Chapter 2
Sensitivity Analysis: Differential Calculus of Models

Abstract Models in remote sensing—and in science and engineering, in general—are, essentially, functions of discrete model input parameters, and/or functionals of continuous model input parameters. In this sense, the sensitivities of model output parameters are, essentially, derivatives—partial derivatives with respect to discrete input parameters, and variational derivatives with respect to continuous input parameters. Specificity of models, as compared to functions and functionals in general, is due to the fact that they have two mandatory components. The first component describes the object or process of study, as is. It is a system of a differential equation, or equations, with initial and/or boundary conditions, which is referred to as a *forward problem*. The second component describes the procedure of deriving the output parameters of the model, which simulate the observed quantities, *observables*, from the solution of the forward problem. In contrast to the first component, it is just an analytic expression, which is referred to as an *observables procedure*. In rare practical cases, the forward problem has an analytic solution, and the output parameters are analytic functions or analytic functionals of the input parameters. Correspondingly, analytic evaluation of sensitivities is possible. In most practical cases, only numerical forward solutions are available, and specific approaches of sensitivity analysis considered in this monograph become indispensable.

Keywords Model input and output parameters · Forward problem · Observables · Observables procedure · Sensitivities

2.1 General Considerations

In the context of this book, we define *forward models* as quantitative tools, which return the desired output parameters for given input parameters. These models are assumed to provide an adequate quantitative description of the objects under study, and this description is specified by given values of the input parameters (*model parameters*). The output parameters of these models simulate the results of

E.A. Ustinov, *Sensitivity Analysis in Remote Sensing*,
SpringerBriefs in Earth Sciences, DOI 10.1007/978-3-319-15841-9_2

observations (*observables*). Thus, in a nutshell, we deal with functions, whose arguments are the model parameters and the values are the observables.

Indeed, as was pointed out in the Introduction, the forward models used in remote sensing consist of two basic components. The first component, the forward problem, specifies the quantitative description of the object under study as is, based on relevant laws of physics, which govern the spatial structure and temporal behavior of this object. This description—the forward problem—is provided by corresponding differential equations and initial and/or boundary conditions. The second component, the observables procedure, specifies the quantitative recipe of drawing the observables from the solution of the forward problem—the *forward solution*. This recipe is provided in the form of a closed-form analytic expression, which converts the forward solution into the observables.

Thus, abstracting from the inner workings of the forward models, they represent essentially functions whose arguments are the model parameters and values are the observables. There is a caveat though. In many practical cases, the models involve the continuous parameters, which are functions themselves—functions of space and/or time. Then the forward models become the functionals defined on these functions. From the viewpoint of practical implementation, there is little or no difference between functionals and functions of many variables, because the practical implementation requires a representation of those functions on an adequate grid of their arguments. But, as we will see in relevant examples below, from the viewpoint of analytic work that is necessary to conduct the sensitivity analysis in each specific case, it is instructive to treat the models with continuous parameters as functionals, and to apply corresponding tools of variational analysis.

In a relatively small number of practical cases, the forward problems used in practical forward models of remote sensing have analytic solutions. For example, this is the case in remote sensing of planetary atmospheres in the thermal spectral region, when atmospheric scattering can be neglected (see Sects. 4.3 and 5.3). In such cases, the forward solution can be represented as a closed-form analytic expression, which after the application of the observables procedure results in an analytic expression of observables directly through the model input parameters. Then, depending upon whether the given input parameter is just a constant or a function of space and/or time variables, the observables are functions or functionals. Accordingly, the sensitivities can be found using standard techniques of the differential calculus or variational calculus.

In most practical cases, though, the corresponding forward problems can be solved only numerically. This means that for given numerical values of the input parameters, the forward solution is obtained using appropriate numerical methods. This means that the analytic relation between the model input parameters and observables does not exist. This is where the methods of sensitivity analysis become indispensable. At this point we need to take a more detailed look at sensitivities with respect to different types of model parameters and observables.

