5

Time-dependent methods – 2

This brief chapter includes a number of extensions of the material in Chapter 4, as well as providing introductions to a number of more specialized topics that would be of interest to anyone attempting to use the methods for large-scale practical problems. References are given for fuller coverage.

5.1 Monte Carlo/ensemble methods

5.1.1 Ensemble methods and particle filters

When a model is non-linear, one of the fundamental computational steps of the Kalman filter (and any related calculation such as a smoother) is no longer possible. Consider a Kalman filter problem in which the initial conditions, $\bar{\mathbf{x}}(0)$, contain errors characterized by the covariance matrix, $\mathbf{P}(0)$, and the zero-mean disturbance or control, $\mathbf{u}(0)$, is unknown with covariance, $\mathbf{Q}(0)$. The state forecast step, Eq. (4.50) proceeds as before. Computation of the forecast error covariance, Eq. (4.51), however, which sums the error owing to the initial conditions and that of the unknown controls, $\mathbf{A}(0)\mathbf{P}(0)\mathbf{A}(0)^{\mathrm{T}} + \boldsymbol{\Gamma}\mathbf{Q}\boldsymbol{\Gamma}^{\mathrm{T}}$, depends directly upon the linearity assumption, and can no longer be carried out rigorously. For weak non-linearities, the extended or linearized Kalman filters and associated smoothers may be adequate. But when linearizing assumptions fail, some other method must be used. A commonly discussed example of a non-linear (but scalar) model is

$$x_t = \frac{1}{2}x_{t-1} + \frac{25x_{t-1}}{1 + x_{t-1}^2} + 8\cos 1.2t + \varepsilon_t,$$
$$y_t = \frac{x_t^2}{20} + \eta_t,$$

which is non-linear in both the evolution equation and in the measurement; ε_t, η_t are Gaussian white noise processes.[1] Extended Kalman filters work badly for this low-dimensional example.

The basic idea behind so-called ensemble or Monte Carlo methods is in some ways even simpler than the use of Eq. (4.51). (In the signal-processing literature, closely related approaches are usually called "sequential Monte Carlo methods," or "particle filtering."[2]) One directly simulates a sufficiently large number of forecasts, $\tilde{\mathbf{x}}^{(i)}(t, -)$, all having the same statistical properties; then $\mathbf{P}(t, -)$ can be estimated by brute force computation from the many simulations. If a sufficiently large ensemble can be generated, one can contemplate estimating not just the second moments, but calculating the empirical frequency function for the forecast step.

To see how this approach might work, generate an ensemble of initial conditions, $\tilde{\mathbf{X}}(0)$, where each column of the $N \times L$, $L < N$ matrix corresponds to a possible initial condition consistent with both $\tilde{\mathbf{x}}(0)$ and $\mathbf{P}(0)$. Form a similar ensemble for $\tilde{\mathbf{u}}(0)$ based upon $\langle \mathbf{u}(0) \rangle = 0$, and $\mathbf{Q}(0)$. (We discuss generation of such ensembles below.) Then one can run the model on each column of $\tilde{\mathbf{X}}(0)$, with a disturbance from the corresponding column of $\tilde{\mathbf{U}}(0)$, and compute the ensemble of forecasts $\tilde{\mathbf{X}}(1, -)$. Assuming that the true mean of $\mathbf{x}(1)$ is zero, estimate

$$\tilde{\mathbf{P}}(1, -) = \frac{1}{L}\tilde{\mathbf{X}}(1, -)\tilde{\mathbf{X}}(1, -)^{\mathrm{T}} = \frac{1}{L}\sum_{j=1}^{L} \tilde{\mathbf{x}}_j(1, -)\tilde{\mathbf{x}}_j(1, -)^{\mathrm{T}}, \tag{5.1}$$

where $\tilde{\mathbf{x}}_j(1, -)$ is column j of $\tilde{\mathbf{X}}(t, -)$, as an estimate of $\mathbf{P}(1, -)$. Note that if the mean is computed from the columns of $\tilde{\mathbf{X}}$, and subtracted from the estimate, the factor in front becomes $1/(L - 1)$. With $\tilde{\mathbf{P}}(1, -)$ known, the filter averaging step (4.52) can be carried out, although if the probability densities of the model and data errors are different, the average may have little meaning. Because averaging is a linear operation, the conventional filter error covariance calculation (4.54) is still appropriate, and one can continue in this fashion through the filter loop. In essence, this approach characterizes the so-called ensemble Kalman filter method. The main issue here concerns the reliability of the estimates for small ensemble sizes.[3] Because of its structure, if L is less than N, the maximum rank of $\tilde{\mathbf{P}}(1, -)$ is $K = L < N$, and the matrix will be singular. Singularity implies that some structures (those in the nullspace of $\tilde{\mathbf{P}}(1, -)$) are impossible in the initial conditions – a potentially troublesome outcome.

In principle, one can use the ensemble members to produce estimates of the complete probability densities of $\tilde{\mathbf{x}}$, $\tilde{\mathbf{u}}$, no matter how non-linear the model – leading to the use of maximum likelihood methods. These are computationally more demanding, however. Even small ensembles provide at least a qualitative indication

of where maximum uncertainty is likely to lie, but their use should not stretch beyond their actual limited information content.

How does one generate ensemble members with zero mean and given spatial covariance, $\mathbf{P}(0)$? Let

$$\mathbf{P}(0) = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{\mathrm{T}},$$

and suppose $\alpha_i^{(p)}$ is white noise from a pseudo-random number generator such that $\langle \alpha_i^{(p)} \rangle = 0$, $\langle \alpha_i^{(p)} a_j^{(p)} \rangle = \delta_{ij}$, where p is the ensemble member label. Form

$$\tilde{\mathbf{x}}_p(0) = \sum_{j=1}^{N} \sqrt{\lambda}_j \alpha_j^{(p)} \mathbf{v}_j.$$

Then it follows that

$$\langle \tilde{\mathbf{x}}^{(p)}(0) \rangle = 0,$$

$$\langle (\tilde{\mathbf{x}}_p(0) - \tilde{\mathbf{x}}(0))(\tilde{\mathbf{x}}_p(0) - \tilde{\mathbf{x}}(0))^{\mathrm{T}} \rangle = \left\langle \left(\sum_{j=1}^{N} \sqrt{\lambda}_j \alpha_j^{(p)} \mathbf{v}_j \right) \left(\sum_{n=1}^{N} \sqrt{\lambda_n} \alpha_n^{(p)} \mathbf{v}_n \right)^{\mathrm{T}} \right\rangle$$

$$= \sum_{j=1}^{N} \lambda_j \langle \alpha_j^{(p)\,2} \rangle \mathbf{v}_j \mathbf{v}_j^{\mathrm{T}} = \mathbf{P}(0),$$

as required. It is readily confirmed too, that the ensemble members are uncorrelated with each other.

The members of the ensemble of initial conditions can have highly non-Gaussian probability densities. One would then select the $\alpha_j^{(p)}$ from populations with whatever is the appropriate probability density.[4] More generally, the initial condition disturbances may have specific structures related to the dynamics. Some of those structures may give rise to particularly rapidly growing disturbances, and which if excited can give an ensemble spread much larger than that obtained from purely random components. A lot of effort in weather forecasting, in particular, has gone into generating small ensembles that are representative of the spread of the true probability density.[5] Unknown model parameters can include initial conditions, including for example, mixing parameterizations, boundary conditions, source/sink components, etc. Ensembles can be generated by calculating solutions from random perturbations to any and all of these problem elements simultaneously.

