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ABSTRACT

A system of M nonlinear equations in N unknowns with M≥N may be considered as a vector function F(X) mapping R^N into R^M. The technique of differentiation with respect to a parameter is applied in a general fashion to solve the equation F(X) = 0. This approach reduces the problem to integrating a system of first order differential equations. In general, numerical integration which yields approximate solutions to F(X) = 0 must be used.

A non-linear least squares error function $E(X) = \sum_{i=1}^{M} f_i^2(X)$ is minimized by applying the above procedure to (1) the equation $\frac{\partial E}{\partial X} = 0$ and (2) the system of equations $f_i(X) = 0$ and also by applying to $\frac{\partial E}{\partial X} = 0$ the (3) Newton-Raphson and (4) differential correction algorithms. Each procedure depends on an initial estimate X_o. The range of X_o which yields convergence is evaluated.

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FROM: C. L. Greer

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TECHNICAL MEMORANDUM

INTRODUCTION

A common procedure for solving systems of N equations in N unknowns is Newton's method. In solving a system of equations $F(X) = 0$ by Newton's method, the choice of initial conditions for the technique to converge is often critical. To eliminate the problems associated with the choice of initial conditions, E. Lahaye[1] proposed the introduction of a parameter, t, in the function $F(X)$ and defined a new function $G(X,t)$ so that for $t = t_f$, $G(X,t_f) = F(X)$ and for $t = t_o$ a solution to $G(X,t_o) = 0$ is easily computed. A set of t_i's is chosen such that $t_o < t_1 <\ldots< t_i < t_{i+1} <\ldots< t_n = t_f$, and the equation $G(X,t_{i+1}) = 0$ is solved by Newton's method using the solution of $G(X,t_i) = 0$ as initial conditions. The solution of $G(X,t_n) = 0$ is then a solution of $F(X) = 0$. The difficulties of this technique are determining whether the Newton method is diverging or converging at t_{i+1} and, if diverging, the choice of t_{i+1} to obtain convergence.

D. F. Davidenko[2] observed that, with the introduction of the parameter, the solutions are a function of the parameter and proposed a different technique for solving the equation $G(X,t_i) = 0$ for $i = 1,2,\ldots,n$. If $G(X,t)$ is identically zero, the total variation is zero. Thus

$$[\frac{\partial G}{\partial X}] * [\frac{dX}{dt}] + [\frac{\partial G}{\partial t}] = 0. \qquad (1)$$

If the matrix $\frac{\partial G}{\partial X}$ is nonsingular, equation (1) can be solved for $\frac{dX}{dt}$, in which case

$$[\frac{dX}{dt}] = [\frac{\partial G}{\partial X}]^{-1} * [-\frac{\partial G}{\partial t}]. \qquad (2)$$

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The differential equations describe an integral curve such that $G(X(t),t) = 0$ and $X(t_i)$ are the solutions to $G(X,t_i) = 0$. Therefore, the problem is reduced to one of integrating a set of first order differential equations over the interval $[t_o, t_f]$.

This approach, which has been referred to as the method of differentiation with respect to a parameter[3], is the basis for the present work on solving systems of M equations in N unknowns with $M \geq N$.

Mathematical Method

Let $F(X)$ be a vector function of a vector variable X mapping R^N into R^M with $M \geq N$ such that the second partial derivatives of F with respect to X are continuous. Suppose X is a function of a scalar λ. Define a new vector function $\phi(\lambda) = F[X(\lambda)]-(1-\lambda)F[X(0)]$, which satisfies the conditions $\phi(0) = 0$ and $\phi(1) = F[X(1)]$. Therefore, if $\phi(\lambda)$ is a constant function, $X(1)$ is a solution to $F(X) = 0$. A necessary and sufficient condition that $\phi(\lambda)$ be a constant is that $\frac{d\phi}{d\lambda} = 0$. Thus, $X(1)$ is a solution to $F(X) = 0$ if $X(\lambda)$ satisfies the condition

$$\frac{d\phi}{d\lambda} = \frac{\partial F(X(\lambda))}{\partial X} \frac{dX}{d\lambda} + F(X(0)) = 0 \qquad (3)$$

Let X_o be an arbitrary point in R^N. If $F(X_o) \neq 0$, define $X(0) = X_o$ and $X(\lambda) = X_o + \int_o^\lambda \frac{dX}{d\lambda} d\lambda$, where $0 \leq \lambda \leq 1$ and $\frac{dX}{d\lambda}$ satisfies equation (3). The curve $X(\lambda)$ will be referred to as a solution curve and the point $X(1)$ as a solution point. In general numerical integration must be used which yields approximate solutions.

