Chapter 6

Basic Concepts in Nonlinear Filtering

6.1 Introduction

In this lecture, we are interested in treating the estimation problem for nonlinear systems. Due to the difficulties involved in problems of this type, and the various possible methods to approach them, we will confine this lecture to the study of the case of systems governed by stochastic *ordinary* differential equations. In fact, we assume that the case of atmospheric data assimilation, which the governing equations are a set of *partial* differential equations, can be formulated in terms of a system of ordinary differential equations. In general, this can be done by treating the space variables on a discrete grid, restricting in this manner the infinite dimensional problem to the case of finite dimension. Although this type of argument is in general a good starting point for dealing with the problem of data assimilation in earth sciences, it appears that the best way would be to study the system of governing equations and observational process in the continuum, at least to a very good extent. Discretization leads to modeling errors which have not been treated appropriately so far in that field. For further details related to this point of view the reader is referred to the excellent discussion in Cohn [27].

We saw in Lecture 4, that in many cases of Bayes estimation an estimate of the variable of interest reduces to the conditional mean. As a matter of fact, the estimate of minimum variance is the conditional mean. In case of Gaussian processes, other optimization criteria produces similar estimates to the one given by the minimum variance. Furthermore, we saw in Lecture 5, that when a linear observation process is combined with a linear dynamical process the Kalman filter provides the best linear unbiased estimate (BLUE). When the statistics of errors are Gaussian the Kalman filter estimates correspond to the conditional mean. In the nonlinear case, even with Gaussian error statistics, the resulting estimates are not Gaussian distributed and consequently different Bayes optimization criteria lead to distinct estimates, in particular not necessarily coinciding with the conditional mean. One of the consequences of Gaussian error statistics in the linear case is that only the first two moments are enough to describe the process completely; in the nonlinear case, on the

other hand, moments of higher order may play an important role in describing the process. Ideally, the transition probabilities related to the processes under consideration should be the quantities being calculated, however, in most practical applications calculating these quantities requires computations well beyond available resources.

A precise treatment of the estimation problem for nonlinear systems can be made following statistical arguments. Since the probability density of the variables of the system contain all the necessary information to describe the system, the probabilistic method studies the evolution of the probability density in time, as well as the way by which this quantity is modified as observations become available. In Lecture 3, we obtained evolution equations only for the first two moments of the probability density for nonlinear dynamical systems. In fact, it is possible to show that the probability density evolves according to the Fokker–Planck equation, and once its evolution is determined we can determine any desired moment.

For the continuous–discrete system case, the conditional probability density evolves through the Fokker–Planck equation during the intervals of time in which there are no observations. At observation times the transition undertaken by the probability density due to the observations can be evaluated through Bayes rule. The rigorous mathematical treatment following this procedure can be found, for example, in the classic text books of Jazwinski [84] and Sage & Melsa [121], or in more modern texts such as that of Øksendal's [108]. The precise treatment of nonlinear estimation problems is beyond the scope of our introductory course.

6.2 The Extended Kalman Filter

In this section, we follow the simple treatment of Gelb [60] to derive the so called extended Kalman filter. We consider the continuous–discrete system problem, that is, the case in which the dynamics evolves continuously in time whereas the observations are available at discrete times $t_1, t_2, \ldots$. The modification for the case in which the dynamical system is discrete in time can be derived using the results from Section 3.2.2.

The continuous–time dynamical process, corresponding to the evolution of the n–vector $\mathbf{w}^t(t)$ — the variable of interest — is written here as

$$\frac{d\mathbf{w}^t(t)}{dt} = \mathbf{f}(\mathbf{w}^t, t) + \mathbf{b}^t(t) \tag{6.1}$$

and the discrete–time observation process, at times $t_{k-1} \leq t < t_k$, is written as

$$\mathbf{w}_k^o = \mathbf{h}(\mathbf{w}_k^t) + \mathbf{b}_k^o \tag{6.2}$$

where the $\mathbf{w}_k^t \equiv \mathbf{w}^t(t = t_k)$, and the m–vector $\mathbf{w}_k^o$ corresponds to the observation vector. We assume the n–vector process noise $\{\mathbf{b}^t(t)\}$ is white in time, Gaussian, with mean zero and (co)variance $\mathbf{Q}(t)$. Similarly, we assume the m–vector observation noise $\{\mathbf{b}_k^o\}$ is white in time, Gaussian, with mean zero and (co)variance $\mathbf{R}_k$. Moreover, the processes $\{\mathbf{b}^t(t)\}$ and $\{\mathbf{b}_k^o\}$ are assumed to be uncorrelated at all times. Analogously to what we have done in the previous lecture, let us indicate by $\mathbf{W}_k^o = \{\mathbf{w}_k^o, \mathbf{w}_{k-1}^o, \cdots, \mathbf{w}_1^o\}$ the set of all observations

up to and including time t_k. The n–vector function $\mathbf{f}$ corresponds to the dynamics of the system and the m–vector function $\mathbf{h}$ corresponds to the observation operator.

The most common procedure to deal with estimation problems for nonlinear systems is that of minimum variance. Since the estimate with minimum variance corresponds to the conditional mean, we choose to calculate the conditional mean during the interval of time in which there are no observations. In this way, we want to calculate $\mathcal{E}\{\mathbf{w}^t(t)|\mathbf{W}^o_{k-1}\}$ during the interval of time $t_{k-1} \leq t < t_k$. According to to (6.1) it follows that

$$\frac{d\mathcal{E}\{\mathbf{w}^t(t)|\mathbf{W}^o_{k-1}\}}{dt} = \mathcal{E}\{\mathbf{f}[\mathbf{w}^t(t),t]|\mathbf{W}^o_{k-1}\} \tag{6.3}$$

where we used the fact that the process $\{\mathbf{b}(t)\}$ is white and has mean zero.

