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Note

Pointwise Feature Sensitivity Analysis

I. INTRODUCTION

Mathematical models in chemistry, physics, biology and engineering have become increasingly more complicated. In order to assess the quality and effectiveness of an assumed model and also to gain further insight into the model's nature, investigations are often undertaken for the purpose of unravelling the relationship between the output and input of the model. The effective and efficient exploration of this relationship forms the domain of *sensitivity analysis* [1, 2]. Here we will be concerned in particular with the question of how input parameters affect structural features of the output. The model in its simplest form is considered to be a function of some variable, say x. The features of interest then arise in a plot of the output versus x over some domain in x. The relationship between these features and model input parameters, α_j ($j = 1,..., L$) is the focus of this paper.

The plotting of output as a function of some independent variable such as energy, frequency, time, angle, quantum number, etc., is a very common practice in the analysis of physical problems. Such plots are particularly important in exhibiting interesting characteristics or trends in a system. Interest in the dependence of this behavior on other input parameters of the system then naturally follows. In recent work [3, 4], a sensitivity analysis approach has been developed for examining such dependencies and applied to problems in molecular dynamics and kinetics. The approach involves first fitting the output over the domain in x by a judiciously chosen function that contains several parameters, each of which controls a particular feature of interest. Then by combining the fitting with knowledge of certain so-called elementary sensitivities (i.e., partial derivatives of output with respect to input) sensitivities of the feature parameters with respect to the input parameters are determined. In this paper an alternative approach is explored, one that does not depend upon any fitting procedure.

The alternative approach is based on the fact that features can be typically described by the behavior of just a few representative points or characteristics of the graphed observable. Thus, for example, one might describe an oscillatory output in terms of its extrema or frequency. The values and positions of such critical points will then depend on the input parameter values and hence viewed from this perspective, feature analysis reduces to the determination of pointwise sensitivity information. A special case of this perspective is given in our work [3] and by Cacuci *et al.* [5], where sensitivities at an extremum are used to determine the effect of parameter variations on its position. More recently, Cacuci [6] has given a very

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general procedure for determining feature sensitivities. The feature of interest which may depend on an extremum, saddle *or* inflection point of the output, is written as an objective functional containing the output and the critical point. Sensitivity expressions are then determined for such features. The same functional perspective is also mentioned in our earlier work [4]. It is worth pointing out [6] that considerable computational savings can be achieved if: (i) the desired objectives can be identified prior to the sensitivity calculation and (ii) the number of such objectives does not exceed the number of system variables or parameters. Unfortunately, in many real problems one or both of these criteria are not satisfied. When the latter circumstances arise the procedures in the present paper offer the widest realm of computational flexibility. In this paper, we seek to further stimulate interest in the employment of feature sensitivity analysis. In particular, sensitivity expressions are presented and applied which, while they may in the main be derived from the analysis of [6], make transparent the simplicity of the approach for a great variety of problems in the sciences and engineering.

In Section II the basic theory is presented for the determination of feature sensitivity coefficients from a pointwise analysis and Section III gives a simple example. Concluding remarks are contained in Section IV.

II. Theory

Consider an output $O_{\boldsymbol{\alpha}}(x)$, where x is the variable as a function of which $O_{\boldsymbol{\alpha}}(x)$ exhibits features[1] and $\boldsymbol{\alpha}$ is the input parameter vector with components α_l ($l = 1,..., L$). For the purpose of illustration suppose that our interest lies in the value and position of a feature defined by the constraint that

$$O_{\boldsymbol{\alpha}}(x) = h \tag{II.1}$$

where h is assumed to be independent of x and $\boldsymbol{\alpha}$. From Eq. (II.1) we then obtain a solution for the position of the feature

$$x^* = x^*(\boldsymbol{\alpha}, h) \tag{II.2}$$

or possibly a set of solutions

$$x_1^*(\boldsymbol{\alpha}, h),..., x_N^*(\boldsymbol{\alpha}, h). \tag{II.3}$$

Let us examine what happens when one of the parameters in $\boldsymbol{\alpha}$, say $\alpha_{l'}$, $l' \in \{1,..., L\}$, is varied by an amount $\Delta\alpha_{l'}$. Clearly by definition the value of the feature will be unchanged. Its position x^*, however, will change and the variation in position may be expanded as a power series in $\Delta\alpha_{l'}$, i.e.,

$$x^*(\boldsymbol{\alpha} + \Delta\boldsymbol{\alpha}, h) = x^*(\boldsymbol{\alpha}, h) + \frac{\partial x^*}{\partial \alpha_{l'}} \Delta\alpha_{l'} + \cdots \tag{II.4a}$$