It is shown that, if $X(\lambda)$ for $0 \leq \lambda \leq 1$ is a solution to equation 3 and the rank of $\frac{\partial F(X(\lambda))}{\partial X}$ is N, the solution curve is unique. For $M > N$, equation (3) may not have a solution even though the rank of $\frac{\partial F(X(\lambda))}{\partial X}$ is N. However, there exists a unique solution to equation (3) in the least squares sense and the behavior of the resulting curve is described. The following notation will be used: J_λ denotes the Jacobian matrix $\frac{\partial F(X(\lambda))}{\partial X}$, $\rho(A)$ denotes the rank of matrix A, and A^T denotes the transpose of matrix A.

Proposition 1. If $\rho(J_\lambda) = N$ for $0 \leq \lambda \leq 1$ and $X(\lambda)$ satisfies equation (3), then the solution curve $X(\lambda)$ is unique.

Proof: The curve $X(\lambda)$ is a solution to the differential equation $\frac{\partial F}{\partial X}\frac{dX}{d\lambda} = F(X_o)$ in a domain D with initial conditions $X(0) = X_o$. If $\rho(\frac{\partial F}{\partial X}) = N$ in D, the equation can be transformed into the form $\frac{dX}{d\lambda} = H(X)$. The function $H(X)$ is described in proposition 2. The functions $\frac{\partial F_j}{\partial X_i}$ have continuous derivatives $\frac{\partial^2 F_j}{\partial X_i \partial X_k}$ which implies $H(X)$ is a continuously differentiable function of X. Therefore $H(X)$ satisfies a Lipshitz condition which implies the equation $\frac{dX}{d\lambda} = H(X)$ with $X(0) = X_o$ has a unique solution.

Clearly $\frac{dX}{d\lambda} = J_\lambda^{-1} F(X_o)$ when M=N. For M>N the problem of determining $\frac{dX}{d\lambda}$ is slightly more difficult. The procedure used is described below.

Proposition 2. If $\rho(J_\lambda) = N$ and $\frac{dX}{d\lambda}$ is a solution to equation (3) then $\frac{dX}{d\lambda} = -[J_\lambda^T J_\lambda]^{-1} J_\lambda^T F(X_o)$.

Proof: If $J\frac{dX}{d\lambda} + F(X_o) = 0$ then $J_\lambda^T J_\lambda \frac{dX}{d\lambda} = -J_\lambda^T F(X_o)$. The matrix coefficient of $\frac{dX}{d\lambda}$ is nonsingular, hence $\frac{dX}{d\lambda}$ has the form described.

The solution point $X(1)$ is dependent on the starting point X_o. It would be interesting to know the relationship between points which determine the same solution. Only one result in this direction has been obtained.

Theorem 3. If $\rho(J_\lambda) = N$, then every point on the solution curve $X(\lambda)$ determines the same solution point when taken as a starting point X_o.

Proof: Let $X(a)$ be a point on the solution curve $X(\lambda)$. Then $X(a) = X_o + \int_o^a A_\lambda F(X_o)d\lambda$ where $A_\lambda = -[J_\lambda^T J_\lambda]^{-1} J_\lambda^T$. Taking $X(a)$ as a starting point defines $X(1) = X(a) + \int_o^1 A_\lambda F(X(a))d\lambda$. The function $\phi(\lambda)$ is identically zero, thus $F(X(\lambda)) = (1-\lambda)F(X_o)$. Substituting for $F(X(a))$ in the

integral expression gives $X(1) = X(a) + \int_o^1 A_\lambda F(X_o)(1-a)d\lambda$.

