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The Kantorovich Theorem and Two-Point Boundary Value Problems

Two-point boundary value problems for nonlinear ordinary differential equations occur naturally and frequently in applied mathematics, physics and engineering. For example, many problems in flight mechanics, optimization, and control theory, when attacked by the calculus of variations, lead to two-point boundary value problems.

An often cited method for the solution of two-point boundary value problems by the systematic variation of arbitrarily chosen initial conditions is given in the paper by Goodman and Lance.[1] However, such questions as convergence and the rate of convergence are not discussed in their paper.

One of the purposes of this communication is to show how the Goodman-Lance method can be cast into a form to which Kantorovich's theorem[2] on Newton's method[3] for the solution of nonlinear operator equations in Banach space can be applied. Kantorovich's theorem thus furnishes sufficient conditions for the convergence of the Goodman-Lance method and estimates of the rate of convergence.

Kantorovich has also shown how the abstract Newton's method can be applied to the solution of nonlinear differential equations to give a sequence of linear differential equations whose solutions converge, under appropriate conditions, to the desired solution. The idea has been exploited by Bellman and Kalaba[4] as "quasilinearization" and by McGill and Kenneth[5] as the "generalized Newton-Raphson method." McGill and Kenneth also give an independent proof of convergence for a particular class of two-point boundary problems. Thus, the Goodman-Lance method and quasilinearization as applied to nonlinear, two-point boundary value problems are two concrete realizations of the abstract Newton's method.

Utilization of the Kantorovich theorem as a diagnostic tool for two-point boundary value problems which fail to converge is suggested. Our numerical experience has shown that whenever the two-point boundary value problems fail to converge, the conditions of the Kantorovich theorem are violated.

Goodman-Lance method

A set of n nonlinear ordinary differential equations is given:

$$\dot{y}_i(t) = g_i(y_1, y_2, \cdots, y_n, t), \quad i = 1, 2, \cdots, n \quad (1)$$

where the functions g_i are twice differentiable with respect to all the y_i. The initial conditions are specified at $t = t_0$ for r variables, which by relabeling, if necessary, can be considered to be $y_1, \cdots, y_r$, while the terminal conditions are specified at $t = t_f$ for $n - r$ variables y_{i_m}, where $m = 1, 2, \cdots, n - r$. The indexed subscripts i_m on y_{i_m} are $n - r$ integers chosen from the set $(1, 2, \cdots, n)$. If, for example, we are given in a six dimensional problem, the initial conditions $y_1(0)$, $y_2(0)$, $y_3(0)$ and the terminal conditions $y_3(t_f)$, $y_4(t_f)$, $y_6(t_f)$, then $i_1 = 3$, $i_2 = 4$, $i_3 = 6$.

At the kth stage of the Goodman-Lance method, estimates of the missing initial values $y_{r+1}^{(k)}(t_0), \cdots, y_n^{(k)}(t_0)$ are available, which with the given initial values $y_1(t_0), \cdots, y_r(t_0)$, permit Eq. (1) to be integrated forward as an initial value problem. If the estimated initial conditions are close enough to the true initial conditions, the difference

$$\delta y_i^{(k)}(t) = y_i(t) - y_i^{(k)}(t), \qquad i = 1, 2, \cdots, n, \quad (2)$$

satisfies the system of variational equations

$$\delta \dot{y}_i^{(k)}(t) = \sum_{j=1}^{n} \left(\frac{\partial g_i}{\partial y_j}\right)^{(k)} \delta y_j^{(k)}(t), \qquad i = 1, 2, \cdots, n, \quad (3)$$

where the superscript (k) denotes evaluation at $y_j^{(k)}(t)$, $j = 1, \cdots, n$. Between the solutions of Eq. (3) and the solutions of its adjoint equations

$$\dot{x}_i^{(k)} = -\sum_{j=1}^{n} \left(\frac{\partial g_j}{\partial y_i}\right)^{(k)} x_j^{(k)}, \quad i = 1, 2, \cdots, n, \quad (4)$$

the relation

$$\sum_{i=1}^{n} x_i^{(k)}(t_f)\delta y_i^{(k)}(t_f) = \sum_{i=1}^{n} x_i^{(k)}(t_0)\delta y_i^{(k)}(t_0) \tag{5}$$

