Chapter 2
Forward Sensitivity Method: Scalar Case

In this chapter, using a simple deterministic nonlinear, scalar model, we derive the dynamics of evolution of the first-order and second-order forward sensitivities of the solution or model forecast with respect to control (the initial condition and parameters). It is assumed that the given model is perfect and the forecast errors, if any, are due only to the errors in the control consisting of the initial condition and the parameters. Refer to Sect. 1.5 for a discussion on classification of forecast errors. Given a set of N noisy observations of the phenomenon that the given model is expected to capture, we introduce a new data assimilation strategy called the forward sensitivity method (FSM). As the name implies, this strategy relies on evolution of model sensitivities—the changes in forecast as a function of changes in the control vector. These sensitivities march forward in time in step with the model forecast.

In Sect. 2.1 we derive equations governing the evolution of the first-order forward sensitivities. The basis for the FSM is developed in Sect. 2.2. The equations governing evolution of the second-order forward sensitivities are derived in Sect. 2.3. Discrete time analogs of the dynamics of evolution for first-order and second-order forward sensitivities are given in Sect. 2.4. A class of second-order methods for deterministic dynamic data assimilation using the second-order forward sensitivity is developed in Sect. 2.5. The last Sect. 2.6 contains a discussion of the computation of the Lyapunov index which is the long term average rate of growth of small errors in the initial conditions which in turn depends on the evolution of the first-order forward sensitivity.

S. Lakshmivarahan et al., *Forecast Error Correction using Dynamic Data Assimilation*, Springer Atmospheric Sciences, DOI 10.1007/978-3-319-39997-3_2

2.1 Evolution of First-Order Sensitivities

Let $f : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ and consider a continuous time dynamical system described by a scalar, non-linear, first-order, autonomous, ordinary differential equation of the type

$$\dot{x} = f(x, \alpha), \tag{2.1.1}$$

with $x(0) = x_0 \in \mathbb{R}$ as the initial condition and $\alpha \in \mathbb{R}$ as a real parameter. It is assumed that $f(x, \alpha)$ satisfies the conditions necessary (such as Lipschitz condition) for the existence and uniqueness of the solution that continuously depends on the initial condition x_0, parameter α and the time variable t. Thus, the solution

$$x(t) = x\left(t, x(0), \alpha\right) = x\left(t, \mathbf{c}\right), \tag{2.1.2}$$

where $\mathbf{c} = (x(0), \alpha)^T \in \mathbb{R}^2$ is called the control vector. The partial derivatives $\partial x(t)/\partial x(0)$ and $\partial x(t)/\partial \alpha$ are respectively the sensitivities of the solution $x(t)$ at time $t(> 0)$ with respect to x_0 and α. Hence these derivatives are called forward sensitivities. Likewise, the second partial derivatives $\partial^2 x(t)/\partial x^2(0)$, $\partial^2 x(t)/\partial \alpha^2$ and $\partial^2 x(t)/\partial x(0)\partial \alpha$ are known as the second-order forward sensitivities. Our goal in this section is to derive the dynamics of evolution of the first-order forward sensitivities.

To this end, taking the partial derivatives of both sides of (2.1.1) with respect to the initial condition $x(0)$, we get

$$\frac{\partial \dot{x}}{\partial x(0)} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x(t)}{\partial x(0)}\right) = \left(\frac{\partial f(x, \alpha)}{\partial x(t)}\right)\left(\frac{\partial x(t)}{\partial x(0)}\right). \tag{2.1.3}$$

To simplify the notation, define

$$u_1(t) = \frac{\partial x(t)}{\partial x(0)}, \; D_{x(t)}(f) = \frac{\partial f(x, \alpha)}{\partial x}, \tag{2.1.4}$$

where subscript 1 refers to the first-order sensitivity.

Using these definitions (2.1.3) becomes

$$\dot{u_1}(t) = D_{x(t)}(f)u_1(t), \tag{2.1.5}$$

which is a scalar, linear, first-order, homogeneous, non-autonomous, ordinary differential equation that describes the evolution of the first-order sensitivity $u_1(t)$ when $D_x(f)$ is the Jacobian of f that varies along the trajectory of (2.1.1). Since

$$u_1(0) = \frac{\partial x(0)}{\partial x(0)} = 1, \tag{2.1.6}$$

the initial condition for (2.1.5) is $u_1(0) = 1$.

The solution $u_1(t)$ of (2.1.5) is given by

$$u_1(t) = e^{\int_0^t D_{x(\tau)}(f(x(\tau),\alpha)d\tau} u_1(0). \tag{2.1.7}$$

Again differentiating (2.1.1) with respect to α we obtain

$$\frac{\partial \dot{x}}{\partial \alpha} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x(t)}{\partial \alpha}\right) = \left(\frac{\partial f}{\partial x(t)}\right)\left(\frac{\partial x(t)}{\partial \alpha}\right) + \frac{\partial f}{\partial \alpha} \tag{2.1.8}$$

as the sum of two terms. The first term on the right hand side of (2.1.8) arises from the implicit dependence of $f(x, \alpha)$ on α through $x(t)$ and the second term arises from the explicit dependence of $f(x, \alpha)$ on α. Define

$$v_1(t) = \frac{\partial x(t)}{\partial \alpha}, \text{ and } D_\alpha(f) = \frac{\partial f(x,\alpha)}{\partial \alpha.} \tag{2.1.9}$$

Using (2.1.4) and (2.1.9), we can rewrite (2.1.8) succinctly as

$$\dot{v}_1(t) = D_{x(t)}(f)v_1(t) + D_\alpha(f), \tag{2.1.10}$$

which is again a scalar, linear, first-order, non-homogeneous, non-autonomous ordinary differential equation with a forcing term $D_\alpha(f)$, which is the Jacobian of f with respect to α that also varies along the trajectory of (2.1.1).

Thus $u_1(t)$ and $v_1(t)$ as solutions of (2.1.5) and (2.1.10) are called first-order forward sensitivity functions and are computed using the algorithm given in Algorithm 2.1.

Algorithm 2.1 Computation of the forward sensitivity function

Given $f(x, \alpha)$, the initial condition $x(0)$, the value of the parameter α, and $T > 0$.
Step 1: Compute the Jacobian $\mathbf{D}_x(f)$ and $\mathbf{D}_\alpha(f)$
Step 2: Solve (2.1.1) analytically, if possible, or numerically using some discretization scheme—Euler method, 4th-order Runge-Kutta method and compute $x(t)$ for $0 \le t \le T$
Step 3: Evaluate $\mathbf{D}_x(f)$ along the trajectory computed in Step 2 and solve (2.1.5) and compute the evolution of the forward sensitivity function $u_1(t), 0 \le t \le T$.
Step 4: Evaluate $\mathbf{D}_\alpha(f)$ along the trajectory computed in Step 2 and solve (2.1.10) and compute the evolution of the forward sensitivity function $v_1(t), 0 \le t \le T$.

The following example illustrates the computation of the first-order forward sensitivity functions.

Example 1. Consider the case where cold continental air moves out over an ocean of constant surface temperature. We follow a column of air in a Lagrangian frame; that is, the column of air moves with the prevailing low-level wind speed. Turbulent transfer of heat from the ocean to air warms the column. The governing linear dynamics is taken to be

$$\frac{dx}{dt} = \frac{C_T V}{H}(\theta - x) \tag{2.1.11}$$

where

- x : temperature of the air column (°C),
- θ : sea surface temperature (SST, °C),
- C_T : turbulent heat exchange coefficient (nondimensional),
- V : speed of air column ($\mathrm{m\,s^{-1}}$),
- H : height of the column – the mixed layer (m)
- t : time (h).

Assuming the following scales for the physical variables,
$H \sim 150\,\mathrm{m}$, $V \sim 10\,\mathrm{m\,s^{-1}}$, $C_T \sim 10^{-3}$,
we get

$$\frac{C_T V}{H} \sim 0.25\,\mathrm{h^{-1}}.$$

Let $c = \dfrac{C_T V}{H}$, then (2.1.11) becomes

$$\frac{\mathrm{d}x}{\mathrm{d}t} = c\,(\theta - x) = f(x, \alpha),$$

whose analytic solution is

$$x(t, x_0, \alpha) = (x_0 - \theta)e^{-ct} + \theta \tag{2.1.12}$$

where x_0 is the initial condition and the parameters are θ and c.

There are three elements of control: initial condition, $x(0)$, boundary condition θ, and parameter, c. The Jacobians of f with respect to x and α are given by

$$D_x(f) = -c, \quad D_\theta(f) = c, \quad D_c(f) = \theta - x(t). \tag{2.1.13}$$

The evolution of the forward sensitivity with respect to the initial condition is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x(t)}{\partial x(0)}\right) = -c\left(\frac{\partial x(t)}{\partial x(0)}\right), \tag{2.1.14}$$

and that with respect to the parameters θ and c are given by

$$\left.\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x(t)}{\partial \theta}\right) &= -c\frac{\partial x(t)}{\partial \theta} + c, \\ \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x(t)}{\partial c}\right) &= -c\frac{\partial x(t)}{\partial c} + \theta - x(t), \end{aligned}\right\} \tag{2.1.15}$$

where

$$\left[\frac{\partial x(t)}{\partial \theta}\right]_{t=0} = 0 = \left[\frac{\partial x(t)}{\partial c}\right]_{t=0}, \quad \text{and} \quad \left[\frac{\partial x(t)}{\partial x(0)}\right]_{t=0} = 1.$$

Either by solving (2.1.14) and (2.1.15) or by computing directly from (2.1.12), it can be verified that the required sensitivities evolve according to

$$\begin{aligned} \frac{\partial x(t)}{\partial x(0)} &= e^{-ct}, \\ \frac{\partial x(t)}{\partial \theta} &= 1 - e^{-ct}, \\ \frac{\partial x(t)}{\partial c} &= [\theta - x(0)]\, te^{-ct}. \end{aligned} \tag{2.1.16}$$

The plots of the solution and the three sensitivities when $x(0) = 1$, $x_s = 11$ and $c = 0.25$ are given in Figs. 2.1, 2.2, 2.3, and 2.4.

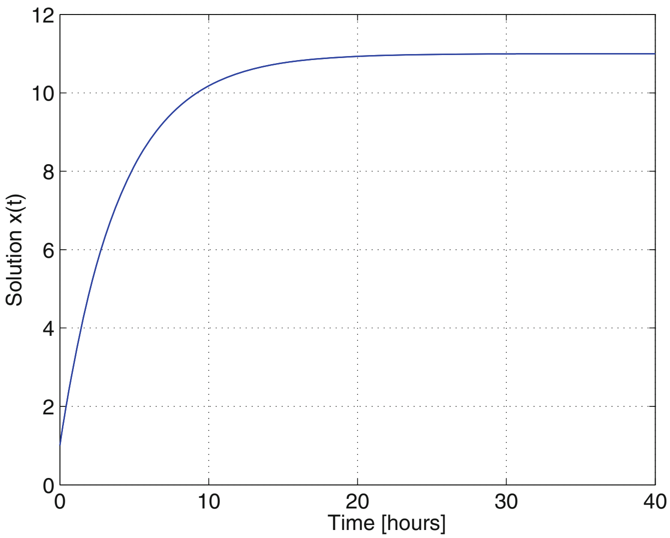


Fig. 2.1 Evolution of the solution of $x(t)$ in (2.1.12)

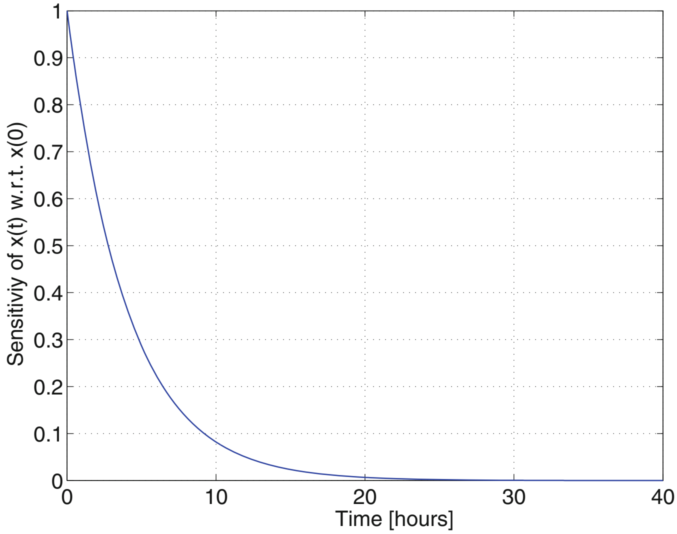


Fig. 2.2 Evolution of the sensitivity of $x(t)$ with respect to the initial condition $x(0)$