Example *Let the initial estimate for the mass–spring oscillator of the Example on p. 183, be* $\tilde{\mathbf{x}}(0) = [1, 1]^{\mathrm{T}}$, *and have error covariance*

$$\mathbf{P}(0) = \begin{Bmatrix} 1 & 0 \\ 0 & 1 \end{Bmatrix}.$$

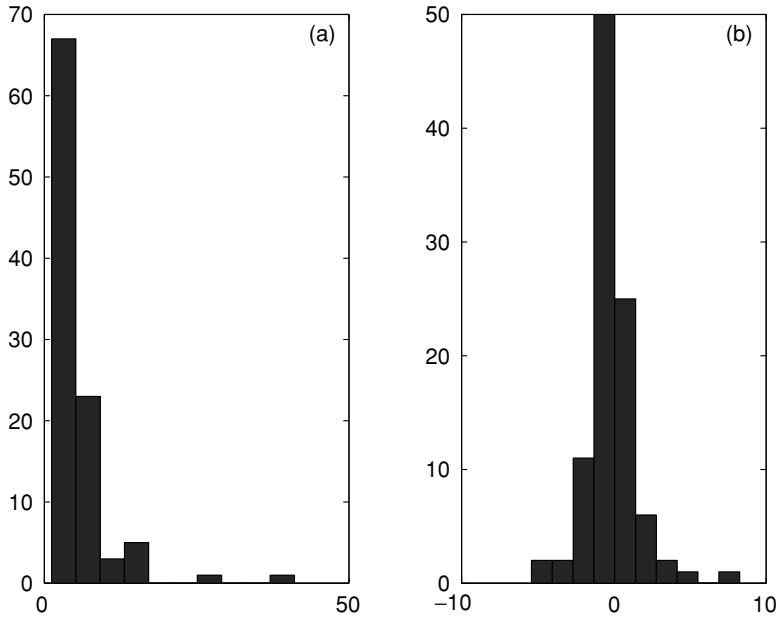

Figure 5.1 (a) Empirical histogram of an ensemble of 100 values of $\tilde{x}_1(0)$ obtained from a log-normal distribution with parameters (1, 1). A similar ensemble of values was generated for $x_2(0)$, with no correlation between the two. The random variables are regarded as different realizations of the noise occurring in the true value $\mathbf{x}(0) = [1, 1]^{\mathrm{T}}$. (b) Histogram of 100 realizations of $x_1(t = 500)$ from the mass–spring oscillator ($k = 0.1$, $\Delta t = 1$, $r = 0.01$). Note the tendency for the frequency function to tend towards Gaussian.

It is thought, however, that the errors follow a log-normal distribution,

$$p(\xi) = \frac{1}{\sqrt{2\pi}\xi} \exp(-(\ln \xi - 1)^2/2). \tag{5.2}$$

An ensemble of initial conditions of the form $\tilde{\mathbf{x}}(0) = [1, 1]^{\mathrm{T}} + \boldsymbol{\xi}$ *was generated, producing a frequency function (histogram) of values for* $\tilde{x}_1(0)$ *as shown in Fig. 5.1. After 500 time steps (with* $k = 0.1, r = 0.01, \Delta t = 1$) $\tilde{x}_1(500)$ *tends to become Gaussian in this linear system, and it would be reasonable to calculate the mean position as* $\overline{\tilde{x}_1(500)}$ *where the overbar indicates an average of the ensemble, and the error of the mean position is computed simply from its standard deviation in the ensemble. The latter can be used in the Kalman averaging step. But in a highly non-Gaussian distribution, as seen in the left panel of Fig. 5.1, the sample mean and variance may differ greatly from the true mean and variance owing to the presence of a few strong outliers. (One would be strongly advised to work with the logarithm of* $\tilde{x}_1(0)$;[6] *such a transformation would not be possible with* $\tilde{x}_1(500)$ *because it can be negative.)*

Calculation of probability densities, or the defining low moments of the probability densities for filter/smoother solutions can also be approached by solving equations for the evolution of the densities or moments. Dynamical evolution equations can be used to write an explicit equation (the so-called Fokker–Planck, or Kolmogorov equation in the physics and mathematics literature, respectively) for the evolution of the state probability density.[7] Because the solution of such equations in high dimensions is forbidding, one can alternatively seek approximate equations for the evolution of the low moments.

This subject is a large and sophisticated one; a growing literature describes applications at various levels of approximation in oceanography and meteorology. But we must leave it to the references to deal with it further.[8]

5.2 Numerical engineering: the search for practicality

Estimation theory is comparatively straightforward in its goals, and in the methods of solution. When it comes to real problems, particularly those involving fluids, the main issues tend to be much less the principle of what one wants to do (it is usually reasonably clear), and more the problems of practicality. Even linear three-dimensional fluid models, particularly those arising in the geophysical world, readily overwhelm the largest available computers and storage devices. Investigators exploiting the special structure of the simultaneous equations represented by time-evolving models may still have serious computational difficulties. The major issues are then primarily those of "numerical engineering" – finding approximate practical methods adequate for a particular goal, while keeping the underlying theory in mind as a guideline. Engineering involves all aspects of the problem, including the forward model, the algorithms for doing minimization, representation and computation of weight matrices, finding adequate estimates of model, and overall system errors. Because of the diversity of the problems that arise, only some very general description of various applications and remedies can be described here.

5.2.1 Meteorological assimilation

"Data assimilation" is a term widely used in numerical weather prediction (NWP) to describe the process of combining a forecast with current observations for the primary purpose of updating a dynamical model – usually in preparation for another forecast. In this book, we use the term "state estimation" for the more general problem of forming model/data combinations, and reserve "assimilation" for the specific meteorological application. For fluid models, forecasting is probably more highly developed in meteorology than in any other field. Astronomers forecasting planetary or cometary positions have a longer history, and ballistic engineers are

greatly experienced with a range of trajectory and impact prediction problems. But the meteorological problem is of much greater dimension than any of these, and the economic stakes are so high, that many person-years have been devoted to making and improving weather forecasts. The field is thus a highly developed one and a correspondingly large literature on meteorological assimilation exists and is worth examining.[9] The specialized terminology used by meteorologists can, however, be a major problem. For example, what we are calling the method of Lagrange multipliers (or adjoint method) is known in meteorology as 4DVAR, to imply four-dimensional models and variational techniques. As has been seen, however, the methodology operates in arbitrary dimensions and as used in practice, is least-squares rather than variational in derivation.