Performing the change of variable $s = (1-a)\lambda+a$, gives $\int_o^1 A_\lambda F(X_o)(1-a)d\lambda = \int_a^1 A_s F(X_o)ds$. Thus

$$X(1) = X_o + \int_o^a A_\lambda F(X_o)\, d\lambda + \int_a^1 A_s F(X_o)\, ds = X_o + \int_o^1 A_t F(X_o)dt.$$

There is no assurance that the starting point X_o determines a solution curve. As might be expected, the scalar function $F^T(X)F(X)$ provides some useful information on the curve $X(\lambda)$. It is shown that the curve $X(\lambda)$ proceeds to minimize the scalar function $F^T(X)F(X)$ and that the solution curve fails to exist at nonzero minima of $F^T(X)F(X)$.

Proposition 4. The solution curve $X(\lambda)$ fails to exist at nonzero minima of the function $F^T(X)F(X)$.

Proof: On a solution curve $X(\lambda)$, $F(X(\lambda)) = (1-\lambda)F(X_o)$ which implies $F^T(X(\lambda))F(X(\lambda)) = (1-\lambda)^2F^T(X_o)F(X_o)$ and $\frac{d}{d\lambda}(F^T(X(\lambda))F(X(\lambda))) = -2(1-\lambda)F^T(X_o)F(X_o) < 0$ for $0\leq\lambda<1$. Suppose $X(t)$ minimizes $F^T(X)F(X)$ for $0\leq t<1$. Then $\frac{d}{d\lambda}(F^T(X(\lambda))F(X(\lambda))\Big|_{\lambda=t} = 0$, hence there does not exist a curve $X(\lambda) = X(t) + \int_o^\lambda \frac{dX}{d\lambda}d\lambda$ such that $F(X(\lambda)) = (1-\lambda)F(X(t))$. By theorem 3, the solution curve fails to exist.

When $M = N$, the condition that $\rho(J_\lambda) = N$ guarantees a solution to equation (3), thus $\rho(J_\lambda)<N$ at nonzero minima of $F^T(X)F(X)$. Such is not the case for $M>N$ and in proposition 2 it was necessary to assume a solution to equation (3) exists. If a solution to (3) does not exist and $\rho(J_\lambda) = N$ the form of $\frac{dX}{d\lambda}$ from proposition 2 represents a least squares solution to equation (3). The behavior of the resulting curve $X(\lambda)$ is described below.

Proposition 5. If $\rho(J_\lambda) = N$ on the curve $X(\lambda) = X_o + \int_o^\lambda - [J_\lambda{}^T J_\lambda]^{-1}J_\lambda{}^T F(X_o)d\lambda$, then $F^T(X_o)F(X(\lambda))$ is a monotone decreasing function.

Proof: Let $S(\lambda) = F^T(X_o)F(X(\lambda))$. Then $\frac{dS}{d\lambda} = F^T(X_o)J_\lambda\frac{dX}{d\lambda} = -F^T(X_o)J_\lambda[J_\lambda{}^TJ_\lambda]^{-1}J_\lambda{}^TF(X_o)$. The matrix $J_\lambda{}^TJ_\lambda$ is positive semi-definite and nonsingular, hence positive definite. Therefore the matrix $[J_\lambda{}^TJ_\lambda]^{-1}$ is positive definite and admits a decomposition of the form $[J_\lambda{}^TJ_\lambda]^{-1} = PDP^T$, where the columns of P are the eigenvectors and D is a diagonal matrix of the respective positive eigenvalues. Thus $\frac{dS}{d\lambda} = -F^T(X_o)J_\lambda PDP^TJ_\lambda{}^TF(X_o) = -(D^{1/2}P^TJ_\lambda{}^TF(X_o))^T(D^{1/2}P^TJ_\lambda{}^TF(X_o))$ where $D^{1/2}$ is the diagonal matrix with entries $(d_{ii})^{1/2}$. The scalar $(D^{1/2}P^TJ_\lambda{}^TF(X_o))^T(D^{1/2}P^TJ_\lambda{}^TF(X_o))$ is nonnegative, hence $\frac{dS}{d\lambda} \leq 0$.

