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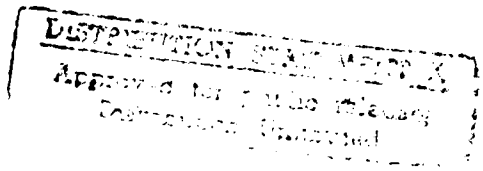

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On the Sensitivity of Solutions of Parametrized Equations *

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Abstract: *The sensitivity of a solution of a parametrized equation $F(z,\lambda) = 0$ with respect to the parameter vector λ is usually defined as the change of the state z in dependence of λ. In other words, for any solution expressible in the form $(z(\lambda), \lambda)$ with some smooth function $z = z(\lambda)$ the sensitivity is the derivative $Dz(\lambda)$. Typically the solutions form a manifold M in the product of the state-space and the parameter space and this sensitivity is available only at those points of M where the parameters can be used to define a local coordinate system. This paper introduces a general sensitivity concept which applies at all solutions on M and which includes the earlier definition. Some general geometric interpretations of the new measure are presented and it is shown that the sensitivity analysis can be easily integrated into the solution process. The theory also suggests the introduction of a readily computable second-order sensitivity measure reflecting the curvature-behavior of M. Two numerical examples illustrate the discussion.*

1. Introduction

Mathematical models for many scientific and engineering problems have the form of a nonlinear equation

$$F(z,\lambda) = 0, \tag{1.1}$$

involving some (often infinite-dimensional) state variable z and a finite-dimensional vector λ of parameters. The computational tasks then include not only the calculation of suitable solutions but also the determination of their sensitivity under variations of the parameters.

In recent years the literature on methods for a sensitivity analysis of specific problems has been growing rapidly (see, e.g., [7], [11] and the references given there). Most of this

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work is based on the assumption that near a given solution (z_0, λ_0) of (1.1) the state z depends smoothly on the parameter vector λ; that is, the solutions of (1.1) can be witten in the form $(z(\lambda), \lambda)$ with some smooth function $z = z(\lambda)$. Then the derivative $Dz(\lambda_0)$ of z at λ_0 is a natural measure of the sensitivity of the solution $(z(\lambda_0), \lambda_0)$. For suffiently smooth F this sensitivity measure has to satisfy the linearized equation

$$D_z F(z_0, \lambda_0) Dz(\lambda_0) + D_\lambda F(z_0, \lambda_0) = 0. \tag{1.2}$$

If this equation is explicitly available and $D_z F(z_0, \lambda_0)$ is invertible then $Dz(\lambda_0)$ can be computed from (1.2). Codes for solving (1.2) for various applications in molecular dynamics are cited in [7]. When the partial derivatives $D_z F$ and $D_\lambda F$ are not explicitly known we may consider the use of some difference approximations for them in which case there is also a need for studying the influence of these approximations upon the desired solution of (1.2). Alternately, if the sensitivity $Dz(\lambda_0)\mu$ in the direction of a parameter vector μ is required then one may compute approximations of $z(\lambda_0 + \tau\mu)$ for several values of the scalar τ near $\tau = 0$ and then apply some numerical differentiation formula for approximating $Dz(\lambda_0)\mu$.

Generally, this definition of sensitivity does not reflect any of the underlying geometric aspects; moreover, the indicated methods do not take much account of information that may be available during the computation of the original solution (z_0, λ_0) itself. In fact, sensitivity analysis is usually considered to be a "post-processing" technique which is applied only after a suitable solution has already been found. The purpose of this paper is to give some general geometric interpretations of the sensitivity concept and to show that the sensitivity analysis can be easily integrated into the primary solution process without adding unduly to the computational cost. The approach is based on the application of some differential-geometric considerations which have been shown earlier to be very natural in connection with parameterized equations (1.1), (see e.g. [3], [8], [9]).

2. Background

The operator F in (1.1) may represent a system of nonlinear equations in several real variables or some boundary value problem in the state variable z. In the latter case, a discretization has to be introduced for the computational solution of the problem, and thus in either case we arrive at a finite-dimensional equation.

It is useful to combine the state variable z and parameter variable λ of (1.1) into a single vector x and hence to write the equation in the form

$$F(x) = 0. \tag{2.1}$$

Here we assume that $F : E \subset R^n \mapsto R^m$, $d = n - m \geq 1$, is of class C^r, $r \geq 1$ on an open subset $E \subset R^n$ and $0 \in R^m$ is a regular value of F; that is, rank $DF(x) = m$ for all x in the inverse image $F^{(-1)}(0)$.