A measure of the error in the estimate can be obtained by means of the conditional error (co)variance matrix $\mathbf{P}(t)$, defined as

$$\mathbf{P}(t) \equiv \mathcal{E}\{[\mathbf{w}^t(t) - \mathcal{E}\{\mathbf{w}^t(t)|\mathbf{W}^o_{k-1}\}]\,[\mathbf{w}^t(t) - \mathcal{E}\{\mathbf{w}^t(t)|\mathbf{W}^o_{k-1}\}]^T\,|\mathbf{W}^o_{k-1}\} \tag{6.4}$$

for $t_{k-1} \leq t < t_k$. The evolution equation of this matrix between two consecutive observation times can be determined as in Lecture 3. Integrating (6.3) between t_{k-1} and t_k, substituting the result in the definition of $\mathbf{P}$, differentiating the resulting expression and using the properties of the processes $\{\mathbf{w}^t(t)\}$ and $\{\mathbf{b}^t(t)\}$ we obtain (see Exercise 6.1):

$$\begin{aligned}\dot{\mathbf{P}}(t) &= \mathcal{E}\{\mathbf{w}^t(t)\mathbf{f}^T[\mathbf{w}^t(t),t]|\mathbf{W}^o_{k-1}\} - \mathcal{E}\{\mathbf{w}^t(t)|\mathbf{W}^o_{k-1}\}\mathcal{E}\{\mathbf{f}[\mathbf{w}^t(t),t]|\mathbf{W}^o_{k-1}\}^T \\ &+ \mathcal{E}\{\mathbf{f}[\mathbf{w}^t(t),t]\mathbf{w}^{tT}(t)|\mathbf{W}^o_{k-1}\} - \mathcal{E}\{\mathbf{f}[\mathbf{w}^t(t),t]|\mathbf{W}^o_{k-1}\}\mathcal{E}\{\mathbf{w}^t(t)|\mathbf{W}^o_{k-1}\}^T \\ &+ \mathbf{Q}(t)\end{aligned} \tag{6.5}$$

which is often written in the more compact form,

$$\begin{aligned}\dot{\mathbf{P}}(t) &= \mathcal{E}\{\mathbf{w}^t\mathbf{f}^T\}_{k-1} - \mathcal{E}\{\mathbf{w}^t\}_{k-1}\mathcal{E}\{\mathbf{f}\}^T_{k-1} \\ &+ \mathcal{E}\{\mathbf{f}\mathbf{w}^{tT}\}_{k-1} - \mathcal{E}\{\mathbf{f}\}_{k-1}\mathcal{E}\{\mathbf{w}^t\}^T_{k-1} + \mathbf{Q}(t)\end{aligned} \tag{6.6}$$

where we wrote the conditional ensemble mean operator in the compact form: $\mathcal{E}\{(.)\}_{k-1} = \mathcal{E}\{.|\mathbf{W}^o_{k-1}\}$, and we omitted the explicit functional dependencies of $\mathbf{w}^t$ and $\mathbf{f}$. The equations for the mean and error (co)variance are not ordinary differential equations in the usual sense because they depend on the ensemble mean. To solve these equations it is necessary to know the probability density of the process $\{\mathbf{w}^t(t)\}$, which in general is not known. Moreover, we should calculate the corresponding moments depending on the function $\mathbf{f}[\mathbf{w}^t(t)]$.

The simplest approximation to the equation for the evolution of the mean (6.3) and to the equation for the evolution of the second moment (6.6), follows what we have seen in Lecture 3. That is, let us introduce the forecast vector $\mathbf{w}^f_k$ as a suitable approximation for the conditional mean, that is,

$$\mathbf{w}^f(t) \approx \mathcal{E}\{\mathbf{w}^t(t)|\mathbf{W}^o_{k-1}\} \tag{6.7}$$

In the extended Kalman filter, we expand the function $\mathbf{f}[\mathbf{w}^t(t)]$ as a Taylor series about the approximate mean $\mathbf{w}^f(t)$, and retain only up to the the first order term. Thus, in the time interval $t_{k-1} \leq t < t_k$, between two consecutive observations, we write

$$\mathbf{f}[\mathbf{w}^t(t),t] \approx \mathbf{f}[\mathbf{w}^f(t),t] + \mathcal{F}'[\mathbf{w}^f(t),t](\mathbf{w}^t(t) - \mathbf{w}^f(t)) \tag{6.8}$$

where, as in Lecture 3, $\mathcal{F}$ is the $n \times n$ Jacobian matrix defined as

$$\mathcal{F}'[\mathbf{w}^f(t), t] \equiv \left. \frac{\partial \mathbf{f}[\mathbf{w}^t(t), t]}{\partial [\mathbf{w}^t(t)]^T} \right|_{\mathbf{w}^t(t)=\mathbf{w}^f(t)} \tag{6.9}$$

Consequently, using the expansion and (6.7) the forecast equation becomes

$$\dot{\mathbf{w}}^f(t) = \mathbf{f}[\mathbf{w}^f(t), t] \tag{6.10}$$

valid for the times t in the interval between t_{k-1} and t_k: Using the expansion (6.8) in (6.6) we obtain that

$$\dot{\mathbf{P}}^f(t) = \mathcal{F}[\mathbf{w}^f(t), t]\mathbf{P}^f(t) + \mathbf{P}(t)\mathcal{F}^T[\mathbf{w}^f(t), t] + \mathbf{Q}(t) \tag{6.11}$$

which is identical to what we saw in Lecture 3, with the additional restriction that this expression applies only when $t \in [t_{k-1}, t_k)$. Notice that here,

$$\mathbf{P}^f(t) \equiv \mathcal{E}\{[\mathbf{w}^t(t) - \mathbf{w}^f(t)\}][\mathbf{w}^t(t) - \mathbf{w}^f(t)\}]^T\} \approx \mathbf{P}(t) \tag{6.12}$$

that is, $\mathbf{P}^f(t)$ is an approximation to the conditional error (co)variance matrix $\mathbf{P}(t)$.