[1] The analysis here can be readily extended to consider features appearing in several dimensions.

where

$$\Delta\boldsymbol{\alpha} = (0, \ldots, 0, \Delta\alpha_{l'}, 0, \ldots, 0) \tag{II.4b}$$

and $\Delta\alpha_{l'}$ appears in the l'th position in the vector $\Delta\boldsymbol{\alpha}$. The quantity $\partial x^*/\partial\alpha_{l'}$ in Eq. (II.4a) is an example of a so-called feature sensitivity coefficient in that it quantifies how in particular the position of a feature responds to variations in input parameters. It is determined by first noticing that according to the constraint of Eq. (II.1)

$$O_{\boldsymbol{\alpha}+\Delta\boldsymbol{\alpha}}\left(x^* + \frac{\partial x^*}{\partial\alpha_{l'}}\Delta\alpha_{l'} + \cdots\right) = h. \tag{II.5}$$

It follows that to first order in $\Delta\alpha_{l'}$ that

$$\left.\frac{\partial O_{\boldsymbol{\alpha}}}{\partial\alpha_{l'}}\right|_{x=x^*}\Delta\alpha_{l'} + \left.\frac{\partial O_{\boldsymbol{\alpha}}}{\partial x}\right|_{x=x^*}\frac{\partial x^*}{\partial\alpha_{l'}}\Delta\alpha_{l'} = h - O_{\boldsymbol{\alpha}}(x^*) = 0 \tag{II.6}$$

so that

$$\frac{\partial x^*}{\partial\alpha_{l'}} = -\left.\frac{\partial O_{\boldsymbol{\alpha}}}{\partial\alpha_{l'}}\right|_{x=x^*}\Big/\left.\frac{\partial O_{\boldsymbol{\alpha}}}{\partial x}\right|_{x=x^*}. \tag{II.7}$$

This argument applies to any of the points in (II.3) so that finally

$$\frac{\partial x_j^*}{\partial\alpha_{l'}} = -\left.\frac{\partial O_{\boldsymbol{\alpha}}}{\partial\alpha_{l'}}\right|_{x=x_j^*}\Big/\left.\frac{\partial O_{\boldsymbol{\alpha}}}{\partial\alpha_{l'}}\right|_{x=x_j^*} \qquad (j=1, \ldots, N). \tag{II.8}$$

The analysis presented thus far in this section is now extended. We begin by defining the feature of interest in terms of the constrained operator equation

$$\hat{F}(O_{\boldsymbol{\alpha}} \mid x) = 0 \tag{II.9}$$

where $\hat{F}$ is an arbitrary operator. The previous analysis could then be invoked by introducing a particular operator $\hat{F}'$ such that

$$\hat{F}'(O_{\boldsymbol{\alpha}} \mid x) = O_{\boldsymbol{\alpha}} - h. \tag{II.10}$$

The purpose of the generalization is to provide the tools to enable us to examine features which are described in terms of minima, maxima, points of inflexion, integral transforms, etc. For example, in the case of an extremum we would introduce the derivative operator

$$\hat{F}''(O_{\boldsymbol{\alpha}} \mid x) = \frac{d}{dx} O_{\boldsymbol{\alpha}}(x) \tag{II.11}$$

or for a point of inflexion

$$\hat{F}'''(O_\alpha \mid x) = \frac{d^2 O_\alpha(x)}{dx^2}. \tag{II.12}$$

Similarly $\hat{F}(O_\alpha \mid x)$ could be a functional of O_α such as

$$\hat{F}''''(O_\alpha \mid x) = \int W(x, x')\, O_\alpha(x')\, dx' \tag{II.13}$$

where $W(x, x')$ is an appropriate weighting function. Consider then Eq. (II.9). Suppose that one of the input parameters, $\alpha_{l'}$ say, is varied by an amount $\Delta\alpha_{l'}$ where $l' \in \{1,..., L\}$. Assuming that x^* is a solution to Eq. (II.9) (and that $\hat{F}$ is independent of $\alpha_{l'}$) we find that

