Chapter 4
Derivative Approximations

4.1 First-order approximations

At this point we have identified a quantity of interest (QoI) and the uncertain parameters in our system, and we want to start understanding how variations in those parameters affect the QoI. In this section we will look at how we can quantify the sensitivity of the QoI to changes in the parameters near some point in parameter space. To do this we think of the QoI as a function of the p parameters represented by a vector θ, i.e., $Q(\theta)$. We can then expand this function in a Taylor series about some nominal value of θ that we denote as $\bar{\theta}$:

$$\begin{aligned} Q(\theta) = Q(\bar{\theta}) &+ \Delta_1 \frac{\partial Q}{\partial \theta_1}\bigg|_{\bar{\theta}} + \Delta_2 \frac{\partial Q}{\partial \theta_2}\bigg|_{\bar{\theta}} + \cdots + \Delta_p \frac{\partial Q}{\partial \theta_p}\bigg|_{\bar{\theta}} \\ &+ \frac{\Delta_1^2}{2}\frac{\partial^2 Q}{\partial \theta_1^2}\bigg|_{\bar{\theta}} + \frac{\Delta_1 \Delta_2}{2}\frac{\partial^2 Q}{\partial \theta_1 \theta_2}\bigg|_{\bar{\theta}} + \cdots + \frac{\Delta_{p-1}\Delta_p}{2}\frac{\partial^2 Q}{\partial \theta_{p-1}\theta_p}\bigg|_{\bar{\theta}} + \frac{\Delta_p^2}{2}\frac{\partial^2 Q}{\partial \theta_p^2}\bigg|_{\bar{\theta}} \\ &+ \text{higher order terms.} \end{aligned} \tag{4.1}$$

In this equation $\Delta_i = \theta_i - \bar{\theta}_i$. The value of $\bar{\theta}$ is typically chosen to be the mean or median of the uncertain parameters. We can write Eq. (4.1) in shorthand form as

$$Q(\theta) = Q(\bar{\theta}) + \sum_{i=1}^{p} \Delta_i \frac{\partial Q}{\partial \theta_p}\bigg|_{\bar{\theta}} + \sum_{i=1}^{p}\sum_{j=1}^{p} \frac{\Delta_i \Delta_j}{2}\frac{\partial^2 Q}{\partial \theta_i \theta_j}\bigg|_{\bar{\theta}} + O(\Delta^3) \tag{4.2}$$

4.1.1 Scaled Sensitivity Coefficients and Sensitivity Indices

Therefore, if we know the derivatives of the QoI with respect to the uncertain parameters we can say something about how we expect the QoI to vary around a nominal value. As in many analyses, the first order behavior will be the most important. The first-order derivatives of the QoI are often called the first-order sensitivities of the QoI. By ranking the sensitivities by magnitude, we can gauge which uncertain parameters are likely to have the largest impact. To compare the sensitivities we need to cast them in the same units because, for example, the units of sensitivity i will have the inverse units of θ_i. One way to do this is with *scaled sensitivity coefficients* . The scaled sensitivity coefficient for parameter i is the mean of parameter i, μ_i, multiplied by the derivative of the QoI with respect to θ_i:

$$(\text{Scaled Sensitivity Coefficient})_i = \mu_i \frac{\partial Q}{\partial \theta_i}\bigg|_{\bar{\theta}}. \tag{4.3}$$

The scaled sensitivity coefficients indicate which parameters are most sensitive about the mean value of the parameter. This can be misleading however, because it is possible that a parameter has a large scaled sensitivity coefficient, but a small overall uncertainty, i.e, we know that parameter to within a small degree of uncertainty. To correct this case, *sensitivity indices* are used. In this case we multiply by the standard deviation of parameter i, σ_i, rather than the mean:

$$\text{(Sensitivity Index)}_i = \sigma_i \frac{\partial Q}{\partial \theta_i}\bigg|_{\bar{\theta}}. \tag{4.4}$$

The parameter with the largest product of the derivative and the standard deviation will have the highest sensitivity index.