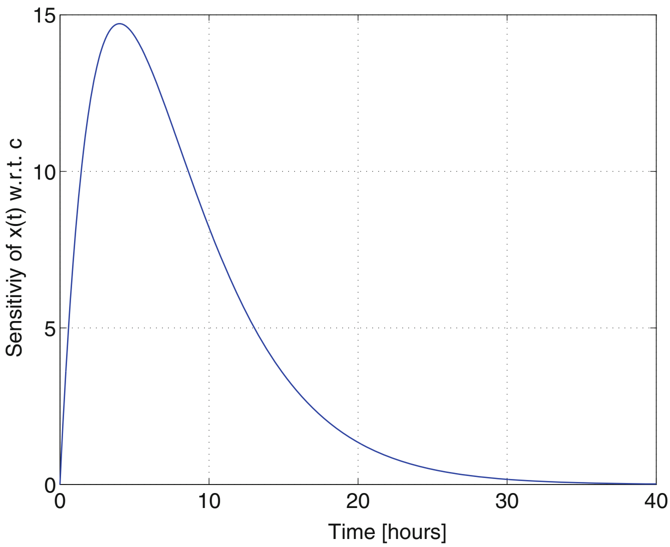


Fig. 2.3 Evolution of the sensitivity of $x(t)$ with respect to c

2.2 First-Order Sensitivities Used in FSM

Referring to Sect. 1.5, it is assumed that the model field, $f(x, \boldsymbol{\alpha})$, the forward operator $h(x)$, the control $\mathbf{c} = (x(0), \boldsymbol{\alpha})^T \in \mathbb{R}^2$, the actual observation $z(t)$ and its error covariance $R(t)$ are given. It is assumed that the current value of the control $\mathbf{c}$ is

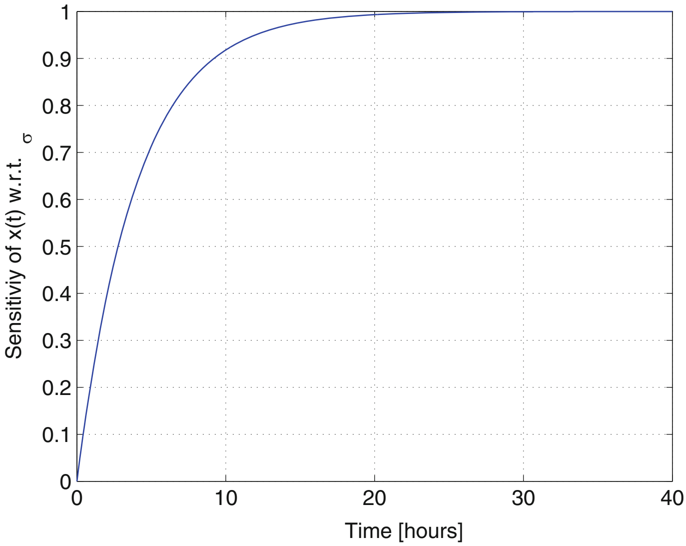


Fig. 2.4 Evolution of the sensitivity of $x(t)$ with respect to the boundary condition, θ

not exact which in turn induces error in the model forecast. Our goal is to find the correction, $\delta\mathbf{c}$ to the control vector $\mathbf{c}$, such that the new model forecast starting from $(\mathbf{c}+\delta\mathbf{c})$ will render the forecast error, $\mathbf{e}_p(t)$ purely random. That is, we wish to remove the systematic part of the forecast error induced by the erroneous control. To this end, we start by quantifying the actual change Δx in the solution $x(t) = x(t,\mathbf{c})$ resulting from a change $\delta\mathbf{c}$ in $\mathbf{c}$. Using the standard Taylor series expansion, we get

$$\Delta x = x(t, \mathbf{c} + \delta\mathbf{c}) - x(t, \mathbf{c}) = \sum_k \delta^k x, \tag{2.2.1}$$

where the kth variation of $x(t)$ is given by

$$\delta^k x = g\left(\frac{\partial^k x}{\delta \mathbf{c}^k}, \delta\mathbf{c}\right) \tag{2.2.2}$$

and g is a known function of the kth partial derivative of $x(t)$ with respect to $\mathbf{c}$ and the perturbation $\delta\mathbf{c}$. While using higher-order correction terms in (2.2.1) would lead to improved accuracy, inclusion of higher order terms invariably leads to a more complex inverse problem as will become evident from the following analysis. Recognizing this trade-off between complexity and accuracy, a useful compromise is to restrict the sum in (2.2.1) to the first two terms at the most, that is

$$\Delta x = \delta x + \delta^2 x, \tag{2.2.3}$$

where δx is the first-order and $\delta^2 x$ is the second-order correction term. In the following, we first illustrate the first-order analysis, where Δx is approximated by δx. Inclusion of the second-order analysis is justified in cases where the field, $f(x, \boldsymbol{\alpha})$ and/or the forward operator $h(x)$, are highly nonlinear and warrant use of second-order correction. Further, it is shown below that iterative application of first-order method can be used in lieu of second-order methods in many cases.

2.2.1 *First-Order Analysis*

Let $\bar{x}(t)$ be the solution of (2.1.1) starting from the true initial value of the control $\mathbf{c} = (x(0), \alpha)^T$. Let $x(t)$ be the solution of (2.1.1) starting from the perturbed value of the control

$$\mathbf{c} + \delta\mathbf{c} = \ (x(0) + \delta x(0), \alpha + \delta\alpha)^T .$$

Let $\delta x(t)$ be the first-order approximation to the actual change $x(t) - \bar{x}(t)$—see Fig. 2.5. From first principles, that is, applying the first-order Taylor expansion to (2.1.2), we have

$$\Delta x \approx \delta x = D_{x(0)}(x)\delta x(0) + D_\alpha(x)\delta\alpha \tag{2.2.4}$$

where

$$\mathbf{D}_{\mathbf{x(0)}}(\mathbf{x}) = \frac{\partial x(t)}{\partial x(0)} = u_1(t),\ \mathbf{D}_{\boldsymbol{\alpha}}(x) = \frac{\partial x(t)}{\partial \alpha} = v_1(t), \tag{2.2.5}$$

are the first-order sensitivities of $x(t)$ with respect to the initial condition $x(0)$ and the parameter α, respectively.

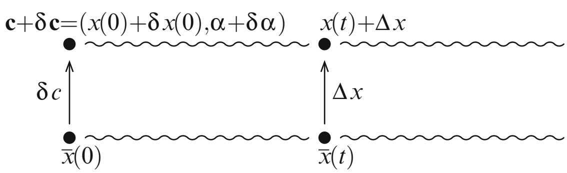
Knowing the first-order forward sensitivities, we compute the corrections $\delta x(0)$ and $\delta\alpha$ by fitting the model to a given set of noisy observations in a least squares framework.

Case 1: Single Observation

Let $z(t)$ be a given single observation. Recall that

$$z(t) = h\,(x(t)) + v(t), \tag{2.2.6}$$

Fig. 2.5 An illustration of an initial perturbation and its impact on the solution at time t



where $\nu(t) \sim N(0, \sigma_0^2)$. If the model counterpart to the observation is strictly the model variable, then $h(x(t)) = x(t)$. The first variation δx in $x(t)$ induces a first variation δh in $h\,(x(t))$ given by

$$\delta h = \mathbf{D_x}(h)\delta x, \tag{2.2.7}$$

where

$$\mathbf{D_x}(h) = \frac{\partial h(x)}{\partial x}. \tag{2.2.8}$$

Again, if $h(x) = x$, then $\mathbf{D}_x(h) = 1$.
Substituting (2.2.4) into (2.2.7) yields

$$\delta h = H_1(t)\delta x(0) + H_2(t)\delta\alpha, \tag{2.2.9}$$

where

$$\begin{aligned} H_1(t) &= \mathbf{D_x}(h)\mathbf{D_{x(0)}}(x) = \mathbf{D_x}(h)u_1(t), \\ H_2(t) &= \mathbf{D_x}(h)\mathbf{D}_{\boldsymbol{\alpha}}(x) = \mathbf{D_x}(h)v_1(t). \end{aligned} \tag{2.2.10}$$

Now, define

$$\mathbf{H}(t) = [H_1(t), H_2(t)] \in \mathbb{R}^{1\times 2}, \text{ and } \boldsymbol{\zeta} = (\boldsymbol{\zeta}_1, \boldsymbol{\zeta}_2)^T, \tag{2.2.11}$$

where $\boldsymbol{\zeta}_1 = \delta x(0)$, and $\boldsymbol{\zeta}_2 = \delta\alpha$. Then (2.2.9) can be succinctly written as

$$\delta h = \mathbf{H}(t)\boldsymbol{\zeta}. \tag{2.2.12}$$

Given an operating point $\mathbf{c}$, our goal is to find the perturbation $\delta\mathbf{c} = \boldsymbol{\zeta}$ such that the given observation $z(t)$ matches its model counterpart to a first-order accuracy, that is

$$z(t) = h\,(x(t) + \delta x) \approx h\,(x(t)) + \delta h, \tag{2.2.13}$$

Thus, the forecast error $e_F(t)$ when viewed from the observation space becomes

$$e_F(t) \equiv z(t) - h\,(x(t)) \approx \delta h, \tag{2.2.14}$$

where $x(t)$ is the forecast computed from the incorrect control $\mathbf{c}$. From (2.2.12) and (2.2.14), the perturbation $\delta\mathbf{c} = \boldsymbol{\zeta}$ is required to satisfy

$$\mathbf{H}(t)\boldsymbol{\zeta} = \mathbf{e}_F(t). \tag{2.2.15}$$

But $\boldsymbol{\zeta}$ has two or more components—two if the parameter space has dimension one. Thus, $\boldsymbol{\zeta}$ cannot be determined from a single observation and the associated single equation. The problem as stated is under-determined.

The approach summarized in Box 2.1 offers a least squares solution to the problem by requiring that the norm of the corrections be minimized. In short, for the case of two unknowns, the requirement that the sum of the squared adjustments be a minimum yields an expression for the optimal (least squares) adjustment.

Box 2.1 Method of Lagrangian multipliers.
Lagrangian multiplier method: under-determined case.
Let the model counterpart matrix $\mathbf{H} : [h_1, h_2] \in \mathbb{R}^{1\times 2}, \mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^2$ and $z \in \mathbb{R}$. Let $z = \mathbf{Hx}$ or $h_1x_1 + h_2x_2 = z$. Rewriting this as $x_1 = \frac{1}{h_1}[z - h_2x_2]$, it follows that for each $x_2 \in \mathbb{R}$, there is a unique x_1 satisfying this relation. Hence, we are left with a problem admitting infinitely many solutions (Lewis et al. 2006, Chap. 5).
The method of Lagrangian multipliers helps to find a unique solution by seeking the one with the minimum norm (same as energy) subject to the constraint. To this end, for $\lambda \in \mathbb{R}$ define the Lagrangian

$$L(\mathbf{x}, \lambda) = \frac{1}{2}\mathbf{x}^T\mathbf{x} + \lambda(z - \mathbf{Hx})$$

Here λ is called the undetermined Lagrangian multiplier. The necessary conditions for the minimum of $L(x, \lambda)$ are given by

$$\nabla_x L(\mathbf{x}, \lambda) = \mathbf{x} - \mathbf{H}^T\lambda = 0$$

$$\nabla_\lambda L(\mathbf{x}, \lambda) = \mathbf{z} - \mathbf{Hx} = 0$$

Substituting the first equation in the second, we get

$$\lambda = \left(\mathbf{HH}^T\right)^{-1} z$$

which when substituted back into the first equation yields the unique solution

$$x_{LS} = \mathbf{H}^T\left(\mathbf{HH}^T\right)^{-1} z$$

$$\boldsymbol{\zeta}_{LS} = \mathbf{H}^T\left(\mathbf{HH}^T\right)^{-1} e_F(t), \tag{2.2.16}$$

which can be computed using the algorithm given in Algorithm 2.2.