holds. Let Eqs. (4) be integrated backwards from t_f to t_0 with conditions at t_f:

$$x_i^{(k)}(t_f) = \begin{cases} 0 & \text{if} \quad i \neq i_m \\ 1 & \text{if} \quad i = i_m; \end{cases}$$

do this successively for $m = 1, \cdots, n - r$, and call the resulting solutions $x_{i,m}^{(k)}(t_f)$. Then Eqs. (5) become

$$\delta y_{i_m}^{(k)}(t_f) = \sum_{i=r+1}^{n} x_{i,m}^{(k)}(t_0)\ \delta y_i^{(k)}(t_0),$$

$$m = 1, 2, \cdots, n - r, \tag{6}$$

or, setting

$$w_m^{(k)} \equiv y_{i_m}^{(k)}(t_f),$$

$$z_j^{(k)} \equiv y_{r+j}^{(k)}(t_0),$$

the equation is written:

$$\delta w_m^{(k)} = \sum_{j=1}^{n-r} x_{r+j,m}^{(k)}(t_0)\ \delta z_j^{(k)};$$

note that

$$\delta y_1^{(k)}(t_0) = \cdots = \delta y_r^{(k)}(t_0) = 0, \text{ since } y_i(t_0),$$

$$i = 1, \cdots, r \text{ are the specified initial conditions.}$$

This system of $n - r$ linear algebraic equations can, in general, be solved for $\delta z_j^{(k)}$ which, substituted into Eq. (2), give a new and hopefully better estimate of the missing initial conditions $z_j^{(k+1)} \equiv y_{r+j}^{(k+1)}(t_0)$, $j = 1, 2, \cdots, n - r$. The process is repeated until the values of $w_m^{(k)} \equiv y_{i_m}^{(k)}(t_f)$, $m = 1, 2, \cdots, n - r$, obtained on successive iterations differ by less than a preassigned quantity or until a predetermined number of iterations has been performed.

The Kantorovich theorem

Kantorovich established sufficient conditions for the convergence of Newton's method in the solution of nonlinear operator equations in Banach space. In this section we will state Kantorovich's theorem in the form applicable to systems of nonlinear algebraic equations, where the underlying Banach space is the familiar n-dimensional Cartesian space treated as a vector space over the real field, and the nonlinear operators are vector-valued, nonlinear functions. In the next section we show that the theorem in this form is also applicable to two-point boundary value problems for systems of nonlinear ordinary differential equations. Consider the set of n nonlinear algebraic equations

$$\varphi_i(y_1, y_2, \cdots, y_n) = 0, \qquad i = 1, 2, \cdots, n. \tag{7}$$

Newton's method for solving this set leads to the successive approximations

$$\mathbf{y}^{(k+1)} = \mathbf{y}^{(k)} - [A^{(k)}]^{-1}\boldsymbol{\varphi}^{(k)}, \tag{8}$$

where

$\mathbf{y}^{(k)}$ = the kth approximation to the solution of Eq. (7), an $n \times 1$ vector with components $y_1^{(k)}, y_2^{(k)}, \cdots, y_n^{(k)}$;

$A^{(k)} \equiv A(\mathbf{y}^{(k)}) = n \times n$ matrix, whose component in the ith row, jth column is $(\partial\varphi_i/\partial y_j)$, evaluated at $\mathbf{y}^{(k)}$; $A^{(k)}$ is assumed nonsingular;

$\boldsymbol{\varphi}^{(k)} \equiv \boldsymbol{\varphi}(\mathbf{y}^{(k)}) = n \times 1$ vector with components $\varphi_i(\mathbf{y}^{(k)})$, $i = 1, 2, \cdots, n$ from Eq. (7).