2.2 Input and Output Parameters of Models

Without losing any generality, the model input parameters can be divided into two broad groups: discrete parameters and continuous parameters. Discrete parameters are constants, which do not depend on any arguments, such as space, time, etc. Continuous parameters are functions with essentially the same domain of arguments, as the forward solutions. Consider a couple of simplified examples.

Motion of a material point in the planetary gravity field. If the finite size of the material object in the gravity field can be neglected as compared to the scale of spatial variation of the gravity field of the planet, then this object can be considered as a material point, and its motion, assumed here to be non-relativistic, is described by a forward problem in the form:

$$\begin{cases} \dfrac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = \mathbf{g}(\mathbf{r}, t) \\ \left.\dfrac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\right|_{t=0} = \mathbf{v}_0 \\ \mathbf{r}|_{t=0} = \mathbf{r}_0 \end{cases} \tag{2.1}$$

The model input parameters here consist of two discrete parameters, $\mathbf{v}_0$ and $\mathbf{r}_0$, and one continuous parameter $\mathbf{g}(\mathbf{r}, t)$. The forward solution $\mathbf{r}(t)$ is a function of time t.

Transfer of thermal radiation in the non-scattering planetary atmosphere. Neglecting the vertical span of the planetary atmosphere as compared to the radius of the planet, the radiative transfer in the non-scattering atmosphere can be described by a forward problem in the form:

$$\begin{cases} u\dfrac{\mathrm{d}I}{\mathrm{d}z} + \alpha(z)I(z,u) = \alpha(z)B(z) \\ I(z,u) = 0, \quad \text{for } z = 0, u > 0 \\ I(z,u) = 2A\int\limits_0^1 I(z,u')\, u'\mathrm{d}u' + B_s, \quad \text{for } z = z_0, u < 0 \end{cases} \tag{2.2}$$

Here we have two discrete parameters, albedo A and source function B_s of the underlying surface, and two continuous parameters, extinction coefficient $\alpha(z)$, and source function $B(z)$ of the atmosphere itself. The forward solution $I(z,u)$ is a function of the vertical coordinate z and of cosine u of the nadir angle of propagation.

The practical implementation of the retrieval algorithms in the form of computer programs intended for the interpretation of practical data involves the representation of the continuous parameters as finite-dimensional arrays with values corresponding to an appropriate grid of argument values of those continuous parameters. But in many practical cases, the analytic work, which is necessary to be done in order to derive the analytic background of the retrieval algorithms, is easier to perform in terms of continuous parameters considered as functions, using appropriate tools of variational analysis. This will be demonstrated in the sections to follow.

On the other hand, the output parameters, the observables R, are always discrete parameters due to the nature of measurements themselves. In the first example above, such observables may be relative distances and velocities of the material point as measured from some known location of the observer. At each instant of observation:

$$\begin{aligned} \mathbf{R} &= |\mathbf{r} - \mathbf{r}_i| \\ \mathbf{S} &= |\mathbf{V} - \mathbf{V}_i| \end{aligned} \tag{2.3}$$

In practice, the measured values are always integrated over some finite span of arguments of the forward solution: time, space, viewing angle, etc. But the integration results are always benchmarked by some instant values of these arguments. More information will be provided in the sections to follow.

2.3 Sensitivities: Just Derivatives of Output Parameters with Respect to Input Parameters

As mentioned in the Introduction, sensitivity of any output parameter with respect to any input parameter is merely a derivative of a suitable type. Sensitivity of the observable R with respect to a discrete input parameter p isa partial derivative:

$$K = \frac{\partial R}{\partial p} \tag{2.4}$$

Sensitivity of the observable R with respect to a continuous input parameter $p(x)$ is a variational derivative:

$$K(x) = \frac{\delta R}{\delta p(x)} \tag{2.5}$$

There are a few different definitions of the variational derivative, which sometimes is also called the functional derivative. For all practical purposes in this book, the variational derivative with respect to the continuous parameter $p(x)$ is defined as a kernel of the linear integral expression

$$\delta_p R = \int_{D_x} \frac{\delta R}{\delta p(x)} \delta p(x) \, \mathrm{d}x \tag{2.6}$$

Here, the integration is conducted over the domain D_x of arguments x of the parameter $p(x)$; $\delta p(x)$ is the variation of the input parameter $p(x)$, and $\delta_p R$ is the variation of the output parameter R caused by the variation $\delta p(x)$.