Algorithm 2.2 Algorithm for computing the forecast error correction

Step 1: Compute $\mathbf{D_x}(h)$
Step 2: Using $\mathbf{D_{x(0)}}(x) = u(t)$ and $\mathbf{D}_{\boldsymbol{\alpha}}(x) = v(t)$ computed in Algorithm 2.1, now assemble $H_1 = \mathbf{D_x}(h)\mathbf{D_{x(0)}}$ and $H_2 = \mathbf{D_x}(h)\mathbf{D}_{\boldsymbol{\alpha}}(x)$ and form $\mathbf{H} = [H_1, H_2]$.
Step 3: Using $x(t)$ computed in Algorithm 2.1, compute the forecast error
$\mathbf{e_F}(t) = \mathbf{z}(t) - \mathbf{h}(\mathbf{x}(t))$.
Step 4: Solve the under-determined linear least-squares problem using (2.2.16) (Lewis et al. 2006, Chap. 5).

Remark 2.1 (Structure of Optimal Correction).

In this case where there is only one observation, $\mathbf{H}$ is a row matrix of size 1×2 and hence

$$\mathbf{H}\mathbf{H}^T = \mathbf{H}_1^2(t) + \mathbf{H}_2^2(t) = \|\mathbf{H}\|^2$$

Consequently we can rewrite (2.2.16) as a product of a vector and a scalar given by

$$\boldsymbol{\zeta}_{LS} = \frac{\mathbf{H}^T}{\|\mathbf{H}\|}\,\frac{\mathbf{e_F}(t)}{\|\mathbf{H}\|}, \tag{2.2.17}$$

Since the second factor on the right hand side is a scalar that is proportional to the forecast error, $e_F(t)$, it follows that the optimal least squares correction, $\boldsymbol{\zeta}_{LS}$, is proportional to the unit vector

$$\frac{\mathbf{H}^T}{\|\mathbf{H}\|} = \frac{1}{\left[u_1^2(t) + v_1^2(t)\right]^{1/2}} \begin{bmatrix} u_1(t) \\ v_1(t) \end{bmatrix}$$

whose components are uniquely determined by the forward sensitivities $u_1(t)$ and $v_1(t)$. In other words, the optimal correction to the control is uniquely determined by the normalized forward sensitivity vector and the scaled forecast error.

Case 2: Multiple Observations

We now extend the above analysis to the case when there are observations available at N different times, beyond the initial time ($t = 0$). Let $0 < t_1 < t_2 < \ldots < t_N$ be the N different times and $z(t_1), z(t_2), \ldots, z(t_N)$ be the observations at these times. If $x(t)$ is the current model forecast, then the forecast errors at time t_i, for $1 \le i \le N$ are given by

$$\mathbf{e}_F(t_i) = \mathbf{z}(t_i) - \mathbf{h}\left(x(t_i)\right). \tag{2.2.18}$$

If δc is the initial perturbation in the control c, the sequence of N induced perturbations are given by

$$\delta x(t_i) = \mathbf{D}_{\mathbf{x(0)}}(x(t_i))\delta x(0) + \mathbf{D}_{\alpha}(x(t_i))\delta\alpha,\ 1 \leq i \leq N. \tag{2.2.19}$$

The first variation $\delta h(i)$, the model counterpart of the observation at time t_i, is given by

$$\delta h(i) = D_{x(t_i)}(h)\delta x(t_i) \tag{2.2.20}$$

Combining these we obtain

$$\delta h(i) = H_1(t_i)\delta x(0) + H_2(t_i)\delta\alpha, \tag{2.2.21}$$

where

$$\begin{aligned} H_1(t_i) &= D_{x(t_i)}(h)D_{x(0)}\left(x(t_i)\right), \\ H_2(t_i) &= D_{x(t_i)}(h)D_{\alpha}\left(x(t_i)\right). \end{aligned} \tag{2.2.22}$$

Hence, at time t_i, we have

$$\mathbf{H}(t_i)\boldsymbol{\zeta} = e_F(t_i), \tag{2.2.23}$$

where

$$\begin{aligned} \mathbf{H}(t_i) &= [H_1(t_i), H_2(t_i)] \in \mathbb{R}^{1\times 2}, \\ \boldsymbol{\zeta} &= (\delta x(0), \delta c)^T \in \mathbb{R}^2. \end{aligned} \tag{2.2.24}$$

Now define an $N \times 2$ matrix $\mathbf{H}$ obtained by stacking $H(t_i)$ in rows and the vector $\mathbf{e}_F$ by stacking $e_F(t_i)$ in rows:

$$\mathbf{H} = \begin{bmatrix} H(t_1) \\ H(t_2) \\ \vdots \\ H(t_N) \end{bmatrix} \in \mathbb{R}^{N\times 2},\ \mathbf{e}_F = \begin{bmatrix} e_F(t_1) \\ e_F(t_2) \\ \vdots \\ e_F(t_N) \end{bmatrix} \in \mathbb{R}^N. \tag{2.2.25}$$

Then, (2.2.23) becomes

$$\mathbf{H}\boldsymbol{\zeta} = \mathbf{e}_F. \tag{2.2.26}$$

Again, from Sect. 1.5 it follows that $\mathbf{e}_F$ contains a systematic deterministic error and a random observation noise. Assuming that the matrix $\mathbf{H}$ is of full rank, that is, Rank($\mathbf{H}$) $= 2$, we get two special cases. When $N = 2$, (2.2.26) can be solved uniquely by the standard method for solving linear systems. Refer to Lewis et al. (2006, Chap. 9) for details.

We now consider the overdetermined case when $N \geq 3$. In such a case, (2.2.26) is solved by minimizing the weighted sum of squared errors

$$J(\boldsymbol{\zeta}) = \frac{1}{2}(\mathbf{e}_F - H(t_i)\boldsymbol{\zeta})^T \mathbf{R}^{-1}(t_i)(\mathbf{e}_F - H(t_i)\boldsymbol{\zeta}), \tag{2.2.27}$$

where $\mathbf{R} \in \mathbb{R}^{N\times N}$ diagonal matrix where the ith diagonal element represents the variance of the ith observation $z(t_i)$.

By taking gradient $J(\boldsymbol{\zeta})$ with respect to $\boldsymbol{\zeta}$ (refer to Appendix A for details) and equating it to zero, we readily see that the minimized $\boldsymbol{\zeta}_{LS}$ is given by the solution of the linear system

$$\left(\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\right)\boldsymbol{\zeta} = \mathbf{H}^T\mathbf{R}^{-1}\mathbf{e}_F, \tag{2.2.28}$$

where the system matrix $\left(\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\right)$ is symmetric and positive definite. It follows (refer to Appendix A for details) that the Hessian of $J(\boldsymbol{\zeta})$ in (2.2.27) is given by

$$\nabla^2 J(\boldsymbol{\zeta}) = \left(\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\right), \tag{2.2.29}$$

which is symmetric and positive definite. The least squares (LS) solution $\boldsymbol{\zeta}_{LS}$ of (2.2.28) is

$$\boldsymbol{\zeta}_{LS} = \left(\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{e}_F.$$

Referring to Lewis et al. (2006, Chap. 5 and 6), it follows that the vector $\mathbf{H}\boldsymbol{\zeta}_{LS}$ is the (oblique) projection of $\mathbf{e}_F$ onto the subspace spanned by the columns of $\mathbf{H}$.

2.3 Evolution of Second-Order Sensitivities

For later use, we derive equations for evolution of second-order forward sensitivities associated with the solution of (2.1.1)—$x(t) = x(t, \mathbf{c})$ where $\mathbf{c} = (x(0), \alpha)^T$. In principle there are three equations of interest to us: one for each of $\frac{\partial^2 x(t)}{\partial x^2(0)}$, $\frac{\partial^2 x(t)}{\partial \alpha^2}$ and $\frac{\partial^2 x(t)}{\partial x(0)\partial \alpha}$ which are respectively the second partial derivations of $x(t)$ with respect to $x(0), \alpha$ and the mixed partial derivative that captures the interaction between $x(0)$ and α.

2.3.1 Evolution of $\partial^2 x(t)/\partial x^2(0)$

Since we already know the evolution of the first-order sensitivity of $x(t)$ with respect to $x(0)$, we start with this equation given in (2.1.3). We reproduce this equation here for convenience:

$$\frac{d}{dt}\left(\frac{\partial x(t)}{\partial x(0)}\right) = \left(\frac{\partial f(x,\alpha)}{\partial x(t)}\right)\left(\frac{\partial x(t)}{\partial x(0)}\right). \tag{2.3.1}$$

Now, differentiate both sides with respect to $x(0)$ to get

$$\frac{\partial}{\partial x(0)}\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x(t)}{\partial x(0)}\right)\right] = \frac{\partial}{\partial x(0)}\left[\left(\frac{\partial f(x,\alpha)}{\partial x(t)}\right)\left(\frac{\partial x(t)}{\partial x(0)}\right)\right].$$

Invoking the product rule, we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left[\left(\frac{\partial^2 x(t)}{\partial x^2(0)}\right)\right] &= \left[\frac{\partial}{\partial x(0)}\left(\frac{\partial f(x,\alpha)}{\partial x(t)}\right)\right]\frac{\partial x(t)}{\partial x(0)} \\ &\quad + \left(\frac{\partial f(x,\alpha)}{\partial x(t)}\right)\frac{\partial}{\partial x(0)}\left(\frac{\partial x(t)}{\partial x(0)}\right) \\ &= \frac{\partial f^2(x,\alpha)}{\partial x^2(t)}\left(\frac{\partial x(t)}{\partial x(0)}\right)^2 + \frac{\partial f(x,\alpha)}{\partial x(t)}\left(\frac{\partial^2 x(t)}{\partial x^2(0)}\right).\end{aligned} \tag{2.3.2}$$

Define

$$u_2 = \frac{\partial^2 x(t)}{\partial x^2(0)},\ \mathbf{D}_x^2(f) = \frac{\partial^2 f}{\partial x^2}. \tag{2.3.3}$$

Substituting (2.3.3) in (2.3.2), the required dynamics takes the form

$$\frac{\mathrm{d}u_2}{\mathrm{d}t} = \mathbf{D}_x(f)u_2 + \mathbf{D}_x^2(f)u_1^2 \tag{2.3.4}$$

with the initial conditions

$$u_2(0) = \left.\frac{\partial^2 x(t)}{\partial x^2(0)}\right|_{t=0} = \left.\frac{\partial}{\partial x(0)}\left(\frac{\partial x(t)}{\partial x(0)}\right)\right|_{t=0} = \frac{\partial}{\partial x(0)}(1) = 0 \tag{2.3.5}$$

which is a scalar, linear, non-autonomous, non-homogeneous, first-order ordinary differential equation.

2.3.2 Evolution of $\partial^2 x(t)/\partial\alpha^2$

Now consider the evolution of the first-order sensitivity of $x(t)$ with respect to α given in (2.1.8), which is reproduced here for convenience:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x(t)}{\partial\alpha}\right) = \left(\frac{\partial f(x,\alpha)}{\partial x(t)}\right)\left(\frac{\partial x(t)}{\partial\alpha}\right) + \frac{\partial f}{\partial\alpha}. \tag{2.3.6}$$

Differentiating both sides with respect to α, using product rule, we get

$$\begin{aligned}\frac{d}{dt}\left[\left(\frac{\partial^2 x(t)}{\partial\alpha^2}\right)\right] = {} & \frac{\partial}{\partial\alpha}\left[\left(\frac{\partial f(x,\alpha)}{\partial x(t)}\right)\right]\frac{\partial x(t)}{\partial\alpha} \\ & + \left(\frac{\partial f(x,\alpha)}{\partial x(t)}\right)\left(\frac{\partial^2 x(t)}{\partial\alpha^2}\right) + \frac{\partial}{\partial\alpha}\left(\frac{\partial f}{\partial\alpha}\right).\end{aligned} \tag{2.3.7}$$

While the first-order sensitivity dynamics in (2.1.3) is linear, homogeneous and non-autonomous, this second-order sensitivity equation is linear, non-homogeneous and non-autonomous.

