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COMPUTATION OF PERIODIC SOLUTIONS OF NONLINEAR ODEs

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Dedicated to Germund Dahlquist, on the occasion of his 60th birthday.

Abstract.

The paper proposes a new Gauss-Newton algorithm for the computation of periodic orbits in autonomous nonlinear ODEs. On the basis of Floquet theory, the new algorithm is shown to converge quadratically in a neighbourhood of the solution. Nontrivial examples are included.

0. Introduction.

Periodic solutions of nonlinear ODEs play an important role in several fields of application such as chemistry, epidemiology, or electronics. Mathematical problems in this context are existence, uniqueness, parameter dependence, and stability of periodic orbits of given dynamical systems. The present paper deals with a new Gauss-Newton algorithm for the actual computation of such solutions. In section 1, the key idea of the method to be proposed is derived on the basis of Floquet theory. In section 2, the basic algorithm and its multiple shooting implementation are worked out. The suggested Gauss-Newton technique for autonomous problems is shown to converge *locally* and *quadratically*. Non-trivial numerical examples are documented in section 3.

1. Preliminary considerations.

Consider the system of n, in general nonlinear, ordinary differential equations (ODEs):

$$y' = f(t, y). \tag{1.1}$$

The problem is to compute possible *periodic* solutions, with some period $T > 0$.

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The periodicity is reflected in the boundary conditions

$$y(T) = y(0). \tag{1.2}$$

Throughout the paper, critical points with $f(t, y) = 0$ will be excluded. In a first-order perturbation analysis any perturbations $\delta y(t)$ of the solution will satisfy the *variational equation*

$$\delta y' = f_y(y(t))\delta y. \tag{1.3}$$

This linear ODE system can be formally solved in terms of the Wronskian matrix $W(t, 0)$ with $W(0, 0) = I$. Hence

$$\delta y(T) = W(T, 0)\delta y(0). \tag{1.3'}$$

A rather general analytic discussion of periodic solutions can be found in the textbook of Coddington-Levinson [2].

Non-autonomous systems. If $f_t \not\equiv 0$, then the right-hand side f is periodic

$$f(t+T) = f(t)$$

with *given* T. Thus any periodic solutions y will have periods, which are just integer multiples of T. The conditions (1.1) and (1.2) define a periodic boundary value problem (BVP) with an associated *sensitivity matrix* (at $t = 0$, say):

$$E(0) := W(T, 0) - I. \tag{1.4}$$

If E is nonsingular, then the periodic solution y will be locally unique – compare e.g. Lemma 1 in [6]. Usually, the periodic solutions are characterized in terms of the (in general complex) eigenvalues of $W(T, 0)$, say $\mu_1, \ldots, \mu_n$, also called *Floquet multiplies*. Note that $E(0)$ just has eigenvalues $\mu_i - 1$. Then, under the assumption

$$|\mu_i| < 1, \qquad i = 1, \ldots, n \tag{1.5}$$

the periodic solution y is *stable*, i.e. any perturbation $\delta y(0)$ eventually dies out by virtue of (1.3').

Generally speaking, $E(0)$ is nonsingular as long as none of the μ_i equals 1. Under this assumption, the periodic BVP (1.1)–(1.2) can be treated by any standard BVP code. Therefore the rest of the paper will concentrate on autonomous systems, which are known to violate this assumption.

Autonomous systems. If $f_t \equiv 0$, then the period T is unknown. Moreover, f is now a solution of the variational equation (1.3) so that

$$f(y(t)) = W(t,0)f(y(0)). \tag{1.6}$$

Upon inserting (1.2) into (1.6) for $t = T$ one obtains

$$f(y(0)) = W(T,0)f(y(0)), \tag{1.7}$$

or, equivalently

$$E(0)f(y(0)) = 0 \quad \text{for} \quad f(y(0)) \neq 0. \tag{1.7'}$$

This means the Wronskian has an eigenvalue 1 (say μ_1) and E is singular. As a consequence, this type of problem cannot be solved by just applying any BVP code to (1.1)–(1.2) directly. In fact, additional consideration is needed.

The condition (1.7) reflects the fact that in an autonomous system the phase of the solution is undetermined, i.e. with $y(t)$ a T-periodic solution $y(t+t_0)$ with $t_0 \neq 0$ is also a T-periodic solution. For this reason, most authors (see [17], [10] or [16]) suggest to fix the phase by fixing a selected component of the initial values [10, 17], say

$$y_j(0) := \alpha,$$

or by setting a component f_j of the right-hand side to zero [16]. Such approaches, however, require a careful choice of the index j (and the parameter α).