For a continuous parameter specified on a grid of its arguments, there exists a simple relationship between values of the variational derivative on this grid and values of partial derivatives with respect to grid values of the continuous parameter. The accuracy of this relationship depends on the mesh width of this grid. As an example, assume that $p(x)$ is defined on an interval $x \in [a, b]$ represented by a set of grid values $p_j = p(x_j)$, $(j = 1, \ldots n)$. Then, the output parameter R becomes a function of n variables $\{x_j\}$, and Eq. (2.6) can be approximated in the form:

$$\delta_p R = \int\limits_{D_x} \frac{\delta R}{\delta p(x)} \delta p(x)\ \mathrm{d}x \approx \sum_j \left(\frac{\delta R}{\delta p(x)}\right)\bigg|_{x_j} \delta p_j \Delta_j x \tag{2.7}$$

From Eq. (2.7) we immediately obtain:

$$\frac{\partial R}{\partial p_j} \approx \left(\frac{\delta R}{\delta p(x)}\right)\bigg|_{x_j} \Delta_j x, \text{ or vice versa, } \left(\frac{\delta R}{\delta p(x)}\right)\bigg|_{x_j} \approx \frac{1}{\Delta_j x}\frac{\partial R}{\partial p_j} \tag{2.8}$$

The definition of variational derivative, Eq. (2.6), has an important practical value. Throughout this book we will derive the expressions for sensitivities to continuous parameters—which are variational derivatives—by transforming the expressions for variations of the output parameters to the form of Eq. (2.6) and obtaining the sensitivities as kernels of resulting integral expressions. Equations (2.5) and (2.6) will serve as a definition of sensitivities to continuous parameters.

Consider a special kind of a functional: the value of a function $f(\xi)$ defined on the interval $[a, b]$ at the specified value of its argument $\xi = x$. Representing $f(x)$ in the form

$$f(x) = \int\limits_a^b \delta(\xi - x) f(\xi)\ \mathrm{d}\xi \tag{2.9}$$

we take the variations of both sides of Eq. (2.9):

$$\delta f(x) = \int\limits_a^b \delta(\xi - x) \delta f(\xi)\ \mathrm{d}\xi \tag{2.10}$$

Comparing Eq. (2.10) with the definition of variational derivative, Eqs. (2.5) and (2.6), we obtain:

$$\frac{\delta f(x)}{\delta f(\xi)} = \delta(\xi - x) \tag{2.11}$$

In a similar fashion, one can derive an expression for the variational derivative of the ordinary derivative of the function $f'(x)$ with respect to the function $f(x)$ itself:

$$\frac{\delta f'(x)}{\delta f(\xi)} = -\delta'(\xi - x) \tag{2.12}$$

where $\delta'(x) = \mathrm{d}\delta(x)/\mathrm{d}x$ is the derivative of the δ-function. We have:

$$\delta f'(x) = \int_a^b \delta(\xi - x)\delta f(\xi)\ \mathrm{d}\xi \tag{2.13}$$

Integrating by parts we obtain:

$$\delta f'(x) = \delta(\xi - x)\delta f(\xi)|_a^b - \int_a^b \delta'(\xi - x)\delta f(\xi)\ \mathrm{d}\xi \tag{2.14}$$

The off-integral term in Eq. (2.14) equals zero for all values of x within the interval $[a, b]$. Comparing the resulting Eq. (2.14) with the definition of variational derivative, Eqs. (2.5) and (2.6), we see that Eq. (2.12) is valid everywhere within this interval.