Recall that, $f = f(x,\alpha)$ and $x(t) = x(t, x_0, \alpha)$. Hence,

$$\frac{\partial}{\partial\alpha}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial^2 f}{\partial x^2}\frac{\partial x}{\partial\alpha} + \left(\frac{\partial^2 f}{\partial x\partial\alpha}\right)$$

and

$$\frac{\partial}{\partial\alpha}\left(\frac{\partial f}{\partial\alpha}\right) = \left(\frac{\partial^2 f}{\partial x\partial\alpha}\right)\frac{\partial x}{\partial\alpha} + \frac{\partial^2 f}{\partial\alpha^2}.$$

Substituting (2.3.8) in (2.3.7) and simplifying, we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial^2 x(t)}{\partial\alpha^2}\right) = {} & \left(\frac{\partial^2 f}{\partial x^2(t)}\right)\left(\frac{\partial x}{\partial\alpha}\right)^2 + \left(\frac{\partial^2 f}{\partial x(t)\partial\alpha}\right)\left(\frac{\partial x(t)}{\partial\alpha}\right) \\ & + \left(\frac{\partial f}{\partial x(t)}\right)\left(\frac{\partial^2 x(t)}{\partial\alpha^2}\right) + \left(\frac{\partial^2 f}{\partial\alpha\partial x(t)}\right)\left(\frac{\partial x(t)}{\partial\alpha}\right) \\ & + \left(\frac{\partial^2 f}{\partial\alpha^2}\right).\end{aligned} \tag{2.3.8}$$

Define

$$v_2 = \frac{\partial^2 x(t)}{\partial\alpha^2}, \qquad \mathbf{D}^2_\alpha(f) = \frac{\partial^2 f}{\partial\alpha^2}, \qquad \mathbf{D}^2_{x\alpha}(f) = \frac{\partial^2 f}{\partial x\partial\alpha}. \tag{2.3.9}$$

Substituting (2.2.5), (2.3.3) and (2.3.9) in (2.3.8), the dynamics of evolution of the second-order sensitivity of $x(t)$, with respect to α is given by

$$\frac{\mathrm{d}v_2}{\mathrm{d}t} = \mathbf{D}_x(f)v_2 + \mathbf{D}_x^2(f)v_1^2 + 2\mathbf{D}_{x\alpha}^2(f)v_1 + \mathbf{D}_\alpha{}^2(f), \tag{2.3.10}$$

which is a scalar, linear, non-autonomous and non-homogeneous ordinary differential equation, with the initial condition

$$v_2(0) = \left.\frac{\partial^2 x(t)}{\partial\alpha^2}\right|_{t=0} = \frac{\partial}{\partial x(0)}\left(\frac{\partial x(t)}{\partial\alpha}\right)\Bigg|_{t=0} = \frac{\partial}{\partial\alpha}(0) = 0$$

2.3.3 Evolution of $\partial^2 x(t)/\partial\alpha\partial x(0)$

The evolution of this second-order cross sensitivity can be derived starting either from (2.3.1) or (2.3.6). For definiteness, we start with (2.3.6). Now differentiate both sides of (2.3.6) with respect to $x(0)$, we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial^2 x(t)}{\partial x(0)\partial\alpha}\right) &= \left[\frac{\partial}{\partial x(0)}\left(\frac{\partial f}{\partial x(t)}\right)\right]\left(\frac{\partial x(t)}{\partial\alpha}\right)\\ &\quad+\left(\frac{\partial f}{\partial x(t)}\right)\frac{\partial}{\partial x(0)}\left(\frac{\partial x(t)}{\partial\alpha}\right)+\frac{\partial}{\partial x(0)}\left(\frac{\partial f}{\partial\alpha}\right)\\ &= \left(\frac{\partial^2 f}{\partial x^2(t)}\right)\left(\frac{\partial x(t)}{\partial x(0)}\right)\left(\frac{\partial x(t)}{\partial\alpha}\right)\\ &\quad+\left(\frac{\partial f}{\partial x(t)}\right)\left(\frac{\partial^2 x(t)}{\partial x(0)\partial\alpha}\right)+\left(\frac{\partial^2 f}{\partial\alpha\partial x}\right)\frac{\partial x(t)}{\partial x(0)}\end{aligned} \tag{2.3.11}$$

Using (2.2.5), (2.3.3) and (2.3.9) in (2.3.11), the required dynamics becomes

$$\frac{d}{dt}\left(\frac{\partial^2 x(t)}{\partial x(0)\partial\alpha}\right) = \mathbf{D}_x(f)\left(\frac{\partial^2 x(t)}{\partial x(0)\partial\alpha}\right) + \mathbf{D}_x^2(f)u_1v_1 + \mathbf{D}_{x\alpha}^2(f)u_1, \tag{2.3.12}$$

where the initial condition

$$\left.\frac{\partial^2 x(t)}{\partial x(0)\partial\alpha}\right|_{t=0} = \frac{\partial}{\partial\alpha}\left(\frac{\partial x(t)}{\partial x(0)}\right)\Bigg|_{t=0} = \frac{\partial}{\partial x(0)}(1) = 0. \tag{2.3.13}$$

2.4 Data Assimilation Using FSM: A Second-Order Method

Referring to (2.2.3), a second-order approximation to Δx given by

$$\Delta x \approx \delta x(k) + \delta^2 x(k) \tag{2.4.1}$$

where, as before

$$\delta x(k) = \left[\frac{\partial x(k)}{\partial x(0)}, \frac{\partial x(k)}{\partial \alpha}\right]\begin{bmatrix}\delta x(0)\\ \delta\alpha\end{bmatrix} = \mathbf{D}_c(x)\boldsymbol{\zeta} \tag{2.4.2}$$

and $\mathbf{D_c}$ is the Jacobian of $x(k)$ with respect to $\boldsymbol{\zeta}$. Similarly

$$\begin{aligned}\delta^2 x(k) &= \frac{1}{2}\left(\delta x(0), \delta\alpha\right)\begin{bmatrix}\frac{\partial^2 x(k)}{\partial x^2(0)} & \frac{\partial^2 x(k)}{\partial\alpha\,\partial x(0)}\\ \frac{\partial^2 x(k)}{\partial x(0)\partial\alpha} & \frac{\partial^2 x(k)}{\partial\alpha^2}\end{bmatrix}\begin{bmatrix}\delta x(0)\\ \delta\alpha\end{bmatrix}\\ &= \frac{1}{2}\boldsymbol{\zeta}^T\mathbf{D}_c^2(x)\boldsymbol{\zeta}\end{aligned} \tag{2.4.3}$$

where $\mathbf{D}^2_{\mathbf{c}}(x)$ is the Hessian of x with respect to $\mathbf{c}$. For simplicity in algebra, again consider case of a single observation $z(k)$ at time k where

$$z(k) = h\left(x(k)\right) + \nu(k) \tag{2.4.4}$$

Again, from first principles, the second-order change Δh in $h(x)$ induced by the change Δx in x is given by

$$\Delta h = h\left(x + \Delta x\right) - h(x) = \delta h + \delta^2 h \tag{2.4.5}$$

where

$$\begin{aligned}\delta\mathbf{h} &= \left(\frac{\partial h}{\partial x}\right)\delta x = \mathbf{D}_x(h)\delta x \text{ and}\\ \delta^2 h &= \frac{1}{2}\left(\frac{\partial^2 h}{\partial x^2}\right)(\delta x)^2 = \frac{1}{2}\mathbf{D}_x^2(h)(\delta x)^2\end{aligned} \tag{2.4.6}$$

Now, substituting (2.4.1)–(2.4.3) into (2.4.5) we get

$$\begin{aligned}\Delta\mathbf{h} =\ & \mathbf{D}_x(h)\left[\mathbf{D}_c(x)\boldsymbol{\zeta} + \frac{1}{2}\boldsymbol{\zeta}^T\mathbf{D}_c^2(x)\boldsymbol{\zeta}\right]\\ & + \frac{1}{2}\mathbf{D}_x^2(h)\left[\mathbf{D}_c(x)\boldsymbol{\zeta} + \frac{1}{2}\boldsymbol{\zeta}^T\mathbf{D}_c^2(x)\boldsymbol{\zeta}\right]^2\end{aligned} \tag{2.4.7}$$

which is already a 4th-degree polynomial in the components of $\boldsymbol{\zeta}$.

Since we are interested in the second-order approximation, dropping the terms of degree 3 or more in $\boldsymbol{\zeta}$ from (2.4.7), we obtain[1]

$$\Delta\mathbf{h} = \mathbf{H}\boldsymbol{\zeta} + \boldsymbol{\zeta}^T A\boldsymbol{\zeta} \tag{2.4.8}$$

where

$$\begin{aligned}
\mathbf{H} &= \mathbf{D}_x(h)\mathbf{D}_c(x) \in \mathbb{R}^{1\times 2} \\
\mathbf{A} &= \mathbf{a}_1\mathbf{D}_c^2(x) + \mathbf{a}_2\,\mathbf{D}_c^T(x)\,\mathbf{D}_c(x) \in \mathbb{R}^{2\times 2} \\
\mathbf{a}_1 &= \frac{1}{2}D_x(h) \quad \text{and} \quad \mathbf{a}_2 = \frac{1}{2}\mathbf{D}_x^2(h).
\end{aligned} \tag{2.4.9}$$

If $h(x) = x$, then $\mathbf{D_x}(h) = 1$ and $\mathbf{D}_x^2(h) = 0$. In this case, $a_1 = 1/2$ and $a_2 = 0$, and A is the Hessian multiplied by 0.5. Our goal is to find $\boldsymbol{\zeta}$ such that

$$\mathbf{z}(k) \approx h(x(k) + \Delta x) = \mathbf{h}(x(k)) + \Delta h \tag{2.4.10}$$

or

$$\Delta\mathbf{h} = \mathbf{e}_F(k) = \mathbf{z}(k) - \mathbf{h}(x(k)).$$

Substituting for Δh from (2.4.8), we obtain the following constraint associated with the FSM process.

$$\mathbf{g}(\boldsymbol{\zeta}) = \mathbf{H}\boldsymbol{\zeta} + \boldsymbol{\zeta}^T A\boldsymbol{\zeta} = \mathbf{e}_F. \tag{2.4.11}$$

We do not demand that this constraint be satisfied exactly, but that the squares of the residual associated with this equation be minimized. This condition is expressed as minimization of

$$\mathbf{f}(\boldsymbol{\zeta}) = \frac{1}{2}\left[\mathbf{e}_F - H\boldsymbol{\zeta} - \boldsymbol{\zeta}^T\mathbf{A}\boldsymbol{\zeta}\right]^2, \tag{2.4.12}$$

which is a polynomial of degree 4 in the components of $\boldsymbol{\zeta}$ (Lakshmivarahan et al. 2003). We drop all terms of degree 3 or more from the right hand side of (2.4.12), and obtain the full quadratic approximation $\mathbf{Q}(\boldsymbol{\zeta})$ to $\mathbf{f}(\boldsymbol{\zeta})$ given by

$$\begin{aligned}
\mathbf{Q}(\boldsymbol{\zeta}) &= \frac{1}{2}\left[\mathbf{e}_F - 2\mathbf{e}_F\left(\mathbf{H}\boldsymbol{\zeta} + \boldsymbol{\zeta}^T\mathbf{A}\boldsymbol{\zeta}\right) + \boldsymbol{\zeta}^T\mathbf{H}^T\mathbf{H}\boldsymbol{\zeta}\right] \\
&= \frac{1}{2}\left[\mathbf{e}_F^2 - 2\mathbf{e}_F\mathbf{H}\boldsymbol{\zeta} + \boldsymbol{\zeta}^T\left(\mathbf{H}^T\mathbf{H} - 2\mathbf{e}_F\mathbf{A}\right)\boldsymbol{\zeta}\right].
\end{aligned} \tag{2.4.13}$$

[1] Using $(\mathbf{a}^T\mathbf{x})^2 = \mathbf{a}^T\mathbf{x}\,\mathbf{a}^T\mathbf{x} = \mathbf{x}^T(\mathbf{a}\mathbf{a}^T)\mathbf{x}$, where $\mathbf{a}$ and $\mathbf{x}$ are column vectors.

Setting the gradient of $Q(\boldsymbol{\zeta})$ with respect to $\boldsymbol{\zeta}$ equal to zero, we obtain

$$\left[\mathbf{H}^T\mathbf{H} - 2\mathbf{e}_F\mathbf{A}\right]\boldsymbol{\zeta} = \mathbf{H}^T\mathbf{e}_F \tag{2.4.14}$$

The solution of (2.4.14) is indeed a minimum provided, the Hessian of $\mathbf{Q}(\boldsymbol{\zeta})$, using (2.4.9), is given by

$$\begin{aligned}\nabla^2\mathbf{Q}(\boldsymbol{\zeta}) &= \mathbf{H}^T\mathbf{H} - 2\mathbf{e}_F\mathbf{A}\\ &= \mathbf{H}^T\mathbf{H} - \mathbf{e}_F\left[\mathbf{D}_x(h)\mathbf{D}^2_{\zeta}(x) + \mathbf{D}^2_x(h)\mathbf{D}^T_{\zeta}(x)\mathbf{D}_{\zeta}(x)\right]\end{aligned} \tag{2.4.15}$$

is positive definite.

