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On a Newton-Moser Type Method

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Abstract. We prove that a variant of Moser's iterative method for solving nonlinear equations is quadratically convergent and give error bounds. We estimate the amount of arithmetic for the method and compare it to Newton's method. Finally we use the method to solve a problem with small divisors.

1. Introduction

In this paper we will discuss an iterative technique, due to Jürgen Moser, for finding the roots of a single nonlinear equation $f(x)=0$. Consider the following method:

$$x_{n+1}=x_n-y_n f(x_n), \tag{1.1}$$

$$y_{n+1}=y_n-y_n[f'(x_n)y_n-1]. \tag{1.2}$$

The first equation is similar to Newton's method, in which case y_n is equal to $1/f'(x_n)$. The second equation is Newton's method applied to $g(y)=1/y-f'(x_n)=0$. Thus, if y_n is close to $1/f'(x_n)$ then y_{n+1} is even closer. It can be shown that the rate of convergence for the above scheme is $(1+\sqrt{5})/2=1.62\ldots$, provided the root is simple, see [4, pp. 149–151]. However, this is unsatisfactory from a numerical point of view because the scheme uses the same amount of information per step as Newton's method, yet, it converges no faster than the secant method.

Moser's method was developed as a technical tool for investigating the stability of the N-body problem in Celestial Mechanics. The main difficulty in this and similar problems involving small divisors is the solution of a system of nonlinear partial differential equations, which on the Fourier side can be written in the form $F(w)=w+T(w)=0$ where T is a nonlinear unbounded operator and w is a vector with infinite many components. Thus we can not expect the contraction method

$$w_{k+1}=-T(w_k) \tag{1.3}$$

to converge to a solution. The application of Newton's method is also dubious since it is not clear whether $F'(w_k)=I+T'(w_k)$ is invertible. In essence, Moser's idea is to solve the problem by a sequence of changes of variables, see Section 3. An alternative device has recently been proposed by Rüssmann, see [6].

In Section 2 we will prove that a modification of (1.2) leads to a quadratically convergent scheme, see also [4, pp. 151–152] and [12]. In Section 3 this scheme will be interpreted in terms of an approximation to the inverse function of $f(x)$. In Section 4 we will discuss the natural generalization of the method to systems of nonlinear equations, and also give error bounds. The computational aspects are considered in Section 5. Finally, in Section 6 we compare several methods for investigating stability problems involving small divisors.

2. The Improved Scheme

We will now consider a modified version of Moser's method:

$$x_{n+1} = x_n - y_n f(x_n), \tag{2.1}$$

$$y_{n+1} = y_n - y_n [f'(x_{n+1}) y_n - 1]. \tag{2.2}$$

We note that (2.2) differs from (1.2) in that the latest available information is used. This is crucial for obtaining fast convergence.

Let α be a simple root of $f(x) = 0$. We assume that f is twice differentiable in an open interval B with midpoint α and let

$$m = \inf_B |f'|, \qquad M = \sup_B |f''|.$$

If B is sufficiently small then m is positive. Our main objective is to investigate how fast x_n converges to α and not how fast y_n converges to $1/f'(\alpha)$. We regard $e_n = x_n - \alpha$ and $d_n = 1 - y_n f'(x_n)$ as the errors in the n-th step. Convergence properties for the y_n can easily be obtained once the rate of convergence for e_n and d_n have been found, see Corollary 2.

We can now formulate our first result.

Theorem 1. Let $c = \dfrac{9M}{4m}$ and define $s_n = |d_n| + c|e_n|$. If x_0 is in B and $s_0 < \frac{1}{2}$, then $s_{n+1} \leqq 2s_n^2$ for all n.

Remark. This result shows that s_n converges quadratically. However, we do not claim that e_{n+1}/e_n^2 converges to a constant, which is the normal way of expressing the quadratic convergence of an iterative method for a single nonlinear equation, see [10, p. 9]. Nevertheless e_n converges rapidly to zero, see Corollary 1.

Proof. We will prove the result by induction and consider the $(n+1)$-th step. Suppose that x_n is in B and that $s_n < \frac{1}{2}$. We will then show that x_{n+1} is in B and that $s_{n+1} \leqq 2s_n^2$. From this follows that $s_{n+1} < \frac{1}{2}$.

By expanding f in a Taylor series around x_n we get

$$0 = f(\alpha) = f(x_n) - f'(x_n)\, e_n + \tfrac{1}{2} f''\, e_n^2.$$

Here f'' is evaluated at a point between x_n and α and thus $|f''| \leqq M$. From this and formula (2.1) we obtain an expression for the error in step $n+1$,

$$\begin{aligned} e_{n+1} &= e_n - y_n [f'(x_n)\, e_n - \tfrac{1}{2} f''\, e_n^2] \\ &= d_n\, e_n + \tfrac{1}{2} y_n f''\, e_n^2. \end{aligned}$$

To estimate y_n we use that $|d_n| = |1 - y_n f'(x_n)| < \frac{1}{2}$. Because $|f'(x_n)| \geqq m$ we can conclude that $|y_n| < 3/(2m)$. Combining these estimates with the above equation for e_{n+1} we find

$$\begin{aligned}|e_{n+1}| &\leqq |d_n|\,|e_n| + \frac{1}{2}\,\frac{3}{2m}\,M|e_n|^2 \\ &\leqq s_n|e_n|. \end{aligned} \tag{2.3}$$

Since $s_n < \frac{1}{2}$ we see that $|e_{n+1}| < \frac{1}{2}|e_n|$ and thus x_{n+1} is in B.

We will now estimate d_{n+1}. From (2.2) follows that

$$\begin{aligned} d_{n+1} &= \{1 - y_n f'(x_{n+1})\}^2 \\ &= \{1 - y_n f'(x_n) + y_n [f'(x_n) - f'(x_{n+1})]\}^2. \end{aligned}$$

The first term in the last paranthesis simply equals d_n. From the mean value theorem follows that $f'(x_n) - f'(x_{n+1}) = f'' \cdot (x_n - x_{n+1})$ where f'' now is evaluated at a point between x_n and x_{n+1}. Both points are in B and we therefore have $|f''| \leqq M$. Moreover we conclude from (2.3) that $|x_n - x_{n+1}| < \frac{3}{2}|e_n|$. By using these estimates and the fact that $|y_n| < 3/(2m)$ we obtain the following inequalities

$$\begin{aligned} |d_{n+1}| &\leqq \left\{ |d_n| + \frac{3}{2m}\,M\,\frac{3}{2}\,|e_n| \right\}^2 \\ &\leqq s_n^2. \end{aligned} \tag{2.4}$$

From (2.3) follows that $c|e_{n+1}| \leqq s_n^2$. We can finally conclude that $s_{n+1} \leqq 2s_n^2$ by combining this result with (2.4). This completes the proof.

