Particle Accelerators, 1986, Vol. 19, pp. 73–81
0031-2460/86/1904–0073/$15.00/0

Printed in the United States of America

ON DETERMINING IMPORTANT ASPECTS OF TRAJECTORY DESIGN PROBLEMS†

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(Received March 7, 1985)

The design of particle accelerators aims to produce machines with stable particle trajectories over many orbits. A real machine will consist of discrete focusing and accelerating elements which inherently will be flawed due to various physical effects or manufacturing errors. Even when such defects are minimal, the question remains as to which physical or engineering factors are critically important or conversely may be neglected in relation to machine performance. Questions of this nature may be addressed in a practical fashion by the techniques of sensitivity analysis, and the present paper reviews these concepts especially for trajectory issues. The Hamiltonian for the particles within the accelerator is assumed to be described either in terms of discrete parameters or more generally in terms of a potential function. The response of system performance with respect to variations of initial conditions, system parameters, and features on the potential surface will be treated. Practical calculations giving quantitative insight may be performed with existing codes. Finally, a discussion will be presented concerning global design or error propagation associated with finite alterations of an existing Hamiltonian.

I. INTRODUCTION

A broad class of generic questions arises when performing orbital-dynamics calculations either for design purposes or for probing the fundamental physics involved. Calculations performed for either of the latter purposes will be referred to as modeling throughout this paper. Often the physical model contains imprecisely known components for a variety of reasons. Even after a design is chosen, one must also consider the fact that the ultimately constructed device will not have ideal components, and such "apparatus" flaws can affect operating performance. The latter problem is statistical in nature and could also be stochastic if temporal fluctuations occur during the orbital cycles. Finally, even if the physical model is precisely known and no other errors are anticpiated, there still remains the important question as to which components of the model are responsible for physically interesting observations or performance.

Although the above questions were couched in terms of accelerator orbital-dynamics problems, exactly the same issues will arise in any area involving trajectories such as in electrical circuits or molecular dynamics. Traditional stability-analysis techniques are just a special case of the broader sensitivity matters being considered here. In particular, stability analysis is normally defined with regard to sensitivity of a trajectory to its initial conditions. The material in Section II will clearly show the relation between stability analysis, sensitivity

† The author acknowledges support from the Department of Energy.

analysis, and broader parametric concerns. In addition, when dealing with complicated multidimensional phase-space problems, it can be of considerable interest to understand which dynamical coordinates or momenta are important for controlling the overall behavior of the remainder. This question may be addressed by a variant of stability analysis discussed below. In general, beyond the realm of stability matters, sensitivity analysis will be concerned with the interrelationship between the input model and its output observables. In the case of trajectories these observables may be merely the particle trajectories themselves or perhaps some function (or functional) of the coordinates and/or momenta. The input model may be characterized by a discrete set of parameters describing, for example, components of a Hamiltonian. In more general terms trajectory problems are best expressed in terms of an input potential function in coordinate space, although additional parametric variables may also enter. Regardless of whether the input information consists of discrete parameters or continuous functions, the main context of this paper will focus on gradient concepts for probing sensitivity issues. These gradients will accordingly be partial derivatives or functional derivatives. This approach is inherently local around an operating point in the space of input parameters or potential functions. Questions concerning system performance in response to finite excursions in the parameter space involve issues of global sensitivity analysis. If the questions of concern focus on merely "what's important" in the dynamical system, then local techniques are generally quite adequate. However, matters of finite error propagation or general system design (parameter searching) inevitably fall into the category of global analysis. Less is known about the latter topic due to its inherently more complicated nature. Accordingly, this paper will primarily focus on local gradient techniques although an introduction to some of the global matters will also be included.

The present paper is not intended to be a thorough treatment on all aspects of sensitivity analysis which might be relevant to orbital dynamics particularly for accelerator design. The goal of this paper is to give the accelerator community an introduction to the tools and also present some classes of questions which may be accordingly addressed. Many of these questions are uniquely treated by the specialized tools of sensitivity analysis and to the author's knowledge they have not been broached in the accelerator-design area. Much of the relevant developments in sensitivity analysis have occurred in diverse fields of chemistry,[1] physics,[2] and engineering.[3] The reader should be reminded of the generic nature of sensitivity-analysis tools when reading the focused developments in the latter areas of the literature. The bulk of the paper in Section II below is divided into various subcategories after introductory comments regarding the nature of the dynamical equations.