The problem of producing an estimate $\mathbf{w}_k^a$ in t_k of the state of the system, using the observation $\mathbf{w}_k^o$, is what we want to solve in order to obtain a filtered estimate. Motivated by the results obtained in the linear case, we assume that such an estimate can be obtained as a linear combination among the observations. Hence, we write

$$\mathbf{w}_k^a = \mathbf{u}_k + \tilde{\mathbf{K}}_k \mathbf{w}_k^o \tag{6.13}$$

where the n–vector $\mathbf{u}_k$ and the $n \times m$ matrix $\tilde{\mathbf{K}}_k$ are deterministic (non-stochastic) quantities to be determined from statistical and optimization arguments, just as we did in the linear case.

Introduce the analysis and forecast estimation errors, that is, $\mathbf{e}_k^a$ is the error in the estimate at time t_k which includes the current observation, while $\mathbf{e}_k^f$ is the error in the estimate at time t_k which includes observations only up to time t_{k-1}:

$$\mathbf{e}_k^a \equiv \mathbf{w}_k^a - \mathbf{w}_k^t \tag{6.14a}$$

$$\mathbf{e}_k^f \equiv \mathbf{w}_k^f - \mathbf{w}_k^t \tag{6.14b}$$

By adding and subtracting $\mathbf{w}_k^t$ from the left–hand–side of expression (6.13), and using (6.2) we can write

$$\begin{aligned} \mathbf{e}_k^a &= \mathbf{w}_k^a - \mathbf{w}_k^t \\ &= \mathbf{u}_k + \tilde{\mathbf{K}}_k \left[\mathbf{h}(\mathbf{w}_k^t) + \mathbf{b}_k^o\right] - \mathbf{w}_k^t \end{aligned} \tag{6.15}$$

Now, adding and subtracting $\mathbf{w}_k^f$ from the right–hand–side of last equality above we get

$$\mathbf{e}_k^a = \mathbf{u}_k + \tilde{\mathbf{K}}_k \left[\mathbf{h}(\mathbf{w}_k^t) + \mathbf{b}_k^o\right] + \mathbf{e}_k^f - \mathbf{w}_k^f \tag{6.16}$$

According to Bayes estimation, one of the desired properties of an estimate is that it be unconditionally unbiased. This means that we want $\mathcal{E}\{\mathbf{e}_k^a\} = \mathbf{0}$. Therefore, applying the ensemble mean operator to the expression above it follows that

$$\mathcal{E}\{\mathbf{e}_k^a\} = \mathcal{E}\{\left[\mathbf{u}_k + \tilde{\mathbf{K}}_k\mathbf{h}(\mathbf{w}_k^t) - \mathbf{w}_k^f\right]\} + \mathcal{E}\{\mathbf{b}_k^o\} + \mathcal{E}\{\mathbf{e}_k^f\} \tag{6.17}$$

Recall that the sequence $\{\mathbf{b}_k^o\}$ has mean zero, thus $\mathcal{E}\{\mathbf{b}_k^o\} = \mathbf{0}$. Moreover, inspired by the linear case, we assume that the forecast error is unbiased. A word of caution is appropriate here: it is important to recognize that this is an assumption we know can only be approximately correct since the forecast is only an approximation to the conditional mean, that is,

$$\begin{aligned}
\mathcal{E}\{\mathbf{e}_k^f\} &= \mathcal{E}\{\mathbf{w}_k^f - \mathbf{w}_k^t\} \\
&\approx \mathcal{E}\{\mathcal{E}\{\mathbf{w}_k^t|\mathbf{W}_{k-1}^o\}\} - \mathcal{E}\{\mathbf{w}_k^t\} \\
&= \mathcal{E}\{\mathbf{w}_k^t\} - \mathcal{E}\{\mathbf{w}_k^t\} \\
&= \mathbf{0}
\end{aligned} \tag{6.18}$$

thus $\mathcal{E}\{\mathbf{e}_k^f\} \approx \mathbf{0}$. With that in mind, from (6.17) we see that for the estimate to be (approximately) unbiased we should satisfy:

$$\mathcal{E}\{\left[\mathbf{u}_k + \tilde{\mathbf{K}}_k\mathbf{h}(\mathbf{w}_k^t) - \mathbf{w}_k^f\right]\} = \mathbf{0} \tag{6.19}$$

Since $\mathbf{u}_k$ was assumed to be deterministic we have

$$\begin{aligned}
\mathbf{u}_k &= \mathcal{E}\{\left[\mathbf{w}_k^f - \tilde{\mathbf{K}}_k\mathbf{h}(\mathbf{w}_k^t)\right]\} \\
&= \mathbf{w}_k^f - \tilde{\mathbf{K}}_k\mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\}
\end{aligned} \tag{6.20}$$