The following norms are employed. For a vector $\mathbf{v}$ whose elements are $v_1, v_2, \cdots, v_n$, define a norm

$$||\mathbf{v}|| = \max_{1 \le i \le n} |v_i|. \tag{9}$$

For an $n \times n$ matrix A with elements a_{ij}, define the norm

$$||A|| = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|. \tag{10}$$

The Kantorovich theorem in the version given by Henrici[6] has four hypotheses:

a. For the initial approximation $\mathbf{y}^{(0)}$ to the solution of Eq. (7)

$$A^{(0)} \equiv A(\mathbf{y}^{(0)}) \text{ has an inverse } \Gamma_0 \text{ such that } ||\Gamma_0|| \le \beta_0; \tag{11}$$

b. $\mathbf{y}^{(0)}$ satisfies Eq. (7) approximately in the sense that

$$||\Gamma_0\boldsymbol{\varphi}^{(0)}|| \le \eta_0; \tag{12}$$

c. In the region defined by inequality (15), the components of the vector $\boldsymbol{\varphi}(\mathbf{y})$ are twice continuously differentiable with respect to the components of $\mathbf{y}$ and satisfy

$$\sum_{j,s=1}^{n} \left|\frac{\partial^2\varphi_i}{\partial y_j\,\partial y_s}\right| \le K \qquad \text{for each } i. \tag{13}$$

d. The constants β_0, η_0, K satisfy

$$h_0 \equiv \beta_0\eta_0 K \le \tfrac{1}{2}. \tag{14}$$

When hypotheses (a)–(d) are satisfied, the Kantorovich theorem asserts that the system of equations, Eq. (7), has a solution $\mathbf{Y}$ which is located in the cube

$$||\mathbf{y} - \mathbf{y}^{(0)}|| \le \frac{1 - \sqrt{1 - 2h_0}}{h_0}\,\eta_0. \tag{15}$$

Moreover, the successive approximations $\mathbf{y}^{(k)}$ defined by Eq. (8) exist and converge to $\mathbf{Y}$ and the speed of convergence may be estimated by the inequality

$$||\mathbf{y}^{(k)} - \mathbf{Y}|| \le \frac{1}{2^{k-1}}(2h_0)^{2^k-1}\eta_0. \tag{16}$$

Equivalence of Newton's method and Goodman-Lance method

As usually thought of and employed, Newton's method is applicable to the solution of systems of nonlinear "algebraic" equations, when algebraic is taken to mean that the solution is a point in n-space, $(y_1, y_2, \cdots, y_n)$, rather than a function, say $[y_1(t), y_2(t), \cdots, y_n(t)]$. However, Newton's method and the Kantorovich theorem can be applied to the solution of two-point nonlinear boundary value problems, Eq. (1), if the problem is thought of as the search for those missing initial conditions $y_{r+1}(t_0), \cdots, y_n(t_0)$ which drive to zero the final "miss distances"

$$\varphi_m \equiv Y_m - w_m, \qquad m = 1, 2, \cdots, n - r, \tag{17}$$

where Y_m are the $n - r$ given final values and w_m are the final values of the solution of Eq. (1) with initial values $y_1(t_0), \cdots, y_r(t_0), y_{r+1}(t_0), \cdots, y_n(t_0)$. Since the final values of the solution $y_1(t), \cdots, y_n(t)$ of Eq. (1) are continuous functions of the initial values, φ_m may be considered to be functions of $\mathbf{y}(t_0)$ and solving Eq. (1) equivalent to finding the solution to the system

$$\varphi_m[\mathbf{y}(t_0)] = 0, \qquad m = 1, 2, \cdots, n - r, \tag{18}$$

or

$$\boldsymbol{\varphi}[\mathbf{y}(t_0)] = 0.$$

Assume that the kth approximation to the vector of $n - r$ missing initial conditions $\mathbf{z}^{(k)}$ (with components $z_j^{(k)} \equiv y_{r+j}^{(k)}(t_0)$, $j = 1, 2, \cdots, n - r$) has been found. Newton's method gives as the $(k + 1)$st approximation

$$\mathbf{z}^{(k+1)} = \mathbf{z}^{(k)} - [A^{(k)}]^{-1}\boldsymbol{\varphi}^{(k)}, \tag{19}$$

where $\boldsymbol{\varphi}^{(k)}$ is the column vector with components $\varphi_m^{(k)} \equiv \varphi_m[\mathbf{y}^{(k)}(t_0)]$; and $A^{(k)}$ is the $(n - r) \times (n - r)$ matrix whose element $A_{mj}^{(k)}$ in the mth row, jth column is $(\partial\varphi_m/\partial z_j)^{(k)}$. Note that the superscript (k) always indicates evaluation of the quantity superscripted at $\mathbf{y}^{(k)}(t_0)$.