$$\hat{F}\left(O_{\alpha+\Delta\alpha} \,\middle|\, x^* + \frac{\partial x^*}{\partial \alpha_{l'}} \Delta\alpha_{l'} + \cdots\right) = 0 \tag{II.14}$$

where $\Delta\boldsymbol{\alpha} = (0,..., 0, \Delta\alpha_{l'}, 0,..., 0)$. To first order in $\Delta\alpha_{l'}$ Eq. (II.14) now becomes

$$\hat{F}(O_\alpha \mid x^*) + \frac{\partial}{\partial \alpha_{l'}} \hat{F}(O_\alpha \mid x)\bigg|_{x=x^*} \Delta\alpha_{l'} + \frac{\partial}{\partial x} \hat{F}(O_\alpha \mid x)\bigg|_{x=x^*} \frac{\partial x^*}{\partial \alpha_{l'}} \Delta\alpha_{l'} = 0 \tag{II.15}$$

so that the feature sensitivity coefficient $\partial x^*/\partial\alpha_{l'}$ is given by

$$\frac{\partial x^*}{\partial \alpha_{l'}} = -\frac{\partial \hat{F}(O_\alpha \mid x)}{\partial \alpha_{l'}}\bigg|_{x=x^*} \bigg/ \frac{\partial \hat{F}(O_\alpha \mid x)}{\partial x}\bigg|_{x=x^*}. \tag{II.16}$$

In the case that Eq. (II.9) has several solutions, say $x_1^*,..., x_N^*$ the equivalent argument yields the sensitivity coefficients for any of the solutions. Thus,

$$\frac{\partial x_j^*}{\partial \alpha_{l'}} = -\frac{\partial \hat{F}(O_\alpha \mid x)}{\partial \alpha_{l'}}\bigg|_{x=x_j^*} \bigg/ \frac{\partial \hat{F}(O_\alpha \mid x)}{\partial x}\bigg|_{x=x_j^*} \qquad (j=1,..., N). \tag{II.17}$$

Although the actual observable associated with the features may not be O_α itself the sensitivity of the latter "elementary" observable at the point x_j^*, $j \in \{1,..., N\}$, will often be of interest. This gradient may be calculated by combining the direct variation of $\alpha_{l'}$ with the one implicitly contained in x_j^* to obtain

$$\frac{\partial O_\alpha}{\partial \alpha_{l'}}(x_j^*) = \frac{\partial O_\alpha}{\partial \alpha_{l'}}\bigg|_{x=x_j^*} + \frac{\partial O_\alpha}{\partial x}\bigg|_{x=x_j^*} \frac{\partial x_j^*}{\partial \alpha_{l'}} \qquad (j=1,..., N). \tag{II.18}$$

The above analysis can be further extended to deal with the situation where a feature of interest is constrained by the value and/or position of another feature. An example of this might be the width at half-maximum of a peaking function. Mathematically this reduces in general to the two operator equations

$$\hat{F}(O_\alpha \mid x) = 0 \tag{II.19a}$$

$$R(O_\alpha \mid x) = K_\alpha(\mathbf{x}^*) \tag{II.19b}$$

where $\mathbf{x}^* = (x_1^*,..., x_N^*)$ are solutions of Eq. (II.19a). Then following the same analysis as before, i.e., varying a parameter $\alpha_{l'}$ by say $\Delta\alpha_{l'}$, $l' \in \{1,..., L\}$, and equating the first order terms in $\Delta\alpha_{l'}$ on the left-hand side and right-hand side of the resulting equation

$$\left.\frac{\partial K_\alpha}{\partial \alpha_{l'}}\right|_{\mathbf{x}^*} + \sum_{j=1}^{N} \left.\frac{\partial K_\alpha}{\partial x_j}\right|_{\mathbf{x}^*} \frac{\partial x_j^*}{\partial \alpha_{l'}} - \left.\frac{\partial R_\alpha}{\partial \alpha_{l'}}\right|_{s_P^*} - \left.\frac{\partial R_\alpha}{\partial x}\right|_{s_P^*} \frac{\partial s_P^*}{\partial \alpha_{l'}} = 0 \tag{II.20}$$