Under these conditions it is well-known that the set of all regular solutions,

$$M = \{\ x \in E; \quad F(x) = 0\ \} \tag{2.2}$$

is either empty or a d-dimensional C^r-manifold in R^n without boundary. We assume always that $M \neq \emptyset$. For simplicity the tangent space $T_x M$ at any point x of M will be identified here with the d-dimensional affine space

$$T_x M = \{(x,p) \in \{x\} \times R^n; \quad DF(x)p = 0\}. \tag{2.3}$$

For numerical purposes a computationally feasible scheme is required for fixing local coordinate systems at a given point $x_0 \in M$. We consider only orthogonal coordinate systems and call a linear map

$$V = (V_m, V_d) \in L(R^m \times R^d, R^n); \quad V^T V = I_{m+d},\ VV^T = I_n, \tag{2.4}$$

a local basis at $x_0 \in M$ if

$$T^\perp \cap \ker DF(x_0) = \{0\},\ T = \text{rge } V_d,\ T^\perp = \text{rge } V_m. \tag{2.5}$$

In terms of (2.4), the condition (2.5) is equivalent with

$$DF(x_0)V_m \in \text{Isom } (R^m), \tag{2.6}$$

or, alternately, with

$$\begin{pmatrix} DF(x_0) \\ V_d^T \end{pmatrix} \in \text{Isom } (R^n). \tag{2.7}$$

We introduce the function

$$G : V^T(E - x_0) \subset R^m \times R^d \mapsto R^m, \quad G(y, \tau) = F(x_0 + V_d\tau + V_m y). \tag{2.8}$$

Then, by the implicit function theorem applied to the equation

$$G(y, \tau) = 0, \tag{2.9}$$

there are open neighborhoods $S_d \subset R^d$ of $0 \in R^d$ and $S_n \subset R^n$ of x_0, respectively, such that for any $\tau \in S_d$ there exists exactly one solution y of (2.9) with $x_0 + V_d\tau + V_m y \in S_n$ and that the mapping $\phi : S_d \mapsto R^m$, $\phi(\tau) = y$ is of class C^r on S_d. Evidently, we have $\phi(0) = 0$ and

$$\Phi : S_d \subset R^d \mapsto R^n, \ \Phi(\tau) = x_0 + V_d\tau + V_m\phi(\tau), \quad \forall \tau \in S_d, \tag{2.10}$$

is a C^r-diffeomorphism from S_d onto $M \cap S_n$. In other words, Φ^{-1} is a chart of M at x_0 and we call Φ the local coordinate map at x_0 induced by the local basis V and refer to ϕ as the corresponding corrector function.

For any d-dimensional subspace $T \subset R^n$ we can choose an orthonormal basis $v_1, \ldots, v_n$ of R^n such that $T = \text{span } \{v_{m+1}, \ldots, v_n\}$ and then set $V = (v_1, \ldots, v_n)$. Since the condition (2.5) depends only on T, it makes sense to speak of a local coordinate system induced by the subspace T. A point $x_0 \in M$ is called a foldpoint with respect to the subspace T if the condition (2.5) is violated; that is, if T does not induce a local coordinate system.

Obviously (2.5) always holds for the d-dimensional subspace $T = \ker DF(x_0)$. In view of our definition (2.3) of the tangent spaces, a local coordinate map induced by $\ker DF(x_0)$ shall be called a tangent-coordinate map and the corresponding local basis a tangential local basis. We shall always denote tangential bases by $U = (U_m, U_d)$ and their induced local coordinate map by

$$\Psi : S_d \subset R^d \mapsto R^n, \ \Psi(\omega) = x_0 + U_d\omega + V_m\psi(\omega), \quad \forall \omega \in S_d, \tag{2.11}$$

Note that any tangential local basis U is characterized by (2.4) together with the condition $DF(x_0)U_d = 0$ which automatically implies (2.5).

As suggested by (1.1), in many applications the equation (2.1) typically represents some multi-parameter problem which means that some natural d-dimensional parameter subspace $\Lambda \subset R^n$ has been identified. Then Λ defines a natural local coordinate system at all those points $x \in M$ where $\Lambda^\perp \cap \ker DF(x) = \{0\}$.

3. First Order Sensitivity

Suppose that a local basis map (2.4/5) has been chosen at the point $x_0 \in M$ and that (2.10) denotes the induced local coordinate mapping. Then the derivative

$$D\Phi(0)\mu = V_d\mu + V_m D\phi(0)\mu, \ \mu \in R^d, \tag{3.1}$$

represents the "change" of the solution x_0 in the local coordinate direction $\mu \in R^d$. Accordingly, it is natural to define the derivative of the corrector function $\phi : S_d \mapsto R^m$; that is, the linear map

$$\Sigma \in L(R^d, R^m), \quad \Sigma = D\phi(0), \tag{3.2}$$

as the sensitivity map at x_0 with respect to the local basis V and to call the image vector $\Sigma\mu \in R^m$ the sensitivity of the solution $x_0 \in M$ in the direction μ. It is essential to observe that this definition of sensitivity depends intrinsically on the choice of the local basis V.

In applications where a natural, d-dimensional parameter subspace $\Lambda \subset R^n$ is given, the sensitivity map can be defined at all those points of M where Λ induces a local coordinate system. In that case we speak of the sensitivity mapping at these points with respect to natural parameter changes.