Both of these measures of sensitivity are useful in eliminating parameters that do not appear to be important to the QoI, at least near their nominal value. The utility of such knowledge is most evident in a system where there is a large number of uncertain parameters. Knowing the sensitivities allows the UQ practitioner to narrow the focus to a smaller number of parameters and then apply the more time consuming techniques we shall discuss later, e.g. sampling methods or polynomial chaos expansions. One must keep in mind, however, the fact that sensitivities are only local quantities and extrapolating far from the nominal value of θ may require understanding of higher order terms and the interactions between different parameters.

4.1.2 Variance Estimation

The sensitivities also allow us to estimate the variance in the QoI. To do this the value of $\bar{\theta}$ should be the mean of the parameters. Recall that the variance of a random variable $Q(\theta)$ with joint PDF, $f(\theta)$, is written as

$$\begin{aligned} \text{Var}(Q) &= \left(\int d\theta\, Q(\theta)^2 f(\theta)\right) - \left(\int d\theta\, Q(\theta) f(\theta)\right)^2 \\ &= \left(\int d\theta\, Q(\theta)^2 f(\theta)\right) - Q(\bar{\theta})^2. \end{aligned} \tag{4.5}$$

To estimate the expectation, of $Q(\theta)^2$ we use the first-order Taylor expansion in Eq. (4.2) and ignore the second-derivative and higher terms:

$$\begin{aligned} &Q(\theta)^2 \approx \\ &\quad Q(\bar{\theta})^2 + \left(\sum_i (\theta_i - \bar{\theta}_i) \frac{\partial Q}{\partial \theta_i}\bigg|_{\theta_i = \bar{\theta}_i}\right)^2 + 2Q(\bar{\theta})\left(\sum_i (\theta_i - \bar{\theta}_i) \frac{\partial Q}{\partial \theta_i}\bigg|_{\theta_i = \bar{\theta}_i}\right). \end{aligned} \tag{4.6}$$

Using the expansion in Eq. (4.6) we get, to second order,

$$\mathrm{Var}(Q) = -Q(\bar{\theta})^2 + \int d\theta \left[Q(\bar{\theta})^2 + \left(\sum_i (\theta_i - \bar{\theta}_i) \frac{\partial Q}{\partial \theta_i}\bigg|_{\theta_i=\bar{\theta}_i} \right)^2 + 2Q(\bar{\theta}) \left(\sum_i (\theta_i - \bar{\theta}_i) \frac{\partial Q}{\partial \theta_i}\bigg|_{\theta_i=\bar{\theta}_i} \right) \right] f(\theta), \tag{4.7}$$

We notice that

$$\int d\theta\, Q(\bar{\theta})^2 f(\theta) = Q(\bar{\theta})^2, \tag{4.8}$$

and this will cancel the other quadratic Q term. In addition, the cross term will integrate to zero by the definition of the mean of θ_i. The remaining term to deal with is

$$\int d\theta\, f(\theta) \left(\sum_i (\theta_i - \bar{\theta}_i) \frac{\partial Q}{\partial \theta_i}\bigg|_{\theta_i=\bar{\theta}_i} \right)^2 = \sum_i \sum_j \frac{\partial Q}{\partial \theta_i}\bigg|_{\theta_i=\bar{\theta}_i} \frac{\partial Q}{\partial \theta_j}\bigg|_{\theta_j=\bar{\theta}_j} \int d\theta_i \int d\theta_j\, f_{ij}(\theta_i, \theta_j)(\theta_i - \bar{\theta}_i)(\theta_j - \bar{\theta}_j) \tag{4.9}$$

where

$$f_{ij} = \int d\theta_{ij}\, f(\theta) \tag{4.10}$$

The integral in Eq. (4.9) is the covariance matrix that we previously defined. The covariance matrix indicates how parameters vary together and was defined in Section 2.3 as

$$\sigma_{ij} = \int d\theta_i \int d\theta_j\, f_{ij}(\theta_i, \theta_j)(\theta_i - \bar{\theta}_i)(\theta_j - \bar{\theta}_j) \tag{4.11}$$