When two or more observations are considered, the stacked form of the sensitivities and error as found in (2.2.25) come into play. In place of (2.4.14), we get

$$\left[\mathbf{H}^T\mathbf{H} - 2e_F(t_1)A(t_1) - e_F(t_2)A(t_2)\cdots - e_F(t_N)A(t_N)\right]\zeta = \mathbf{H}^T\mathbf{e}_F \tag{2.4.16}$$

2.5 FSM: Discrete Time Formulation

In Sects. 2.1 and 2.2 we have illustrated the basic principles that underlie the first-order forward sensitivity method (FSM) using a simple, scalar model in continuous time. However, in practice without exception, all the large scale models operate in discrete time. As a prelude to this transition, we derive the dynamics of first-order and second-order sensitivity evolution in discrete time.

2.5.1 Discrete Evolution of First-Order Forward Sensitivities

Discretizing equation (2.1.1) using the standard Euler scheme (Richtmyer and Morton 1967), we obtain

$$x(k+1) = \mathbf{M}(x(k), \alpha). \tag{2.5.1}$$

where $M : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a nonlinear function given by

$$M(x(k), \alpha) = x(k) + \Delta t f(x(k), \alpha) \tag{2.5.2}$$

where Δt is the length interval used in time discretization. Differentiating (2.5.1) with respect to $x(0)$, we readily obtain the dynamics of evolution of the first-order forward sensitivity $\partial x(k)/\partial x(0)$ as

$$\frac{\partial x(k+1)}{\partial x(0)} = \frac{\partial M\,(x(k),\alpha)}{\partial x(k)}\frac{\partial x(k)}{\partial x(0)} \tag{2.5.3}$$

with

$$\left.\frac{\partial x(k)}{\partial x(0)}\right|_{k=0} = 1$$

as the initial condition. Much like its continuous time counterpart, (2.5.3) is a linear, homogeneous and non-autonomous first-order difference equation. Setting

$$u_1(k) = \frac{\partial x(k)}{\partial x(0)}, \quad \text{and } \mathbf{D}_x(M) = \frac{\partial M\,(x(k), \alpha)}{\partial x(k)}, \tag{2.5.4}$$

the discrete time evolution in (2.5.3) can be written as

$$u_1(k+1) = \mathbf{D}_{x(k)}(\mathbf{M})\, u_1(k) \;\text{ with }\; u_1(0) = 1. \tag{2.5.5}$$

Alternatively, one could also obtain (2.5.3) by discretizing (2.1.3) using the Euler scheme (Problem 2.1)

$$\mathbf{D}_x(M) = 1 + \Delta t \mathbf{D}_x(f). \tag{2.5.6}$$

Similarly, differentiating (2.5.1) with respect to α, we get

$$\frac{\partial x(k+1)}{\partial \alpha} = \frac{\partial M\,(x(k), \alpha)}{\partial x(k)} \frac{\partial x(k)}{\partial \alpha} + \frac{\partial M\,(x(k), \alpha)}{\partial \alpha} \tag{2.5.7}$$

Setting

$$v_1(k) = \frac{\partial x(k)}{\partial \alpha} \quad \text{and} \quad \mathbf{D}_\alpha = \frac{\partial M\,(x(k), \alpha)}{\partial \alpha} \tag{2.5.8}$$

in (2.5.7), the latter becomes

$$v_1(k+1) = \mathbf{D}_{x(k)}(M) v_1(k) + \mathbf{D}_\alpha(M) \tag{2.5.9}$$

which is the discrete time analog of (2.1.8) for the evolution of the forward sensitivity $v_1(k)$. Derivation of (2.5.9) by directly discretizing (2.1.8) is left as the Problem 2.1.

Example 2. Consider the discrete time version of the logistic model for population dynamics given by

$$x(k+1) = \alpha x(k)\,(1 - x(k)) \;\text{ for }\; \alpha > 0. \tag{2.5.10}$$

Then $M(x, \alpha) = \alpha x(1 - x)$ and $\mathbf{D}_x(M) = \alpha(1 - 2x)$, and $\mathbf{D}_\alpha(M) = x(1 - x)$.

Hence

$$\frac{\partial x(k+1)}{\partial x(0)} = \alpha\,(1-2x(k))\,\frac{\partial x(k)}{\partial x(0)} \quad \text{with} \quad \frac{\partial x(0)}{\partial x(0)} = 1, \tag{2.5.11}$$

and

$$\begin{aligned} \frac{\partial x(k+1)}{\partial \alpha} &= \alpha\,(1-2x(k))\,\frac{\partial x(k)}{\partial \alpha} + x(k)(1-x(k)), \text{ with} \\ \frac{\partial x(0)}{\partial \alpha} &= 0. \end{aligned} \tag{2.5.12}$$

Plots of the solution of (2.5.11) and (2.5.12) are given in Figs. 2.6 and 2.7. Figure 2.8 contains the plot of the asymptotic state $x(0)$ for various values of $1 \leq \alpha \leq 4$. Figure 2.8 is obtained by fixing a value of the parameter in the range $1 \leq \alpha \leq 4$ in steps of 0.001 and running the model 2.5.10 for a long time until steady state $x(\infty)$ is reached. For $1 \leq \alpha \leq 3$, there is a unique steady state. For $3 < \alpha \leq 3.45$, we observe the first bifurcation, called periodic doubling where $x(\infty)$ oscillates between two values. Further periodic doubling occurs where $3.45 \leq \alpha \leq 3.54$ and the system exhibits non-chaotic behavior for $\alpha < 3.57$. When α is around 3.57, there is a cascading of periodic doubling behavior which signals the onset of chaos. An expanded view of Fig. 2.8 for $3 \leq \alpha \leq 4$ is given in Fig. 2.9

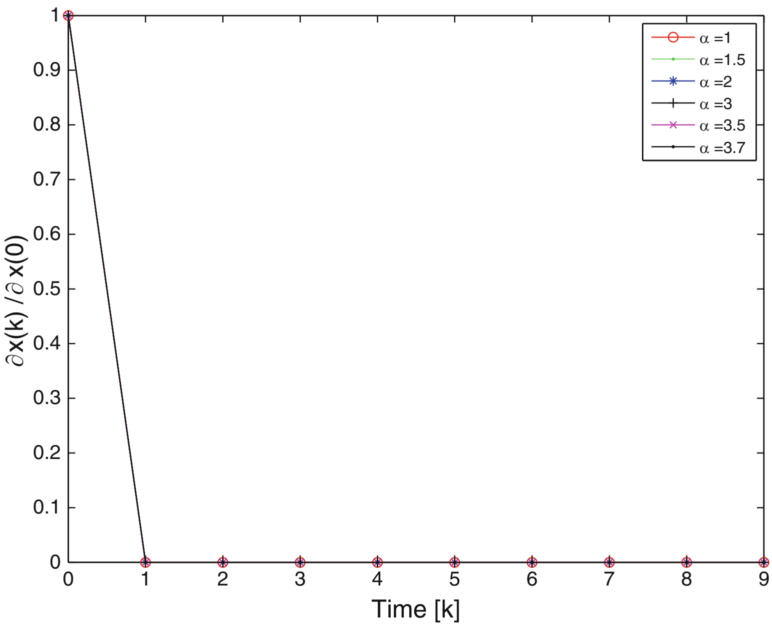


Fig. 2.6 Sensitivity to initial condition $x(0)$

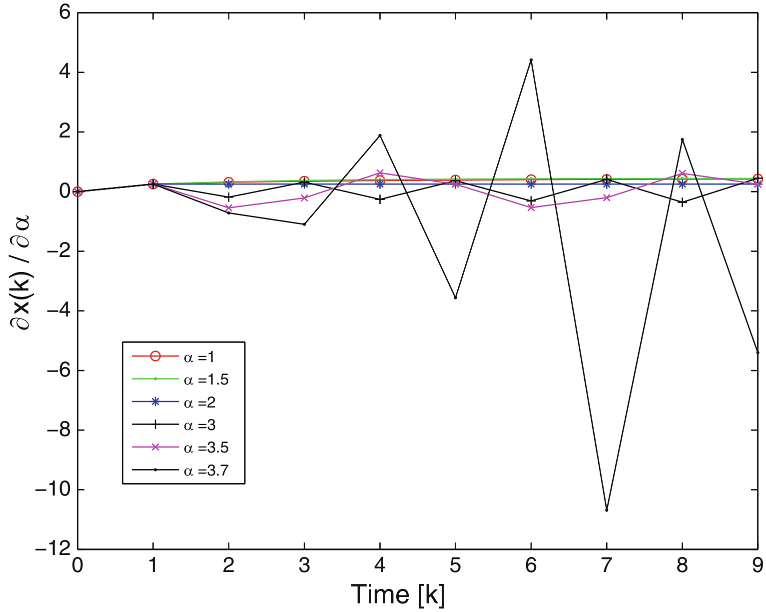


Fig. 2.7 Sensitivity to value of α

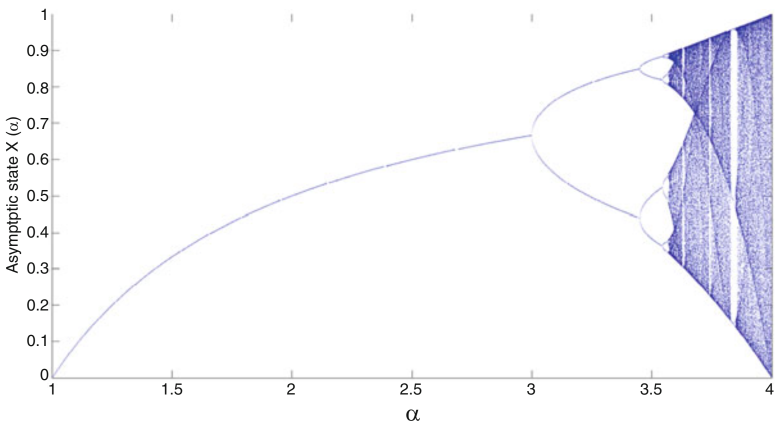


Fig. 2.8 Asymptotic state for various values of $1 \leq \boldsymbol{\alpha} \leq 4$

where one can identify gaps in the final state diagram. These gaps are due to the so called "intermittency" of the chaotic behavior. Refer to Peitgen et al. (1992) for more details.