II. ON DETERMINING IMPORTANT ASPECTS OF MODELING FROM A LOCAL SENSITIVITY PERSPECTIVE

The differential equations describing orbital dynamics would nominally be Hamilton's equations for a conservative system. However, there are physical

circumstances where a broader perspective is required. For example, dissipation through synchrotron radiation may be present, as may collective spatial effects described by Fokker–Planck equations. The relevant equations could also be stochastic if temporal fluctuations existed due to various uncontrollable laboratory events while the particles are traversing their trajectories. For the purposes of this paper it suffices to consider purely temporal initial-value problems of the following form:

$$\frac{d\mathcal{O}_i}{dt} = f_i(\mathcal{O}, \boldsymbol{\alpha}), \tag{1}$$

where elements of the vector $\mathcal{O}(t, \boldsymbol{\alpha})$ may be thought of as basic system observables, and the vector $\boldsymbol{\alpha}$ includes all relevant system parameters residing in the differential equations. Equation (1) would be completely specified with the addition of a set of initial conditions. These initial conditions may also be thought of as additional system parameters. Hamilton's equations are clearly of the type in Eq. (1), and dissipative processes may be readily included without any further modification. The trajectory modeling process alone would consist of solving Eq. (1) to a desired time limit. This task is a serious problem in itself for orbital mechanics, but in the present context it is assumed that a viable code is available for the solution. Our purpose here is to explore the information content in the solutions with regard to the system parameters. In some cases this problem may take on a modified form if the actual laboratory objective is a function or functional of the solution to Eq. (1). In either case the analysis follows along similar lines.

If we consider the parameters in Eq. (1) to be time independent, then the simplest form of sensitivity analysis can be addressed by taking the partial derivative of Eq. (1) with respect to an arbitrary parameter α_j:

$$\frac{d}{dt}\left(\frac{\partial \mathcal{O}_i}{\partial \alpha_j}\right) - \sum_l J_{il}\left(\frac{\partial \mathcal{O}_l}{\partial \alpha_j}\right) = \frac{\partial f_i}{\partial \alpha_j}. \tag{2}$$

For the particular case of α_j being an element of the initial condition vector $\mathcal{O}(0)$, the inhomogeneity in Eq. (2) will not be present. The Jacobian matrix $\mathbf{J}$ has elements

$$J_{il}(t) = \frac{\partial f_i}{\partial \mathcal{O}_l}. \tag{3}$$

Since Eq. (2) is a linear inhomogeneous differential equation, it is convenient to define the system Green's function which satisfies the equation:

$$\begin{aligned} &\frac{d}{dt} G_{ij}(t, t') - \sum_l J_{il} G_{lj}(t, t') = \delta_{ij}\, \delta(t - t'), \\ &G_{ij}(t', t') = \delta_{ij}, \\ &G_{ij}(t, t') = 0, \qquad t < t'. \end{aligned} \tag{4}$$

The physical interpretation of $\mathbf{G}$ will be discussed more extensively below, but for

now we may use the existence of **G** to solve Eq. (2):

$$\frac{\partial \mathcal{O}_i(t)}{\partial \alpha_j} = \sum_n \int_0^t dt' G_{in}(t, t') \frac{\partial f_n(t')}{\partial \alpha_j}, \tag{5}$$

where α_j is understood not to be an initial condition for Eq. (1). A numerical algorithm may be generated based on Eq. (5) for obtaining the parametric sensitivities,[4] but, regardless of how the sensitivities are calculated, it is evident that they are a simple convolution of the system Green's function. The temporal behavior of the sensitivities is therefore essentially dictated by that of the Green's function, and for this reason it will be discussed more extensively below. The sensitivity coefficient on the left-hand side of Eq. (5) is simply interpreted as the sensitivity of the ith observable at time t with respect to a variation of the jth system parameter. This interpretation is clearly significant with regard to relating orbital-trajectory behavior to underlying particle-accelerator design parameters.

The formulation in Eq. (1) tacitly assumed that the system parameters formed a set of time-independent constants. However, there is another approach based on a functional view which is especially important when considering Hamiltonian systems.[5] Without loss of generality we will use Newton's equations:

$$\begin{aligned} \frac{d}{dt} p_i &= -\frac{\partial V(\mathbf{q})}{\partial q_i} = F_i(\mathbf{q}), \\ m_i \frac{d}{dt} q_i &= p_i, \end{aligned} \tag{6}$$

where V and **F** are the potential and force. Although in many cases these latter quantities will be expressed in terms of a set of discrete parameters, it is more general and informative to consider the force (or potential) *function* for variation. In other words, we desire to understand how the trajectory at time t is affected by a disturbance in the force at position $\mathbf{q}'$. In analogy with the case of discrete variations, we may define functional sensitivity densities with respect to the force:

$$\delta q_i(t)/\delta F_j(\mathbf{q}') \quad \text{and} \quad \delta p_i(t)/\delta F_j(\mathbf{q}'). \tag{7}$$