Therefore, if we know the covariance of the parameters, we can directly compute the variance of our QoI as

$$\mathrm{Var}(Q) = \sum_i \sum_j \frac{\partial Q}{\partial \theta_i}\bigg|_{\theta_i=\bar{\theta}_i} \frac{\partial Q}{\partial \theta_j}\bigg|_{\theta_j=\bar{\theta}_j} \sigma_{ij}.$$

In this chapter, we will once use the advection-diffusion-reaction (ADR) equation as our test bench for the methods. In this case we will use a steady ADR equation in one-spatial dimension with a spatially constant diffusion coefficient, a linear reaction term, and a prescribed source:

$$v\frac{du}{dx} - \omega \frac{d^2 u}{dx^2} + \kappa(x) u = S(x), \tag{4.12}$$

$$u(0) = u(10) = 0,$$

where v and ω are spatially constant with means

$$\mu_v = 10, \quad \mu_\omega = 20,$$

and variances

$$\mathrm{Var}(v) = 0.0723493, \quad \mathrm{Var}(\omega) = 0.3195214.$$

The reaction coefficient, $\kappa(x)$, is given by

$$\kappa(x) = \begin{cases} \kappa_l & x \in (5, 7.5) \\ \kappa_h & \text{otherwise} \end{cases},$$

with $\mu_{\kappa_h} = 2$, $\mathrm{Var}(\kappa_h) = 0.002778142$ and $\mu_{\kappa_l} = 0.1$, $\mathrm{Var}(\kappa_l) = 8.511570 \times 10^{-6}$. The value of the source is given by

$$S(x) = qx(10 - x),$$

with $\mu_q = 1$, $\mathrm{Var}(q) = 7.062353 \times 10^{-4}$. These functions are shown graphically in Fig. 4.1. The QoI for this example will be the total reaction rate in the problem:

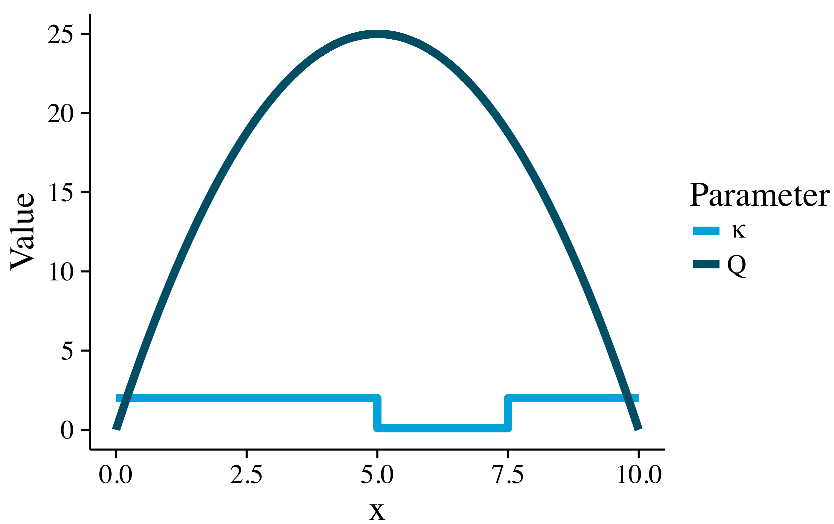

Fig. 4.1 Values as a function of x for ω and Q for our ADR example.

$$Q = \int_0^{10} dx\, \kappa(x) u(x). \tag{4.13}$$

At the nominal values of parameters, that, evaluating v, ω, κ_l, κ_h, and q at their mean values, the solution $u(x)$ is shown in Fig. 4.2. Using a solution with 2000 equally spaced spatial zones ($\Delta x = 0.005$), we get $Q(\bar{\theta}) = 52.3903954692$. The Python code used to produce these solutions is given in Algorithm 4.1.