Much data assimilation involves simplified forms of objective mapping, in which the model dynamics are used in a primitive fashion to help choose covariances in both time and space for interpolation as in Chapter 2.[10] The formal uncertainties of the forecast are not usually computed – the forecaster learns empirically, and very quickly, how accurate his forecast is. If something works, then one keeps on doing it; if it doesn't work, one changes it. Because of the short timescale, feedback from the public, the military, farmers, the aviation industry, etc., is fast and vehement. Theory often takes a backseat to practical experience. It is important to note that, despite the dense fog of jargon that has come to surround meteorological practice, the methods in actual use remain, almost universally, attempts at the approximate least-squares fitting of a time-evolving atmospheric model to the oncoming observations. The primary goal is forecasting, rather than smoothing. Ensemble methods are used to obtain semi-quantitative understanding of the uncertainty of the forecast. They are semi-quantitative primarily because the ensembles tend to be small in size compared to the model dimension, although useful methods exist for determining the most uncertain elements of short-term forecasts.[11]

5.2.2 Nudging and objective mapping

A number of meteorological schemes can be understood by referring back to the Kalman filter averaging step,

$$\tilde{\mathbf{x}}(t) = \tilde{\mathbf{x}}(t, -) + \mathbf{K}(t)[\mathbf{y}(t) - \mathbf{E}\tilde{\mathbf{x}}(t, -)]. \tag{5.3}$$

This equation has the form of a predictor–corrector – the dynamical forecast of $\tilde{\mathbf{x}}(t, -)$ is compared to the observations and corrected on the basis of the discrepancies. Some assimilation schemes represent guesses for $\mathbf{K}$ rather than the computation of the optimum choice, which we know – for a linear model – is given by the

Kalman gain, replacing (5.3) with

$$\tilde{\mathbf{x}}(t) = \tilde{\mathbf{x}}(t, -) + \mathbf{K}_m[\mathbf{y}(t) - \mathbf{E}\tilde{\mathbf{x}}(t, -)], \tag{5.4}$$

where $\mathbf{K}_m$ is a modified gain matrix. Thus, in "nudging," $\mathbf{K}_m$ is diagonal or nearly so, with elements that are weights that the forecaster assigns to the individual observations.[12] To the extent that the measurements have uncorrelated noise, as might be true of pointwise meteorological instruments like anemometers, and the forecast error is also nearly spatially uncorrelated, pushing the model values pointwise to the data may be very effective. If, in (5.4), the observations $\mathbf{y}(t)$ are direct measurements of state vector elements (e.g., if the state vector includes the density and $\mathbf{y}(t)$ represents observed densities), then $\mathbf{E}(t)$ is very simple – but only if the measurement point coincides with one of the model grid points. If, as is common, the measurements occur between model grid points, $\mathbf{E}$ is an interpolation operator from the model grid to the data location. Usually, there are many more model grid points than data points, and this direction for the interpolation is the most reasonable and accurate. With more data points than model grid points, one might better interchange the direction of the interpolation. Formally, this interchange is readily accomplished by rewriting (5.3) as

$$\tilde{\mathbf{x}}(t) = \tilde{\mathbf{x}}(t, -) + \mathbf{K}_m\mathbf{E}[\mathbf{E}^+\mathbf{y}(t) - \mathbf{x}(t, -)], \tag{5.5}$$

where $\mathbf{E}^+$ is any right inverse of $\mathbf{E}$ in the sense of Chapter 2, for example, the Gauss–Markov interpolator or some plausible approximation to it.

There are potential pitfalls of nudging, however. If the data have spatially correlated errors, as is true of many real observation systems, then the model is being driven toward spatial structures that are erroneous. More generally, the expected great variation in time and space of the relative errors of model forecast and observations cannot be accounted for with a fixed diagonal gain matrix. A great burden is placed upon the skills of the investigator who must choose the weights. Finally, one can calculate the uncertainty of the weighted average (5.4), using this suboptimal gain, but it requires that one specify the true covariances. As noted, however, in NWP formal uncertainty estimates are not of much interest. User feedback is, however, rarely available when the goal is understanding – the estimation problem – rather than forecasting the system for public consumption. When forecasts are made in many contexts, e.g., for decadal climate change, the timescale is often so long as to preclude direct test of the result.

As with the full Kalman filter, in the "analysis step," where the model forecast is averaged with the observations, there is a jump in the state vector as the model is pulled toward the observations. Because the goal is usually forecasting, this state vector discontinuity is not usually of any concern, except to someone instead interested in understanding the fluid physics.

Another more flexible, approximate form of time-dependent estimation can also be understood in terms of the Kalman filter equations. In the filter update equation (4.52), all elements of the state vector are modified to some degree, given any difference between the measurements and the model-prediction of those measurements. The uncertainty of the statevector is *always* modified whenever data become available, even if the model should perfectly predict the observations. As time evolves, information from measurements in one part of the model domain is distributed by the model dynamics over the entire domain, leading to correlations in the uncertainties of all the elements.

One might suppose that some models propagate information in such a way that the error correlations diminish rapidly with increasing spatial and temporal separation. Supposing this to be true (and one must be aware that fluid models are capable of propagating information, be it accurate or erroneous, over long distances and times), static approximations can be found in which the problem is reduced back to the objective mapping methods employed in Chapter 2. The model is used to make an estimate of the field at time t, $\tilde{\mathbf{x}}(t,-)$, and one then finds the prediction error $\Delta\mathbf{y}(t) = \mathbf{y}(t) - \mathbf{E}\tilde{\mathbf{x}}(t,-)$. A best estimate of $\Delta\mathbf{x}(t)$ is sought based upon the covariances of $\Delta\mathbf{y}(t)$, $\Delta\mathbf{x}(t)$, etc. – that is, objective mapping – and the improved estimate is

$$\tilde{\mathbf{x}}(t) = \tilde{\mathbf{x}}(t,-) + \Delta\tilde{\mathbf{x}}(t) = \tilde{\mathbf{x}}(t,-) + \mathbf{R}_{xx}\mathbf{E}^{\mathrm{T}}(\mathbf{E}\mathbf{R}_{xx}\mathbf{E}^{\mathrm{T}} + \mathbf{R}_{nn})^{-1}\Delta\mathbf{y}\,, \tag{5.6}$$

which has the form of a Kalman filter update, but in which the state uncertainty matrix, $\mathbf{P}$, is replaced in the gain matrix, $\mathbf{K}$, by $\mathbf{R}_{xx}$ representing the prior covariance of $\Delta\mathbf{x}$. $\mathbf{R}_{xx}$ is fixed, with no dynamical evolution of the gain matrix permitted. Viewed as a generalization of nudging, this approach permits one to specify spatial structure in the noise covariance through choice of a non-diagonal $\mathbf{R}_{nn}$. The weighting of the $\Delta\mathbf{y}$ and the modification for $\tilde{\mathbf{x}}$ is potentially more complex than in pure nudging.

The major issues are the specification of $\mathbf{R}_{xx}$, $\mathbf{R}_{nn}$. Most attempts to use these methods have been simulations by modelers who were content to ignore the problem of determining $\mathbf{R}_{nn}$ or to assume that the noise was purely white. In principle, estimates of $\mathbf{R}_{xx}$ can be found either from observations or from the model itself.

Methods that permit data to be employed from finite-time durations, weighting them inversely with their deviation from some nominal central time, are localized approximations to smoothing algorithms of the Wiener type. Many variations on these methods are possible, including the replacement of $\mathbf{R}_{xx}$ by its eigenvectors (the singular vectors or EOFs), which again can be computed either from the model or from data. Improvements could be made by comparison of the covariance matrices used against the estimates emerging from the calculations of $\tilde{\mathbf{x}}(t)$, $\tilde{\mathbf{n}}(t)$.

All practical linearized assimilation methods are a weighted average of a model estimate of the fluid state with one inferred from the observations. If the model and the observations are physically inconsistent, the forced combination will be impossible to interpret. Thus, the first step in any assimilation procedure has to be to demonstrate that model physics and data represent the same fluid – with disagreement being within the error bounds of both. Following this confirmation of physical consistency, one recognizes that the weighted average of model and data will be useful only if the weights make sense – chosen to at least well-approximate the relative uncertainties of these two. Otherwise, the result of the combination is an average of "apples and oranges."