From the definition of s_n follows that $|e_n| \leqq s_n/c$ and $|d_n| \leqq s_n$, and we can therefore use Theorem 1 to estimate the rate of convergence of e_n and d_n. Slightly sharper estimates can also be obtained as in

Corollary 1. If x_0 is in B and $s_0 < \frac{1}{2}$, then

$$|e_n| \leqq \frac{(2s_0)^{2^n}}{2^{n+1}} \cdot \frac{1}{c}, \qquad |d_n| \leqq \frac{(2s_0)^{2^n}}{4}.$$

Remark. We can express this result by saying that the convergence of the iterative method (2.1), (2.2) is R-quadratic at the point α which means that $\limsup_n |e_n|^{2^{-n}}$ is less than one. For a definition and an analysis of this concept see [5, pp. 287–294].

Proof. To find the bound for $|e_n|$ we use the inequality (2.3) and obtain

$$|e_n| \leqq s_{n-1}\, s_{n-2} \cdots s_0 |e_0|.$$

Let $q_k = 2s_k$. From Theorem 1 follows that $q_{k+1} \leqq q_k^2$ and consequently $q_k \leqq (q_0)^{2^k}$. We can therefore estimate the products of the s_k as

$$\begin{aligned} \prod_{k=0}^{n-1} s_k &\leqq \prod_{k=0}^{n-1} \tfrac{1}{2}(q_0)^{2^k} \\ &= 2^{-n} (q_0)^{2^n - 1}. \end{aligned}$$

By combining this estimate with the inequality for $|e_n|$ and by using that $|e_0| \leqq s_0/c$ we arrive at the bound as stated in the corollary.

From (2.4) follows that $|d_n| \leqq \frac{1}{4} q_{n-1}^2$ and the proof is completed by using the inequality for q_k with $k = n-1$.

The next corollary shows that y_n converges quadratically to $1/f'(\alpha)$.

Corollary 2. Let $\delta_n = 1/f'(\alpha) - y_n$. If x_0 is in B and $s_0 < \frac{1}{2}$, then

$$|\delta_n| \leqq \frac{(2s_0)^{2^n}}{2m}.$$

Proof. The corollary is an easy consequence of the inequality $|\delta_n| \leqq s_n/m$. From the mean value theorem follows

$$\begin{aligned}\delta_n f'(\alpha) &= 1 - y_n f'(x_n) + y_n [f'(x_n) - f'(\alpha)] \\ &= d_n + y_n f'' e_n\end{aligned}$$

where f'' is evaluated at a point between x_n and α. Thus $|f''| \leqq M$. Since $|y_n| \leqq 3/(2m)$ we get the estimate

$$\begin{aligned}|\delta_n|\,|f'(\alpha)| &\leqq |d_n| + \frac{3}{2m} M |e_n| \\ &\leqq s_n\end{aligned}$$

and the proof is completed by using that $|f'(\alpha)| \geqq m$.

3. An Alternative Formulation

Moser's original derivation and presentation of his method was in terms of an approximation to the inverse function of $f(x)$. The formulas (1.1), (1.2) is a later interpretation, see [4, pp. 121–126]. We will now show that the modified method (2.1), (2.2) also can be expressed in this manner.

Let the initial guess x_0 be in the neighborhood B of α and assume that $s_0 < \frac{1}{2}$ such that the iteration will converge according to Theorem 1. By a change of variables we may assume that x_0 is zero and consequently that B is a neighborhood of zero. Since f' does not vanish in B there exists an inverse function ϕ of f such that $(f \circ \phi)(\xi) = \xi$ for all ξ in B. If ϕ was known, $\alpha = \phi(0)$ would be the root of $f(x) = 0$. The basic idea is to find a good approximation to $\phi(\xi)$.

Let $f_0 = f$ and define the sequence of function f_n recursively by

$$g_n(\xi) = f_n(\xi) - \xi, \tag{3.1}$$

$$w_n(\xi) = -[g_n(0) + g_n'(-g_n(0))\xi], \tag{3.2}$$

$$v_n(\xi) = \xi + w_n(\xi), \tag{3.3}$$

$$f_{n+1}(\xi) = f_n(v_n(\xi)). \tag{3.4}$$

To interpret this scheme we introduce the composite function

$$u_n(\xi) = v_0 \circ v_1 \circ \cdots \circ v_{n-1}$$

and using this notation we can rewrite Eq. (3.4) in the form

$$f_n(\xi) = f(u_n(\xi)). \tag{3.5}$$

By a slight modification of Moser's proof, see [4, pp. 123–126], it can be shown that $f_n(0)$ and $f_n'(0) - 1$ converge rapidly to zero. Thus, if n is large and ξ small then the functions $f_n(\xi)$ and ξ are close and it follows from (3.5) that u_n is a good approximation to the inverse function ϕ in a neighborhood of zero.

To bring forth the connection between the schemes (2.1), (2.2) and (3.1)–(3.4) we observe that all the functions v_n depend linearly on ξ. The functions u_n are therefore linear, i.e. $u_n(\xi) = x_n + a_n\xi$. On the other hand the u_n satisfy $u_{n+1}(\xi) = u_n(v_n(\xi))$ and by identifying the coefficients of ξ in this equation and by using (3.2) and (3.3) we see that

$$x_{n+1} = x_n - a_n g_n(0),$$
$$a_{n+1} = a_n - a_n g_n'(-g_n(0)).$$

From Eqs. (3.1) and (3.5) follow that $g_n(0) = f(u_n(0))$ and $g_n'(\xi) = f'(u_n(\xi))a_n - 1$. Moreover, $u_n(0) = x_n$ and $u_n(-g_n(0)) = x_{n+1}$. Thus the last two equations are identical with Eqs. (2.1), (2.2).