The Kantorovich theorem is thus applicable to the two-point boundary value problem.

We now proceed to show that the Goodman-Lance method is equivalent to Newton's method as applied to the two-point nonlinear ordinary differential equation boundary value problem.

Since w_m is a function of $y_1(t_0), y_2(t_0), \cdots, y_n(t_0)$, the total variation can be expressed as

$$\delta w_m^{(k)} = \sum_{j=1}^{n-r} \left(\frac{\partial w_m}{\partial z_j}\right)^{(k)} \delta z_j^{(k)}.$$

$$m = 1, 2, \cdots, n - r. \tag{20}$$

Forming the partial derivatives of Eq. (17) and substituting into Eq. (20):

$$\delta w_m^{(k)} = -\sum_{j=1}^{n-r} \left(\frac{\partial \varphi_m}{\partial z_j}\right)^{(k)} \delta z_j^{(k)}, \text{ or}$$

$$\delta \mathbf{w}^{(k)} = -A^{(k)}\,\delta\mathbf{z}^{(k)}. \tag{21}$$

If we now equate for the mth integration of the adjoint equations, Eq. (6) with Eq. (21), we find that

$$x_{r+j,m}^{(k)}(t_0) = -\left(\frac{\partial\varphi_m}{\partial z_j}\right)^{(k)} = -A_{mj}^{(k)},$$

$$m, j = 1, 2, \cdots, n - r. \tag{22}$$

Equations (6) may be written, using the notation of this section, $\delta\mathbf{w}^{(k)} = -A^{(k)}\delta\mathbf{z}^{(k)}$, with solution

$$\delta\mathbf{z}^{(k)} = -[A^{(k)}]^{-1}\,\delta\mathbf{w}^{(k)}. \tag{23}$$

On comparing the definitions of the variation in Eq. (2) and the miss distance in Eq. (17), we note that

$$\delta w_m^{(k)} = \varphi_m^{(k)} \equiv \varphi_m[\mathbf{y}^{(k)}(t_0)]. \tag{24}$$

Substituting Eq. (24) into (23) yields

$$\delta\mathbf{z}^{(k)} = -[A^{(k)}]^{-1}\boldsymbol{\varphi}^{(k)} \tag{25}$$

as the correction vector in the Goodman-Lance method. Referring to Eq. (20) we see that this is the same correction vector obtained by applying Newton's method to solving $\boldsymbol{\varphi}[\mathbf{y}(t_0)] = 0$.

The Kantorovich sufficiency theorem can, therefore, be applied to the Goodman-Lance method, furnishing a theoretical basis for the convergence of the process and an estimate of the rate of convergence. In practice, assuming an initial estimate of the missing initial values $y_{r+1}^{(0)}(t_0), \cdots, y_n^{(0)}(t_0)$ is available, the matrix $\Gamma_0 = [A^{(0)}]^{-1}$ can be calculated after one integration of the system, Eq. (1), and $n - r$ integrations of the adjoint system, Eq. (4), and then the norm, $||\Gamma_0|| = \beta_0$, determined. Since $\varphi_i(\mathbf{y}^{(0)})$ is also known at this stage, the vector $\Gamma_0\boldsymbol{\varphi}(\mathbf{y}^{(0)})$ can be formed and from it the norm, $||\Gamma_0\boldsymbol{\varphi}(\mathbf{y}^{(0)})|| = \eta_0$. However, there are practical problems in computing K defined in Eq. (13), as the next section indicates.

Numerical results

A double precision FORTRAN program for the IBM 7094 was written for the Goodman-Lance method. The method was applied to a variety of two-point boundary values for the two-body equations of motion. In addition, the Kantorovich theorem norms were evaluated for each iteration of the Goodman-Lance method.