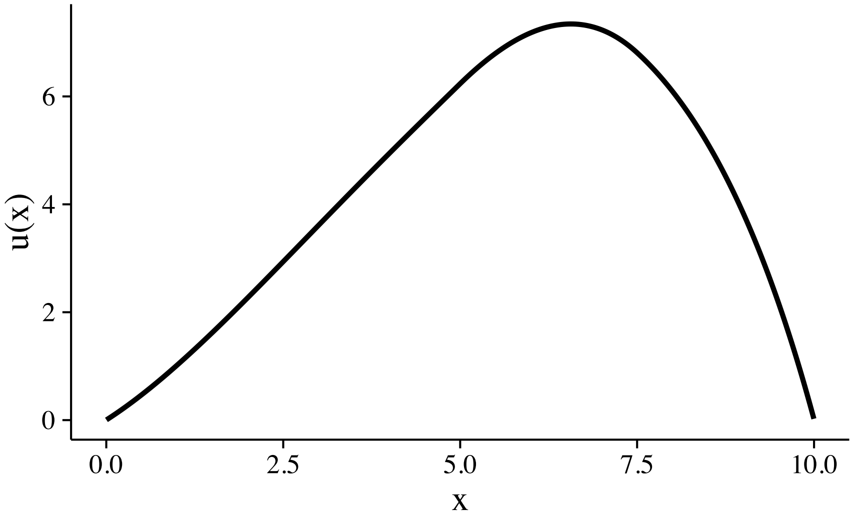

Fig. 4.2 The solution $u(x)$ evaluated at $\bar{\theta}$.

Algorithm 4.1 Numerical method to solve the advection-diffusion-reaction equation that will be used in this chapter.

```
def ADRSource(Lx, Nx, Source, omega, v, kappa):
    #Solves the diffusion equation with Generalized Source
    A = sparse.dia_matrix((Nx,Nx))
    dx = Lx/Nx
    i2dx2 = 1.0/(dx*dx)
    #fill diagonal of A
    A.setdiag(2*i2dx2*omega + np.sign(v)*v/dx + kappa)
    #fill off diagonals of A
    A.setdiag(-i2dx2*omega[1:Nx] + 0.5*(1-np.sign(v[1:Nx]))*v[1:Nx]/dx,1)
    A.setdiag(-i2dx2*omega[0:(Nx-1)] - 0.5*(np.sign(v[0:(Nx-1)])+1)*v[0:(Nx-1)]/dx,-1)
    #solve A x = Source
    Solution = linalg.spsolve(A,Source)
    return Solution
```

4.2 Difference Approximations

As discussed above, the scaled sensitivity coefficients and sensitivity index require the derivative of the QoI with respect to each θ_i. We can approximate these derivatives easily using finite differences:

$$\left.\frac{\partial Q}{\partial \theta_i}\right|_{\bar{\theta}} \approx \frac{Q(\bar{\theta}+\delta_i \hat{e}_i)-Q(\bar{\theta})}{\delta_i}, \tag{4.14}$$

where δ is a small, positive parameter and $\hat{e}_i$ is a vector that is one in the i^{th} position. Given that we need to compute I derivatives we need to compute the QoI at $I+1$ points (i.e., $I+1$ runs of the code): 1 for the mean value, $\bar{\theta}$, and 1 for each of the i parameters.

For our ADR example, we will compute the sensitivities to each parameter using the same mesh used above ($\Delta x = 0.005$). For each parameter we compute the derivative using $\delta_i = \mu_i \times 10^{-6}$. The results from the 6 simulations needed to compute the

Parameter	Sensitivity	Scaled Sensitivity Coef.	Sensitivity Index
v	-1.74063662044	-17.4063662044	-0.468193395375
ω	-0.970209745432	-19.4041949086	-0.548422933999
κ_l	12.8679549505	1.28679549505	0.0375417375611
κ_h	17.761320219	35.522640438	0.936165138013
q	52.3903956022	52.3903956022	1.39227937131

Table 4.1 Sensitivities to the five parameters in the ADR reaction.

5 sensitivities are shown in Table 4.2. Based on the scaled sensitivity coefficient and the sensitivity index, q has the largest sensitivity. Also, both measures indicate that ω_h is the second most important parameter. This table gives many digits for each number so that we can compare with other approaches for computing the derivatives in later chapters.