5.2.3 Approximate filter/smoother methods

This book has been primarily devoted to the principles underlying various state estimation methods, rather than to addressing practical issues of implementation. A few methods were introduced to reduce computation (Lagrange multipliers, and ensemble methods), avoiding the calculation of the covariance matrices using the model. Lagrange multiplier methods are attractive because they do not demand the covariance matrices; but their main weakness is that they therefore do not provide them.

Unsurprisingly, numerous approaches have attempted to approximate the full results of the filter/smoother algorithms, both to reduce the burden of the state estimates themselves and of the corresponding error covariances. We examine some examples of such approaches.[13]

Steady-state approximation

Consider, as an example, the Kalman filter, Eqs. (4.50)–(4.54) of Chapter 4. The error covariances, $\mathbf{P}(t, -)$, $\mathbf{P}(t)$ are propagated as

$$\mathbf{P}(t, -) = \mathbf{A}(t-1)\mathbf{P}(t-1)\mathbf{A}(t-1)^{\mathrm{T}} + \mathbf{\Gamma}\mathbf{Q}(t-1)\mathbf{\Gamma}^{\mathrm{T}}, \tag{5.7}$$

$$\mathbf{P}(t) = \mathbf{P}(t, -) - \mathbf{P}(t, -)\mathbf{E}(t)^{\mathrm{T}}[\mathbf{E}(t)\mathbf{P}(t, -)\mathbf{E}(t)^{\mathrm{T}} + \mathbf{R}(t)]^{-1}\mathbf{E}(t)\mathbf{P}(t, -), \tag{5.8}$$

and do not involve the actual data. These equations can be simply time-stepped from $\mathbf{P}(0)$ to any time t, assuming the availability of $\mathbf{R}(t)$, $\mathbf{E}(t)$ and $\mathbf{P}(0)$. Knowledge of $\mathbf{P}(t)$ then permits the finding of $\mathbf{K}(t)$, and both are determined before any observations actually exist.

Let the model and data stream be time independent, $\mathbf{A}(t) = \mathbf{A}$, $\mathbf{E}(t) = \mathbf{E}$, $\mathbf{Q}(t) = \mathbf{Q}$, $\mathbf{R}(t) = \mathbf{R}$. Substituting for $\mathbf{P}(t, -)$, one has the matrix Riccati

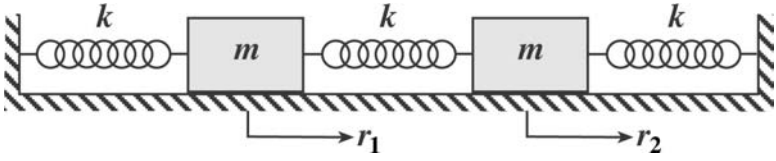

Figure 5.2 Coupled mass-spring oscillator. Rest positions of the two masses define the coordinates $r_{1,2}$. (After McCuskey, 1959.)

equation,

$$\begin{aligned}\mathbf{P}(t) = {} & \mathbf{A}\mathbf{P}(t-1)\mathbf{A}^{\mathrm{T}} + \mathbf{\Gamma}\mathbf{Q}\mathbf{\Gamma}^{\mathrm{T}} \\ & - [\mathbf{A}\mathbf{P}(t-1)\mathbf{A}^{\mathrm{T}} + \mathbf{\Gamma}\mathbf{Q}\mathbf{\Gamma}^{\mathrm{T}}]\mathbf{E}^{\mathrm{T}}\{\mathbf{E}[\mathbf{A}\mathbf{P}(t-1)\mathbf{A}^{\mathrm{T}} + \mathbf{\Gamma}\mathbf{Q}\mathbf{\Gamma}^{\mathrm{T}}]\mathbf{E}^{\mathrm{T}} + \mathbf{R}\}^{-1} \\ & \times \mathbf{E}[\mathbf{A}\mathbf{P}(t-1)\mathbf{A}^{\mathrm{T}} + \mathbf{\Gamma}\mathbf{Q}\mathbf{\Gamma}^{\mathrm{T}}],\ t = 0, 1, \ldots .\end{aligned} \tag{5.9}$$

Suppose the difference equation (5.9) approaches a steady state. That is, as $t \to \infty$, $\mathbf{P}(t) = \mathbf{P}(t-1) \equiv \mathbf{P}_\infty$. Then it follows from Eq. (4.53) that $\mathbf{K}(t) = \mathbf{K}_\infty$ also becomes steady. Once $\mathbf{P}$ and $\mathbf{K}$ cease to change, the computational load of the filter is much reduced: the model must be run only once at each time-step. This reduction in load leads one to understand under which circumstances Eq. (5.9) will asymptote to a steady state, and, when it does, to find methods for determining that state. With $\mathbf{K}_\infty$ known, one can, if one chooses, use it in place of $\mathbf{K}(t)$, *even during the period when the steady state is invalid*. To the extent that the system "forgets" its initial conditions, experience suggests that eventually the estimated state will converge to the correct one, even though the initial transient is not properly computed. A steady-Kalman filter is a "Wiener filter"; they are usually applied by fast convolution methods (which we omit).[14] Similar considerations apply to the problem of obtaining steady-state solutions to the evolution equation for the RTS smoother (Wiener smoother); further discussion can be found in the references.

Example *Consider two masses coupled to each other and to the boundaries as indicated in Fig. 5.2. A governing set of differential equations for the position, r_i, of each oscillator is readily shown to be*

$$\mathbf{M}\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} + \mathbf{D}\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} + \mathbf{L}\mathbf{r} = \mathbf{f}. \tag{5.10}$$

Here, $\mathbf{M}, \mathbf{D}, \mathbf{L}$ are matrices, $\mathbf{r}(t) = [r_1(t), r_2(t)]^{\mathrm{T}}$ is the non-equilibrium displacement of the masses, and $\mathbf{f}$ is the forcing vector. To generate the simplest case, take $\mathbf{M} = m\mathbf{I}_2$, so that the masses are identical; $\mathbf{D} = \varepsilon\mathbf{I}_2$, so that the dissipation is of ordinary Rayleigh type, and that

$$\mathbf{L} = \begin{Bmatrix} 2k & -k \\ -k & 2k \end{Bmatrix}$$

couples the masses through the connecting springs. Using a one-sided discretization of Eq. (5.10), a canonical state space approximation is

$$\begin{aligned}
\mathbf{x}(n+1) &= \mathbf{A}\mathbf{x}(n) + \mathbf{f}_d(n), \\
\mathbf{A} &= \begin{Bmatrix} 2\mathbf{I}_2 - \mathbf{L}(\Delta t)^2/m & (-1+\varepsilon\Delta t)\mathbf{I}_2 \\ \mathbf{I}_2 & \mathbf{0} \end{Bmatrix}, \\
\mathbf{x}(n) &= [\, r_1(n)\; r_2(n)\; r_1(n-1)\; r_2(n-1)\,]^{\mathrm{T}}, \\
\mathbf{f}_d(n) &= (\Delta t)^2 [\, \mathbf{f}(n)^{\mathrm{T}} \quad \mathbf{0}\,]^{\mathrm{T}}.
\end{aligned}$$