where the points, s_p^* $(p = 1,..., Q)$ are solutions of Eq. (II.19b). Rewriting Eq. (II.20) in order to obtain an explicit expression for the feature sensitivity coefficient $\partial s_P^*/\partial\alpha_{l'}$, $p \in \{1,..., Q\}$, we derive

$$\frac{\partial s_P^*}{\partial \alpha_{l'}} = \frac{\left.\frac{\partial K_\alpha}{\partial \alpha_{l'}}\right|_{\mathbf{x}^*} + \sum_{j=1}^{N} \left.\frac{\partial K_\alpha}{\partial x_j}\right|_{\mathbf{x}^*} \frac{\partial x_j^*}{\partial \alpha_{l'}} - \left.\frac{\partial R_\alpha}{\partial \alpha_{l'}}\right|_{s_P^*}}{\left.\frac{\partial R_\alpha}{\partial x}\right|_{s_P^*}}. \tag{II.21}$$

The choice of constraining operator equation is in a sense arbitrary. It will depend upon the kind of information or parameter dependence that the observer is seeking to obtain.

III. Example: Elastic Differential Scattering

The simple example here serves to elucidate the basic concepts in Section II. We focus in particular on scattering from a (12, 6) Lennard–Jones potential and consider how features in the differential scattering cross section depend on two reduced parameters. The radial Schrödinger equation is solved with the potential $V(\rho) = (\rho^{-12} - \rho^{-6})$. Here the reduced system parameters are given by $A = kR_m$, $B = 2\mu\varepsilon R_m/\hbar^2$, where μ is the reduced mass, k the wave vector and R_m is the location of the potential minimum of depth ε. The differential scattering cross section was generated using the JWKB result for the partial wave phase shift [7] and the input parameters A and B were set equal to 200 and 40,000/3, respectively. The resulting cross section $I_{A,B}(\theta)$ is given in Fig. 1. We have chosen to focus on the slow overriding pattern of the rainbow centered around $\theta = 35°$ and the supernumerary rainbows centered around $\theta = 24°$ and $\theta = 17.5°$. This was accomplished by filtering out the high frequency oscillatory structure with the window function $f_\sigma(\theta, \theta') = (1/\sigma(2\pi)^{1/2}) \exp[-(\theta - \theta')^2/2\sigma^2]$. This function filters both the cross section and its

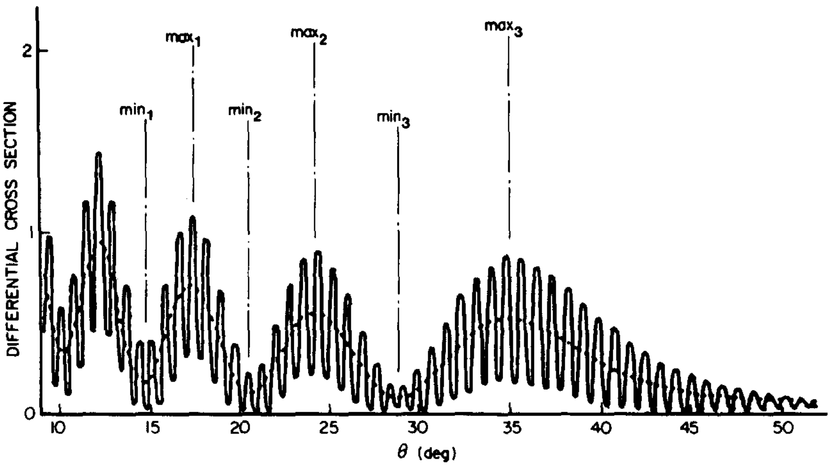

FIG. 1. Differential cross section $I_{A,B}(\theta)$ for scattering from a (12-6) Lennard-Jones potential (——) in units of R_m^2 and filtered differential cross section $I^f_{A,B}(\theta)$ (---). Various maxima and minima of $I^f_{A,B}(\theta)$ are labelled.