Finally we mention that if the argument of g_n' in (3.2) is zero instead of $-g_n(0)$, then the scheme (3.1)–(3.4) reduces to Moser's original method (1.1), (1.2).

4. A Generalization. Error Bounds

It is easy to generalize Moser's method to a system of nonlinear equations $F(x) = 0$. Let x_0 be given and chose $A_0 = [F'(x_0)]^{-1}$, where F' is the Fréchet derivative of F at x_0, see [5, p. 61]. We consider the following scheme

$$x_{n+1} = x_n - A_n F(x_n),$$
$$A_{n+1} = A_n - A_n[F'(x_{n+1})A_n - I].$$

If F' is nonsingular in a neighborhood of a solution α of $F(x) = 0$ then minor modifications of the proof of Theorem 1 shows that the method converges quadratically provided $x_0 - \alpha$ is sufficiently small. The convergence of this scheme and a related method has also been discussed by Zehnder, see [12].

We will now estimate the error in the $(n+1)$-th step in terms of computable quantities from the n-th step. This bound can be used as a stopping criteria. The proof is based on Kantorovich's theorem for Newton's method, see [5, p. 421–423].

Theorem 2. Let B be a neighborhood of x_n and assume that

$$\|F'(x) - F'(y)\| \leqq \gamma \|x - y\|$$

for all x and y in B, where $\|\cdot\|$ denotes the max-norm for vectors and the corresponding matrix norm. Suppose that

$$\varepsilon = \|A_{n-1}F'(x_n) - I\| < 1$$

and define

$$\beta = (1-\varepsilon^2)^{-1}\|A_n\|, \qquad \eta = (1-\varepsilon^2)^{-1}\|A_n F(x_n)\|.$$

If $\beta\gamma\eta < \frac{1}{2}$ and the sphere with center x_n and radius $(1 - \sqrt{1 - 2\beta\gamma\eta})/(\beta\gamma)$ is in B, then

$$\|x_{n+1} - \alpha\| \leqq (2\beta\gamma\eta + \varepsilon^2)\eta.$$

Remark. The constants ε, β and η which depend on n can be calculated in each step of the iteration, whereas γ must be estimated from the beginning. If F is twice differentiable in B then we can choose

$$\gamma = \sup_B \max_l \Sigma_{i\,j} \left| \frac{\partial^2 f_l}{\partial x_i \partial x_j} \right|$$

where f_l are the components of F. We will not prove this result, but refer to [5, pp. 74–78] for the necessary tools.

Proof. We consider the $(n+1)$-th step in the iteration and write

$$A_n = A_{n-1} - [A_{n-1} J_n - I] A_{n-1} \tag{4.1}$$

$$x_{n+1} = x_n - A_n F_n \tag{4.2}$$

where $J_n = F'(x_n)$ and $F_n = F(x_n)$. From Eq. (4.1) follows that

$$I - A_n J_n = (I - A_{n-1} J_n)^2, \tag{4.3}$$

which shows that A_n and J_n are nonsingular matrices since by our initial assumption the norm of the right hand side is less than one. We can therefore rewrite (4.2) in the form

$$x_{n+1} - [(A_n J_n)^{-1} - I] A_n F_n = x_n - J_n^{-1} F_n. \tag{4.4}$$

We can interpret the left hand side, which we denote by $\bar{x}_{n+1}$, as the result of one step of Newton's method.

By using Kantorovich's result for Newton's method we can find a bound for $\bar{x}_{n+1} - \alpha$ in terms of γ and the norm of J_n^{-1} and $J_n^{-1} F_n$. From (4.3) follows that

$$\begin{aligned} J_n^{-1} &= (A_n J_n)^{-1} A_n \\ &= [I - (I - A_{n-1} J_n)^2]^{-1} A_n \end{aligned}$$

and we can therefore estimate J_n^{-1}, using the definitions of ε and β by

$$\|J_n^{-1}\| \leqq (1 - \varepsilon^2)^{-1} \|A_n\| = \beta.$$

Since $J_n^{-1} F_n = (A_n J_n)^{-1} A_n F_n$ we obtain by using the same technique that

$$\|J_n^{-1} F_n\| \leqq (1 - \varepsilon^2)^{-1} \|A_n F_n\| = \eta.$$

We can now refer to Kantorovich's theorem, see [5, p. 421], which states that if $\beta\gamma\eta < \frac{1}{2}$ and the sphere with center x_n and radius $(1 - \sqrt{1 - 2\beta\gamma\eta})/(\beta\gamma)$ is in B, then Newton's method converges to α with x_n as initial guess. In particular the first iterate satisfies

$$\|\bar{x}_{n+1} - \alpha\| \leqq 2\beta\gamma\eta^2.$$

To estimate the second term on the left hand side of (4.4) we note that it follows from (4.3) that

$$(A_n J_n)^{-1} - I = [I - (I - A_{n-1} J_n)^2]^{-1} (I - A_{n-1} J_n)^2.$$

By using this identity and the definition of η we conclude that

$$\begin{aligned} \|\bar{x}_{n+1} - x_{n+1}\| &\leqq (1 - \varepsilon^2)^{-1} \varepsilon^2 \|A_n F_n\| \\ &\leqq \varepsilon^2 \eta. \end{aligned}$$

The proof is completed by combining the last two inequalities.

5. Numerical Aspects

In this section we will compare Moser's method to Newton's method from a computational point of view. We write Newton's method in the implicit form

$$F'(x_k)(x_{k+1} - x_k) = -F(x_k) \tag{5.1}$$

and assume that F has n components, so F' is a n by n matrix. To find x_{k+1} we must solve the linear systems of Eq. (5.1). For the sake of illustration we choose two examples. We are not concerned with the existence of a solution to the problems, rather we will estimate the amount of arithmetic for the two methods.

The first example is Urysohn's integral equation

$$u(s) = \psi(s) + \int_0^1 K\big(s, t, u(t)\big)\, dt.$$

The natural discretization of this integral equation leads to a system of nonlinear equations for which the Fréchet derivative is, in general, a dense unsymmetric matrix. In Newton's method we solve (5.1) by Gaussian elimination which requires $\frac{1}{3}n^3 + n^2$ multiplicative operations, see [3, p. 36]. To get started in Moser's method we must invert $F'(x_0)$ at a cost of n^3 operations, see [3, p. 36]. Thereafter each step of (4.1) and (4.2) requires $2n^3$ and n^2 operations respectively if we use the standard way of multiplying two matrices.