*(**A** includes block sub-matrices.) Taking $k = 1$, $m = 1$, $\varepsilon = 0.01$, $\Delta t = 0.25$, and f to be a unit variance zero mean forcing of r_1 alone (no forcing applied to r_2), a realization of $r_1(t), r_2(t)$ is shown in Fig. 5.3. Now assume that $\mathbf{E} = [\,1\;0\;0\;0\,]$ so that each time step, only $x_1(n)$, that is the position r_1, is measured. Assume $\mathbf{P}(0) = \mathrm{diag}(\,1\;1\;1\;1\,)$, $\mathbf{R} = \mathrm{diag}\,([1, 0])$, and $\mathbf{Q} = \mathbf{I}_4$. Then time-stepping Eq. (5.9) leads to the results for the diagonal elements of $\mathbf{P}(n)$ as depicted in Fig. 5.3. Both P_{11}, P_{12} (and the off-diagonal elements as well) reach steady-state values before $t = n\Delta t = 10$. At that time, $\mathbf{K}(t)$ has become a constant, and one can cease updating either it or the $\mathbf{P}(t)$. ($\mathbf{P}(t, -)$ would also have reached a steady state.)*

How might one find the steady state of Eq. (5.9) – if it exists? Several methods are known. One of them has been used in the above example: time-step the equation until it asymptotes. Other algorithms exist, including a remarkable one called "doubling." In this algorithm, one time steps the equation from $t = 0$, $\mathbf{P}(0)$, to obtain $\mathbf{P}(1\Delta t)$. One then doubles the time step to compute $\mathbf{P}(3\Delta t)$, doubles again for $\mathbf{P}(6\Delta t)$, etc. With this geometric increase in the time step, convergence, if it occurs, is extremely rapid. A simplified equation is treated this way in the Appendix to this chapter.[15]

When does a steady state exist? In general, uncertainty grows because of errors in initial conditions, and the unknown system perturbations (unknown controls, $\mathbf{u}$). Information that reduces uncertainty is provided by the incoming data stream. Under the right circumstances, one can reach an equilibrium where the new information just balances the new uncertainties. A quantitative answer to the question depends directly upon the discussion in Chapter 4 of the observability of the system. Although we omit the formal derivation, one can understand physically why those requirements must be met. Suppose, as in Chapter 4, there is an element of the model which is not observable. Then any error, e.g., in its initial conditions, could grow indefinitely, undetected, without bound. Such growth would mean that the corresponding elements of $\mathbf{P}$ would have to grow, and there would be no steady state. Suppose to the contrary, that such growth *is* observed. Then if those elements are controllable, one can find controls, $\mathbf{u}(t)$, such that the growth is halted. Note that neither $\mathbf{x}(t)$, nor $\mathbf{u}(t)$ will generally become steady – the state continues to evolve.

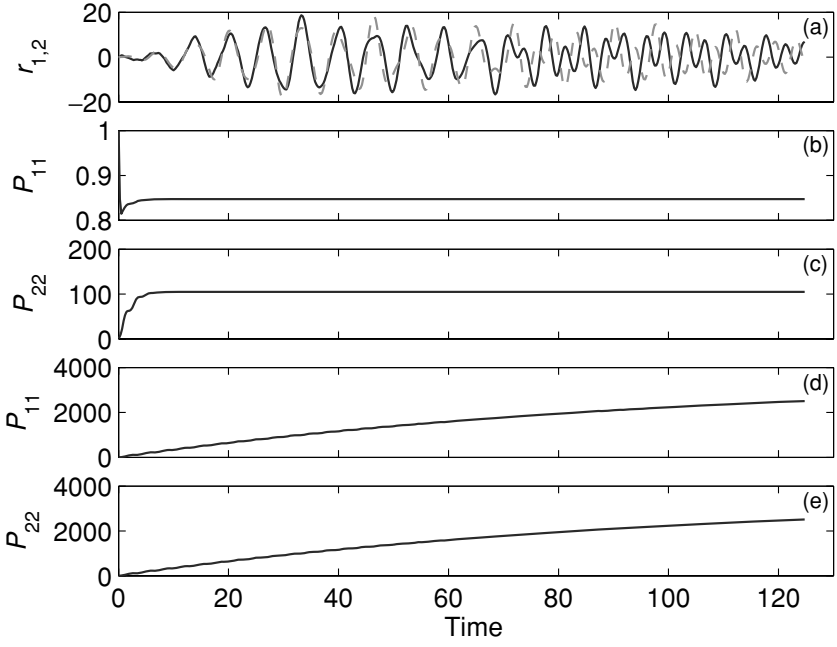

Figure 5.3 (a) Graph of the positions $r_i(t)$, $i = 1, 2$, for the coupled mass–spring oscillator. (b), (c) Graph of $P_{11}(t)$, $P_{22}(t)$ under the assumption that $\mathbf{E} = [1\ 0\ 0\ 0]$, that is, only $r_1(t)$ is measured (with noise). Both $P_{11}(t)$, $P_{22}(t)$ asymptote to a steady state, albeit $P_{11}(t) \ll P_{22}(t)$. (d), (e) Graph of $P_{11}(t)$, $P_{22}(t)$ when the observation matrix is changed to $\mathbf{E} = [-1\ 1\ 0\ 0]$ – that is, the observation is of the relative separation of the two masses. In this case, the uncertainty in the absolute positions continues to grow and a steady state is not reached (there is no dissipation in this example).

In the situation shown in Fig. 5.3, when there is a single measurement of the position, $r_1(t)$, the eigenvalues of the observability matrix, $\mathbf{O}$, range in magnitude from 1.9 down to 0.0067. Albeit there will be considerable uncertainty involved, one can fully determine the initial conditions from the observations. In contrast, when only the relative position, $r_2(t) - r_1(t)$ is measured, two of the eigenvalues of O vanish identically, the system is not completely observable, as seen in Fig. 5.3, and the uncertainties continue to grow without bound. If one were discussing the smoothing algorithm errors, the structure of $\mathbf{\Gamma}$ would enter similarly.[16]

5.2.4 Reduced state methods

The computational load of the Kalman filter and smoothers grows approximately as the cube of the state vector dimension. Thus either decoupling the problem into several smaller problems, or removing elements of the state vector, can have a very

large payback in terms of the computational load reduction. (If one could solve the problem as two $(n/2)^3$ problems rather than as one n^3 problem the difference in load is a factor of four.) One method for solving large fluid state problems is based upon the assumption that large spatial scales in a fluid flow evolve largely independent of small scales, and that it is the largest scales that are of primary interest.[17] Let $\mathbf{D}$ be a matrix operator that has the effect of averaging a vector spatially, so that $\mathbf{x}'(t) = \mathbf{D}\mathbf{x}(t)$ is a spatial average of $\mathbf{x}(t)$, with an equivalent reduced dimension, N'. (We refer to the "coarse state" and "fine state".) Then if $\mathbf{P}(t)$ is the error covariance of $\mathbf{x}(t)$,

$$\langle(\tilde{\mathbf{x}}' - \mathbf{x}')(\tilde{\mathbf{x}}' - \mathbf{x}')^{\mathrm{T}}\rangle = \mathbf{P}'(t) = \mathbf{D}\mathbf{P}(t)\mathbf{D}^{\mathrm{T}}$$

will be of dimension $N' \times N'$ rather than $N \times N$. Now assume further that $\mathbf{D}$ has a left-inverse, $\mathbf{D}^{+}$, as described in Chapter 2, that would map the coarse state to the finer one. Suppose further that one has a coarse resolution model capable of propagating $\mathbf{x}'$. This model might be obtained from the fine-resolution model:

$$\mathbf{D}\mathbf{x}\,(t+1) = \mathbf{D}\mathbf{A}\,(t)\,\mathbf{D}^{+}\mathbf{x}'\,(t) + \mathbf{D}\mathbf{B}\mathbf{D}^{+}\mathbf{u}'\,(t) + \mathbf{D}\Gamma\mathbf{D}^{+}\mathbf{q}'(t),$$

or

$$\mathbf{x}'\,(t+1) = \mathbf{A}'\mathbf{x}'\,(t) + \mathbf{B}'\mathbf{u}'(t),$$

where $\mathbf{u}'\,(t) = \mathbf{D}\mathbf{u}(t)$, $\mathbf{A}' = \mathbf{D}\mathbf{A}\,(t)\,\mathbf{D}^{+}$, $\mathbf{B}' = \mathbf{D}\mathbf{B}\mathbf{D}^{+}$, etc. Then the Kalman filter (and smoother) can be applied to $\mathbf{x}'(t)$ and the filtered data, $\mathbf{D}\mathbf{y}(t)$. One can estimate that

$$\tilde{\mathbf{x}}\,(t) = \mathbf{D}^{+}\tilde{\mathbf{x}}'(t),$$

and

$$\mathbf{P}\,(t) = \mathbf{D}^{+}\mathbf{P}'\,(t)\,\mathbf{D}^{+\mathrm{T}}. \tag{5.11}$$

Given $\mathbf{P}\,(t)$, one has $\mathbf{K}\,(t)$ for the fine state, under the assumption that Eq. (5.11), based wholly upon the large scales, is adequate. One can put any small scales in the fine-state observations into the data error of the coarse state. A further reduction in computational load can be made by assuming a steady state for $\mathbf{P}'(t)$, $\mathbf{P}(t)$, and finding it using the doubling algorithm. In Chapter 7 we will describe an application of this method. The main issue with its general validity would lie with the assumption that errors in the fine state do not strongly influence the error budget of the coarse state. This assumption cannot in general be correct: spatially averaged equations of fluid motion are not proper representations of the equations governing the averaged fields. One must carefully assess the behavior of the algorithm as it evolves.

Determination of $\mathbf{D}$, $\mathbf{D}^+$ is important. In principle, the Gauss–Markov mapping procedures, as described in Chapter 2, would be appropriate (and would include error estimates should one choose to use them). Various strategies for reducing storage and computation are available.[18]

Other approaches to state reduction

The Eckart–Young–Mirsky theorem, described in Chapter 2, shows that sometimes a comparatively small number of singular vectors can represent a field with considerable accuracy. Here "small" is measured relative to the number of grid points or basis functions used by the underlying model.[19] Suppose that the state vector $\mathbf{x}(t) = \mathbf{V}\boldsymbol{\alpha}(t)$, where $\mathbf{V}$ is the matrix of $\mathbf{v}_i$, the singular vectors of a large span of model – that is, the matrix to which the Eckart–Young–Mirsky theorem is applied is $\{\mathbf{x}(0) \quad \mathbf{x}(2) \quad \ldots \quad \mathbf{x}(t_N)\}$ – is then truncated to some acceptable sub-set,

$$\mathbf{x}(t) \approx \mathbf{V}_K \alpha(t).$$

Taking the canonical, full, model,

$$\mathbf{V}_K \mathbf{x}(t+1) = \mathbf{V}_K \mathbf{A}(t) \mathbf{V}_K \alpha(t) + \mathbf{V}_K \mathbf{B} \mathbf{V}_K \mathbf{u}(t) + \mathbf{V}_K \boldsymbol{\Gamma} \mathbf{V}_K \mathbf{q}(t),$$

or

$$\boldsymbol{\alpha}(t+1) = \mathbf{A}'(t)\alpha(t) + \mathbf{B}'\mathbf{u}(t) + \Gamma'\mathbf{q}(t),$$

where $\mathbf{A}'(t) = \mathbf{V}_K \mathbf{A}(t) \mathbf{V}_K$, $\mathbf{B}' = \mathbf{V}_K \mathbf{B} \mathbf{V}_K$, etc., is an evolution equation for the new state vector $\boldsymbol{\alpha}(t)$ whose dimension is $K \ll N$. (If $\mathbf{A}$ is time-independent, an alternative is to diagonalize it in the canonical equation by using its singular vector decomposition.[20]) Then each mode can be handled independently. As with the coarse-to-fine resolution transformation, one is assuming that the suppressed singular vectors (those banished to the nullspace are being assumed zero) do not significantly affect the errors of those retained. One must test the original assumptions against the solution obtained.

5.3 Uncertainty in Lagrange multiplier method

When using the Lagrange multiplier approach, the issue remains of estimating the uncertainty of the solution, even if the system is linear. One approach is to calculate it from the covariance evolution equation of the filter/smoother. When one wishes to avoid that computational load, some limited information about it can be obtained from the Hessian of the cost function at the solution point.[21]

Understanding of the Hessian is central to quadratic norm optimization problems in general. Let $\boldsymbol{\xi}$ represent all of the variables being optimized, including $\mathbf{x}(t)$, $\mathbf{u}(t)$

for all t. Let $\boldsymbol{\xi}^*$ be the optimal value that is sought. Then, as with the static problems of Chapter 2, if we are close enough to ξ^* in the search process, the objective function is locally

$$J = \text{constant} + (\boldsymbol{\xi} - \boldsymbol{\xi}^*)^{\mathrm{T}} \cdot \mathcal{H} \cdot (\boldsymbol{\xi} - \boldsymbol{\xi}^*) + \Delta J,$$

where $\mathcal{H}$ is the Hessian (see Eq. (2.31)) and ΔJ is a higher-order correction. The discussion of the behavior of the solution in the vicinity of the estimated optimal value proceeds then, exactly as before, with row and column scaling being relevant, and issues of ill-conditioning, solution variances, etc., all depending upon the eigenvalues and eigenvectors of $\mathcal{H}$.[22] One of the important future applications of automatic differentiation (AD) tools as described in Chapter 4 would be to calculate the second derivatives of objective functions to produce the Hessian.

The only problem, albeit a difficult one, is that the dimensions of $\mathcal{H}$ are square of the dimensions of $\mathbf{x}(t)$ plus $\mathbf{u}(t)$ over the entire time history of the model and data. Finding ways to understand the solution structure and uncertainty with realistic fluids and large-scale datasets remains as one of the most important immediate challenges to results such as those described in Chapter 7.