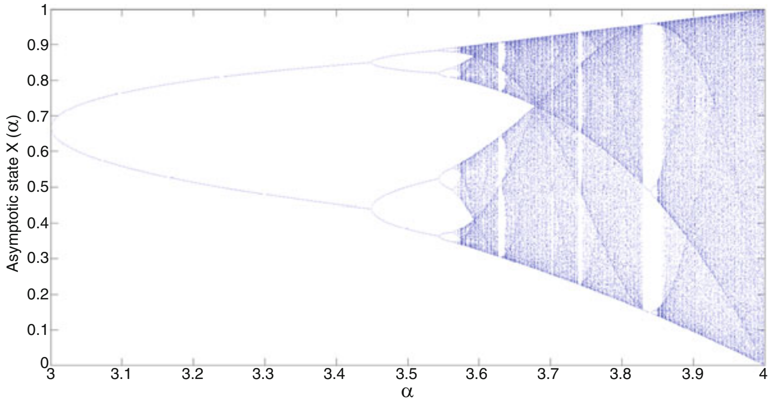


Fig. 2.9 Asymptotic state for various values of $3 \le \boldsymbol{\alpha} \le 4$

2.5.2 Discrete Evolution of Second-Order Forward Sensitivity

By following the first principles used in the derivation of dynamics of evolution of second-order forward sensitivities in Sect. 2.5, it can be verified that the discrete time evolution of second-order sensitivities are given by (Problem 2.2).

$$\frac{\partial^2 x(k+1)}{\partial x^2(0)} = \frac{\partial M}{\partial x(k)} \frac{\partial^2 x(k)}{\partial x^2(0)} + \frac{\partial^2 M}{\partial x^2(k)} \left(\frac{\partial x(k)}{\partial x(0)} \right)^2 \tag{2.5.13}$$

$$\begin{aligned} \frac{\partial^2 x(k+1)}{\partial \alpha^2} &= \frac{\partial M}{\partial x(k)} \frac{\partial^2 x(k)}{\partial \alpha^2} + \frac{\partial^2 M}{\partial x^2(k)} \left(\frac{\partial x(k)}{\partial \alpha} \right)^2 \\ &\quad + 2 \left(\frac{\partial^2 M}{\partial x(0) \partial \alpha} \right) \left(\frac{\partial x(k)}{\partial \alpha} \right) + \frac{\partial^2 M}{\partial \alpha^2} \end{aligned} \tag{2.5.14}$$

and

$$\begin{aligned} \frac{\partial^2 x(k+1)}{\partial x(0) \partial \alpha} &= \left(\frac{\partial M}{\partial x(k)} \right) \left(\frac{\partial^2 x(k)}{\partial x(0) \partial \alpha} \right) \\ &\quad + \frac{\partial^2 M}{\partial x^2(k)} \frac{\partial x(k)}{\partial \alpha} \frac{\partial x(k)}{\partial x(0)} + \left(\frac{\partial^2 M}{\partial x(k) \partial \alpha} \right) \frac{\partial x(k)}{\partial x(0)} \end{aligned} \tag{2.5.15}$$

2.6 Sensitivity to Initial Conditions and Lyapunov Index

As stated in Chap. 1, some models exhibit extreme sensitivity to initial conditions for certain ranges of values of the parameter. The logistic model is an example we discussed in Sect. 2.5 (Example 2)—a text book case known to exhibit extreme sensitivity to initial conditions when $\alpha = 4$. In such situations, a slight perturbation to the initial condition grows with time and masks the quality forecast. This growth of error naturally leads to predictability limits as discussed further in this section. The Lyapunov index is a natural measure that helps quantify the predictability limit.

2.6.1 Continuous Time Model

Consider the forecast model of the type (2.1.1). Let $\bar{x}(t)$ be the base trajectory of this model starting from the base initial condition $\bar{x}(0)$. Let

$$x(0) = \bar{x}(0) + y(0) \tag{2.6.1}$$

be the modified initial condition obtained by adding a perturbation $y(0)$ to $\bar{x}(0)$. Let $x(t)$ be the solution of (2.1.1) starting from $x(0)$. Then

$$y(t) = x(t) - \bar{x}(t). \tag{2.6.2}$$

Differentiating both sides of (2.6.2) and using (2.1.1), we get

$$\dot{y}(t) = f\,(x(t), \alpha) - f\,(\bar{x}(t), \alpha)\,. \tag{2.6.3}$$

Substituting (2.6.2) into the first term on the right-hand side of (2.6.3) and expanding in the first-order Taylor series, we readily obtain the dynamics of perturbation evolution:

$$\dot{y}(t) = \mathbf{D}_{\bar{x}(t)}(f)y(t). \tag{2.6.4}$$

This is a scalar linear, non-autonomous O.D.E. of the same type as the FSM dynamics in (2.1.5). Equation (2.6.4) is also called the *tangent linear system* or the *variational equation* in the literature. The initial condition for (2.1.5) is $u(0) = \left.\frac{\partial x(t)}{\partial x(0)}\right|_{t=0} = 1$, while that of (2.6.4) is $y(0)$, which is the perturbation on the initial condition $\bar{x}(0)$.

Let $[0, T]$ be the time interval that denotes the forecast horizon. Discretize this time interval into N subintervals of equal length τ, where $T = N\tau$. It is reasonable to assume that the Jacobian $\mathbf{D}_{\bar{x}(t)}(f)$ remains nearly constant in the kth subinterval $[(k-1)\tau, k\tau]$ by choosing an appropriate value of τ. Define

$$L_{k-1} = \left.\mathbf{D}_{\bar{x}(t)}(f)\right|_{t=(k-1)\tau} \tag{2.6.5}$$

Then, on this kth subinterval $(k-1)\tau \leq t \leq k\tau$, we can represent (2.6.4) as

$$\dot{y} = L_{k-1} y \tag{2.6.6}$$

for $k = 1, 2, \ldots, N$. Solving (2.6.6), we get

$$y_k = y_{k-1} e^{L_{k-1}\tau}, \tag{2.6.7}$$

where $y_k = y(t = k\tau)$. Clearly $e^{L_{k-1}\tau}$ is the error magnification during the kth subinterval. Iterating (2.6.7), it follows that

$$y_k = y_0 e^{\left(\sum_{k=0}^{N-1} L_k\right)\tau} \tag{2.6.8}$$

Thus, the perturbation y_k at time k is related to that at time $k = 0$ through a magnification/amplification factor that is given by the exponential term on the right hand side of (2.6.8). The Lyapunov index λ is defined by

$$\lambda = \lim_{T\to\infty} \lim_{N\to\infty} \frac{1}{(N\tau)} \ln\left(\frac{|y_k|}{|y_0|}\right) \tag{2.6.9}$$

Thus, when T is large and τ is very small, at time $t = k\tau$, we can express

$$y_k \approx e^{\lambda t} y_0 \tag{2.6.10}$$

Using (2.6.8) in (2.6.9), it readily follows that

$$\lambda = \lim_{T\to\infty} \lim_{N\to\infty} \frac{1}{N} \left(\sum_{k=0}^{N-1} L_k\right). \tag{2.6.11}$$

Thus, λ denotes the long term average growth rate of errors.

2.6.2 Discrete Time Model

Starting from the discrete time model in (2.5.1), let $\bar{x}(k)$ be the base trajectory starting from $\bar{x}(0)$. If $x(0) = \bar{x}(0) + y(0)$ with $y(0)$ as the initial perturbation, then the perturbation $y(k) = x(k) - \bar{x}(k)$ is given by

$$\mathbf{y}(k) = \mathbf{M}\left(x(k,\alpha)\right) - \mathbf{M}\left(\bar{x}(k),\alpha\right). \tag{2.6.12}$$

Expanding the first term on the right hand side in a first-order Taylor series around $\bar{x}(k)$, the dynamics of evolution of the perturbation is given by the tangent linear system

$$\mathbf{y}(k+1) = \mathbf{D}_{\bar{x}(k)}(\mathbf{M}) y(k) \tag{2.6.13}$$

Iterating, we obtain (refer to Problem 2.5)

$$\mathbf{y}(k) = \left[{\prod_{i=0}^{k-1}}' A(i) \right] y(0). \tag{2.6.14}$$

where $\mathbf{A}(i) = \mathbf{D}_{\bar{x}(i)}(\mathbf{M})$ for simplicity in notation. From Problem 2.5, it can be verified that

$$y(k) = u_1(k)y(0), \tag{2.6.15}$$

where

$$u_1(k) = {\prod_{i=0}^{k-1}}' \mathbf{D}_{x(i)}(M) = \frac{\partial \bar{x}(k)}{\partial \bar{x}(0)}, \tag{2.6.16}$$

the forward sensitivity of the solution $\bar{x}(k)$ with respect to $\bar{x}(0)$. Define

$$\Lambda(k) = \left(\frac{y(k)}{y(0)} \right)^{1/k} = \left[\prod_{i=0}^{k-1} A(i) \right]^{1/k} = [u_1(k)]^{1/k} \tag{2.6.17}$$

which is the geometric mean of the forward sensitivity at time k. Then, from the definition, the expression for the Lyapunov index is given by

$$\begin{aligned} \lambda &= \lim_{k\to\infty} \ln(\Lambda(k)) \\ &= \lim_{k\to\infty} \frac{1}{k} \sum_{i=0}^{k-1} \ln A(i) \\ &= \lim_{k\to\infty} \frac{1}{k} \ln u_1(k), \end{aligned} \tag{2.6.18}$$

which is the long-term average of the logarithm of the first-order forward sensitivities.

2.7 Exercises

Problem 2.1. By directly discretizing (2.1.3) and (2.1.8) using the standard Euler scheme, obtain the corresponding discrete dynamics given in (2.5.3) and (2.5.9) respectively.

Problem 2.2. Starting from (2.5.3) and (2.5.9), derive the dynamics of the evolution of second-order forward sensitivities given in (2.5.13)–(2.5.15) .

Problem 2.3. Consider a linear, first-order, time varying and non-homogeneous recurrence relation

$$\mathbf{y}(k+1) = \mathbf{A}(k)\mathbf{y}(k) + \mathbf{B}(k),$$

where $\mathbf{y}(k) \in \mathbb{R}^n, \mathbf{A}(k) \in \mathbb{R}^{n\times n}$ and $\mathbf{B}(k) \in \mathbb{R}^n$ with $\mathbf{y}(0) \in \mathbb{R}^n$ as the initial condition. We illustrate the *method of substitution* for solving the above recurrence relation. Clearly

$$\begin{aligned}
\mathbf{y}(1) &= \mathbf{A}(0)\mathbf{y}(0) + \mathbf{B}(0),\\
\mathbf{y}(2) &= \mathbf{A}(1)y(1) + \mathbf{B}(1)\\
&= \mathbf{A}(1)\mathbf{A}(0)y(0) + \mathbf{A}(1)B(0) + \mathbf{B}(1),\\
\mathbf{y}(3) &= \mathbf{A}(2)\mathbf{y}(2) + \mathbf{B}(2)\\
&= \mathbf{A}(2)\mathbf{A}(1)\mathbf{A}(0)\mathbf{y}(0) + \mathbf{A}(2)\mathbf{A}(1)\mathbf{B}(0) + \mathbf{A}(2)\mathbf{B}(1) + \mathbf{B}(1).
\end{aligned}$$

Verify inductively that

$$\mathbf{y}(k) = \left[\prod_{i=0}^{k-1}{}' \mathbf{A}(i)\right]\mathbf{y}(0) + \sum_{i=0}^{k-1}\left[\prod_{q=i+1}^{k-1}{}' \mathbf{A}(q)\right]\mathbf{B}(i)$$

where to indicate the order of indices in the product we use two symbols:

$$\begin{aligned}
\prod_{i=0}^{k}\mathbf{A}(i) &= \mathbf{A}(0)\mathbf{A}(1)\ldots\mathbf{A}(k)\text{—natural order}\\
\prod_{i=0}^{k}{}'\mathbf{A}(i) &= \mathbf{A}(k)\mathbf{A}(k-1)\ldots\mathbf{A}(0)\text{—reverse order}
\end{aligned}$$

and

$$\prod_{i=p}^{q}\mathbf{A}(i) = 1 \;\text{ if }\; q < p\text{—vacuous product .}$$

While these two products are the same when $\mathbf{A}(i)$ are scalars, they are distinct when $\mathbf{A}(i)$ are matrices.

Problem 2.4. Consider the linear, first-order, time varying and homogeneous recurrence (2.5.9) that describes the evolution of the first-order sensitivity vector $\mathbf{v}_1(k) \in \mathbb{R}^p$, of $x(k)$ with respect to $\boldsymbol{\alpha} \in \mathbb{R}^p$ given by

$$\mathbf{v}_1(k+1) = \mathbf{A}(k)\mathbf{v}_1(k) + \mathbf{B}(k), \;\text{ with }\; \mathbf{v}_1(0) = 0 \in \mathbb{R}^p$$

where $\mathbf{A}(k) = \mathbf{D}_{x(k)}(\mathbf{M})$ and $\mathbf{B}(k) = \mathbf{D}_\alpha(\mathbf{M}(x(k), \alpha))$ for simplicity in notation. The recurrence is structurally the same as the one in Exercise 2.3 given above. By setting $\mathbf{y}(k) = \mathbf{v}_1(k)$ and knowing that $\mathbf{v}_1(0) = 0$, verify that the solution $\mathbf{v}_1(k)$ is given by

$$\mathbf{D}_\alpha\,(x(k)) = \frac{\partial x(k)}{\partial \alpha} = \mathbf{v}_1(k) = \sum_{i=0}^{k-1}\left[\prod_{q=i+1}^{k-1}\mathbf{A}(q)\right]\mathbf{B}(i).$$

Problem 2.5. Consider the scalar, linear, time varying and homogeneous recurrence relation (2.5.5) that describes the evolution of the first-order sensitivity, $u_1(k) \in \mathbb{R}$ of the solution $x(k)$ with respect to the initial condition $x(0)$. It is given by

$$u_1(k+1) = A(k)u_1(k)$$

with $A(k) = \mathbf{D}_{x(k)}(\mathbf{M})$ and $u_1(0) = 1$. By setting $n = 1, y(k) = u_1(k)$ and $B(k) \equiv 0$ in the solution of the recurrence in Problem 2.3, verify that (since $u_1(0) = 1$) that

$$\mathbf{D}_{x(0)}\,(x(k)) = \frac{\partial x(k)}{\partial x(0)} = u_1(k) = \prod_{i=0}^{k-1}\mathbf{A}(i),$$

which is the product of the sensitivities of $x(k)$ along the trajectory.