In Moser's method the approximate inverse of F' is available and this facilitate the estimate of the error. Even this advantage disappears if we compare it to the following version of Newton's method

$$x_{k+1} = x_k - [F'(x_k)]^{-1} F(x_k),$$

which however requires more work than the conventional form (5.1). From Kantorovich's theorem we can obtain a bound for $x_{k+1} - \alpha$ and the work would be $n^3 + n^2$ operations per step.

Our second example is the differential equation

$$u'' = f(t, u)$$

on the interval $0 \leqq t \leqq 1$ and with $u(0)$ and $u(1)$ given. If we approximate u'' by a second order central difference quotient, we obtain a system of nonlinear equations the Fréchet derivative of which is a tridiagonal matrix. In this case only $5n$ operations are needed to solve (5.1), see [3, p. 57], whereas $\frac{1}{2}n^3 + 3n^2$ operations are required in (4.1), if we use that the matrices A_k are symmetric.

The main weakness in Moser's method is the need for matrix multiplications, and this weakness gets even more pronounced when solving nonlinear elliptic boundary problems. There exist fast methods for computing the product of two matrices, due to Winograd [11] and Strassen [9]. However, these methods can also be adapted to solve a linear system of equations, and we shall therefore not pursue the comparison further in this direction.

In the numerical calculations below we use the following version of the variant of Moser's method

$$w_{k+1} = w_k - A_k F(w_k) \tag{5.2}$$

where $w_0 = 0$ and the linear operators A_k are defined iteratively by

$$A_i u = A_{i-1}[2 - F'(w_i)\, A_{i-1}]\, u \tag{5.3}$$

for $i = 1, 2, \ldots, k$ with $A_0 u = u$. Thus to compute $A_k F(w_k)$ we must save the Fréchet derivative from all the previous steps.

To estimate the amount of arithmetic for this algorithm let c_i and c be the number of multiplicative operations needed to calculate $v = A_i u$ and $F'(w_i)v$ respectively. It follows from (5.3) that $c_i = 2c_{i-1} + c$ and since $c_0 = 0$ we see that $c_k = (2^k - 1)c$. If the cost of computing $F(w_i)$ is less than or equal to c, then the total amount of work for the computation of $w_1, \ldots, w_{k+1}$ is less than $2^{k+1}c$.

The cost per step of method (5.2), (5.3) grows thus exponentially. However, if c is small compared to the number of operations needed to solve (5.1), then we can take several steps of Moser's method in the time needed for one step of Newton's method, see e.g. the case investigated below. It is of course important in this context that the modified method converges quadratically, whereas the rate of convergence of the original method (1.1), (1.2) is only 1.62 .... From a theoretical point of view this difference seems unessential.

6. A Numerical Example

In this section we will illustrate the use of algorithm (5.2), (5.3) on a small divisor problem, see Section 1. We consider two discs of radii r_1 and r_2 respectively, rotating around axes through their centers.

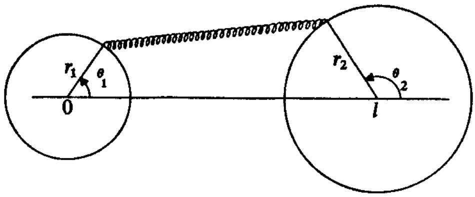

Fig. 1

We let the distance between the axes be l and connect the discs with a spring fixed on the edge of each disc, see Fig. 1.

In the discussion below we will assume that the discs rotate without friction and that the force exerted by the spring is proportional to the lenght of the spring. Let $\dot{\theta}_1 = \frac{d}{dt}\theta_1$ and $\dot{\theta}_2 = \frac{d}{dt}\theta_2$ be the angular velocities of the discs. By using the Euler equations of motions for a rotating rigid body with a fixed point, see [2, p. 157], we get

$$I_1\ddot{\theta}_1 + kr_1\{l\sin\theta_1 + r_2\sin(\theta_1 - \theta_2)\} = 0, \tag{6.1}$$

$$I_2\ddot{\theta}_2 + kr_2\{l\sin\theta_2 + r_1\sin(\theta_2 - \theta_1)\} = 0 \tag{6.2}$$

where k is the spring constant and I_1 and I_2 are the moments of inertia of the discs. We can reverse time, thus if $\theta_1(t)$ and $\theta_2(t)$ are solutions of (6.1) and (6.2) then $\theta_1(-t)$ and $\theta_2(-t)$ will also be solutions.

For convenience we set $l = 1$ and introduce the constants $\mu_1 = kr_1/I_1$ and $\mu_2 = kr_2/I_2$. If we furthermore introduce the functions $\phi_1 = \dot{\theta}_1$ and $\phi_2 = \dot{\theta}_2$

Eqs. (6.1) and (6.2) can be written as a reversible system

$$\dot\theta_1=\phi_1,$$
$$\dot\theta_2=\phi_2,$$
$$\dot\phi_1=-\mu_1\{\sin\theta_1+r_2\sin(\theta_1-\theta_2)\},$$
$$\dot\phi_2=-\mu_2\{\sin\theta_2+r_1\sin(\theta_2-\theta_1)\}.$$

We will now use a general theorem due to Moser, see [4, p. 49]. It states that if μ_1 and μ_2 are sufficiently small, then there exist solutions of the form

$$\theta_1=\xi_1+u_1(\xi_1,\xi_2),\qquad \phi_1=\omega_1+v_1(\xi_1,\xi_2), \tag{6.3}$$

$$\theta_2=\xi_2+u_2(\xi_1,\xi_2),\qquad \phi_2=\omega_2+v_2(\xi_1,\xi_2), \tag{6.4}$$

provided ω_1 and ω_2 are rationally independent. The functions u_1, u_2, v_1 and v_2 are real analytic, 2π periodic in ξ_1 and ξ_2 with

$$\dot\xi_1=\omega_1,\qquad \dot\xi_2=\omega_2. \tag{6.5}$$

Moreover, the reversible character of the system implies that u_1 and u_2 are odd functions of $\xi=(\xi_1,\xi_2)$ whereas v_1 and v_2 are even functions of ξ. The real numbers ω_1 and ω_2 are rationally independent if there exist two positive constants σ and τ such that

$$|\omega_1 j_1+\omega_2 j_2|>\sigma(|j_1|+|j_2|)^{-\tau} \tag{6.6}$$

for all $(j_1, j_2)\neq 0$.