These densities have the following meaning;

$$\delta q_i(t) = \sum_j \int d\mathbf{q}' \frac{\delta q_i(t)}{\partial F_j(q')} \delta F_j(\mathbf{q}'), \tag{8}$$

and analogously for the momentum. Therefore we may interpret $\delta q_i(t)/\delta F_j(\mathbf{q}')$ as the response of the ith coordinate at time t to a disturbance in the jth component of the force at position $\mathbf{q}'$. It is important to understand that the disturbance is at a point in coordinate space and not at a point in time. It would be possible to consider the latter variation, but it is physically entirely different. Equation (8) would correspond to a synchrotron having a fixed deviation $\delta\mathbf{F}(\mathbf{q}')$ in the force field from the nominal design optimum. Upon each orbit a particle would repeatedly experience the same force deviation, and the cumulative effects could be substantial. In contrast, a deviation $\delta\mathbf{F}[\mathbf{q}'(t')]$ would correspond to a pulse at time t', and this might be most applicable to the introduction of laboratory

controlled disturbances. Taking the former perspective we may now functionally differentiate Eq. (6) with respect to the force to produce the following differential equations:

$$\begin{aligned} \frac{d}{dt}\left(\frac{\delta p_i(t)}{\delta F_j(\mathbf{q}')}\right) &= \sum_l \left(\frac{\partial F_i}{\partial q_l}\right)\left(\frac{\delta q_l(t)}{\delta F_j(\mathbf{q}')}\right) + \delta_{ij}\,\delta(\mathbf{q}(t)-\mathbf{q}'), \\ m_i \frac{d}{dt}\left(\frac{\delta q_i(t)}{\delta F_j(\mathbf{q}')}\right) &= \left(\frac{\delta p_i(t)}{\delta F_j(\mathbf{q}')}\right). \end{aligned} \tag{9}$$

An analogous set of equations may also be derived for variations of the potential. The solution to Eq. (9) produces a sensitivity-response function for a particular trajectory with regard to a disturbance of the force. In general, if the observable of interest, $\mathcal{O}(\mathbf{p}, \mathbf{q})$, is a function (a functional may also be treated) of the system coordinates and momenta, we may simply derive $\delta\mathcal{O}(\mathbf{p}(t), \mathbf{q}(t))/\delta\mathbf{F}(\mathbf{q}')$ from the solution of Eq. (9). Typically, it will also be necessary to average over initial conditions or phases to obtain the true laboratory observable of interest, and its subsequent sensitivity response would be assembled from repeated independent trajectory solutions of Eqs. (6) and (9).

As stated earlier, more general differential equations or circumstances could be analogously handled. Many such situations have already been examined to some degree in the available literature. The remainder of this section will deal with particular specialized aspects and physical questions addressable with these techniques.

Stability Analysis and Green's Functions

The Green's functions satisfying Eq. (4) may be identified with the traditional stability matrix in a dynamical system.[6] This connection is evident by differentiating Eq. (1) with respect to an arbitrary initial condition and comparing with Eq. (4). However, an instructive alternative approach consists of first introducing a source flux $\delta\mathcal{J}_i(t)$ of the ith dependent variable into Eq. (1):

$$\frac{d\mathcal{O}_i}{dt} = f_i(\boldsymbol{\mathcal{O}}, \boldsymbol{a}) + \delta\mathcal{J}_i(t). \tag{10}$$

Functional differentiation of this equation with respect to the jth flux will produce:

$$\frac{d}{dt}\left(\frac{\delta\mathcal{O}_i(t)}{\delta\mathcal{J}_j(t')}\right) - \sum_l J_{il}\left(\frac{\delta\mathcal{O}_l(t)}{\sigma\mathcal{J}_j(t')}\right) = \delta_{ij}\,\delta(t-t'). \tag{11}$$

Equations (4) and (11) are identical and provide an immediate physical interpretation of the Green's function elements $G_{ij}(t, t') = \delta\mathcal{O}_i(t)/\delta\mathcal{J}_j(t')$ as being the response of the ith dependent variable at time t with respect to the *flux* of the jth dependent variable at prior time t'. This latter quantity is a functional density and is therefore dimensionless, taking into account the units of flux. Therefore it has been common (but somewhat misleading) to use the identification $G_{ij}(t, t') \equiv \partial\mathcal{O}_i(t)/\partial\mathcal{O}_j(t')$.