Since the Kantorovich theorem is a sufficiency theorem, it only tells us that the problem will converge if certain conditions, Eqs. (11)–(14), are satisfied. If thesec onditions are not satisfied, the theorem makes no pronouncements either for or against convergence. The calculation of the Kantorovich norms is not without difficulties. The norms η_0, β_0 are "point norms," that is, norms evaluated at the trial vector $\mathbf{y}^{(0)}$, which is a point in the n-dimensional vector space of the $\mathbf{y}$. K, however, is an upper bound for a certain set of expressions over the interval given by inequality (15). This interval itself depends on h_0 which depends on K through Eq. (14). Note further from Eqs.

Table 1 Kantorovich norms and calculated initial velocity vector and final position vector for two-point, two-body boundary value problem.

Goodman-Lance method iteration number	*Kantorovich norms* h_i	β_i	η_i	K_i
0	$6.763579(10^{2})$	3.659561	1.069325	$1.728374(10^{2})$
1	$6.536509(10^{1})$	3.444090	1.663449	$1.140937(10^{1})$
2	$5.233003(10^{-1})$	$7.149846(10^{-1})$	$2.365853(10^{-1})$	3.093615
3	$8.472580(10^{-1})$	1.124802	$3.827557(10^{-2})$	$1.967965(10^{1})$
4	$3.273678(10^{-2})$	1.017268	$2.250358(10^{-3})$	$1.430042(10^{1})$
5	$4.037952(10^{-5})$	1.013542	$2.822407(10^{-6})$	$1.411560(10^{1})$
6	$4.537566(10^{-8})$	1.013534	$3.171723(10^{-9})$	$1.411526(10^{1})$
	Calculated missing initial conditions			
	$\dot{x}(0)$	$\dot{y}(0)$	$\dot{z}(0)$	
0	$-5.379999(10^{-1})$	$2.879999(10^{-1})$	$4.988299(10^{-1})$	
1	-1.376313	$5.242722(10^{-1})$	$9.080641(10^{-1})$	
2	$3.236898(10^{-1})$	$5.779965(10^{-1})$	1.001111	
3	$8.720452(10^{-2})$	$4.489073(10^{-1})$	$7.775289(10^{-1})$	
4	$1.017630(10^{-1})$	$4.709831(10^{-1})$	$8.157667(10^{-1})$	
5	$1.016559(10^{-1})$	$4.722822(10^{-1})$	$8.180167(10^{-1})$	
6	$1.016588(10^{-1})$	$4.722833(10^{-1})$	$8.180185(10^{-1})$	
	Calculated terminal conditions			
	$x(2)$	$y(2)$	$z(2)$	
0	$6.086336(10^{-1})$	$-3.733722(10^{-1})$	$-6.466988(10^{-1})$	
1	-2.218209	$-1.837729(10^{-1})$	$-3.183034(10^{-1})$	
2	$7.165604(10^{-1})$	$9.196269(10^{-1})$	1.592828	
3	$-8.591061(10^{-2})$	$5.013211(10^{-1})$	$8.683122(10^{-1})$	
4	$-2.289911(10^{-3})$	$5.726597(10^{-1})$	$9.918756(10^{-1})$	
5	$-9.427341(10^{-6})$	$5.759951(10^{-1})$	$9.976526(10^{-1})$	
6	$-7.212622(10^{-9})$	$5.759999(10^{-1})$	$9.976609(10^{-1})$	

(11), (12), (14) and (15) that both the center point and length of the interval depend on $\mathbf{y}^{(0)}$. For a poor choice of $\mathbf{y}^{(0)}$, it may not be possible to satisfy Kantorovich's conditions and the process described may diverge. Since it is not practical to seek K over an interval, we evaluated instead the point norm, K_i, that is, we computed the expression in Eq. (13) for the value $\mathbf{y}^{(i)}$. In other words, β_i, η_i, $K = K_i$, h_i are all evaluated at each iteration at vector $\mathbf{y}^{(i)}(t_0)$. While in all probability K_0 will not be the upper bound needed for applying the theorem, the computations of K_i are useful. For a process where the sequence $\{\mathbf{y}^{(i)}\}$ converges, the sequence $\{K_i\}$ will usually decrease monotonically, which indicates that K_0 is close to the required K. If the $\{\mathbf{y}^{(i)}\}$ does not converge, we may find one or more K_i much larger than K_0. In general, both of these possibilities are found in practice.