Substituting this result in (6.13) we obtain

$$\mathbf{w}_k^a = \mathbf{w}_k^f + \tilde{\mathbf{K}}_k\left[\mathbf{w}_k^o - \mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\}\right] \tag{6.21}$$

Moreover, the analysis error can be re–written as

$$\mathbf{e}_k^a = \mathbf{e}_k^f + \tilde{\mathbf{K}}_k\left[\mathbf{h}(\mathbf{w}_k^t) - \mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\} + \mathbf{b}_k^o\right] \tag{6.22}$$

As in the linear case, we want to minimize the analysis error variance (6.22). We introduce the analysis error (co)variance matrix

$$\mathbf{P}_k^a \equiv \mathcal{E}\{\mathbf{e}_k^a\,(\mathbf{e}_k^a)^T\} \tag{6.23}$$

and the problem of minimization is reduced to the problem of minimizing the trace of this matrix,

$$\mathcal{J}_k^a \equiv \mathrm{Tr}(\mathbf{P}_k^a) \tag{6.24}$$

as in (5.19), but using $\mathbf{E}_k = \mathbf{I}$ in that expression, without loss of generality.

From (6.22) it follows that

$$\begin{aligned}
\mathbf{P}_k^a &= \mathbf{P}_k^f + \tilde{\mathbf{K}}_k\mathcal{E}\left\{\left[\mathbf{h}(\mathbf{w}_k^t) - \mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\}\right]\left[\mathbf{h}(\mathbf{w}_k^t) - \mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\}\right]^T\right\}\tilde{\mathbf{K}}_k^T \\
&+ \mathcal{E}\left\{\mathbf{e}_k^f\left[\mathbf{h}(\mathbf{w}_k^t) - \mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\}\right]^T\right\}\tilde{\mathbf{K}}_k^T \\
&+ \tilde{\mathbf{K}}_k\mathcal{E}\left\{\left[\mathbf{h}(\mathbf{w}_k^t) - \mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\}\right](\mathbf{e}_k^f)^T\right\} + \tilde{\mathbf{K}}_k\mathbf{R}_k\tilde{\mathbf{K}}_k^T
\end{aligned} \tag{6.25}$$

Applying the trace operator to this expression and using the rules from matrix calculus introduced earlier in this lecture, we can solve

$$\frac{\partial \mathcal{J}_k^a}{\partial \tilde{\mathbf{K}}_k} = 0 \tag{6.26}$$

to find that the gain matrix minimizing $\mathcal{J}_k^a$ is given by

$$\begin{aligned} \tilde{\mathbf{K}}_k \equiv \mathbf{K}_k &= \mathcal{E}\left\{\mathbf{e}_k^f \left[\mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\} - \mathbf{h}(\mathbf{w}_k^t)\right]^T\right\} \\ &\quad \times \left\{\mathcal{E}\{\left[\mathbf{h}(\mathbf{w}_k^t) - \mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\}\right]\left[\mathbf{h}(\mathbf{w}_k^t) - \mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t)\}\right]^T\} + \mathbf{R}_k\right\}^{-1} \end{aligned} \tag{6.27}$$

Substituting this gain matrix in the general equation for the analysis error (co)variance at time t_k we have

$$\mathbf{P}_k^a = \mathbf{P}_k^f - \mathbf{K}_k \mathcal{E}\left\{\left[\mathcal{E}\{\mathbf{h}(\mathbf{w}_k^t) - \mathbf{h}(\mathbf{w}_k^t)\}\right](\mathbf{e}_k^f)^T\right\} \tag{6.28}$$

(see Exercise 6.2). Equations (6.22), (6.27) and (6.28) provide the minimum variance estimate, optimal gain and corresponding error (co)variance at time t_k. These expressions involve the ensemble average operator and consequently cannot be used directly. Analogously to the Taylor expansion used for $\mathbf{f}[\mathbf{w}^t(t), t]$, when deriving a closed form for the evolution of the first and second moments in the interval of time between two consecutive observations, we expand the function $\mathbf{h}[\mathbf{w}^t(t)]$ about the estimate of the state of the system available at time t_k before the observations are processed, that is, $\mathbf{w}_k^f$. Therefore,

$$\begin{aligned} \mathbf{h}[\mathbf{w}^t(t)] &\approx \mathbf{h}[\mathbf{w}^f(t)] - \mathcal{H}'[\mathbf{w}^f(t), t](\mathbf{w}^f(t) - \mathbf{w}^t(t)) \\ &= \mathbf{h}[\mathbf{w}^f(t)] - \mathcal{H}'[\mathbf{w}^f(t), t]\mathbf{e}^f(t) \end{aligned} \tag{6.29}$$

where $\mathcal{H}'$ is the $m \times m$ Jacobian matrix defined as

$$\mathcal{H}'[\mathbf{w}^f(t), t] \equiv \left.\frac{\partial \mathbf{h}[\mathbf{w}^t(t), t]}{\partial [\mathbf{w}^t(t)]^T}\right|_{\mathbf{w}^t(t) = \mathbf{w}^f(t)} \tag{6.30}$$

of the m–vector function $\mathbf{h}$. The substitution of this approximation in expressions (6.22), (6.27) and (6.28) produces

$$\mathbf{w}_k^a = \mathbf{w}_k^f + \mathbf{K}_k\left[\mathbf{w}_k^o - \mathbf{h}(\mathbf{w}_k^f)\right] \tag{6.31a}$$