The eigenvalues of the G matrix (actually their logarithms) may be identified as the Lyapounov stability exponents[6,7]:

$$\lambda_n(t, t') = \mathbf{U}_n^T(t, t')\mathbf{G}(t, t')\mathbf{U}_n(t, t'), \tag{12}$$

where $\mathbf{U}_n(t, t')$ is the nth eigenvector and $\lambda_n(t, t')$ is the associated eigenvalue. These latter quantities depend on the current time as well as the time of initial condition specification. Although many turns of the accelerator would be relevant in realistic problems, the ultimate asymptotic $t \to \infty$ behavior of the stability eigenvalues is not actually of interest (i.e., the particles need only be tracked for a finite period of time). Dynamic instability is indicated by any of the eigenvalues satisfying $|\lambda_n| > 1$. As a final comment, it could be misleading to merely examine the eigenvalue spectrum of the Jacobian $\mathbf{J}$ rather than $\mathbf{G}$ since the former coefficient matrix in Eq. (4) does not include the integrated time history of the system stability which is contained in $\mathbf{G}$.

In addition to calculating the stability eigenvalues, one may also probe for which physical variables contribute to the system stability.[7] This information can be obtained by differentiating Eq. (12) with respect to a system parameter:

$$\frac{\partial \lambda_n(t, t')}{\partial \alpha_j} = \mathbf{U}_n^T(t, t') \frac{\partial \mathbf{G}(t, t')}{\partial \alpha_j} \mathbf{U}_n(t, t'). \tag{13}$$

An accompanying expression may also be established for the sensitivity of the eigenvectors. This approach may be viewed as either a parametric sensitivity analysis of the system stability or equivalently a stability analysis of the parametric sensitivity. This type of knowledge should be especially important when the parameters are of a design nature and controllable in the laboratory. In this fashion design alterations could be identified leading to enhanced trajectory stability.

A related set of reduced or constrained system Green's functions may also be calculated for the purpose of gaining additional insight into dynamic coupling. In order to understand this approach first note that the terms on the right-hand side of Eq. (1) will represent the *kinematic* coupling in the system. However, upon solution of the differential equation, the actual *dynamic* coupling may differ due to complex nonlinear interactions. Therefore, a significant issue to probe is the dynamic coupling arising in many particle systems. Such an analysis can be carried out by considering variations of a portion of the dependent variables while holding another portion constrained as fixed. Therefore upon consideration of the dependent-variable vector, we may decompose it into two parts $\mathcal{O} \equiv (\mathcal{O}', \mathcal{O}'')$ where variations of the second portion are constrained to be $\delta\mathcal{O} = \mathbf{0}$. We accordingly may calculate the elements of the reduced Green's function

$$G'_{ij}(t, t') = \delta\mathcal{O}_i(t')/\delta\mathcal{J}'_j(t')|_{\delta\mathcal{O}''=\mathbf{0}}.$$

In practice this constrained matrix satisfies an equation of exactly the same form as Eq. (4), except now the Jacobian is of reduced dimension with the columns and rows associated with $\mathcal{O}''$ removed. Elements of this reduced stability matrix probe the system dynamic response fostered by restraining the variables of $\mathcal{O}''$. A significant point to understand in this regard is that the latter variables are still

retained in the calculation at their nominal value, despite the fact that their response to variations of $\mathcal{O}'$ is not allowed. By selectively decomposing the system into parts $\mathcal{O}'$ and $\mathcal{O}''$ along with an examination of the corresponding Green's function elements, one may conclude which dynamic couplings are critical for system performance.

Oscillatory Systems

Dynamic oscillators are of interest in a host of areas, including accelerator physics. In principle, sensitivity analysis of such problems follows along exactly the same lines discussed above since the differential equations are of the type in Eq. (1). However, a new sensitivity issue arises due to the secular nature of the sensitivity Eq. (2). In particular, the inhomogeneous forcing term on the right-hand side of Eq. (2) will be in exact resonance with the oscillatory Jacobian. The physical origin of the secular response may also be understood by considering an idealized simple sinusoidal observable $\mathcal{O}(t, \alpha) = A(\alpha) \exp[i\omega(\alpha)t]$ with amplitude A and frequency ω. Differentiation of this equation with respect to the parameter α produces

$$\frac{\partial A}{\partial \alpha} = \frac{dA}{d\alpha} \exp[i\omega(\alpha)t] + it \frac{d\omega}{d\alpha} A \exp[i\omega(\alpha)t]. \tag{15}$$