Problem 2.6. Consider the logistic equation in continuous-time form with carrying capacity 1 ($0 \le x \le 1$) and growth parameter α given by

$$\frac{\partial x}{\partial t} = \alpha x\,(1-x) \quad \text{with} \quad x(0) = x_0.$$

a) Verify that the solution is given by

$$x(t) = \frac{x_0 e^{\alpha t}}{1 - x_0 + x_0^{\alpha t}}.$$

Plot $x(t)$ versus t when $x_0 = 0.5$ and $\alpha = 1.0$.

b) Compute $\partial x(t)/\partial x_0$ and $\partial x(t)/\partial \alpha$ and plot their evolutions.

c) Compute $\partial^2 x(t)/\partial x_0^2$, $\partial^2 x(t)/\partial \alpha^2$ and $\partial^2 x(t)/\partial x_0 \partial \alpha$ and also plot their evolutions.

Problem 2.7. [From Rabitz et al. (1983)] Consider a partial differential equation of type

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u, \alpha). \quad (*)$$

where D is a diffusion constant. When $u = u(x,0),\ t \geq 0,\ x_1 \leq x \leq x_2, f(u,\alpha)$ is some (nonlinear) function of u and the scalar parameter α. The initial condition for $u(x,t)$ is given by $u(x,0) = g(x)$ for all $x_1 \leq x \leq x_2$ and the boundary condition for $u(x,t)$ is given by

$$a_1 \frac{\partial u}{\partial x}\bigg|_{x=x_1} + b_1 u(x,t)\bigg|_{x=x_1} = A_1,$$
$$a_2 \frac{\partial u}{\partial x}\bigg|_{x=x_2} + b_2 u(x,t)\bigg|_{x=x_2} = A_2$$

where $a_i, b_i, A_i\,(1 \leq i \leq 2)$ are constants. Let $s(x,t) = \partial u(x,t)/\partial \alpha$ denote the sensitivity of the solution $u(x,t)$ with respect to α. Differentiating both sides of the partial differential equation ($*$) to verify that $s(x,t)$ is given by the solution of the following system

$$\frac{\partial s}{\partial t} = D\frac{\partial^2 s}{\partial x^2} + \frac{\partial f}{\partial u}s + \frac{\partial f}{\partial \alpha},$$

where $s(x,0) = \partial g/\partial \alpha$ is the initial condition and the boundary conditions are given by

$$a_1 \frac{\partial s}{\partial \alpha}\bigg|_{x=x_1} + b_1 s\bigg|_{x=x_1} = 0,$$
$$a_2 \frac{\partial s}{\partial \alpha}\bigg|_{x=x_2} + b_2 s\bigg|_{x=x_2} = 0.$$

Problem 2.8. Using (2.6.18) compute and plot the variation of the Lyapunov index with respect to the parameter α for the discrete time logistic model in Example 2 of Sect. 2.4.

2.7.1 Demonstrations

Demonstration: Air–Sea Interaction Model

Using the development in Example 1, Sect. 2.1, we solve the FSM data assimilation problem based on the dynamics of air–sea interaction. The solution take the analytic form

$$x(t, x_0, \theta, c) = (x(0) - \theta)e^{-ct} + \theta$$

as previously shown in (2.1.12). The development of formulas for first and second-order sensitivities, applicable to the air–sea interaction dynamics, appears in Sect. 2.1 and 2.3, respectively. The form of the FSM data assimilation process has been developed in Sect. 2.2 (first-order) and 2.4 (second-order).

In this demonstration, we test the FSM using: (i) first-order sensitivity (1 iteration), (ii) first-order sensitivity (2 iterations), (iii) second-order sensitivity dropping terms of power 3 and 4 in the functional [labeled second-order I], and (iv) second-order sensitivity including all power of control (up to power 4) [labeled second-order II]. The true control $\boldsymbol{c}$ $(x, \theta, \boldsymbol{c})$ and erroneous control $\boldsymbol{c}'$ are taken to be:

$$\boldsymbol{c} = (1.0, 11.0, 0.25)$$
$$\boldsymbol{c}' = (3.0, 9.0, 0.35)$$

Forecast is made from erroneous control in the presence of four observations. The observations, forecast, and increment (observation minus forecast) are displayed in Table 2.1.

Table 2.1 Observation (obs, x), forecast (fcst, x) and increment (obs–fcst) for numerical experiments

obs index	Time (h)	obs	fcst	Increment
1	1.0	3.49	4.77	−1.27
2	2.0	5.31	6.02	−0.71
3	8.0	8.93	8.64	0.29
4	12.0	10.28	8.91	1.37

Display of the forecast and observations is shown in Fig. ASI.1 where the Guess temperature is the forecast from erroneous control. The optimally adjusted forecasts from the four experiments are displayed in the two panels of Fig. ASI.2 (first-order FSM) and Fig. ASI.3 (second-order FSM). The optimal adjusted control for each case is shown in Table 2.2.

Table 2.2 Control for the various experiments

Control	X_0	θ	c
True	1.0	11.0	0.25
Erroneous	3.0	9.0	0.35
First-order (1 iter)	1.89	10.32	0.17
First-order (2 iter)	2.14	10.90	0.20
Second-order I	1.61	10.64	0.14
Second-order II	2.0	10.52	0.22

Results indicate that the 2-step first-order sensitivity method gives an excellent result. The 1-step first order method is acceptable. The second-order I is biased low. The second-order II is nearly perfect.

It may at first seem puzzling that the second-order method (full quadratic form) gave such a poor result. But the general philosophy of second order methods is that they provide value if the operating point is "close" to the local minimum—near the "well". Thus, FSM first-order method can be used to move close to the local minimum, and then use the second-order (full quadratic) to get closer to the minimum. We leave this as an exercise for the student. For most problems, the second-order method using all terms up to fourth order is extremely difficult or impossible to solve. In this case, steepest descent algorithm was used.

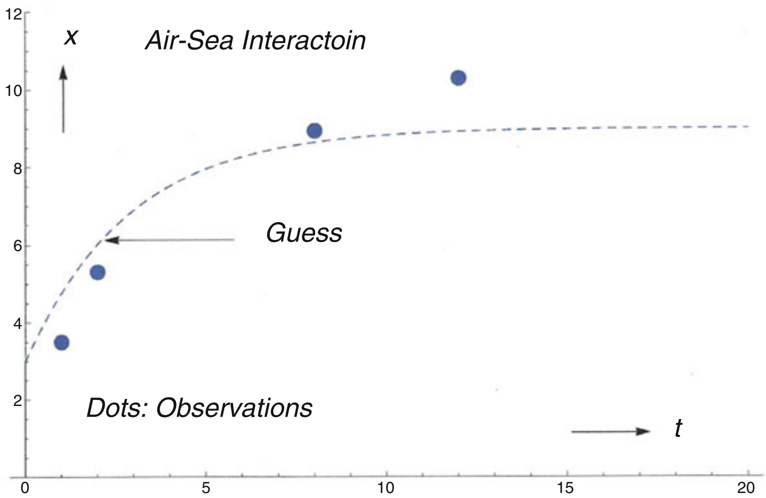


Fig. ASI.1 Guess temperature [$x(t)$] evolution with observations superimposed—sea–air interaction

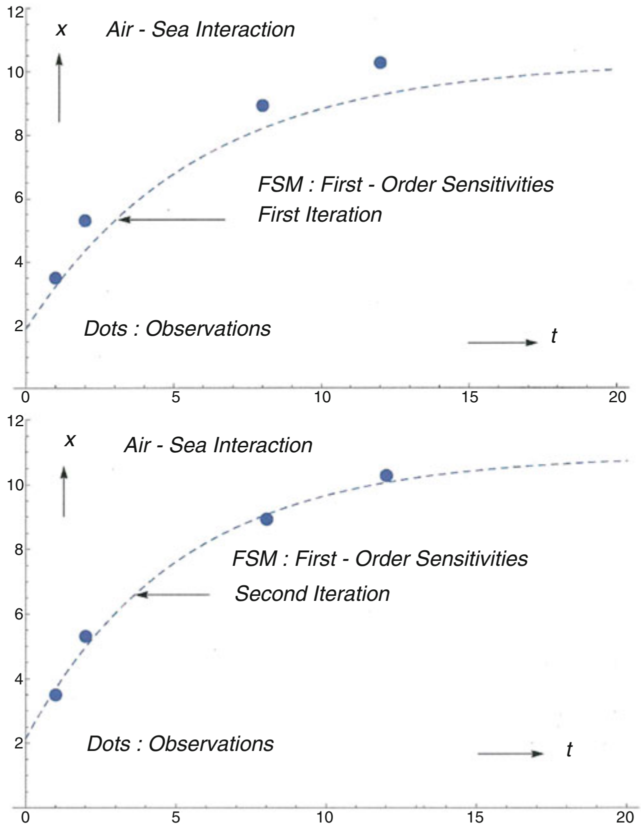


Fig. ASI.2 *Top panel*: Adjusted profile using FSM first-order sensitivity, first iteration. *Bottom panel*: Adjusted profile using FSM first-order sensitivity, 2 iterations

Demonstration: Gauss' Problem

In Lewis et al. (2006), a detailed account of Carl Friedrich Gauss' discovery of the method of least squares under dynamical constraint has been presented. The method was developed when Gauss succeeded in forecasting the time and place of reappearance of the "unknown planet" after its conjunction with the sun. There was only a limited number of observations of this celestial object between January 1, 1801, and February 11, 1801—a 42-day period of observation. The object was actually a large asteroid later named Ceres. Gauss' theoretical development of methodology that led to accurate prediction

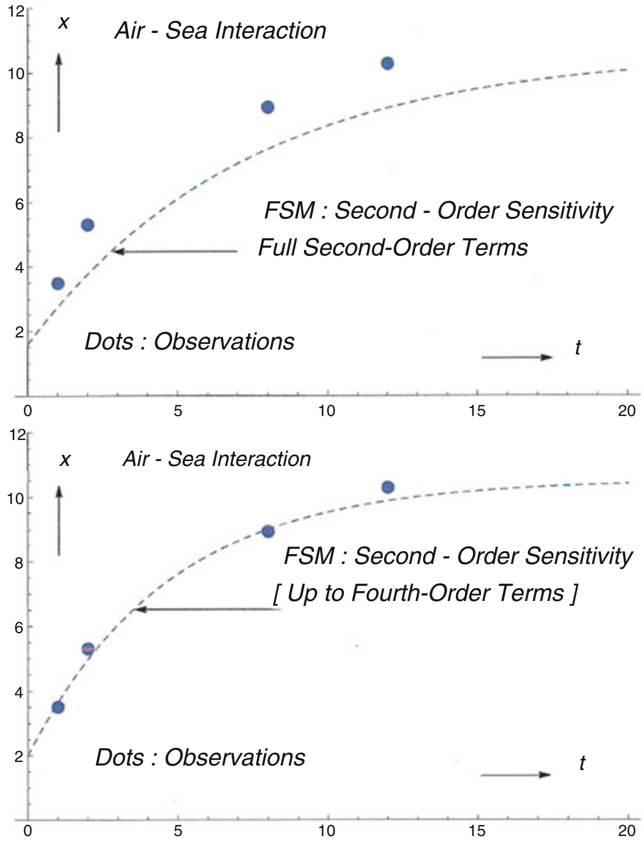


Fig. ASI.3 Adjusted profile using FSM second-order sensitivity (full quadratic form). *Bottom panel*: Adjusted profile using FSM second-order sensitivity (including terms up to fourth order in the functional)

of Ceres' orbit was published in November of the same year. Gauss' results were used to locate the asteroid on January 1, 1802, exactly 1 year after its first sighting. Figure GS.1 is a drawing of Gauss where the background schematic depicts three observations of Ceres' location relative to earth before it comes into conjunction with the sun.