Corollary 6. If X_o is not a minimum of $F^T(X)F(X)$, the function $F^T(X(\lambda))F(X(\lambda))$ is monotone decreasing for suitably small values of λ.

Proof: Let $G(\lambda) = F^T(X(\lambda))F(X(\lambda))-F^T(X_o)F(X(\lambda))$. Then $G(0) = 0$ and $\frac{dG(0)}{d\lambda} = [2F^T(X_o)J_o-F^T(X_o)]\frac{dX(0)}{d\lambda}$ $= -F^T(X_o)J_o[J_o{}^TJ_o]^{-1}J_o{}^TF(X_o) < 0$. For small λ, $G(\lambda) \leq 0$ which implies $F^T(X(\lambda))F(X(\lambda)) \leq F^T(X_o)F^T(X(\lambda))$.

It is necessary to check the monotonicity of $F^T(X)F(X)$ and to redefine $F(X_o)$ at points where it is not satisfied. In problems studied, the monotonicity has been satisfied for $0\leq\lambda\leq.9$.

Programming Results

The mathematical procedure previously described was programmed using the fourth order variable step-size Adams-Moulton integration formulas, with a fourth order Runge-Kutta formula for starting values. The technique experienced great difficulty in integrating over the interval $.9\leq\lambda\leq1$. Because of this difficulty an iteration algorithm was defined by integrating over the interval $0\leq\lambda\leq.9$ and then restarting the solution curve with X(.9). The upper limit of .9 was chosen because it permits an easy check of how well the solution curve has been followed since $F(X(.9)) = .1*F(X_o)$. The number

of iterations to be performed is determined by how accurately the solution is to be computed and by the maximum component of $F(X_o)$. The iteration algorithm has largely been used in solving the nonlinear least squares error problem. To evaluate the technique a comparison with other procedures on a planetary orbit determination problem was conducted[4]. The results are described below.

The nonlinear least squares problem is to minimize a function of the form $E(X) = \sum_{i=1}^{M} f_i^2(X) = F^T(X)F(X)$. The minimum of such a function occurs when the set of first partial derivatives is zero and the matrix of second partial derivatives is positive definite. There are two approaches to the problem: (1) to solve the equation $\frac{\partial E}{\partial X} = 0$ and (2) to minimize the scalar function $E(X)$ directly.

Taking the first approach requires solving N equations in N unknowns. Substituting $\frac{\partial E(X)}{\partial X}$ for $F(X)$ in the derivation of the preceding section defines the solution to be

$$X(1) = X_o + \int_o^1 - \left[\frac{\partial^2 E(X(\lambda))}{\partial X^2}\right]^{-1} \frac{\partial E}{\partial X}(X_o) d\lambda \qquad (4)$$

By using a first order integration procedure a recursive formula may be defined as

$$X_{i+1} = X_i - h \left[\frac{\partial^2 E(X_i)}{\partial X^2}\right]^{-1} \frac{\partial E(X_i)}{\partial X} \qquad (5)$$

For the case of unity step-size the recursive formula is the familiar Newton-Raphson formula for N dimensions. The solution curve defined by equation (4) will be referred to as the generalized Newton-Raphson method.

The function $E(X)$ is nonnegative, thus zero is a minimum. Clearly $E(X)$ is zero if and only if $F(X) = 0$. By virtue of corollary 6, attempting to solve the equation $F(X) = 0$ may produce a minimum. The resulting curve is of the form

$$X(1) = X_o + \int_o^1 - \left[J_\lambda^T J_\lambda\right]^{-1} J_\lambda^T F(X_o) d\lambda \qquad (6)$$

Using a first order integration formula with unity step-size produces a recursive formula of the form

$$X_{i+1} = X_i - \left[\frac{\partial F(X_i)}{\partial X}^T \frac{\partial F(X_i)}{\partial X}\right]^{-1} \frac{\partial F(X_i)}{\partial X}^T F(X_i) \qquad (7)$$

which is the classical differential correction formula. The solution defined by equation (6) will be referred to as the Generalized Differential Correction Method.