$$\mathbf{K}_k = \mathbf{P}_k^f \mathcal{H}'^T(\mathbf{w}_k^f)\left[\mathcal{H}'(\mathbf{w}_k^f)\mathbf{P}_k^f \mathcal{H}'^T(\mathbf{w}_k^f) + \mathbf{R}_k\right]^{-1} \tag{6.31b}$$

$$\mathbf{P}_k^a = \left[\mathbf{I} - \mathbf{K}_k \mathcal{H}'(\mathbf{w}_k^f)\right]\mathbf{P}_k^f \tag{6.31c}$$

which correspond to a closed set of equations for the update of the state estimate, gain matrix and corresponding error (co)variance. The equations above, together with (6.10) and (6.11), form the set of equations constituting the *extended* Kalman filter. In case the functions $\mathbf{f}$ and $\mathbf{h}$ are linear, these equations reduced to those of the standard Kalman filter, derived in the previous lecture. The results obtained above can be extended to the case of continuous–time observation processes. Also, higher order expressions can be derived by considering higher order terms in the Taylor expansions for the functions $\mathbf{f}$ and $\mathbf{h}$ (see Gelb [60], Jazwinski [84], and Sage & Melsa [121]). Equations for the case of discrete–time

Table 6.1: Extended Kalman filter: discrete–discrete systems.

Dynamical Process	$\mathbf{w}_k^t = \boldsymbol{\psi}(\mathbf{w}_{k-1}^t) + \mathbf{b}_{k-1}^t$
Observational Process	$\mathbf{w}_k^o = \mathbf{h}(\mathbf{w}_k^t) + \mathbf{b}_k^o$
Estimate Propagation	$\mathbf{w}_k^f = \boldsymbol{\psi}(\mathbf{w}_{k-1}^a)$
Error Covariance Propagation	$\mathbf{P}_k^f = \mathcal{F}'(\mathbf{w}_{k-1}^a)\mathbf{P}_{k-1}^a\mathcal{F}'^T(\mathbf{w}_{k-1}^a) + \mathbf{Q}_{k-1}$
Gain Matrix	$\mathbf{K}_k = \mathbf{P}_k^f\mathcal{H}'^T(\mathbf{w}_k^f)\left[\mathcal{H}'(\mathbf{w}_k^f)\mathbf{P}_k^f\mathcal{H}'^T(\mathbf{w}_k^f) + \mathbf{R}_k\right]^{-1}$
Estimate Update	$\mathbf{w}_k^a = \mathbf{w}_k^f + \mathbf{K}_k\left[\mathbf{w}_k^o - \mathbf{h}(\mathbf{w}_k^f)\right]$
Estimate Error Covariance Update	$\mathbf{P}_k^a = \left[\mathbf{I} - \mathbf{K}_k\mathcal{H}'(\mathbf{w}_k^f)\right]\mathbf{P}_k^f$
Definitions	$\mathcal{F}'(\mathbf{w}_k^a) \equiv \left.\frac{\partial\boldsymbol{\psi}(\mathbf{w})}{\partial\mathbf{w}^T}\right\|_{\mathbf{w}=\mathbf{w}_k^a}$ $\mathcal{H}'(\mathbf{w}_k^f) \equiv \left.\frac{\partial\mathbf{h}(\mathbf{w})}{\partial\mathbf{w}^T}\right\|_{\mathbf{w}=\mathbf{w}_k^f}$

dynamics and discrete–time observations which can be derived simply by using the equations for mean and (co)variance evolution given in Section 3.2.2, are displayed in Table 6.2, which is an adaptation of Table 9.4-3 of Sage & Melsa [121]. Applications of the extended Kalman filter in the contexts of atmospheric and oceanic data assimilation are those of Bürger & Cane [21], Daley [38], Evensen [52], Ménard [104], Miller et al. [107], to cite just a few.

It is important to notice that, contrary to what we saw in Section 5.1.3, The analysis and forecast error (co)variance matrices now depend on the observations – therefore expressions (5.41)–(5.42) is not valid in the nonlinear case. The error (co)variance matrices are functions of the Jacobian matrices $\mathcal{F}'$ and $\mathcal{H}'$, which are functions of the current estimate — which in turn depends on the observations themselves. Thus, the gain matrix $\mathbf{K}_k$ and the error (co)variances $\mathbf{P}_k^f$ and $\mathbf{P}_k^a$ are random, due to the fact that they depend on the set of observations $\mathbf{W}^o$. But most importantly is the fact that neither one of these covariance matrices correspond to the conditional error (co)variance matrices, but are rather approximations to these quantities. The same is true about the estimates $\mathbf{w}_k^f$ and $\mathbf{w}_k^a$ provided by the extended Kalman filter, that is, they represent only approximations to the conditional mean, in particular these estimates are only approximately unbiased. Therefore, precisely putting it, the extended Kalman filter provides biased state estimates.

6.3 An Approach to Parameter Estimation

In this section we want to briefly point out that extensions of the Kalman filter to nonlinear systems, such as the extended Kalman filter discussed in last section, can be used to estimate unknown system parameters, even when the dynamics and observation process are linear. These parameters can be either related to the dynamics, that is, to the vector function $\mathbf{f}$ or to the observation operator $\mathbf{h}$. It is also possible to estimate parameters related to the statistics of the errors involved in the problem.