In order to relate our sensitivity definition to that indicated in the Introduction, let $V = (V_m, V_d)$ be a local basis at x_0 with corresponding local coordinate map (2.10). Recall, that $y = \phi(\tau)$ is for any $\tau \in S_d$ the unique solution y of the equation (2.9) such that $x_0 + V_d\tau + V_m y \in S_n$. Evidently, we have

$$D_\tau G(0,0) = DF(x_0)V_d, \quad D_y G(0,0) = DF(x_0)V_m, \tag{3.3}$$

and by differentiation of $G(\Phi(\tau), \tau) = 0$ it follows that

$$D_y G(0,0) D\,\Phi(0) + D_\tau G(0,0) = 0. \tag{3.4}$$

This agrees exactly with the definition (1.2) when applied to the mapping G at a point where the natural parameter space Λ may be used to induce the local coordinate map. From (3.3),(3.4), and (2.6) we obtain the explicit representation

$$\Sigma = -(DF(x_0)V_m)^{-1} DF(x_0)V_d, \tag{3.5}$$

which plays a central role in many sensitivity studies.

As a typical simple example consider the cubic

$$F : R^3 \mapsto R^1; \quad F(x) = x_1^3 - x_1 x_2 - x_3, \ \forall x \in R^3.$$

Since $DF(x_0) = (3x_1^2 - x_2, -x_1, -1)$ we see that $V = I_3$ defines a local coordinate mapping on M for all $x \in M$ with $3x_1^2 - x_2 \neq 0$ and (3.5) provides that

$$\Sigma = \frac{1}{(3x_1^2 - x_2)}(x_1, -1).$$

Note that $x_0 = 0$ is a foldpoint with respect to V where Σ indeed is not defined.

Suppose that $U = (U_m, U_d)$ defines a tangential local basis at x_0 with corresponding local coordinate map (2.11). Then by (3.5) and the tangency property $DF(x_0)U_d = 0$ we obtain $\Sigma = 0$. In other words, with respect to any tangential local basis the sensitivity mapping always has the value zero.

Let $V = (V_m, V_d)$ again be any local basis at x_0 with corresponding local coordinate map (2.10). Then the relation

$$x = x_0 + V_d\tau + V_m\phi(\tau) = x_0 + U_d\omega + U_m\psi(\omega), \tag{3.6}$$

has to hold for all x in some neighborhood of x_0 on M. From (3.6) it follows that the coordinate transformation relating ω and τ is given by

$$\tau = \gamma(\omega) := V_d^T U_d\omega + V_d^T U_m\psi(\omega). \tag{3.7}$$

Hence, from $D\psi(0) = 0$ it follows that $D\gamma(0) = V_d^T U_d$. Note that by (2.7)

$$\begin{pmatrix} DF(x_0) \\ V_d^T \end{pmatrix} \begin{pmatrix} DF(x_0) \\ U_d^T \end{pmatrix}^T = \begin{pmatrix} DF(x_0)DF(x_0)^T & 0 \\ (DF(x_0)V_d)^T & V_d^T U_d \end{pmatrix} \in \text{Isom}\,(R^n)$$

and hence, because of $DF(x_0)DF(x_0)^T \in \text{Isom}\,(R^m)$, that $D\gamma(0) = V_d^T U_d \in \text{Isom}\,(R^d)$, as expected.

From (3.6) we see that

$$\phi(\tau) = V_m^T U_d\omega + U_m\psi(\omega)$$

which together with $D\psi(0) = 0$ provides the new representation

$$\Sigma = V_m^T U_d(V_d^T U_d)^{-1}. \tag{3.8}$$

for the sensisitivity mapping with respect to V. The equivalence of (3.5) and (3.8) can also be established directly. In fact, from the relation

$$VV^T = V_d V_d^T + V_m V_m^T = I_n, \tag{3.9}$$

it follows that

$$DF(x_0)(V_d V_d^T + V_m V_m^T)U_d = DF(x_0)U_d = 0,$$

and therefore that

$$-(DF(x_0)V_m)^{-1}DF(x_0)V_d = V_m^T U_d (V_d^T U_d)^{-1},$$

as claimed.

For the computation of the sensitivity map Σ by means of the representations (3.5) or (3.8) we have to solve an $m \times m$ system or a $d \times d$ system of linear equations, respectively. In practice, n is large while d is relatively small. Thus the computational cost for (3.5) generally exceeds that of (3.8). In this connection, it is important to observe also that (3.8) does not depend on the orthogonality property $U_d^T U_d = I_d$ but only on the fact that the columns of U_d span the null-space $\ker DF(x_0)$. Indeed, for any $\hat{U}_d \in L(R^d, R^n)$ with $DF(x_0)\hat{U}_d = 0$ and $\operatorname{rank} \hat{U}_d = d$ there exists some $A \in \operatorname{Isom} R^d$ such that $\hat{U}_d = U_d A$ whence

$$V_m^T \hat{U}_d (V_d^T \hat{U}_d)^{-1} = V_m^T U_d A A^{-1} (V_d^T U_d)^{-1} = V_m^T U_d (V_d^T U_d)^{-1}.$$