One can show that the sum of the kinetic energies of the discs and the potential energy of the spring is constant in time. If the spring constant is small then the potential energy contained in the spring is small, but large amounts of kinetic energy could possible be transferred from one disc to the other. However, Moser's theorem implies that the kinetic energies of the discs, i.e. $\frac{1}{2}I_1\dot\theta_1^2$ and $\frac{1}{2}I_2\dot\theta_2^2$, remain almost constant in time provided the spring is sufficiently weak. In this sense the system is stable.

To find the stable solutions we insert (6.3) and (6.4) in (6.1) and (6.2) and by using (6.5) we obtain the following system of nonlinear partial differential equations

$$(\omega_1\partial_{\xi_1}+\omega_2\partial_{\xi_2})^2u_1+\mu_1\{\sin(\xi_1+u_1)+r_2\sin(\xi_1-\xi_2+u_1-u_2)\}=0,$$
$$(\omega_1\partial_{\xi_1}+\omega_2\partial_{\xi_2})^2u_2+\mu_2\{\sin(\xi_2+u_2)+r_1\sin(\xi_2-\xi_1+u_2-u_1)\}=0.$$

These equations present difficult computational problems. For computational convenience we let u_1 and u_2 have period one instead of 2π by introducing the new variables $\zeta=(x,y)$ where $\xi=2\pi\zeta$. Since u_1 and u_2 are odd, real analytic functions we look for solutions of the form

$$u_1=\sum_{j\neq 0}\alpha_j e^{2\pi i(j,\zeta)},\qquad u_2=\sum_{j\neq 0}\beta_j e^{2\pi i(j,\zeta)}$$

where $\alpha_j=-\alpha_{-j}$ and $\beta_j=-\beta_{-j}$. Here $j=(j_1, j_2)$ is a multiindex. Inserting these expressions in the above partial differential equation we get

$$-\sum_{j\neq 0}\alpha_j(\omega,j)^2e^{2\pi i(j,\zeta)}+\mu_1\{\sin(2\pi x+u_1)+r_2\sin\big(2\pi(x-y)+u_1-u_2\big)\}=0,$$
$$-\sum_{j\neq 0}\beta_j(\omega,j)^2e^{2\pi i(j,\zeta)}+\mu_2\{\sin(2\pi y+u_2)+r_1\sin\big(2\pi(y-x)+u_2-u_1\big)\}=0$$

where $\omega=(\omega_1,\omega_2)$ and $(\omega,j)=\omega_1 j_1+\omega_2 j_2$. The functions within the parenthesis are odd and periodic in x and y with period one. We can therefore expand them in a Fourier series and by equating the coefficients we finally obtain

$$\alpha+\mu_1 \Lambda \mathscr{F}\{\sin(2\pi x+\hat{\alpha})+r_2\sin(2\pi(x-y)+\hat{\alpha}-\hat{\beta})\}=0, \tag{6.7}$$

$$\beta+\mu_2 \Lambda \mathscr{F}\{\sin(2\pi y+\hat{\beta})+r_1\sin(2\pi(y-x)+\hat{\beta}-\hat{\alpha})\}=0 \tag{6.8}$$

where α and β are the Fourier coefficients of u_1 and u_2 respectively, i.e. $\alpha=\mathscr{F}u_1$ and $\beta=\mathscr{F}u_2$, and we have used the notation $u_1=\mathscr{F}^{-1}\alpha=\hat{\alpha}$ and $u_2=\mathscr{F}^{-1}\beta=\hat{\beta}$. In addition we define the operator Λ such that if $\gamma=\{\gamma_j\}$ are the Fourier coefficients corresponding to an odd function, then the j-th term of $\Lambda\gamma$ is $-\gamma_j/(\omega,j)^2$. At this point it becomes clear why ω_1 and ω_2 must be kept rationally independent. While it is almost inconceivable that the stability of the physical system actually depends on whether ω_1/ω_2 is a rational number, the analytic formalism breaks down. The existence of α and β which satisfy Eqs. (6.7) and (6.8) is a consequence of Moser's theorem, see [4, Chap. V].

To find α and β numerically we will apply the variant of Moser's method in the form (5.2) and (5.3) to Eqs. (6.7) and (6.8). Let η and ϑ be the Fourier coefficients corresponding to two odd, real analytic functions with period one. The Fréchet derivative $F'(\alpha,\beta)$ corresponding to (6.7) and (6.8) is a linear operator on (η,ϑ) with components

$$\eta+\mu_1 \Lambda \mathscr{F}\{\cos(2\pi x+\hat{\alpha})\hat{\eta}+r_2\cos(2\pi(x-y)+\hat{\alpha}-\hat{\beta})(\hat{\eta}-\hat{\vartheta})\}, \tag{6.9}$$

$$\vartheta+\mu_2 \Lambda \mathscr{F}\{\cos(2\pi y+\hat{\beta})\hat{\vartheta}+r_1\cos(2\pi(y-x)+\hat{\beta}-\hat{\alpha})(\hat{\vartheta}-\hat{\eta})\}. \tag{6.10}$$

So far the problem has infinite many unknowns α_j and β_j. However, in the numerical calculations we will only consider functions $\hat{\alpha}$ and $\hat{\beta}$ in the periodicity interval $0\leqq x<1$, $0\leqq y<1$ on the discrete set of points $x=j_1/N$ and $y=j_2/N$ where $j_1, j_2=0,1,\ldots,N-1$ and N is a power of two. On this mesh we can represent a function u by a discrete Fourier transform, see [1, p. 151],

$$u(j_1,j_2)=\sum_{n_1,n_2=0}^{N-1}\gamma(n_1,n_2)\,e^{2\pi i(j_1n_1+j_2n_2)/N} \tag{6.11}$$

where the Fourier coefficients γ are determined by

$$\gamma(n_1,n_2)=\frac{1}{N^2}\sum_{j_1,j_2=0}^{N-1}u(j_1,j_2)\,e^{-2\pi i(j_1n_1+j_2n_2)/N}. \tag{6.12}$$

If the coefficients γ are given we can evaluate the function u defined by (6.11) for all integers j_1 and j_2 and this periodic continuation of u will have period N in both variables. Similarly we can continue γ, defined by (6.12), as a periodic function. The mesh function u is odd if $u(j_1,j_2)=-u(-j_1,-j_2)=-u(N-j_1, N-j_2)$. Thus, u is odd if and only if γ is odd. To compute u from γ and vice versa we use the fast Fourier transform in an implementation by Singleton [7]. All indices in the expansion (6.11) and (6.12) are positive. This is convenient from a programming point of view, but our definition of the operator Λ must be changed accordingly.