As a simple illustration, consider the discrete–discrete system described by

$$\mathbf{w}_k^t = \Psi(\boldsymbol{\theta})\mathbf{w}_{k-1}^t + \mathbf{b}_{k-1}^t \tag{6.32a}$$

$$\mathbf{w}_k^o = \mathbf{H}\mathbf{w}_k^t + \mathbf{b}_k^o \tag{6.32b}$$

where the sequence of the noises $\{\mathbf{b}_k^t\}$ and $\{\mathbf{b}_k^o\}$ are as in the previous section Gaussian with mean zero and given (co)variances, that is, $\mathbf{b}_k^t \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}_k)$ and $\mathbf{b}_k^o \sim \mathcal{N}(\mathbf{0}, \mathbf{R}_k)$, and are mutually uncorrelated. The system (6.32) does not represent the most general form for problems of parameter estimation, since we are assuming that the equations are linear in the state variable. Another simplification in the system studied here is that the observation function is taken as known, with no parameters to be determined to describe it. Also, the noises error (co)variances are assumed to be completely known. Even with all these simplifications, the system above is sufficient to exemplify the main idea of the approach of parameter estimation based on the extended Kalman filter.

In system (6.32) the variable $\boldsymbol{\theta}$ represents an r–vector of constant, but unknown, coefficients that we intend to estimate. Notice from the beginning that the problem of parameter estimation is always nonlinear (expect in the case of additive unknown parameters — see Jazwinski [84], Section 8.4), making essential the use of nonlinear filter procedures. If we imagine that the parameters $\boldsymbol{\theta}$ are functions of time, the fact that they are in reality constant can be expressed as $\boldsymbol{\theta} = \boldsymbol{\theta}_k^t = \boldsymbol{\theta}_{k-1}^t$. This equality produces an extra equation that we can append to the system above, to augment the state vector, that is

$$\mathbf{u}_k^t \equiv \begin{pmatrix} \mathbf{w}_k^t \\ \boldsymbol{\theta}_k^t \end{pmatrix} \tag{6.33}$$

where $n + r$–vector $\mathbf{u}^t$ is now the re–defined state variable. Unfortunately, this procedure does not lead to anything (see Exercise 6.3), in terms of estimating $\boldsymbol{\theta}$.

To be able to actually estimate $\boldsymbol{\theta}$ through, say, the extended Kalman filter it is necessary to treat the vector of deterministic, constant and unknown parameters as if it were a random vector. Thus, we write the equation for the parameters to be estimated as

$$\boldsymbol{\theta}_k^t = \boldsymbol{\theta}_{k-1}^t + \boldsymbol{\epsilon}_k \tag{6.34}$$

where $\boldsymbol{\epsilon}_k$ is an r–random vector with assumed known statistics, $\boldsymbol{\epsilon}_k \sim \mathcal{N}(0, \mathbf{S}_k)$ — taken to be uncorrelated from the errors $\mathbf{b}_k^t$ and $\mathbf{b}_k^o$ — system (6.32) can be re–written in the form

$$\mathbf{u}_k^t = \mathbf{f}(\mathbf{u}_{k-1}^t) + \begin{pmatrix} \mathbf{b}_k^t \\ \boldsymbol{\epsilon}_k \end{pmatrix} \tag{6.35a}$$

$$\mathbf{w}_k^o = \begin{pmatrix} \mathbf{H} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{w}_k^t \\ \boldsymbol{\theta}_k^t \end{pmatrix} + \mathbf{b}_k^o \tag{6.35b}$$

where $\mathbf{f}(\mathbf{u}_{k-1}^t)$ is defined as

$$\mathbf{f}(\mathbf{u}_{k-1}^t) \equiv \begin{pmatrix} \Psi(\boldsymbol{\theta}_{k-1}^t) & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \mathbf{u}_{k-1}^t = \begin{pmatrix} \Psi(\boldsymbol{\theta}_{k-1}^t)\mathbf{w}_{k-1}^t \\ \boldsymbol{\theta}_{k-1}^t \end{pmatrix} \tag{6.36}$$

Let us assume that initially, at $t = t_0$, the estimates $\mathbf{w}_0^t$ and $\boldsymbol{\theta}_0^t$ are

$$\mathbf{u}_0^a \equiv \begin{pmatrix} \mathbf{w}_0^a \\ \boldsymbol{\theta}_0^a \end{pmatrix} = \begin{pmatrix} \mathcal{E}\{\mathbf{w}_0^t\} \\ \bar{\boldsymbol{\theta}}_0 \end{pmatrix} \tag{6.37}$$

with error (co)variance

$$\mathbf{P}_0^a = \begin{pmatrix} cov\{\mathbf{w}_0^t, \mathbf{w}_0^t\} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Theta}_0 \end{pmatrix} \tag{6.38}$$

Following the extended Kalman filter equations listed in Table 6.2, for the discrete–discrete case, we need to calculate the Jacobian of the modified dynamics in (6.35a). That is,

$$\begin{aligned} \mathcal{F}'(\mathbf{u}_k^a) &\equiv \left.\frac{\partial \mathbf{f}(\mathbf{u}_k^t)}{\partial [\mathbf{u}_k^t]^T}\right|_{\mathbf{u}_k^t = \mathbf{u}_k^a} \\ &= \begin{pmatrix} \left.\frac{\partial \Psi(\boldsymbol{\theta}_k^t)\mathbf{w}_k^t}{\partial [\mathbf{w}_k^t]^T}\right|_{\mathbf{u}_k^t = \mathbf{u}_k^a} & \left.\frac{\partial \Psi(\boldsymbol{\theta}_k^t)\mathbf{w}_k^t}{\partial [\boldsymbol{\theta}_k^t]^T}\right|_{\mathbf{u}_k^t = \mathbf{u}_k^a} \\ \left.\frac{\partial \boldsymbol{\theta}_k^t}{\partial [\mathbf{w}_k^t]^T}\right|_{\mathbf{u}_k^t = \mathbf{u}_k^a} & \left.\frac{\partial \boldsymbol{\theta}_k^t}{\partial [\boldsymbol{\theta}_k^t]^T}\right|_{\mathbf{u}_k^t = \mathbf{u}_k^a} \end{pmatrix} \\ &= \begin{pmatrix} \Psi(\boldsymbol{\theta}_k^a) & \left.\frac{\partial \Psi(\boldsymbol{\theta}_k^t)}{\partial [\boldsymbol{\theta}_k^t]^T}\right|_{\boldsymbol{\theta}_k^t = \boldsymbol{\theta}_k^a} \mathbf{w}_k^a \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \end{aligned} \tag{6.39}$$