4. Some Geometrical Aspects

As before, at the given point $x_0 \in M$ let $V = (V_m, V_d)$ be any local basis and $U = (U_m, U_d)$ a tangential local basis. Then by (3.8) the sensitivity at x_0 in the direction $\mu \in R^d$ with respect to V is given by the vector

$$\sigma = \Sigma\mu = V_m^T V_d (V_d^T U_d)^{-1}\mu \in R^n.$$

Let $\nu = (V_d^T U_d)^{-1}\mu$ and introduce the n-dimensional vectors

$$\hat{\nu} = U_d \nu \in \ker DF(x_0),\ \hat{\mu} = V_d \mu \in T = \operatorname{rge} V_d,\ \hat{\sigma} = V_m \sigma \in T^\perp. \tag{4.1}$$

for which evidently

$$\|\hat{\nu}\|_2 = \|\nu\|_2,\ \|\hat{\mu}\|_2 = \|\mu\|_2,\ \|\hat{\sigma}\|_2 = \|\sigma\|_2. \tag{4.2}$$

Then we have

$$V_d V_d^T \hat{\nu} = \hat{\mu},\ V_m V_m^T \hat{\nu} = \hat{\sigma} \tag{4.3}$$

and

$$\hat{\mu} + \hat{\sigma} = U_d U_d^T \hat{\nu} + V_d V_d^T \hat{\nu} = \hat{\nu}. \tag{4.4}$$

In other words, $\hat{\nu}$ is the unique vector in $\ker DF(x_0)$ for which the orthogonal projection onto T equals $\hat{\mu}$, and $\hat{\sigma}$ is the orthogonal projection of $\hat{\nu}$ onto $T^\perp = \text{rge } V_m$.

As a simple scalar measure of the directional sensitivity σ it is natural to compute the norm $\|\sigma\|_2$. For this note that by (4.3)

$$\hat{\mu}^T \hat{\nu} = \hat{\nu}^T U U^T \hat{\nu} = \hat{\nu}^T U U^T U U^T \hat{\nu} = \|\mu\|_2^{\,2}, \tag{4.5}$$

and therefore

$$\cos\Theta = \frac{\hat{\mu}^T \hat{\nu}}{\|\hat{\nu}\|_2 \|\hat{\mu}\|_2} = \frac{\|\mu\|_2}{\|\nu\|_2}$$

where $0 \le \Theta < \pi/2$ represents the angle between $\hat{\mu}$ and $\hat{\nu}$. Moreover, from (4.4) it follows that

$$\hat{\sigma}^T \hat{\nu} = \|\sigma\|_2^{\,2},\ \hat{\sigma}^T \hat{\mu} = 0,$$

whence in view of (4.2)

$$\|\nu\|_2^{\,2} = \|\sigma\|_2^{\,2} + \|\mu\|_2^{\,2}, \tag{4.6}$$

and thus

$$\|\sigma\|_2 = [\frac{1}{\cos^{\,2}\Theta} - 1]^{1/2} \|\mu\|_2 = \frac{\sin\Theta}{[1 - \sin^{\,2}\Theta]^{1/2}} \|\mu\|_2. \tag{4.7}$$

Evidently, for $\Theta = \pi/2$ the condition (2.5) is violated and obviously this occurs exactly when x_0 is a foldpoint with respect to T. Thus the sensitivity provides a measure of the suitability of the local coordinate system induced by T for representing M locally near the current point x_0.

In the special case $d = 1$ of one-dimensional manifolds the angle Θ is explicitly known. In fact, for $d = 1$ suppose that $DF(x_0)u = 0$, $\|u\|_2 = 1$ and that $V = (V_m, w)$, $w \in V_m^{\perp}$, $\|w\|_2 = 1$, is a local basis at x_0. Then $\nu, \mu \in R^1$ and $\hat{\nu}$ and $\hat{\mu}$ are n-vectors in the direction of u and w, respectively; that is, we have

$$\cos \vartheta = w^T u.$$

Generally, the distance between any two, equi-dimensional linear subspaces S_1 and S_2 of R^n is defined by

$$\text{dist } (S_1, S_2) = \|P_1 - P_2\|_2$$

where P_i is the orthogonal projection onto S_i, $i = 1, 2$. In the case of one-dimensional spaces it is easily seen (see e.g. [4]) that

$$\text{dist } (S_1, S_2) = \sin \Theta$$

where Θ is the angle between the two subspaces. Thus for $d = 1$ and with $T_0 = \ker DF(x_0)$ we may write (4.7) as

$$\|\sigma\|_2 = \frac{\text{dist } (T, T_0)}{[1 - \text{dist } (T, T_0)^2]^{1/2}} |u|. \tag{4.8}$$

Moreover, since in this case $\Sigma \in L(R^1, R^m)$, $m = n - 1$, and $\mu \in R^1$, (4.8) implies that

$$\|\Sigma\|_2 = \frac{\text{dist } (T, T_0)}{[1 - \text{dist } (T, T_0)^2]^{1/2}}. \tag{4.9}$$