We will now outline the $(n+1)$-th step of the algorithm, assuming that $\alpha=\alpha^{(n)}$ and $\beta=\beta^{(n)}$ are given. Since α and β are the Fourier coefficients corresponding to real, odd and periodic functions they are purely imaginary. We can therefore find $\hat{\alpha}$ and $\hat{\beta}$ simultaneously by one application of the fast Fourier transform, see [1, p. 7]. Thereafter we evaluate all sin and cos terms used in (6.7)–(6.10) at the points $x=j_1/N$ and $y=j_2/N$. The function $F(\alpha,\beta)$ defined by the left side of (6.7) and (6.8) is computed by a further application of the fast Fourier transform and multiplications with the diagonal matrices $\mu_1\Lambda$ and $\mu_2\Lambda$. Finally we compute the correction term $A_n F(\alpha,\beta)$ in (5.2) by using (5.3) recursively. It follows from (6.9) and (6.10) that if we store all cos terms evaluated at $\alpha^{(i)}$ and $\beta^{(i)}$ for $i=1,2,\dots,n$, then the evaluation of $A_i(\eta,\vartheta)$ involves two applications of the fast Fourier transform. We can therefore estimate the constant c in Section 5 by $6N^2+4N^2\log_2 N^2$ because one step of the fast Fourier transform requires roughly $\frac{1}{2}N^2\log_2 N^2$ complex multiplications, see [1, p. 23 and 152].

We will compare this version of Moser's method to Newton's method. Let η and ϑ be the modifications of $\alpha=\alpha^{(n)}$ and $\beta=\beta^{(n)}$ to be computed in the $(n+1)$-th step, i.e. $(\eta,\vartheta)=[F'(\alpha,\beta)]^{-1}F(\alpha,\beta)$. By reorganizing (6.9) and (6.10) we see that the components of the Fréchet derivative $F'(\alpha,\beta)$ applied to (η,ϑ) can be written as

$$\begin{aligned}&\{I+\mu_1\Lambda\mathcal{F}[\cos(2\pi x+\hat{\alpha})+r_2\cos(2\pi(x-y)+\hat{\alpha}-\hat{\beta})]\}*\eta\\&\quad-\mu_1 r_2\Lambda\mathcal{F}\cos(2\pi(x-y)+\hat{\alpha}-\hat{\beta})*\vartheta\\&\quad-\mu_2 r_1\Lambda\mathcal{F}\cos(2\pi(y-x)+\hat{\beta}-\hat{\alpha})*\eta\\&\quad+\{I+\mu_2\Lambda\mathcal{F}[\cos(2\pi y+\hat{\beta})+r_1\cos(2\pi(y-x)+\hat{\beta}-\hat{\alpha})]\}*\vartheta\end{aligned}$$

where $*$ denotes convolution. If we represent α,β,η and ϑ by discrete Fourier transforms and use the fact that η and ϑ are odd, wee see that (5.1) reduces to a dense system of linear equations with N^2 unknowns. Gaussian elimination requires approximately $N^6/3$ multiplicative operations for this system.

Table 1 contains an approximate estimate of the work involved for the two methods. We see that it is advantageous to use Moser's method if N is large and both methods converge rapidly.

In the computations presented below we have used $\omega_1=\sqrt{2}$ and $\omega_2=1$ which satisfy (6.6) with $\sigma=0.5$ and $\tau=1$. To establish the inequality it is enough to prove that if p and q are positive integers, then

$$|p-\sqrt{2}q|\geqq 0.5(p+q)^{-1}. \tag{6.13}$$

Table 1

	$N=4$	$N=8$	$N=16$
The constant c	350	1.900	9.700
1 step of Newton	1.400	87.000	5.600.000
1 step of Newton > n step of Moser if $n \leqq$	2	5	9
n step of Newton < n step of Moser if $n \geqq$	5	9	13

Table 2. The modified Moser's method

k	Iteration	$N=4$	$N=8$	$N=16$
10^{-2}	2	$1.8\cdot 10^{-2}$	$1.8\cdot 10^{-2}$	$1.8\cdot 10^{-2}$
	3	$5.8\cdot 10^{-5}$	$3.4\cdot 10^{-4}$	$3.7\cdot 10^{-4}$
	4	$1.7\cdot 10^{-9}$	$5.4\cdot 10^{-7}$	$8.4\cdot 10^{-7}$
10^{-3}	2	$1.9\cdot 10^{-3}$	$1.9\cdot 10^{-3}$	$1.9\cdot 10^{-3}$
	3	$5.8\cdot 10^{-8}$	$2.6\cdot 10^{-7}$	$2.6\cdot 10^{-7}$
10^{-4}	2	$1.9\cdot 10^{-4}$	$1.9\cdot 10^{-4}$	$1.9\cdot 10^{-4}$
	3	$5.8\cdot 10^{-11}$	$2.5\cdot 10^{-10}$	$2.5\cdot 10^{-10}$

We consider the following cases, one: p/q and $(p+1)/q<\sqrt{2}$, two: $p/q<\sqrt{2}$ and $(p+1)/q>\sqrt{2}$, and three: $p/q>\sqrt{2}$. The first case is obvious. In the second case we use that $f(x)=x^2-2$ is a convex function and $f(\sqrt{2})=0$. Let x_2 be the approximation to $\sqrt{2}$ computed by one step of the regula falsi method applied to $f(x)$ with $x_1=p/q$ and $x_0=(p+1)/q$ as initial points. We get

$$\sqrt{2}-p/q>x_2-p/q=\frac{1}{q}\cdot\frac{2q^2-p^2}{1+2p}.$$

To establish (6.13) we multiply the above inequality by q and note that the numerator is greater than one, whereas the denominator is smaller than $2(p+q)$. In the third case we use Newton's method with $x_1=p/q$ as initial guess, and the proof is similar.