In Lewis et al. (2006), a simplified version of Gauss' method of solution was discussed in detail with an outline of solution methodology based on 4D-VAR. The simplification was essentially the assumption that the asteroid and the earth moved about the sun along circular trajectories rather than elliptical trajectories.

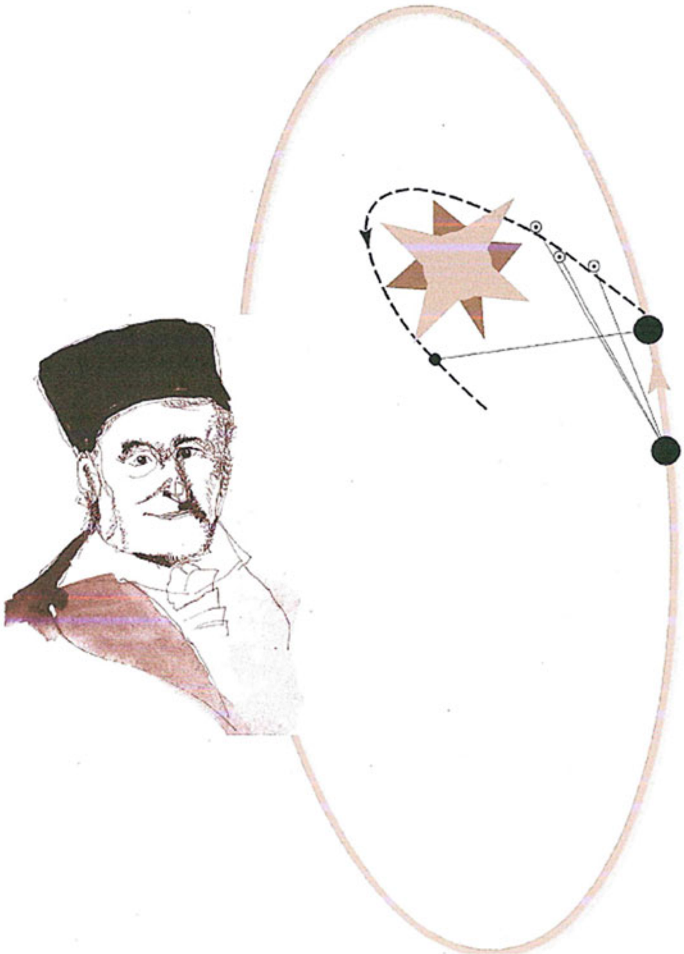


Fig. GS.1 Carl Friedrich Gauss in his academic garb shown aside a schematic showing positions of Ceres as observed from Earth in early 1801 (*small circled dots*) and in early 1802 (*small filled circle*)

We now approach the problem using FSM. The geometry of the problem is shown in Figs. GS.2 and GS.3, exactly the same figures used in Lewis et al. (2006)—Figs. 4.5.1 and 4.5.2 in that book. The nomenclature is described on the insert of Fig. GS.2 where we have assumed that the three bodies are initially co-planar and remain so into the future.

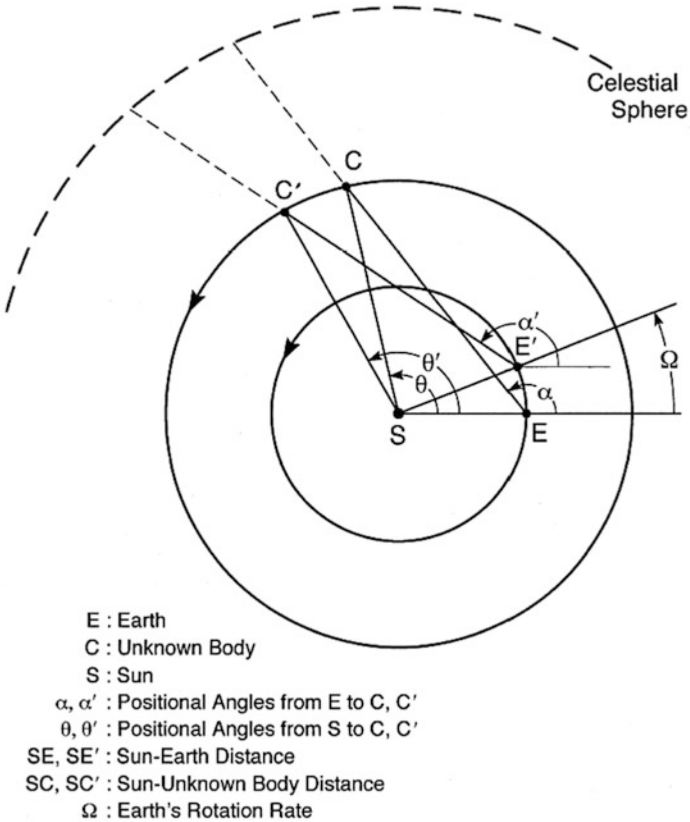


Fig. GS.2 Geometric depiction of the orbits of Earth (E) and Ceres (C) around the Sun (S) with angular measurements from Earth to Ceres against the celestial sphere backdrop

Kepler's third law is the dynamical constraint. Namely, each body in revolution about the sun exhibits constancy of the ratio $\frac{r^3}{T^2}$ where r is the distance from the sun and T is the period of rotation about the sun. We use the orbital elements of earth to evaluate the constant—$r = 1$ A.U. (astronomical unit) and $T = 1$ year. Thus, the constant is 1 $(\text{A.U.})^3(\text{year})^{-2}$.

The asteroid Ceres lies along the line with angle α relative to SE at $t = 0$. At a later time Δt, Fig. GS.2 shows that Ceres lies along the line with angle $\alpha\prime$ relative to SE (earth has rotated through an angle $= \Omega \Delta t$, where $\Omega = 2\pi$ radians/year). The problem reduces to finding Ceres' distance from the sun, its period of revolution about the sun, and its initial angle Θ relative to SE. This is the control vector for the problem. To find these elements of control, at least three observations of the angles $\alpha, \alpha', \ldots$ are required. But since these observations typically include noise (error), the problem is best solved in a least squares context with more than three observations.

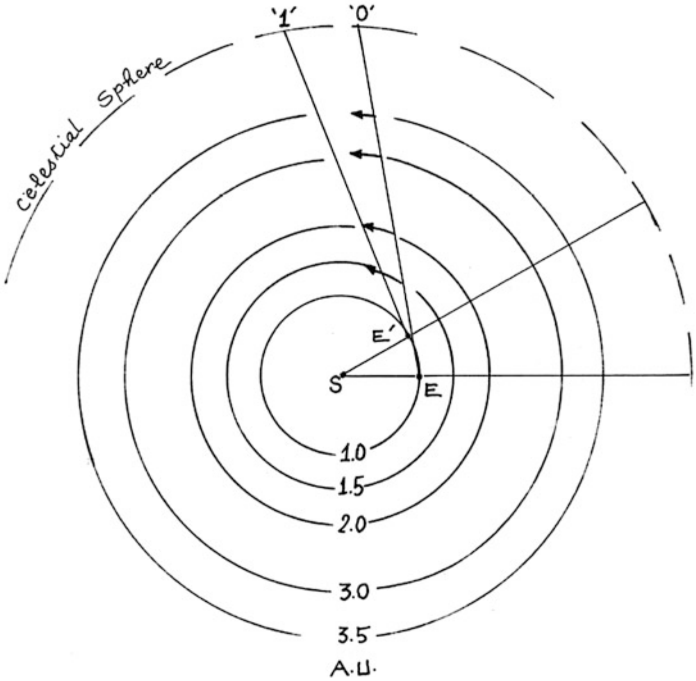


Fig. GS.3 Motion of objects at various distances from the Sun [Earth (E) at 1.0 A.U., other objects at 1.5, 2.0, 3.0, and 3.5 A.U.'s] and their 1-month angular movement according to Kepler's third Law after starting at locations along the line-of-sight EO

Before discussing the mathematical steps involved in solving the problem, it is instructive to qualitatively view the problem for a geometric perspective. Figure GS.3 depicts the case where Ceres is first sighted along the line from E to the point "O" on the celestial sphere—the background of fixed stars. After 1 month, the earth moves 30° along its circular trajectory and is located at E'. As stated earlier, the radius of Earth's trajectory relative to the sun's fixed location is 1 A.U. At $t = 1$ month, we find Ceres along the line from E' to point "1" on the celestial sphere. Now, using Kepler's third law, we move the points initially along EO to points along their respective trajectories 1 month later. These circular displacements are shown by curved arrows from the initial location (tail of arrow) to the location after 1 month (head of arrow). The displacement for the point on the 2 A.U. circle exactly falls on the E'1 line, the other displacements are either too large (1.5 A.U. circle) or too small (3.0 and 3.5 A.U. circles). Thus, in this idealized example, the asteroid is located at 2.0 A.U.'s from the sun. It thus becomes clear that measurement of the "α" angles as a function of time hold the power to determine the control elements.

Now for some mathematical details. The simplest approach to developing formulas for this problem is to make use of theory of complex variables. Let us represent the radius of earth's orbit by $R = 1$ A.U. and the unknown radius of Ceres' orbit by r. The revolution periods of these bodies about the Sun are represented by Ω (Earth) and $\mathrm{d}\Theta/\mathrm{d}t(= \dot{\Theta})$ for Ceres. We measure the angles α and Θ relative to SE (the line from the sun to earth at $t = 0$). Thus the positions of the Earth and Ceres at various times t are

$$\begin{aligned} &R\,\mathrm{e}^{\mathrm{i}\,\Omega t} \quad \text{(earth)} \\ &r\,\mathrm{e}^{\mathrm{i}(\Theta+\dot{\Theta}t)} \quad \text{(Ceres)}\,. \end{aligned} \tag{GS.1}$$

The line in the complex plane connecting Earth and Ceres (line from earth to Ceres) is

$$D(r, \Theta, \dot{\Theta}) = r\,\mathrm{e}^{\mathrm{i}(\Theta+\dot{\Theta}t)} - R\,\mathrm{e}^{\mathrm{i}\,\Omega t} \tag{GS.2}$$

where R and Ω are known. This complex number D can be decomposed into its real and imaginary parts and from these components we can find the angle α as a function of time from Earth to Ceres. Accordingly,

$$\begin{aligned} D &= \begin{cases} r\cos(\Theta + \dot{\Theta}t) - R\cos(\Omega t) \\ +i[r\sin(\Theta + \dot{\Theta}t) - R\sin(\Omega t)] \end{cases} \\ \alpha &= \arctan\frac{r\sin(\Theta + \dot{\Theta}t) - R\sin(\Omega t)}{r\cos(\Theta + \dot{\Theta}t) - R\cos(\Omega t)} \end{aligned} \tag{GS.3}$$

Let

$$\begin{aligned} x &= r\cos(\Theta + \dot{\Theta}t) - R\cos(\Omega t) \\ y &= r\sin(\Theta + \dot{\Theta}t) - R\sin(\Omega t). \end{aligned} \tag{GS.4}$$

Then

$$\alpha = \arctan\left(\frac{y}{x}\right). \tag{GS.5}$$

Taking the derivative of α with respect to time, we get

$$\dot{\alpha} = \frac{\dot{y} - \dot{x}\tan\alpha}{x\sec^2\alpha} \tag{GS.6}$$

This is the forecast equation for the problem. In the FSM approach, we need to find sensitivities of α with respect to the elements of control $r, \dot{\Theta}$, and Θ.

We then minimize the difference between the measured values of α and the adjusted forecast—the guess forecast (using control guess) added to first-order Taylor series terms $\frac{\partial\alpha}{\partial r}\Delta r$, $\frac{\partial\alpha}{\partial\dot{\Theta}}\Delta\dot{\Theta}$, and $\frac{\partial\alpha}{\partial\Theta}\Delta\Theta$.

2.8 Notes and References

This chapter follows the development in Lakshmivarahan and Lewis (2010). The classic review by Rabitz et al. (1983) provides a comprehensive account of the theory of parameter sensitivity and its varied applications to chemical kinetics. A complete and thorough discussion of the concept of Lyapunov index and its computation is given in Peitgen et al. (1992).

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Forecast Error Correction using Dynamic Data Assimilation
Lakshmivarahan, S.; Lewis, J.M.; Jabrzemski, R.
2017, XVI, 270 p. 125 illus., 104 illus. in color., Hardcover
ISBN: 978-3-319-39995-9