5.4 Non-normal systems

Consider a forward model,

$$\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t-1), \tag{5.12}$$

with t again an integer. In general, the underlying physics will fail to be self-adjoint and hence $\mathbf{A}$ will be non-normal, that is, $\mathbf{A} \neq \mathbf{A}^{\mathrm{T}}$. We suppose the system is unforced, but is started with initial conditions $\mathbf{x}(0)$ which are a realization of white noise with variance σ^2. Thus, at time t,

$$\mathbf{x}(t) = \mathbf{A}^t \mathbf{x}(0), \tag{5.13}$$

Recalling the discussion on p. 152, it follows immediately that the eigenvalues and right eigenvectors of $\mathbf{A}^t$ satisfy

$$\mathbf{A}^t \mathbf{g}_i = \lambda_i^t \mathbf{g}_i. \tag{5.14}$$

Expanding,

$$\mathbf{x}(0) = \sum_{i=1}^{N} \alpha_i(0)\, \mathbf{g}_i, \tag{5.15}$$

and

$$\mathbf{x}(t) = \sum_{i=1}^{N} \lambda_i^t \alpha_i(0)\, \mathbf{g}_i. \tag{5.16}$$

Stability of the model demands that all $|\lambda_i| \leq 1$. But the lack of orthogonality of the $\mathbf{g}_i$ means that some of the α_i may be very large, despite the white noise properties of $\mathbf{x}(0)$. This result implies that elements of $\mathbf{x}(t)$ can become very large, even though the limit $\lambda_i^t \to 0$, $t \to \infty$ means that they are actually transients. To an onlooker, the large response of the system to a bounded initial disturbance may make the system look unstable. Furthermore, the disturbance may become so large that the system becomes non-linear, and possibly non-linearly unstable.[23] That is, stable fluid systems may well appear to be unstable owing to the rapid growth of transients, or linearly stable systems may become unstable in the finite amplitude sense if the transients of the linearized system become large enough.

Now consider the forced situation with time-independent $\mathbf{A}$,

$$\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t-1) + \mathbf{q}(t-1). \tag{5.17}$$

Take the Fourier transform of the difference equation (5.17), using the result[24] that if the transform of $\mathbf{x}(t)$ is

$$\hat{\mathbf{x}}(s) = \sum_{t=0}^{\infty} \mathbf{x}(t)\, \mathrm{e}^{-2\pi \mathrm{i} s t}, \tag{5.18}$$

then the transform of $\mathbf{x}(t-1)$ is $\mathrm{e}^{-2\pi \mathrm{i} s}\hat{\mathbf{x}}(s)$. Solving for $\hat{\mathbf{x}}(s)$,

$$\hat{\mathbf{x}}(s) = (\mathrm{e}^{-2\pi \mathrm{i} s}\mathbf{I} - \mathbf{A})^{-1}\hat{\mathbf{q}}(s). \tag{5.19}$$

We call $(\mathrm{e}^{-2\pi \mathrm{i} s}\mathbf{I} - \mathbf{A})^{-1}$ the "resolvent" of $\mathbf{A}$, in analogy to the continuous case terminology of functional analysis.[25] If the resolvent is infinite for real values of $s = s_i$ it implies $\hat{\mathbf{x}}(s_i)$ is an eigenvector of $\mathbf{A}$ and an ordinary resonance is possible. For the mass–spring oscillator of Chapter 2, the complex eigenvalues of $\mathbf{A}$ produce $s_{1,2} = \pm 0.0507 + 0.0008\mathrm{i}$, and the damped oscillator has no true resonance. Should any eigenvalue have a negative imaginary part, leading to $|\mathrm{e}^{-2\pi \mathrm{i} s_i t}| > 1$, the system would be unstable.

Define $z = \mathrm{e}^{-2\pi \mathrm{i} s}$, to be interpreted as an analytic continuation of s into the complex plane. The unit circle $|z| = 1$ defines the locus of real frequencies. The gist of the discussion of what are called "pseudo-spectra" is the possibility that the norm of the resolvent $\|(z\mathbf{I} - \mathbf{A})^{-1}\|$ may become very large, but still finite, on $|z| = 1$ without there being either instability or resonance, giving the illusion of linear instability.

5.4.1 POPs and optimal modes

For any linear model in canonical form, the right eigenvectors of $\mathbf{A}$ can be used directly to represent fluid motions,[26] as an alternative, e.g., to the singular vectors

(EOFs). These eigenvectors were called "principal oscillation patterns," or POPs, by K. Hasselmann. Because $\mathbf{A}$ is usually not symmetric (not self-adjoint), the eigenvalues are usually complex, and there is no guarantee that the eigenvectors are a basis. But assuming that they provide an adequate description – usually tested by trying them – the right eigenvectors are used in pairs when there are complex conjugate eigenvalues. The expansion coefficients of the time-evolving field are readily shown to be the eigenvectors of $\mathbf{A}^{\mathrm{T}}$ – that is, the eigenvectors of the adjoint model. Assuming that the eigenvectors are not grossly deficient as a basis, and/or one is interested in only a few dominant modes of motion, the POP approach gives a reasonably efficient representation of the field.

Alternatively, $\mathbf{A}$ always has an SVD and one can try to use the singular vectors of $\mathbf{A}$ – directly – to represent the time evolving field. The complication is that successive multiplications by non-symmetric $\mathbf{A}$ transfers the projection from the $\mathbf{U}$ vectors to the $\mathbf{V}$ vectors and back again. Write $\mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{V}^{\mathrm{T}}$ and assume, as, is normally true of a model, that it is full rank $K = N$ and $\boldsymbol{\Lambda}$ is square. Using Eqs. (4.99) and (4.101), in the absence of observations,

$$\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t-1), \tag{5.20}$$

$$\boldsymbol{\mu}(t-1) = \mathbf{A}^{\mathrm{T}}\boldsymbol{\mu}(t), \tag{5.21}$$

one can always write

$$\mathbf{x}(t) = \mathbf{V}\boldsymbol{\alpha}(t), \tag{5.22}$$

where $\boldsymbol{\alpha}(t)$ is a set of vector coefficients. Write the adjoint solution as

$$\boldsymbol{\mu}(t) = \mathbf{U}\boldsymbol{\beta}(t). \tag{5.23}$$

Multiply (5.20) by $\boldsymbol{\mu}(t-1)^{\mathrm{T}}$ and (5.21) by $\mathbf{x}(t)^{\mathrm{T}}$, and then subtract,

$$\boldsymbol{\mu}(t-1)^{\mathrm{T}}\mathbf{A}\mathbf{x}(t-1) = \mathbf{x}(t)^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\boldsymbol{\mu}(t) = \boldsymbol{\mu}(t)^{\mathrm{T}}\mathbf{A}\mathbf{x}(t), \tag{5.24}$$

or, using (5.22) and (5.23),

$$\boldsymbol{\beta}(t-1)^{\mathrm{T}}\boldsymbol{\Lambda}\boldsymbol{\alpha}(t-1) = \boldsymbol{\alpha}(t)^{\mathrm{T}}\boldsymbol{\Lambda}\boldsymbol{\beta}(t)^{\mathrm{T}}, \tag{5.25}$$

which can be interpreted as an energy conservation principle, summed over modes.

Assume $\|\mathbf{A}\| < 1$ so that the system is fully stable. We can ask what disturbance of unit magnitude at time $t-1$, say, would lead to the largest magnitude of $\mathbf{x}(t)$? That is, we maximize $\|\mathbf{A}\mathbf{q}(t-1)\|$ subject to $\|\mathbf{q}(t-1)\| = 1$. This requirement is equivalent to solving the constrained maximization problem for the stationary values of

$$J = \mathbf{q}(t-1)^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{q}(t-1) - 2\mu(\mathbf{q}(t-1)^{\mathrm{T}}\mathbf{q}(t-1) - 1), \tag{5.26}$$

where μ is a scalar Lagrange multiplier, and which leads to the normal equations,

$$\mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{q}\,(t-1) = \mu\mathbf{q}(t-1), \tag{5.27}$$

$$\mathbf{q}\,(t-1)^{\mathrm{T}}\,\mathbf{q}\,(t-1) = 1. \tag{5.28}$$

Equation (5.27) shows that the solution is $\mathbf{q}\,(t-1) = \mathbf{v}_1,\ \mu = \lambda_1^2$, which is the first singular vector and value of $\mathbf{A}$ with (5.28) automatically satisfied. The particular choice of μ ensures that we obtain a maximum rather than a minimum. With $\mathbf{q}\,(t-1)$ proportional to the $\mathbf{v}_1$ singular vector of $\mathbf{A}$, the growth rate of $\mathbf{x}(t)$ is maximized.[27] The initial response would be just $\mathbf{u}_1$, the corresponding singular vector. If the time-step is very small compared to the growth rates of model structures, the analysis can be applied instead to $\mathbf{A}^{t_1}$, that is, the transition matrix after t_1 time-steps. The next largest singular value will give the second fastest growing mode, etc.