It is the purpose of the present paper to show that such ad-hoc devices and analytic preparations are unnecessary. The method proposed herein is based on the fact that $\mu_1 = 1$ is a *simple* eigenvalue of the Wronskian $W(T,0)$ – compare [2]. Thus $E(0)$ has rank-deficiency 1. Hence, as a consequence of (1.7'), the extended $(n, n+1)$-matrix $[E, f]$ has full rank, i.e.

$$\operatorname{rank}[E(0), f(y(0))] = n. \tag{1.8}$$

This latter property inspires a special Gauss-Newton technique to be presented in section 2 below.

Homoclinic orbits. A limiting case of periodic orbits are closed orbits with formally *infinite* period T. The method of section 2 will not be able to treat these problems. Instead a time transformation to finite interval will be necessary, which then leads to non-autonomous *singular* BVPs. This case is omitted here.

2. A Gauss-Newton technique for the autonomous case.

In most applications, t is actually the *time* variable so that initial value problem (IVP) approaches to solve the BVP seem to be natural. For stable periodic orbits, and mildly nonlinear ODEs, even *single* shooting might work. For unstable periodic orbits or for highly nonlinear ODEs, a *multiple* shooting technique will be preferable.

2.1. *Basic algorithm.*

This section presents the basic idea in the single shooting context. Let $y(t|x, T)$ denote the T-periodic solution of the IVP

$$y' = f(y), \qquad y(0) := x. \tag{2.1}$$

Then $(n+1)$ unknowns $z := (x, T)$ must be determined from the n equations:

$$F(z) := y(T|x, T) - x = 0. \tag{2.2}$$

To solve these n nonlinear equations, consider the following Gauss-Newton (GN) method: for $z^0 := (x^0, T^0)$ given, let

$$\text{a)} \quad \Delta z^k := -F'(z^k)^+ F(z^k) \tag{2.3}$$

$$\text{b)} \quad z^{k+1} := z^k + \Delta z^k.$$

The superscript $+$ indicates the Moore-Penrose pseudo-inverse. The Jacobian $(n, n+1)$-matrix $F'(z)$ has the following structure:

$$F'(z) = [F_x, F_T] = [E(0), f(y(T))]. \tag{2.4}$$

At a solution point, z^* say, one has

$$F'(z^*) = [E(0), f(y(0))]. \tag{2.4'}$$

The comparison with (1.8) shows that $F'(z^*)$ has full rank n.

THEOREM 1. *Let $F : D \to \mathbb{R}^n$, $F \in C^1(D_0)$ for some convex set $D_0 \subset\subset D \subseteq \mathbb{R}^{n+1}$. Let the Jacobian $F'(z)$ have full rank n for all $z \in D_0$. Then, under the assumptions*

$$\text{a)} \quad \|\Delta z^0\| \leqq \alpha_0, z^0 \in D_0 \tag{2.5}$$

$$\text{b)} \quad \|F'(z_1)^+ (F'(z_2) - F'(z_3))\| \leqq \gamma \|z_2 - z_3\|, \quad \textit{for } z_1, z_2, z_3 \in D_0$$

c) $h_0 := \frac{1}{2}\alpha_0\gamma < 1$,

d) $\bar{S}(z^0, r) := \{z \in \mathbb{R}^{n+1} \mid \|z - z^0\| \leqq r\} \subset D_0$ *for* $r := \alpha_0/(1-h_0)$,

the GN iterates $\{z^k\}$ *defined in* (2.3) *remain in* $\bar{S}(z^0, r)$ *and converge to a point* $z^* = \lim_{k\to\infty} z^k$ *with* $F(z^*) = 0$.

The convergence rate can be estimated by

$$\|z^{k+2} - z^{k+1}\| \leqq (\gamma/2)\|z^{k+1} - z^k\|^2. \tag{2.6}$$

PROOF. Apply Theorem 4 of [8] with $\Gamma_F \equiv F'(z)^+$. The essential part is to verify assumption (3.3.c,d) from [8], which in the special case reads:

$$\|F'(z_1)^+(I_n - F'(z_2))F'(z_2)^+)F(z_2)\| \leqq \kappa(z_2)\|z_1 - z_2\|$$

for some $\kappa(z) \leqq \bar{\kappa} < 1$.

The $(n, n+1)$-matrix F' has a singular value decomposition

$$F'(z) = U\,\Sigma\,V^T,$$

where U is an orthogonal (n, n)-matrix, V an orthogonal $(n+1, n+1)$-matrix and Σ an $(n, n+1)$-matrix of the form

$$\Sigma = [D, 0], \qquad D = \operatorname{diag}(d_1, \ldots, d_n)$$

with $d_i \neq 0$, since $\operatorname{rank}(F'(z)) = \operatorname{rank}(\Sigma) = n$. As a consequence, one obtains

$$F'(z)^+ = V\,\Sigma^+\,U^T, \quad \Sigma^+ = \begin{bmatrix} D^{-1} \\ 0 \end{bmatrix},$$

which implies $F'(z)F'(z)^+ = U\,\Sigma\,V^T V\,\Sigma^+\,U^T = U\,\Sigma\,\Sigma^+\,U^T = UI_nU^T = I_n$.