It turns out that (4.9) holds generally for manifolds of any dimension d. In order to see this let

$$A^T (V_d^T U_d) B = \text{diag } (\cos \Theta_1, \ldots, \cos \Theta_d), \ 0 \leq \Theta_1 \leq \ldots \Theta_d < \pi/2, \tag{4.10}$$

be the singular value decomposition of $V_d^T U_d$ and set again $T_0 = \ker DF(x_0)$. Then it is well known that

$$\text{dist}\,(T, T_0) = \sin \Theta_d, \tag{4.11}$$

(see e.g. [GVL], p24). By (4.6) we have

$$\|\Sigma\mu\|_2^{\,2} = \|(V_d^T U_d)^{-1}\mu\|_2^{\,2} - \|\mu\|_2^{\,2},$$

and hence

$$\|\Sigma\|_2^{\,2} = \max_{\|\mu\|_2=1} \|(V_d^T U_d)^{-1}\mu\|_2^{\,2} - 1 = \|(V_d^T U_d)^{-1}\|_2^{\,2} - 1.$$

By (4.10) we see that

$$\|(V_d^T U_d)^{-1}\|_2 = \frac{1}{\cos \Theta_d}$$

and thus

$$\|\Sigma\|_2^{\,2} = \frac{1}{\cos^{\,2}\Theta_d} - 1 = \frac{\sin^{\,2}\Theta_d}{1 - \sin^{\,2}\Theta_d},$$

which together with (4.11) gives (4.9), as claimed.

5. Second Order Sensitivity

Let $U = (U_m, U_d)$ be a tangential local basis at $x_0 \in M$ and ψ the corresponding corrector function. Then we saw that the sensitivity map $\Sigma = D\psi(0)$ is zero, and hence it is of interest to consider the second derivative $D^2\psi(0)$. For this we assume from now on that our mapping F is at least of class C^r with $r \geq 2$.

The natural inner product of R^n induces a Riemannian structure on the manifold M. In [6] an algorithm was developed for computing the second fundamental tensor on M. Moreover, it was shown that for suitable bases of the tangent and normal spaces this tensor equals the desired second derivative of the corrector function for tangential

local coordinate systems. We shall not detail this approach here but sketch only the basic numerical method of [6] as it applies to the computation of the corrector function.

Let $U = (U_m, U_d)$ be any tangential local basis at $x_0 \in M$ with (2.11) as the induced local coordinate map. For any given $\mu \in R^d$ with $\|\mu\|_2 = 1$ we have $\Psi(t\mu) \in S_d$ for all real t in some interval $J = (-\epsilon, \epsilon)$. Then

$$\xi : J \mapsto M, \quad \xi(t) = x_0 + tU_d\mu + U_m\psi(t\mu),\ t \in J, \tag{5.1}$$

defines a path on M through x_0 which has at x_0 the tangent vector $\{x_0\} \times \xi'(0) = \{x_0\} \times U_d\mu$. Moreover, we have $\xi''(t) = U_m D^2\psi(t\mu)(\mu, \mu)$ and thus $\xi''(0)^T\xi'(0) = 0$.

Let $\eta : J_0 \mapsto J$ be the transformation of the arclength s of the path to the parameter t, and define $\zeta : J_0 \mapsto M$ by $\zeta(s) = \xi(\eta(s)),\ s \in J_0$. Then $\|\zeta'(0)\|_2 = 1$ ensures that $\eta'(0) = 1$ and from

$$0 = 2\zeta''(s)^T\zeta'(s) = 2\eta''(s)\eta'(s)\|\xi'(\eta(s))\|_2^{\,2} + 2\eta'(s)^2\xi''(\eta(s))^T\xi'(\eta(s))$$

it follows that $\eta''(0) = 0$. Therefore we have $\zeta''(0) = \xi''(0)$ and hence

$$k_0 = \|\xi''(0)\|_2 = \|U_m D^2\psi(0)(\mu, \mu)\|_2$$

is the curvature of the path ξ at x_0 and the direction of $\xi''(0)$ equals that of the principal normal of ξ.

With some sufficiently small $t_0 \in J$ set $\omega_1 = t_0\mu$, $\omega_2 = -t_0\mu$ and

$$x_i = x_0 + U_d\omega_i + U_m\psi(\omega_i),\ i = 1, 2, \tag{5.2}$$

If the triangle defined by the points x_0, x_1, x_2 is non-degenerate then the curvature of the circumscribing circle is given by Heron's formula

$$\hat{k} = \frac{4}{abc}[s(s-a)(s-b)(s-c)]^{1/2}$$

where $s = (a+b+c)/2$, $a = \|x_1 - x_0\|_2$, $b = \|x_2 - x_0\|_2$. With the normalization $a_c = a/c$, $b_c = b/c$ this can be re-written as

$$\hat{k} = \frac{1}{c}[\frac{1}{a_c} + \frac{1}{a_c}](1-\delta)^{1/2}\sin\,\alpha, \tag{5.3a}$$

where

$$\delta = a_c - b_c, \quad \alpha = \arccos\,\gamma,\ \gamma = \frac{1}{a_c + b_c}. \tag{5.3b}$$

When $1-\gamma$ falls below the machine precision then, in floating point arithmetic, α will be zero and we set $\hat{k} = 0$. Clearly, if t_0 tends to zero then the circle through x_0, x_1, x_2 tends to the osculating circle of the path at x_0 and hence $\hat{k}$ becomes the curvature k_0. Thus our algorithm produces an approximation $\hat{k}$ of k_0.

