} \right) \qquad (34) \\
L(k+1|k) &= \left[\frac{f(\hat{x}(k|k) + \varepsilon l_1, u(k)) - f(\hat{x}(k|k), u(k))}{\sqrt{2}\varepsilon}, \ldots, \right. \\
&\quad \frac{f(\hat{x}(k|k) + \varepsilon l_q, u(k)) - f(\hat{x}(k|k) l, u(k))}{\sqrt{2}\varepsilon}, \\
&\quad \frac{f(\hat{x}(k|k) - \varepsilon l_1, u(k)) - f(\hat{x}(k|k), u(k))}{\sqrt{2}\varepsilon}, \ldots, \\
&\quad \left. \frac{f(\hat{x}(k|k) - \varepsilon l_q, u(k)) - f(\hat{x}(k|k) l, u(k))}{\sqrt{2}\varepsilon}, FQ^{1/2} \right] \qquad (35)
\end{aligned}$$

For small ε one can also prove also directly that the equations 34 and 35 are equivalent to the truncated second order timestep.

The equations 34 and 35 need $2q + 1$ evaluations of the function f. If $q << n$ the number of computations is reduced considerably. The number of computations about two times that needed for the RRSQRT algorithm, but this timestep is second order accurate.

4 Experiments

To evaluate the performance of the algorithms some experiments were performed. For all experiment the model of section 2 was used. The model area in shown in figure 1. Ten harmonic constituents of the astronomical tide were used at the open boundaries. In a 'truth' model an external surge was simulated by a disturbance on the northern boundary and the wind was neglected. In the 'estimation' model measurements at Scarborough, Lowestoft and Hoek van Holland were assimilated into the model; the other points were used as checks.

Figure 2 and 3 show the results of the RRSQRT algorithm of section 3.2 for 30 modes, which roughly corresponds to a computation time of 30 model runs. It can be seen that the algorithm picks up the signal very well, whereas the model run without data assimilation only shows the astronomical tide after the initial transient.

Figure 4 shows the 2-norm of the error between the estimate and the true state as a function of time for both the first order algorithm of section 3.2 and the second order algorithm of section 3.3. For both algorithms 30 modes,i.e. $q = 30$, were used. It can be seen that the second order algorithm works and performs slightly better than the first order algorithm.

5 Conclusions

In this paper two new algorithms were introduced, that extend the Reduced Rank Square Root algorithm for use with non-linear models. Both models reduce the computation time considerably compared to the 'full' Kalman filter. One algorithm includes second order terms with only relatively few additional computations, the other is comparable to the extended Kalman filter. Experiments were shown that indicate that both algorithms are very efficient and that the second order algorithm indeed provides slightly better estimates.

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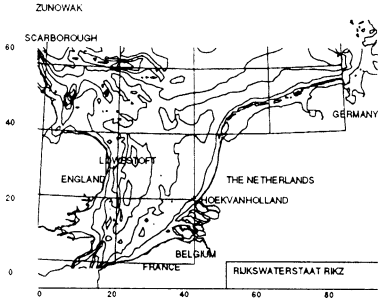

figure 1:

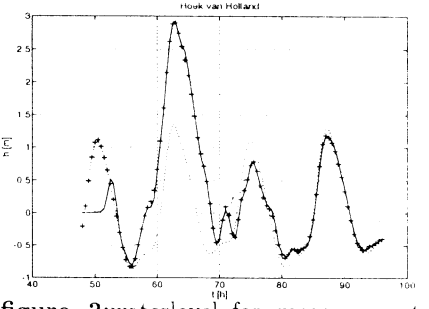

figure 2:waterlevel for measurement station Hoek van Holland: filter (—),measurements (+) and without filter (· · ·)

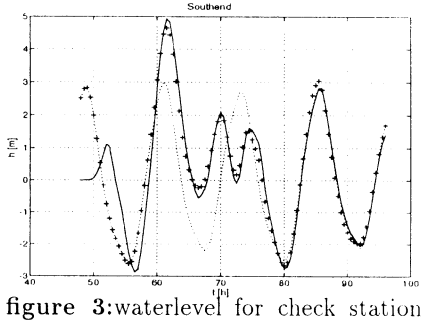

figure 3:waterlevel for check station Southend

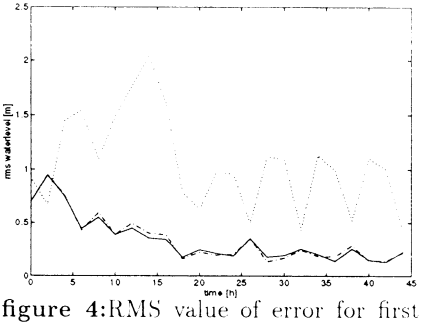

figure 4:RMS value of error for first order (— · —·) and second order (---) RRSQRT filters

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