Hence $\kappa(z) \equiv 0$ for all $z \in D_0$. This proves *local quadratic convergence* to some z^* with $F'(z^*)^+ F(z^*) = 0$.

With (2.4′) and (1.8) one infers that $F(z^*) = 0$. ∎

In order to expand the convergence domain of this ordinary GN method, one may reduce the GN steplength $\|\Delta z^k\|$ by some factor $\lambda_k < 1$. The *damping strategy* as described in [5] applies directly: one must observe, however, that now the operator $F'(z)^+F'(z)$ is a projector in $\mathbb{R}^{n+1}$ of just rank n, which induces a clear modification of the steplength estimates. For details see (2.16.b) in [5].

REMARK. The algorithm above has some connection with a suggestion of Nakhla-Branin [14], who propose a gradient method including the treatment of the autonomous case. In the present notation, their method requires the

computation of

$$\text{grad}\,\varphi = [E(0), f(y(T))]^T r \text{ to minimize } \varphi := \tfrac{1}{2}\|r\|_2^2.$$

This algorithmic approach reduces the computing time per Jacobian evaluation considerably by exploiting

$$E^T r =: u(0) - u(T)$$

where u is the solution of the adjoint variational equation

$$u' = -f_y(y)^T u, \qquad u(T) = r.$$

Hence $u(t) = W^T(T, t)r$.

As in the present paper, these authors also ignore the multiplicity of the periodic solution coming from translation invariance. Numerical comparisons with this algorithm are in preparation.

2.2. *Multiple shooting realization.*

In what follows, certain details of realization are worked out, which have been implemented in a special code called PERIOD. This code is a specification of the general purpose multiple shooting code BVPSOL of Deuflhard-Bader [6]. The notation to be used also follows [6]. This notation naturally includes the single shooting case as well.

Generalized Gauss-Newton method. In order to have fixed shooting nodes, a dimensionless variable

$$\tau := t/T \in [0, 1]$$

is introduced. Let $0 = \tau_1 < \tau_2 < \ldots < \tau_m = 1$ denote the coarse grid and $\Delta\tau_j := \tau_{j+1} - \tau_j$. Then the following conditions must hold:

(2.7) a) $F_j(x_j, x_{j+1}; T) := y(\tau_{j+1}|x_j, T) - x_{j+1} = 0, \quad j = 1(1)m-1$

where $$y(\tau_{j+1}|x_j, T) = x_j + \int_{t=0}^{T\Delta\tau_j} f(y(t))dt$$

b) $r(x_1, x_m) := x_m - x_1 = 0.$

By fixing $x_m := x_1$, the boundary conditions (2.7b) can be formally dropped. In addition to the Wronskian matrices on $[\tau_j, \tau_{j+1}]$

$$G_j := \partial y(\tau_{j+1}|x_j, T)/\partial x_j = W(\tau_{j+1}, \tau_j)|_{y(\tau|x_j, T)}$$

the Jacobian contains the n-vectors

$$\partial F_j/\partial T = \partial y(\tau_{j+1}|x_j, T)/\partial T = \Delta\tau_j \cdot f(y(\tau_{j+1}|x_j, T)) =: g_j. \tag{2.8}$$

The linear system to be solved per GN iteration has the form

$$\begin{cases} \text{a)} & \begin{cases} G_1\Delta x_1 - \Delta x_2 & & + g_1\Delta T & = -F_1 \\ \ddots & & & \vdots \\ & G_{m-1}\Delta x_{m-1} - \Delta x_m + g_{m-1}\Delta T & & = -F_{m-1} \end{cases} \\ \text{b)} & -\Delta x_1 \qquad\qquad + \Delta x_m \qquad\qquad = 0. \end{cases} \tag{2.9}$$

If the associated IVP is not ill-posed, then the so-called *condensing algorithm* may be applied yielding the linear $(n, n+1)$-system

$$E\Delta x_1 + g\Delta T + u = 0 \tag{2.10}$$

with

$$\begin{aligned} E &:= G_{m-1} \dots G_1 - I \\ g &:= g_{m-1} + G_{m-1}g_{m-2} + \dots + G_{m-1} \dots G_2 g_1 \\ u &:= F_{m-1} + G_{m-1}F_{m-2} + \dots + G_{m-1} \dots G_2 F_1. \end{aligned}$$