Then, the forecast step of the extended Kalman filter becomes

$$\begin{pmatrix} \mathbf{w}_k^f \\ \boldsymbol{\theta}_k^f \end{pmatrix} = \begin{pmatrix} \Psi(\boldsymbol{\theta}_{k-1}^a)\mathbf{w}_{k-1}^a \\ \boldsymbol{\theta}_{k-1}^a \end{pmatrix} \tag{6.40a}$$

$$\begin{aligned} \mathbf{P}_k^f = &\begin{pmatrix} \Psi(\boldsymbol{\theta}_{k-1}^a) & \left.\frac{\partial \Psi(\boldsymbol{\theta}_k^t)}{\partial [\boldsymbol{\theta}_k^t]^T}\mathbf{w}_{k-1}^a\right|_{\boldsymbol{\theta}_k^t = \boldsymbol{\theta}_{k-1}^a} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \mathbf{P}_{k-1}^a \\ &\times \begin{pmatrix} \Psi(\boldsymbol{\theta}_{k-1}^a) & \left.\frac{\partial \Psi(\boldsymbol{\theta}_k^t)}{\partial [\boldsymbol{\theta}_k^t]^T}\mathbf{w}_{k-1}^a\right|_{\boldsymbol{\theta}_k^t = \boldsymbol{\theta}_{k-1}^a} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}^T \\ &+ \begin{pmatrix} \mathbf{Q}_{k-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_{k-1} \end{pmatrix} \end{aligned} \tag{6.40b}$$

and analysis step becomes

$$\begin{aligned} \mathbf{K}_k = &\mathbf{P}_k^f \begin{pmatrix} \mathbf{H} & \mathbf{0} \end{pmatrix}^T \\ &\left[\begin{pmatrix} \mathbf{H} & \mathbf{0} \end{pmatrix} \mathbf{P}_k^f \begin{pmatrix} \mathbf{H} & \mathbf{0} \end{pmatrix}^T + \mathbf{R}_k \right]^{-1} \end{aligned} \tag{6.41a}$$

$$\mathbf{P}_k^a = \left[\mathbf{I} - \mathbf{K}_k \begin{pmatrix} \mathbf{H} & \mathbf{0} \end{pmatrix}\right] \mathbf{P}_k^f \tag{6.41b}$$

$$\begin{pmatrix} \mathbf{w}_k^a \\ \boldsymbol{\theta}_k^a \end{pmatrix} = \begin{pmatrix} \mathbf{w}_k^f \\ \boldsymbol{\theta}_k^f \end{pmatrix} + \mathbf{K}_k \left[\mathbf{w}_k^o - \mathbf{H}\mathbf{w}_k^f\right] \tag{6.41c}$$

A few comments are pertinent:

- It is interesting to mention that this type of application of the extended Kalman filter converts the filter into an *adaptive* filter. This means that, at each time step the filter described above improves upon the knowledge of the parameter vector $\boldsymbol{\theta}$. In other words, the system "learns" about itself.

- The technique used here to construct the extended Kalman filter for the parameter estimation problem, that is, that of incorporating the parameter vector into the state vector, is known as *state augmentation* technique. This nomenclature is relatively evident, since in the case studied above, the augmented state $\mathbf{u}_k^t$ contains the system state vector $\mathbf{w}_k^t$ as well as the vector of parameters $\boldsymbol{\theta}_k^t$. State augmentation is a very common and powerful technique in estimation theory. Examples in which this technique is used are in problems of smoothing (e.g., Anderson & Moore [1]); colored noises, that is, noises that are not white (Anderson & Moore [1]); more general parameter estimation problems, as that of estimating parameters related to the noise statistics. Application of these ideas to atmospheric and oceanic data assimilation are those of Hao [71] and Hao & Ghil [72].

- The problem of parameter estimation belongs to a wider class of problems more commonly referred to as *system identification* (e.g., Sage & Melsa [120]). Many alternative methods, which do not use concepts related to the Kalman filter can be found in the literature; some identification methods are based on statistics, but not all (see comments in Gelb [60], pp. 350).

Exercises

1. Following the procedure indicated in Section 6.2, derive equation (6.5) for the forecast (prediction) error covariance evolution.

2. Following the procedure indicated in Section 6.2, derive expression (6.28) for the analysis error covariancia.

3. Consider the following scalar system:

$$\begin{aligned} w_k^t &= \theta w_{k-1}^t \\ w_k^o &= w^t + b^o \end{aligned}$$

where $b_k^o \sim \mathcal{N}(0, \sigma^2)$, and θ is an unknown parameter, with an initial estimate of $\hat{\theta}_0$. Show that if the parameter θ is modeled as a deterministic quantity the state augmentation technique, together with the Kalman filter, give no further information

on the unknown parameter θ, as the filter gets iterated in time. In other words, show that in this case, the extended Kalman filter can be partitioned as

$$\mathbf{K}_k = \begin{pmatrix} g_k \\ 0 \end{pmatrix}$$

and explain why this partition implies nothing is learned about the parameter θ, by the filtering procedure. This is an example of a problem known as identifiability, i.e., θ is non–identifiable.