If $\hat{k}$ is not zero then an approximation $\hat{n}$ of the principal normal of the path at x_0 can be generated by orthogonalizing the sum-vector $(x_1 - x_0) + (x_2 - x_0)$ with respect to $U_d\mu$ and then normalizing the result. In other words, we apply the algorithm

$$\hat{n} := (x_1 - x_0) + (x_2 - x_0); \quad \hat{n} := \hat{n} - [(U_d\mu)^T\hat{n}]U_d\mu; \quad \hat{n} := \hat{n}/\|\hat{n}\|_2. \tag{5.4}$$

Thus altogether

$$U_m D^2\psi(0)(\mu,\mu) \approx \hat{k}\hat{n}. \tag{5.5}$$

The bilinearity and symmetry of $U_m D^2\psi(0)(\mu,\mu)$ implies that for any vectors $\mu_1, \mu_2 \in R^d$ and with $\nu = \mu_1 + \mu_2$ we have

$$U_m D^2\psi(0)(\mu_1,\mu_2) = \frac{1}{2}[U_m D^2\psi(0)(\nu,\nu) - U_m D^2\psi(0)(\mu_1,\mu_1) - U_m D^2\psi(0)(\mu_2,\mu_2)]$$

Hence by applying the above algorithm three times we can compute also $U_m D^2\psi(0)(\mu_1,\mu_2)$. Generally, for the evaluation of this derivative for arbitrary pairs of vectors $\mu_1, \mu_2 \in R^d$ we need to compute only the $d(d+1)/2$ terms $U_m D^2\psi(0)(\mu_i,\mu_j)$, $1 \le i \le j \le d$ for some basis $\mu_1, \ldots, \mu_d$ of R^d, (see [6]).

Now let $V = (V_m, V_d)$ be any other local basis at $x_0 \in M$ with corresponding corrector function ϕ. Then it follows from (3.7) and $D\gamma(0) = V_d^T U_d$ that for any $\mu_1, \mu_2 \in R^d$

$$V_m D^2\phi(0)(V_d^T U_d \mu_1, V_d^T U_d \mu_2) + [V_d + V_m \Sigma] D^2\gamma(0)(\mu_1, \mu_2) = U_m D^2\psi(0)(\mu_1, \mu_2).$$

Hence with

$$D^2\gamma(0)(\mu_1, \mu_2) = V_d^T U_m D^2\psi(0)(\mu_1, \mu_2)$$

and (3.9) it follows readily that

$$V_m D^2\phi(0)(V_d^T U_d \mu_1, V_d^T U_d \mu_2) = [V_m V_m^T - V_m \Sigma V_d^T] U_m D^2\psi(0)(\mu_1, \mu_2). \tag{5.6}$$

Now note that by (3.8)

$$V_m V_m^T - V_m \Sigma V_d^T = V_m V_m^T P, \quad P = I_n - U_d (V_d T U_d)^{-1} V_d^T, \tag{5.7}$$

Since $PV_m = V_m$ and $PU_d = 0$, we see that $P \in L(R^n, R^n)$ is the projection onto rge V_m parallel to rge U_d. Moreover, it follows that $V_m V_m^T P = (I_n - V_d^T V_d) P = P$ whence by (5.6)

$$V_m D^2\phi(0)(V_d^T U_d \mu_1, V_d^T U_d \mu_2) = P U_m D^2\psi(0)(\mu_1, \mu_2), \ \mu_i \in R^d, \ i = 1, 2, \tag{5.8}$$

where the right hand side can be calculated by applying the above algorithm.

6. Some Example Problems

A simple 0-dimensional model of the global energy balance of the earth's climate has been discussed in [2] and [5] (see also [10]). In dimensionless form it can be written as

$$c\frac{d\tau}{dt} = \mu(1 - \alpha(\tau)) - \epsilon a \tau^4, \quad \alpha(\tau) = \max(\min(b - \rho\tau, \alpha_{min}), \alpha_{max}). \tag{6.1}$$

Here the state variable τ is a dimensionless temperature defined as the quotient T/T_0 of an average surface temperature T of a spherical planet and a reference temperature T_0.

The function α is a model of the planetary albedo assumed to depend principally on the extent of the surface snow cover. All constants are dimensionless and, in particular, c characterizes the global heat capacity. The parameter ϵ defines the effective emissivity which incorporates the effect of water vapor, carbon dioxide, dust, etc., upon terrestrial radiation while μ characterizes the variation of the solar radiation from the reference value $\mu = 1$. The model assumes that all quantities are annually averaged to remove the seasonal cycle.

We use the reference temperature $T_0 = 288.6^o K$ of [3] and the constants $a = 1.14$, $b = 2.8$, $\alpha_{min} = 0.2$, $\alpha_{max} = 0.8$. As in [5], for the computation the albedo-definition is replaced by $\alpha(\tau) = \beta(b - \rho\tau)$ where

$$\beta(s) = \begin{cases} 0.2 & \text{if } s \leq 0.2 - \delta, \\ 0.2 + (s - 0.2 + \delta)^2/4\delta & \text{if } |s - 0.2| \leq \delta, \\ s & \text{if } 0.2 + \delta \leq s \leq 0.8 - \delta, \\ s - (s - 0.8 + \delta)^2/4\delta & \text{if } |s - 0.8| \leq \delta, \\ 0.8 & \text{if } s \geq 0.8 + \delta. \end{cases}$$

with $\delta = 10^{-3}$. Then the equilibrium configurations of the model (6.1) are the solutions of the equation

$$f(x) \equiv -a\epsilon\tau^4 + \mu[1 - \beta(b - \rho\tau)] = 0, \quad \forall x = (\tau, \epsilon, \mu, \rho)^T \in R^4. \tag{6.2}$$

and these form a three-dimensional manifold M in R^4.