The second term in Eq. (15) is proportional to the frequency sensitivity and grows linearly with time to eventually totally overcome the first term. In essence, the origin of the secularity can be understood by considering the replacement $\omega(\alpha) \rightarrow \omega(\alpha) + (d\omega/d\alpha)\, d\alpha$, which will cause an arbitrarily large shift in the wave form as time increases regardless of how small the term $(d\omega/d\alpha)\, d\alpha$. Exactly analogous behavior will show up for any oscillator which may always be represented by the Fourier series

$$\mathcal{O}(t, \boldsymbol{\alpha}) = \sum_n A_n(\alpha) \exp[in\omega(\boldsymbol{\alpha})t]. \tag{16}$$

Differentiation of this expression with respect to a system parameter will produce the following relation:

$$\left(\frac{\partial \mathcal{O}}{\partial \alpha_j}\right) = \left(\frac{\partial \mathcal{O}}{\partial \alpha_j}\right)_\omega - \frac{t}{\omega}\left(\frac{\partial \omega}{\partial \alpha_j}\right)\left(\frac{\partial \mathcal{O}}{\partial t}\right). \tag{17}$$

The first term in Eq. (17) may be understood to be the structural or amplitude sensitivity coefficient evaluated with the frequency held fixed.[8] Similarly the last term corresponding to secular growth is associated with the parametric dependence of the oscillator frequency.

Global Sensitivity Issues

All of the analyses discussed above are local in the sense that the gradients were evaluated at an operating point in parameter space. A similar statement would

also apply to functional sensitivities, in which case the gradients are evaluated locally about the nominal input functions. If the goal of the analysis is to determine "what's important," then generally the local-gradient treatment should be quite sufficient. However, matters involving design problems and issues of statistical-error propagation inherently involve the consideration of finite excursions throughout the parameter space. In the case of design problems the goal is to search the parameter space in order to find an optimum set of conditions consistent with a chosen objective. In a similar vein, statistical-error propagation is also associated with finite-parameter excursions. This latter comment follows since a finite variance of the input parameters is necessarily of global concern.

In principle, global sensitivity analysis could be approached by the calculation of higher-order sensitivity gradients. This avenue is computationally intensive, and there is also no guarantee that the resultant Taylor series would be convergent. Of the two global problems discussed above, the case involving design or global mapping is the one computationally most intensive since in the case of error propagation, the goal is typically limited to determining just the covariance properties of the output orbital motion as a result of input statistical errors in the parameters.[9] The central point is that a search is not necessary in contrast to the situation found in design problems.

All global sensitivity problems, to a certain degree, may ultimately be characterized as *inherently* difficult and computationally intensive. Nevertheless, the traditional approach of Monte Carlo sampling of points in the parameter space will often be prohibitively expensive. There is much less known about how to treat global sensitivity analysis in comparison to the developments of the local theory. Two approaches appear promising in this context. First, in the case of statistical-error propagation, the expected value-analysis technique may be applied.[10] This procedure is a Taylor expansion, but it does not entail an expansion of the dependent variables in terms of the parameters. Rather, the parameter dependence of the dependent variables is retained, and a hierarchy of coupled-moment equations is solved ultimately leading to a solution for the statistical mean trajectory and its covariances. In the case of parameter space searching, it appears that Lie-group theoretical methods may have a significant contribution.[11] The essential idea is to identify the infinitesimal operators corresponding to transformations in the parameter space while keeping the original equations of motion invariant. Equations for these generators may be derived with the hope that even their approximate solution will yield valuable information about system behavior over a finite region of parameter space. Much further work still needs to be done in the general area of global analysis, and this topic is expected to be an active area of research.

III. CONCLUSIONS

The present paper has aimed to give a succinct introduction to relevant aspects of sensitivity analysis particularly for orbital dynamics. Extensive numerical calculations with these ideas have been performed on a number of problems outside the

realm of accelerator physics. The only essential difference between the latter area and those already studied concerns the length of the time integrations. Long-time solutions of the dynamic equations can complicate the solution process and should similarly have an impact on seeking sensitivities. The ultimate goal should be the incorporation and simultaneous calculation of sensitivity information while performing the orbital-dynamics calculations. Some real differences may be involved in the numerical aspects of sensitivity analysis in this regard when taking into account the special nature of long-time trajectory problems. Nevertheless the basic tools and concepts of sensitivity analysis are already available and only need to be implemented.

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