4. *Computer Assignment.* Consider again the Lorenz (1960) [1] model of Exercise 3.7. We want to implement an assimilation system based on the extended Kalman filter, and a simple modification of it, for this model. Because this is just a simulation, we have to "define the true model". We take for that the exact same model, that is,

$$\frac{d\mathbf{w}^t}{dt} = \mathbf{f}(\mathbf{w}^t)$$

where $\mathbf{f}$ is the Lorenz model of Exercise 3.7, but we choose a different initial condition that is taken from a realization of $\mathbf{w}_0^t = \bar{\mathbf{w}}_0 + \mathbf{b}_0^t$, where

$$\bar{\mathbf{w}}_0 = \begin{pmatrix} 0.12 \\ 0.24 \\ 0.10 \end{pmatrix}$$

and $\mathbf{b}_0^t \sim \mathcal{N}(\mathbf{0}, \mathbf{P}_0^a)$, with $\mathbf{P}_0^a = (\sigma_0^a)^2\mathbf{I}$. Moreover, we make the perfect model assumption by saying that $\mathbf{b}_k^t = \mathbf{0}$, for all $k = 1, 2, \ldots$. Consequently, $\mathbf{Q}_k = 0$, for all $k = 1, 2, \ldots$.

Let us choose the initial standard deviation error $\sigma_0^a = 0.1$, which is ten times larger than the value we used in our Monte Carlo experiments before. To facilitate your evaluation of different results to be obtained below, fix a seed, in the very beginning of the code, for the random number generator of Matlab.

All experiments that follow are to be performed in the time interval from $t_0 = 0$ to $t_f = 250$, and time step $\Delta t = 0.5$, of Exercise 3.7. With the choice of initial error given above:

True state and approximate mean state evolution: Plot the evolution, of all three variables, of the true state and those produced by a prediction model based on the mean equation, that is,

$$\frac{d\boldsymbol{\mu}}{dt} = \mathbf{f}(\boldsymbol{\mu})$$

where $\mathbf{f}$ is given by the Lorenz model in Exercise 3.7, for all three variables. Take for the initial mean state the value $\boldsymbol{\mu}(0) = \bar{\mathbf{w}}_0$, given above. Does the "predicted" state have any resemblance with the true state?

To construct an assimilation system we need an observation process, which for this problem is taken to be simply

$$\mathbf{w}_k^o = \mathbf{w}_k^t + \mathbf{b}_k^o$$

[1] Lorenz, E.N., 1960: Maximum simplification of dynamical equations. *Tellus,* **12**, 243–254.

for $k = 1, 2, \ldots$. That is, the observation process is linear, with all three variables of the model being observed under noise $\mathbf{b}_k^o \sim \mathcal{N}(\mathbf{0}, \mathbf{R})$, with $\mathbf{R} = (\sigma^o)^2\mathbf{I}$.

The extended Kalman filter: In all cases below plot the true state evolution against the estimate evolution. Also, separately, plot the evolution of the variances for all three variables.

(a) *Low frequency update.* Taking the observation noise level to be $\sigma^o = 0.2$, and the observation interval to be $\Delta t_{obs} = 50$ time units, insert the appropriate equations in your Matlab code to perform the analysis step of the extended Kalman filter. Notice that, between two consecutive observations your program should evolve the mean and (co)variance just as it did in Exercise 3.7. Observe also, that in the extended Kalman filter the mean equation does not include the bias correction term involving the Hessian of the dynamical model. Plot the evolution of the mean on the same frame as that for the true state, for all three variables of the model. Does assimilation improve the prediction you had in the previous item? What do the variance plots tell you?

(b) *More frequent observations.* Reduce the assimilation (observation) interval in the experiment of the previous item to half of what it was. How do the estimates chance? What happens if the observation interval is reduces further to $\Delta t_{obs} = 10$ time units?

(c) *More accurate observations.* The observations considered above are quite lousy — the observation error level is about 100% of the value of the amplitude of the variables of the system — a more sensible observation error level would be considerably smaller. In this way, taking $\sigma^o = 0.05$, repeat the filtering experiment of item (a). Comment on how this changes the estimate, and what the variance plots tell you.

The bias correction term: We saw in the experiments in Exercise 3.7 that the bias correction term can have a considerable influence on the evolution of the mean and (co)variance. In particular, its presence may allow for error variance saturation, avoiding indefinite growth of error. Here, we want to examine the effect of this term in the context of assimilation (filtering). The inclusion of the bias correction term provides a second order filter, which is in principle more accurate than the extended Kalman filter. Repeat items (a) and (b) above when the bias correction term is included in the equation for the evolution of the mean. Compare the results with those found previously in (a) and (b).

Now that you have constructed a small data assimilation system, you might what to change your dynamical model to be a more interesting one, such as the Lorenz (1963)[2] chaotic model. You can use as a guide for some experiments the work of Miller et al. (1994)[3], where the extended Kalman filter was first applied to that model. Have fun.

[2]Lorenz, E.N., 1963: Deterministic non–periodic flow. *J. Atmos. Sci.,* **20**, 130–141.

[3]Miller, R.N., M. Ghil, & F. Gauthiez, 1994: Advanced data assimilation in strongly nonlinear dynamical systems. *J. Atmos. Sci.,* **51**, 1037–1056.