The equilibrium configuration $x \in M$ is (asymptotically) stable if $\eta(x) < 0$ where

$$\eta(x) = \mu \frac{d\beta}{ds}\rho - 4a\epsilon\tau^3,$$

is the derivative of f with respect to τ. Moreover,the foldpoints on M with respect to the space of the three parameters, are the points where $\eta(x)$ vanishes. These foldpoints form the two-dimensional sub-manifold

$$M_0 = \{x \in R^4; \quad x = (\frac{4(b-1)}{3\rho}, \frac{27\mu\rho^4}{256a(b-1)^3}, \mu, \rho)^T \}$$

of M. Observe that on M_0 the albedo has the constant value 0.4. Table 6.1 lists some points of M_0.

τ	ρ	ϵ
1.4	1.714	0.1370μ
1.3	1.846	0.1843μ
1.2	2.000	0.2538μ
1.1	2.182	0.3595μ
1.0	2.400	0.5263μ
0.98	2.449	0.5706μ
0.96	2.500	0.6197μ
0.94	2,553	0.6741μ
0.92	2.609	0.7347μ
0.90	2.666	0.8022μ
0.88	2.727	0.8776μ
0.86	2.791	0.9622μ

Table 6.1 Foldpoint Submanifold

The current climate $x_0 \in M$ is assumed to have the components $\tau_0 = 0.9893, \mu_0 = 1, \epsilon_0 = 0.7071, \rho_0 = 2.6$ where τ_0 corresponds to an absolute temperature of $285.5^o K$ and ρ_0 to the dimensioned slope 0.009 for the albedo decrease used in [10]. Since $\eta(x_0) = -0.5220$ this current point is stable.

In the cited articles interest has focussed on the path on M through x_0 toward M_0 when μ is allowed to decrease while $\epsilon = \epsilon_0$ and $\rho = \rho_0$ are held constant. Some points on this path and the corresponding values of the first-order sensitivity $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are given in Table 6.2.

μ	τ	η	σ_1	σ_2	σ_3	$\|\sigma\|_2$
1.0	0.9894	-0.5226	-2.090	1.478	-1.893	3.184
0.995	0.9816	-0.4500	-2.352	1.672	-2.182	3.618
0.99	0.9730	-0.3703	-2.760	1.971	-2.628	4.290
0.985	0.9623	-0.2733	-3.578	2.569	-3.522	5.639
0.98	0.9501	-0.1658	-5.605	4.044	-5.732	8.979
0.9775	0.9411	-0.8738(-1)	-10.23	7.402	-10.770	16.60
0.9758	0.9307	0.2462(-3)	3474.	-2518.	3780.	5718.

Table 6.2 Decreasing Solar Radiation

These data show clearly how the sensitivity increases as the points approach the foldset M_0. Since ϵ incorporates the so-called greenhouse effect it is also interesting to see the effect of decreasing ϵ. Table 6.3 lists some points on the path on M through x_0 when ϵ is allowed to decrease while $\mu = \mu_0$ and $\rho = \rho_0$ are held constant.

ϵ	τ	η	σ_1	σ_2	σ_3	$\|\sigma\|_2$
0.7	1.003	-0.6236	-1.852	1.297	-1.609	2.775
0.68	1.037	-0.8549	-1.540	1.047	-1.213	2.223
0.66	1.066	-1.046	-1.408	0.9290	-1.019	1.971
0.64	1.093	-1.215	-1.341	0.8582	-0.8998	1.829
0.62	1.120	-1.371	-1.308	0.8110	-0.8170	1.743
0.60	1.146	-1.517	-1.296	0.7776	-0.7555	1.690
0.58	1.172	-1.656	-1.298	0.7530	-0.7078	1.659

Table 6.3 Decreasing Emissivity

As a second example we consider the following model of an exothermic chemical reaction with convective transport

$$-u'' + \nu u' = (1-u)\exp(\alpha - \frac{\lambda}{(1+u)}),\ 0 < t < 1,\ u(0) = u(1) = 0,\ \alpha = 12\ln 10,$$

discussed in [1]. We use the upwind discretization

$$-(1+\nu h)z_{i-1} + (2+\nu h)z_i - z_{i+1} = h^2(1-z_i)\exp(\alpha - \frac{\lambda}{(1+z_i)}), \qquad (6.3)$$
$$i = 1,\ldots,n, \quad z_0 = z_{k+1} = 0.$$