In a number of applications considered in chapters that follow, we will need to convert the linear variational equation

$$L\delta X = \delta S \tag{2.15}$$

into an equation for corresponding variational derivatives with respect to some continuous parameter:

$$L\frac{\delta X}{\delta a} = \frac{\delta S}{\delta a} \tag{2.16}$$

Here, δa is the variation of the parameter $a(x)$, which results in a corresponding variation of the right-hand term $S(x)$, which in turn, results in a corresponding variation of the solution $X(x)$. The linear operator may, in general, be a function of x, too.

In the applications below, at each given value of the argument $x = \xi$, the function $S(x)$ depends on the parameter $a(x)$ only at the same value of the argument $x = \xi$. This means that S is a function of $a(x)$, not a functional of $a(\xi)$. Accordingly,

$$\delta S(x) = \int_a^b \delta(\xi - x) \cdot \frac{\partial S(\xi)}{\partial a(\xi)} \cdot \delta a(\xi)\ \mathrm{d}\xi = \int_a^b \delta(\xi - x) \cdot \frac{\partial S(x)}{\partial a(x)} \cdot \delta a(\xi)\ \mathrm{d}\xi \quad (2.17)$$

Comparing with the definition of the variational derivative, Eqs. (2.5) and (2.6), we have:

$$\frac{\delta S(x)}{\delta a(\xi)} = \delta(\xi - x) \cdot \frac{\partial S(x)}{\partial a(x)} \quad (2.18)$$

Thus, the right-hand term of Eq. (2.12) has the form:

$$\delta S(x) = \frac{\partial S(x)}{\partial a(x)} \delta a(x) \quad (2.19)$$

On the other hand, the solution $\delta X(x)$ of Eq. (2.15) depends on the variation of the parameter $a(\xi)$ in the whole interval $\xi \in [x_0, x_1]$. In other words, $X(x)$ is a functional of $a(\xi)$, while still being a function of x:

$$X(x) = X[a(\xi), x] \quad (2.20)$$

Thus, in the variational equation, Eq. (2.15)

$$\delta X(x) = \int_a^b \frac{\delta X(x)}{\delta a(\xi)} \delta a(\xi) \mathrm{d}\xi \quad (2.21)$$

Substituting Eqs. (2.17) and (2.21) in Eq. (2.15) and moving the right-hand term into the left side, we have:

$$L \int_a^b \frac{\delta X(x)}{\delta a(\xi)} \delta a(\xi) \mathrm{d}\xi - \int_a^b \delta(\xi - x) \cdot \frac{\partial S(x)}{\partial a(x)} \cdot \delta a(\xi) \mathrm{d}\xi = 0 \quad (2.22)$$

Recalling that the operator L may be a function of x, and observing that x is not an integration variable in Eq. (2.22), we can rewrite this equation as

$$\int_a^b \left(L \frac{\delta X(x)}{\delta a(\xi)} - \delta(\xi - x) \cdot \frac{\partial S(x)}{\partial a(x)} \right) \delta a(\xi) \mathrm{d}\xi = 0 \quad (2.23)$$

Finally, demanding that Eq. (2.23) be satisfied for an arbitrary variation δa, we obtain the equation for variational derivatives, Eq. (2.16), which, in a detailed form can be written as

$$L\frac{\delta X(x)}{\delta a(\xi)} = \delta(\xi - x) \cdot \frac{\partial S(x)}{\partial a(x)} \tag{2.24}$$

We will use this result in applications of the linearization approach of sensitivity analysis to various forward problems considered in the chapters that follow.

http://www.springer.com/978-3-319-15840-2

Sensitivity Analysis in Remote Sensing
Ustinov, E.A.
2015, XIII, 128 p. 2 illus., Softcover
ISBN: 978-3-319-15840-2