5.5 Adaptive problems

A major point of concern in estimation procedures based upon Gauss–Markov type methods lies in the specification of the various covariance matrices, especially those describing the model error (here included in $\mathbf{Q}(t)$). Nothing precludes deduction of the covariance matrices from the model and observations, given that adequate numbers of observations are available. For example, it is straightforward to show that if a Kalman filter is operating properly, then the so-called innovation, $\mathbf{y}(t) - \mathbf{E}\tilde{\mathbf{x}}(t,-)$, should be uncorrelated with all previous measurements (recall Chapter 2, Eq. (2.433)):

$$\langle \mathbf{y}(t')\,[\mathbf{y}(t) - \mathbf{E}\tilde{\mathbf{x}}(t,-)]\rangle = 0, \quad t' < t. \tag{5.29}$$

To the extent that (5.29) is not satisfied, the covariances need to be modified, and algorithms can be formulated for driving the system toward this condition. The possibilities for such procedures are known under the title "adaptive estimation."[28]

The major issues here are that accurate determination of a covariance matrix of a field, $\langle \mathbf{z}(t)\mathbf{z}(t')\rangle$, requires a vast volume of data. Note in particular that if the mean of the field $\mathbf{z}(t) \neq \mathbf{0}$, and it is inaccurately removed from the estimates, then major errors can creep into the estimated second moments. This bias problem is a very serious one in adaptive methods.

In practical use of adaptive methods, it is common to reduce the problem dimensionality by *modeling the error covariance matrices*, that is, by assuming a particular, simplified structure described by only a number of parameters much less than the number of matrix elements (accounting for the matrix symmetry). We must leave this subject to the references.[29]

Appendix. Doubling

To make the doubling algorithm plausible,[30] we consider the matrix equation

$$\mathbf{B}_{k+1} = \mathbf{F}\mathbf{B}_k\mathbf{F}^{\mathrm{T}} + \mathbf{C}, \tag{5.30}$$

and seek to time-step it. Starting with $\mathbf{B}_1$, one has, time-stepping as far as $k = 3$,

$$\begin{aligned}
\mathbf{B}_2 &= \mathbf{F}\mathbf{B}_1\mathbf{F}^{\mathrm{T}} + \mathbf{C}, \\
\mathbf{B}_3 &= \mathbf{F}\mathbf{B}_2\mathbf{F}^{\mathrm{T}} + \mathbf{C} = \mathbf{F}^2\mathbf{B}_1\mathbf{F}^{2\mathrm{T}} + \mathbf{F}\mathbf{C}\mathbf{F}^{\mathrm{T}} + \mathbf{C}, \\
\mathbf{B}_4 &= \mathbf{F}\mathbf{B}_3\mathbf{F}^{\mathrm{T}} + \mathbf{C} \\
&= \mathbf{F}^2\mathbf{B}_2\mathbf{F}^{2\mathrm{T}} + \mathbf{F}\mathbf{C}\mathbf{F}^{\mathrm{T}} + \mathbf{C} \\
&= \mathbf{F}^2\mathbf{B}_2\mathbf{F}^{2\mathrm{T}} + \mathbf{B}_2,
\end{aligned}$$

that is, $\mathbf{B}_4$ is given in terms of $\mathbf{B}_2$. More generally, putting $\mathbf{M}_{k+1} = \mathbf{M}_k^2$, $\mathbf{N}_{k+1} = \mathbf{M}_k\mathbf{N}_k\mathbf{M}_k^{\mathrm{T}} + \mathbf{N}_k$, with $\mathbf{M}_1 = \mathbf{F}$, $\mathbf{N}_1 = \mathbf{Q}$, then $\mathbf{M}_{2k} = \mathbf{F}^{2^k}$, $\mathbf{N}_{k+1} = \mathbf{B}_{2^k}$, and one is solving Eq. (5.30) so that the time-step doubles at each iteration. An extension of this idea underlies the doubling algorithm used for the Riccati equation.

Notes

1 See Kitagawa and Sato (2001) for references.
2 See Arulampalam *et al*. (2002). Their development relies on a straightforward Bayesian approach.
3 See Daley (1991) and Evensen and VanLeeuwen (1996) and the references therein for a more complete discussion.
4 See Press *et al*. (1996) for detailed help concerning generating values from known probability distributions.
5 Kalnay (2003) discusses, e.g., "breeding" vectors, which are selected to display fastest growth in the model.
6 See Aitchison and Brown (1957).
7 Gardiner (1985).
8 Evensen (1994) and Evensen and VanLeeuwen (1996) are good starting points for practical applications, insofar as problem dimensions have permitted. See Daley (1991) and Kalnay (2003) for a broad discussion of the specific numerical weather forecasting problem.
9 Reviews are by Lorenc (1986), Daley (1991), Ghil and Malanotte-Rizzoli (1991), or Kalnay (2003).
10 Usually called "3DVAR," by meteorologists, although like "4DVAR" it is neither variational nor restricted to three dimensions.
11 For example, "breeding"; see Kalnay (2003).
12 Anthes (1974).
13 Gelb (1974, Chapters 7 and 8) has a general discussion of the computation reduction problem, primarily in the continuous time context, but the principles are identical.
14 Kalman's (1960) filter derivation was specifically directed at extending the Wiener theory to the transient situation, and it reduces to the Wiener theory when a steady-state is appropriate.)
15 Anderson and Moore (1979) should be consulted for a complete discussion.
16 Fukumori *et al*. (1992) discuss this problem in greater generality for a fluid flow.
17 Fukumori (1995), who interchanges the roles of $\mathbf{D}$, $\mathbf{D}^+$. See also Fukumori (2002).
18 A general discussion of various options for carrying out the transformations between fine and coarse states is provided by Fieguth *et al*. (2003).

19 Used, for example, by Cane *et al*. (1996).
20 For example, Brogan (1991).
21 Thacker (1989), Marotzke and Wunsch (1993).
22 Tziperman *et al*. (1992) grapple with ill-conditioning in their results; the ill-conditioning is interpretable as arising from a nullspace in the Hessian.
23 This potential confusion is the essence of the conclusions drawn by Farrell (1989) and Farrell and Moore (1993), and leads to the discussion by Trefethen (1997, 1999) of pseudo-spectra.
24 Bracewell (2000).
25 Trefethen (1997).
26 Hasselmann (1988), von Storch *et al*. (1988), von Storch and Zwiers (1999).
27 The meteorological literature, e.g., Farrell and Moore (1993), renamed this singular vector as the "optimal" vector.
28 Among textbooks that discuss this subject are those of Goodwin and Sin (1984), Haykin (1986), and Ljung (1987).
29 See Menemenlis and Chechelnitsky (2000) and the references given there.
30 Following Anderson and Moore (1979, p. 67).