on a uniform mesh with step-size $h = 1/(k+1)$. For $k = 9$ the 2-dimensional solution manifold of (6.3) was triangulated by the algorithm of [9] in a neighborhood of the point $x_0 = (z_0, \lambda, \nu) \in R^11$ for which $\lambda = 23.907$, $\nu = 999.978$ and the state vector $z = (z_1,\ldots,9)^T$ has the components

$$z_1 = 4.6067(-3),\ z_2 = 9.7851(-3),\ z_3 = 1.5694(-2),$$

$$z_4 = 2.2570(-2),\ z_5 = 3.0790(-2),\ z_6 = 4.1012(-2),$$

$$z_7 = 5.4582(-2),\ z_8 = 7.5449(-2),\ z_9 = 1.3374(-1),$$

For the first 23 computed nodal points of the triangulation Table 6.4 lists the values of the last (and largest) component z_9 of the state vector and the two (natural) parameters ν and λ together with the Euclidean norm of the sensitivity Σ at each point with respect to the parameters.

node	x_9	ν	λ	$\|\Sigma\|_2$
(1,7)	1.70238(-1)	23.9573	999.957	0.398724
(2,7)	1.70246(-1)	23.9573	1000.00	0.398640
(1,6)	1.67282(-1)	23.9494	999.935	0.435477
(2,6)	1.55214(-1)	23.9248	999.978	0.680829
(3,6)	1.67276(-1)	23.9493	1000.02	0.435561
(1,5)	1.50738(-1)	23.9187	999.913	0.851227
(2,5)	1.50739(-1)	23.9187	999.957	0.851212
(3,5)	1.50739(-1)	23.9186	1000.00	0.851198
(4,5)	1.50740(-1)	23.9186	1000.04	0.851183
(1,4)	1.30793(-1)	23.9070	999.892	16.1791
(2,4)	1.33738(-1)	23.9072	999.935	8.80483
(3,4)	1.33741(-1)	23.9072	999.978	8.79455
(4,4)	1.33743(-1)	23.9072	1000.02	8.78402
(5,4)	1.30793(-1)	23.9069	1000.07	16.1566
(2,3)	1.15878(-1)	23.9132	999.913	1.07936
(3,3)	1.15878(-1)	23.9131	999.957	1.07939
(4,3)	1.15879(-1)	23.9131	1000.00	1.07942
(5,3)	1.15880(-1)	23.9130	1000.04	1.07945
(3,2)	1.13146(-1)	23.9157	999.935	0.922609
(4,2)	1.13132(-1)	23.9156	999.978	0.921912
(5,2)	1.13119(-1)	23.9156	1000.02	0.921225
(6,1)	9.43086(-2)	23.9451	999.957	0.448821
(7,1)	9.43010(-2)	23.9451	1000.00	0.448722

Table 6.4 Sensitivities at Triangulation Nodes

The nodes are indexed by a pair of integers (i,j) where $(3,4)$ is the above given point x_0. They form 30 triangles specified by the following node-triples

$$\langle (i,j),(i,j+1),(i+1,j)\rangle, \quad \langle (i,j),(i+1,j-1),(i+1,j)\rangle,$$

$$1 \le i, i+1 \le 4,\ 1 \le j, j+1 \le 7,\ 5 \le i+j \le 8.$$

In Table 6.4 the nodes $(i,4)$, $i = 1,\ldots,5$ carry a significantly larger value of $\|\Sigma\|_2$. This indicates that this line of nodes should be near a foldline with respect to the natural

parameter space. This is indeed the case. A foldpoint computation with a standard augmentation of the mapping (6.3) started from x_0 converged very quickly and from the resulting point a continuation process readily produced the expected foldline. Table 6.5 gives the values of z_9, λ, and ν of some of the computed points on that foldline.

x_9	ν	λ
1.30771(-1)	23.9074	999.578
1.30773(-1)	23.9071	999.848
1.30773(-1)	23.9070	999.938
1.30774(-1)	23.9070	999.978
1.30774(-1)	23.9069	999.988
1.30774(-1)	23.9069	1000.02
1.30775(-1)	23.9068	1000.11
1.30777(-1)	23.9065	1000.38
1.30780(-1)	23.9061	1000.76

Table 6.5 Foldline

These results certainly show that the sensitivity norms represent an excellent indicator for the existence of nearby foldpoints which could be used effectively in any computational study of the characteristic properties of the solution manifold.

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The sensitivity of a solution of a parametrized equation $F(z, \lambda) = 0$ with respect to the parameter vector λ is usually defined as the change of the state z in dependence of λ. In other words, for any solution expressible in the form $(z(\lambda), \lambda)$ with some smooth function $z = (z(\lambda)$ the sensitivity is the derivative $Dz(\lambda)$. Typically the solutions form a manifold M in the product of the state-space and the parameter space and this sensitivity is available only at those points of M where the parameters can be used to define a local coordinate system. This paper introduces a general sensitivity concept which applies at all solutions on M and which includes the earlier definition. Some general geometric interpretations of the new measure are presented and it is shown that the sensitivity analysis can be easily integrated into the solution process. The theory also suggests the introduction of a readily computable second-order sensitivity measure reflecting the curvature-behavior of M. Two numerical examples illustrate the discussion.

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