We mention that the points (ω_1,ω_2) satisfying (6.6) for some σ and τ are dense in R^2, because every ω_1 and ω_2 can be approximated by $(p_1/q_1)\sqrt{2}$ and p_2/q_2 respectively where p_i and q_i are integers.

The constants in (6.1) and (6.2) have been chosen in the following manner. We assume the discs are made of steel with a density of $7.8\cdot 10^3$ kg/m^3. The discs have radius 0.10 m and 0.15 m respectively and thickness of 0.01 m. The distance between the axes was chosen to be 0.50 m. Thus the discs have masses of 2.45 kg and 5.51 kg respectively and the constants in (6.7) and (6.8) are $r_1=0.2$, $r_2=0.3$ and $\mu_1=4.08\,k$, $\mu_2=1.21\,k$ where k is the spring constant. We tried a variety of choices for k, but settled for a k in the interval 10^{-2} to 10^{-4} N/m. If $k=10^{-2}$ N/m, a weight of one gram will stretch the spring to a length of 0.98 m, so the spring is indeed weak.

All computations were carried out on the IBM 370/155 at Uppsala University. The program was written in Algol. In this language a procedure can call itself recursively, and this facilitates the programming. In accordance with (5.2), (5.3) we choose $\alpha^{(0)}=\beta^{(0)}=0$ and $A_0=I$. In Table 2 we give the relative magnitude of the correction terms for the α component, i.e. for $n=2,3,\ldots$ we evaluate $\|\alpha^{(n)}-\alpha^{(n-1)}\|_\infty/\|\alpha^{(n-1)}\|_\infty$. The correction terms for the β components are smaller in absolute value than those for the α components, but the relative magnitude follows exactly the same pattern.

The numbers in Table 2 indicate quadratic convergence for the modified method. Moreover, from Table 1 follows that with the exception of N equal to 4,

Table 3. The original Moser's method

k	Iteration	$N=4$	$N=8$	$N=16$
10^{-2}	2	$1.8 \cdot 10^{-2}$	$1.8 \cdot 10^{-2}$	$1.8 \cdot 10^{-2}$
	3	$4.1 \cdot 10^{-5}$	$2.5 \cdot 10^{-4}$	$2.7 \cdot 10^{-4}$
	4	$3.5 \cdot 10^{-9}$	$1.9 \cdot 10^{-7}$	$4.4 \cdot 10^{-7}$
10^{-3}	2	$1.9 \cdot 10^{-3}$	$1.9 \cdot 10^{-3}$	$1.9 \cdot 10^{-3}$
	3	$4.1 \cdot 10^{-8}$	$2.7 \cdot 10^{-7}$	$2.7 \cdot 10^{-7}$
10^{-4}	2	$1.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$
	3	$4.1 \cdot 10^{-11}$	$2.7 \cdot 10^{-10}$	$2.7 \cdot 10^{-10}$

one step of Newton's method requires more multiplications than is needed to obtain the final result by Moser's method.

If we replace (5.3) by $A_i u = A_{i-1}[2 - F'(w_{i-1}) A_{i-1}]u$ we get a convenient implementation of the original version of Moser's method. We have compared this method to the modified version. Table 3 contains the relative magnitude of the correction terms for the α components. The rate of convergence is similar to the previous case. The reason is that the Fréchet derivative (6.9), (6.10) at $\alpha^{(0)} = \beta^{(0)} = 0$ is close to F' evaluated at $\alpha^{(1)}$, $\beta^{(1)}$.

Finally we have tried to obtain the solution of (6.7) and (6.8) by using the contraction technique (1.3). This method is rejected in theoretical investigations of stability problems involving small divisors, see [4, p. 120], but in our computations it did converge, though slowly.

We will now give a partial explanation of this phenomena. By using Parseval's identity for the discrete Fourier transform, see [1, p. 11], it is possible to show that the discrete version of (1.3) is a contraction method provided

$$\frac{\max\{\mu_1, \mu_2\}}{\min(\omega, j)^2}(1 + r_1 + r_2) < 1.$$

In this case any α and β can be used as initial values. Since there is only a finite number of frequencies for each fixed N, the inequality can always be satisfied if the spring constant k is sufficiently small. For $N = 16$ we have $|(\omega, j)| \geqq (\sqrt{2} \cdot 5 - 7)$ and by using the values for r_1, r_2, μ_1 and μ_2 we see that (1.3) is a contraction for all $k \leqq 8.2 \cdot 10^{-4}$. This convers the case of the smallest k discussed here. However, it can also be shown by tedious calculations that the l_2 norm of the Fréchet derivative of T is larger than one for $\alpha = \beta = 0$ and $k = 10^{-2}$. Thus (1.3) may be a contraction even with $k = 10^{-2}$, but $\alpha = \beta = 0$ cannot belong to its domain of definition. In Table 4 we present the relative magnitude of the correction terms for the α components.

We have also tested values of k larger than 10^{-2}. Thus for $k = 0.025$ we obtain convergence for $N = 4$ and $N = 8$, but divergence for $N = 16$ for all three methods. If N and k are fixed the two versions of Moser's method give solutions which agree in the first 8 significant digits. If the relative magnitude of the correction term for the contraction method is of order 10^{-d}, the solution agrees with the other two in the first d significant digits.