sensitivities with respect to A and B. The filtered cross section $I^f_{A,B}(\theta)$ and sensitivities are then given by

$$I^f_{A,B}(\theta) = \int_0^\pi f_\sigma(\theta, \theta')\, I_{A,B}(\theta')\, d\theta' \tag{III.1}$$

$$\begin{aligned} \frac{\partial I^f_{A,B}(\theta)}{\partial A} &= \int_0^\pi f_\sigma(\theta, \theta') \frac{\partial I_{A,B}(\theta')}{\partial A}\, d\theta' \\ \frac{\partial I^f_{A,B}(\theta)}{\partial B} &= \int_0^\pi f_\sigma(\theta, \theta') \frac{\partial I_{A,B}(\theta')}{\partial B}\, d\theta'. \end{aligned} \tag{III.2}$$

This example is a particular case of Eq. (II.13) with $W = f_\sigma$. Filtering of this type would also be meaningful for incorporating an instrument resolution function in order to compare theory and experiment. It was found that setting $\sigma = \pi/360$ was sufficient to separate the high and low frequency structure of $I_{A,B}(\theta)$. Thus, in Fig. 1, one sees that $I^f_{A,B}(\theta)$ follows only the low frequency structure of $I_{A,B}(\theta)$. At the same time it is important that our analysis of the low frequency structure not be critically dependent on the actual value of σ, the parameter introduced in the window function. This was confirmed in a sensitivity test of the smoothed cross section with respect to σ.

Table Ia presents results for the normalized sensitivities of the various maxima and minima of interest with respect to A, the reduced wavenumber parameter and B, the so-called quantum parameter. First, we see that increasing B decreases the extrema while increasing A increases them. Second, the sensitivities with respect to A are significantly weaker. Third, the extrema became increasingly sensitive to

TABLE I

(a) Sensitivities of the Filtered Differential Cross Section $I^f_{A,B}(\theta)$ with Respect to the Reduced Parameters A and B

$\partial \ln I^f_{A,B}(\theta_i)/\partial \ln \gamma$

γ \ θ_i	$\max_1$	$\max_2$	$\max_3$	$\min_1$	$\min_2$	$\min_3$
A	5.83(−2)	5.67(−2)	6.25(−2)	8.73(−2)	7.30(−2)	5.49(−2)
B	−1.28	−1.04	−1.15	−2.50	−1.50	−0.97

(b) Sensitivities of the Position of Extrema of the Filtered Differential Cross Section $I^f_{A,B}(\theta)$ with Respect to the Reduced Parameters A and B

$\partial \ln \theta_i/\partial \ln \gamma$

γ \ θ_i	$\max_1$	$\max_2$	$\max_3$	$\min_1$	$\min_2$	$\min_3$
A	−0.75	−0.96	−1.20	−0.70	−0.88	−1.16
B	31.7	36.3	41.2	31.5	35.7	43.8

input parameter variations as we shift to smaller angles and this is particularly marked for the B parameter sensitivities. Table Ib now considers how the variation of the A and B parameters affects the *position* of the extrema. We see that high decreasing angle, the position of each extremum becomes less sensitive to variations of the input parameters. Also, while increasing A shifts the extrema to smaller angles, increasing B shifts the same to higher angles and as in Table Ia has a more significant effect on the extrema than A. Sensitivities to other features in Fig. 1 (e.g., the oscillation widths) may be similarly examined. The results found here are likely system dependent but they clearly serve to show that interesting physical questions can be directly addressed by simple application of the ideas in Section II.

IV. Discussion

We have been concerned with the question of how input parameters affect structural features of output. This was done by characterizing the output in terms of the behavior of just a few representative points. The choice of points will of course depend on the feature being studied. Recently, a more significant and extensive application of the methodology of this paper has been undertaken, involving a study of wet CO oxidation kinetics [8].

It is worth noting again here that in certain circumstances, one may wish to transform the original data into a new representation and then examine the behavior of critical points in the new data. The example of Section III illustrated some of the basic ideas.

The approach to feature sensitivity questions that has been outlined here, has obvious advantages over our alternative sensitivity approach (discussed in Section I) [3, 4]. Thus, the analysis here is simpler and avoids having to invoke the art of curve fitting. At the same time, however, there may be circumstances for which the alternative approach is to be preferred. One may, for example, be interested in detecting the appearance of new features in the data and this is readily done within the alternative framework. In addition, the fitting approach can be used when attempting non-linear parametric scaling of system solutions [9].

Problems in feature analysis have their own particular characteristics determined by the questions of concern and the mathematical structure of the system. It is not unlikely, therefore, that further analytical techniques will be developed reflecting this diversity of character.

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