The Goodman-Lance method will generate, usually, a succession of trial initial vectors which do not satisfy the Kantorovich theorem. If the $\{\mathbf{y}^{(i)}\}$ converges, perhaps the 4th iterate of the Goodman-Lance method will produce the 0th iterate for the application of the Kantorovich theorem; an example of this is found in Table 1. The use of K_i in place of K may give rise to erratic behavior in the numerical evaluation of h_i. For example, h_i may oscillate between numbers larger than and less than 1/2. In all cases we have examined this behavior in h_i can be traced directly to the fact that K_0 is not equal to the upper bound K.

To illustrate a more or less typical numerical experience, we list in Table 1 the Kantorovich norms, the initial velocity vector, and the final position for the two-body version of the problem of McGill and Kenneth.

The two-body equations of motion are

$$\ddot{x}(t) = -\frac{kx(t)}{r^3}$$

$$\ddot{y}(t) = -\frac{ky(t)}{r^3}$$

$$\ddot{z}(t) = -\frac{kz(t)}{r^3},$$

where

$r = [x^2(t) + y^2(t) + z^2(t)]^{1/2}$;

$k = 1.0$, for canonical units.

The boundary conditions, for $t_0 = 0$ and $t_f = 2$, are:

$x(0) = 1.076000 \qquad x(2) = 0.000000$

$y(0) = 0.000000 \qquad y(2) = 0.576000$

$z(0) = 0.000000 \qquad z(2) = 0.997661.$

The trial initial velocity vector is taken as the average velocity vector based on the difference between the final and initial position vectors divided by the time interval; that is, the initial conditions correspond to McGill and Kenneth's starting function. The values are:

$\dot{x}(0) = -0.538000$

$\dot{y}(0) = 0.288000$

$\dot{z}(0) = 0.498830.$

In Table 1 the calculations were made for 20 integration steps over the interval (0, 2) and the h_i were computed using β_i, η_i, K_i in Eq. (14). Fifty integration steps yielded essentially the same results. The h_i are monotone, except for the third iteration of the Goodman-Lance method. As stated above, this behavior can be traced directly to the evaluation of K_i. The 4th iteration of the Goodman-Lance provides the 0th iteration for the application of the Kantorovich theorem. From the 4th iteration on, the h_i are less than 1/2, and the h_i and η_i are monotonic decreasing. We infer that the conditions of the Kantorovich theorem are satisfied, and expect convergence. A check on the computed terminal position vector confirms that the problem indeed converges.

As a matter of interest, we list in Table 2 the computed rate of convergence, the left-hand side of inequality (16) and the estimated rate of convergence, the right-hand side of (16). The calculations are based on using the 4th iteration of the Goodman-Lance method as the 0th iteration for the evaluation of the Kantorovich norms. The 6th iteration of the Goodman-Lance method is assumed to yield the "true" solution. We observe that the estimated rates of convergence are realistic.

Our computational experience suggests the following rules of thumb for similar problems. First, if the problem is going to converge, it will do so, in general, within 5 to 10 iterations of the Goodman-Lance method. Second, it is better to calculate with smaller time steps per iteration of the Goodman-Lance method and employ fewer iterations, than to calculate with larger time steps per iteration and employ more iterations. Another interesting computational observation is that if the computed h_i remains less than 1/2 for two or three consecutive iterations, then the process will probably converge.

Table 2 Comparison of computed and estimated rates of convergence for problem presented in Table 1.

Goodman-Lance method iteration number	*Rates of convergence* Computed (LHS of Eq. (16))	Estimated (RHS of Eq. (16))
4	$2.2518\ (10^{-3})$	$4.500716\ (10^{-3})$
5	$2.8\ (10^{-6})$	$1.473389\ (10^{-5})$
6	0.0	$3.158037\ (10^{-7})$

Acknowledgments

The authors acknowledge discussions with Frank Ditto, IBM Federal Systems Division, Houston and with Henry Decell, NASA, Houston, which served as useful background for this work. M. A. Hyman, IBM Federal Systems Division, Bethesda, carefully reviewed the manuscript and made a number of notational and editorial suggestions to improve the presentation.

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Received May 23, 1966.