Table 4. The contraction method

k	Iteration	$N=4$	$N=8$	$N=16$
10^{-2}	2	$1.9\cdot 10^{-2}$	$1.9\cdot 10^{-2}$	$1.9\cdot 10^{-2}$
	3	$2.8\cdot 10^{-3}$	$3.5\cdot 10^{-3}$	$3.5\cdot 10^{-3}$
	4	$5.6\cdot 10^{-5}$	$2.8\cdot 10^{-4}$	$3.0\cdot 10^{-4}$
	5	$9.3\cdot 10^{-6}$	$4.5\cdot 10^{-5}$	$5.6\cdot 10^{-5}$
	6		$1.2\cdot 10^{-5}$	$1.4\cdot 10^{-5}$
10^{-3}	2	$1.9\cdot 10^{-3}$	$1.9\cdot 10^{-3}$	$1.9\cdot 10^{-3}$
	3	$2.9\cdot 10^{-5}$	$3.5\cdot 10^{-5}$	$3.5\cdot 10^{-5}$
	4	$5.8\cdot 10^{-8}$	$2.5\cdot 10^{-7}$	$2.5\cdot 10^{-7}$
10^{-4}	2	$1.9\cdot 10^{-4}$	$1.9\cdot 10^{-4}$	$1.9\cdot 10^{-4}$
	3	$2.9\cdot 10^{-7}$	$3.5\cdot 10^{-7}$	$3.5\cdot 10^{-7}$

By comparing the solutions for fixed k, but different N, we get an indication of the errors in the calculations. For $k=10^{-2}$ and $N=16$ the solution of (6.7) and (6.8) gives the following Fourier series expansion of u_1 and u_2

$$\begin{aligned} u_1 = {} & 0.02033\sin 2\pi x + 0.07122\sin 2\pi(x-y) \\ & -0.00132\sin 2\pi y + 0.00077\sin 2\pi(2x-2y) \\ & +0.00047\sin 2\pi(2x-y) + 0.00022\sin 2\pi(2x-3y) \\ & +0.00020\sin 2\pi(x-2y) + \cdots \end{aligned}$$

$$\begin{aligned} u_2 = {} & 0.01207\sin 2\pi y + 0.01407\sin 2\pi(y-x) \\ & +0.00029\sin 2\pi(2y-x) + 0.00015\sin 2\pi(2y-2x) + \cdots. \end{aligned}$$

All remaining terms have coefficients less than 10^{-4}. For $N=8$ the Fourier coefficients are, after rounding, identical to those above and the agreement, as expected, is best for the very low frequencies. For $N=4$ the Fourier coefficients agree with those above in the first two significant digits. If k is 10^{-3} or 10^{-4} the solutions for different N differ much less than in the example above, presumably because the Fourier series for u_1 and u_2 converge more rapidly, and u_1 and u_2 can therefore be well represented by few terms.

We observe that the above solutions u_1 and u_2 for $k=10^{-2}$ and $N=16$ are close to the functions we obtain in the first step when we solve (6.7) and (6.8) by any of the three methods discussed here. In fact, we find in the first iteration of (6.7)

$$\alpha_{1,0} = \frac{\mu_1}{(\sqrt{2}+0)^2} = 0.02041, \qquad \alpha_{1,-1} = \frac{\mu_1\gamma_2}{(\sqrt{2}-1)^2} = 0.07143$$

which agrees tolerably with the coefficients of the dominating terms in the expansion of u_1. Similarly, by using (6.8) we obtain an even better agreement with the coefficients in the expansion of u_2

$$\beta_{0,1} = \frac{\mu_2}{(0+1)^2} = 0.01209, \qquad \beta_{-1,1} = \frac{\mu_2\gamma_1}{(-\sqrt{2}+1)^2} = 0.01411.$$

To obtain the solution of the nonlinear partial differential equations we just substitute in u_1 and u_2 the original variables $\xi_1 = 2\pi x$ and $\xi_2 = 2\pi y$. Finally we get the solutions θ_1 and θ_2 of (6.1) and (6.2) by solving (6.5) and using (6.3) and (6.4), i.e.

$$\theta_1(t) = \sqrt{2}t + c_1 + u_1(\sqrt{2}t + c_1, t + c_2),$$
$$\theta_2(t) = t + c_2 + u_2(\sqrt{2}t + c_1, t + c_2)$$

where c_1 and c_2 are arbitrary real constants.

The computational procedure suggested in this section can be improved in several ways. By using the symmetry of α and β we can decrease the number of sin and cos evaluations and the number of multiplications needed in (6.9) and (6.10) by a factor two. In addition, the fast Fourier transform can be speeded up by a factor two. To prove this we assume u is an odd function and write (6.11) in the form

$$\begin{aligned} u(j_1, j_2) &= \sum_{n_2=0}^{N-1} \left[\sum_{n_1=0}^{N-1} \gamma(n_1, n_2)\, e^{2\pi i j_1 n_1/N} \right] e^{2\pi i j_2 n_2/N} \\ &= \sum_{n_2=0}^{N-1} \Gamma(j_1, n_2)\, e^{2\pi i j_2 n_2/N}. \end{aligned} \tag{6.14}$$

Because u is odd, γ is also odd and since γ can be continued periodically with period N we conclude that $\Gamma(j_1, n_2) = -\Gamma(N - j_1, N - n_2)$ for all j_1 and n_2. It is therefore enough to compute $\Gamma(j_1, n_2)$ for $j_1 = 0, \ldots, N-1$ and $n_2 = 0, 1, \ldots, (N/2) - 1$. This can be done by $N/2$ fast Fourier transforms and requires roughly $(N/2) \cdot (N/2) \log_2 N$ complex multiplications. For each j_1 we can consider (6.14) as a discrete Fourier transform with respect to j_2, and if we compute $u(j_1, j_2)$ for $j_1 = 0, 1, \ldots, (N/2) - 1$ and $j_2 = 0, 1, \ldots, N-1$ we can find the remaining coefficients by symmetry, i.e. $u(j_1, j_2) = -u(N - j_1, N - j_2)$. Thus the total cost is $\frac{1}{4} N^2 \log_2 N^2$ complex multiplications, which is only half of the number of operations needed for the ordinary fast Fourier transform. We can therefore solve a given problem twice as fast, or alternatively, take one further step of Moser's method in the same amount of time. Hence the comparison between Newton's and Moser's methods becomes more favorable for the latter method. Additional gain in speed can be obtained by using fast Fourier transforms written specially for the number of points we are interested in, for $N = 8$ see e.g. [8].

The purpose of this example has been to illustrate the application of Moser's method on a problem which is difficult to solve by other methods. At present there is no proof for the convergence of the discrete solution toward the solution of the continuous problem, though the stability of our numerical results strongly indicate such a result.

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