The four procedures (1) Newton-Raphson, (2) generalized Newton-Raphson, (3) differential correction, and (4) generalized differential correction are all dependent on the choice of initial conditions for convergence. A simulation was performed to compare the ranges of X_o which yield convergence for the four procedures. The simulation was to minimize the function $E = (D - H(X))^T (D - H(X))$ where D was a set of simulated data, X^T is the vector (a, e, τ, i, w), $H(X) = -\left[\frac{\mu}{a(1-e^2)}\right]^{1/2} \sin i \, [\cos(w+f) + e \cos w]$, and f is determined by the equation

$$\left(\frac{\mu}{a^3}\right)^{1/2} (t - \tau) = \sin^{-1}\left[\frac{\sqrt{1-e^2}\sin f}{1 + e\cos f}\right] - e\left[\frac{\sqrt{1-e^2}\sin f}{1 + e\cos f}\right].$$

The variable t represents time.

The above equations describe the doppler time history of an orbiter around a stationary planet at an infinite distance from the observer.

The following set of parameters was arbitrarily chosen for the simulation:

$a = 2788$ km

$e = 0.289$

$\tau = 0$ min

$i = 40°$

$w = 283°$

$\mu = 1.77 * 10^7$ km^3/min^2

The parameters were substituted into the expression for H(X) and the observational data D were simulated by rounding the resulting values to three significant figures. Fifty data points were used in the simulation. The results of the simulation are shown in Table I. All results shown are obtained by programming with double precision.

Table I is designed to show the initial estimate range for which the four methods converge to the absolute minimum. It is seen that the generalized differential correction method has the widest range and the classical differential correction method the next. The Newton-Raphson and generalized Newton-Raphson methods have almost the same range. The generalized procedures require about 30 seconds for a solution with 250 data points while the others require about 3 seconds. No detailed time comparisons have been performed.

1014-CLG-llf

C. L. Greer

Attachment
Table I

REFERENCES

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3. Yakoulev, M. N., "Solution of Systems of Nonlinear Equations by the Method of Differentiation with respect to a Parameter," NASA Technical Translation, NASA TT F-254.

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TABLE I

SIMULATION RESULTS

PARAMETERS	THEORETICAL	SOLUTION
a(KM)	2788	2787.9892
e	0.289	0.28897788
τ(MIN)	0	-0.0076632791
i(DEG)	40	40.00886
ω(DEG)	283	282.97972

INITIAL CONDITIONS						SOLUTION PROCEDURE			
a	e	τ	i	ω		G.D.C.	D.C.	N.R.	G.N.R.
2600.0	0.289	0	40	283		C	C	X	X
2677.0	0.289	0	40	283		C	C	X	X
2677.8	0.289	0	40	283		C	C	C	C
2900.0	0.289	0	40	283		C	C	X	X
3300.0	0.289	0	40	283		C	X	X	X
2788.0	0.100	0	40	283		C	C	C	C
2788.0	0.230	0	40	283		C	C	C	C
2788.0	0.250	0	40	283		C	C	C	C
2788.0	0.500	0	40	283		C	C	C	C
2788.0	0.289	0	20	283		C	C	C	C
2788.0	0.289	0	30	283		C	C	C	C
2788.0	0.289	0	60	283		C	C	X	C
2788.0	0.289	0	40	240		C	C	X	X
2788.0	0.289	0	40	260		C	C	C	X
2788.0	0.289	0	40	300		C	C	C	X
2788.0	0.289	0	40	320		C	C	X	X
2000.0	0.500	10	40	270		C	X	X	X
2500.0	0.250	-5	30	250		C	C	X	X
3500.0	0.400	15	60	360		C	X	X	X
4000.0	0.400	15	60	360		C	X	X	X

LEGEND:

C: CONVERGED TO SOLUTION

X: FAILED TO CONVERGE OR CONVERGED TO WRONG SOLUTION

G.D.C.: GENERALIZED DIFFERENTIAL CORRECTION METHOD

D.C.: DIFFERENTIAL CORRECTION METHOD

N.R.: NEWTON-RAPHSON METHOD

G.N.R.: GENERALIZED NEWTON-RAPHSON METHOD