This system is underdetermined. At a solution point $z^* := (x_1^*, \dots, x_m^*, T^*)$ one obtains

$$E^* = W(\tau_m, \tau_1) - I$$

$$g^* = \Delta\tau_{m-1} f(x_m^*) + \Delta\tau_{m-2} W(\tau_m, \tau_{m-1}) f(x_{m-1}^*) + \dots + \Delta\tau_1 W(\tau_m, \tau_2) f(x_2^*).$$

Upon recalling from (1.6) that $f(x_m^*) = W(\tau_m, \tau_j) f(x_j^*)$ and observing that, by definition, $\Delta\tau_1 + \dots + \Delta\tau_{m-1} = 1$, one ends up with $g^* = f(x_1^*)$.

Thus, in comparison with section 1, one has $[E^*, g^*] \equiv [E(0), f(y(0))]$.

Consequently, in view of (1.8) and (2.3), the following generalized GN method is inspired (dropping the iteration index k):

$$\begin{aligned} &\text{a)} \quad \begin{pmatrix} \Delta x_1 \\ \Delta T \end{pmatrix} = -[E, g]^+ u \\ &\text{b)} \quad \Delta x_{j+1} = G_j \Delta x_j + g_j \Delta T + F_j, \qquad j = 1, \dots, m-2. \end{aligned} \tag{2.11}$$

Using standard techniques for a generalized Jacobian inverse J^- as essentially defined in [3], the iterative method above can also be shown to converge *locally* and *quadratically*.

REMARK. Apart from the rank-deficiency in (2.11.a), there are, of course, similarities with the parameter identification technique as suggested by Bock [1].

Note, however, that the period T is a rather special parameter – a fact, which is reflected in the key property (1.8).

Jacobian rank-1 updates. The construction of such updates requires some special attention. Let $\hat{G}_j^{k+1}$ denote the updated Wronskian at the iterate $(k+1)$. Then the Davidon-Fletcher-Powell condition in block row j reads (with damping factor λ_k):

$$(\hat{G}_j^{k+1} - G_j^k)\lambda_k \Delta x_j^k + (g_j^{k+1} - g_j^k)\lambda_k \Delta T^k = F_j^{k+1} - (1-\lambda_k)F_j^k. \tag{2.12}$$

As the g_j can be computed cheaply, only the G_j will be approximated. This leads to

$$\begin{aligned} \hat{G}_j^{k+1} &:= G_j^k + W_j V_j^T \\ W_j &:= F_j^{k+1} - (1-\lambda_k)F_j^k - \lambda_k(g_j^{k+1} - g_j^k)\Delta T^k \\ V_j &:= (\Delta x_j^k)/(\lambda_k \|\Delta x_j^k\|_2^2). \end{aligned} \tag{2.12'}$$

Iterative refinement sweeps (IRS). For *unstable* periodic orbits, the IRS technique as suggested in [6] may be worth performing. As the linear least squares system (2.11a) leads to a zero residual, the technique in [6], Section 2.2., can be directly applied. In order to start the IRS, one merely continues the recursion (2.11.b) up to $j = m-1$ and computes the residual $dr^0 := \Delta\tilde{x}_m - \Delta\tilde{x}_1$.

Floquet multipliers. At the solution point, the computed Wronskian

$$W(T,0) \doteq G_{m-1} \cdots G_1$$

is available. PERIOD calls standard linear algebra software ([12, 13, 14]) to compute the associated eigenvalues μ_i. The standard value $\mu_1 = 1$ is also computed to check for the accuracy of the Jacobian approximations.

3. Numerical experiments.

All subsequent numerical problems have been solved by means of the special multiple shooting code PERIOD using the non-stiff extrapolation integrator DIFEX1 (see e.g. [4]). The common required relative error tolerance was 1.D–6. Throughout the examples $m = 11$ equidistant shooting nodes were chosen. The numerical experiments were run in FORTRAN double precision on the IBM 3081 of the Computing Center of the University of Heidelberg.

3.1. *Nerve membrane model* ([9], [16]).

The model is represented by the ODEs:

$$y_1' = 3(y_2 + y_1 - y_1^3/3 + \lambda); \qquad y_2' = -(y_1 - 0.7 + 0.8y_2)/3. \tag{3.1}$$

Rough initial guesses obtained from Fig. 1 of [16] for $\lambda = -1$ were $(x_1^0, T^0) = (3, 1.5, 12)$. The remaining initial guesses $x_2^0, \ldots, x_{10}^0$ were constructed from the associated IVP solution $y(t|x_1^0)$. The code PERIOD required 12 GN iterations (among which 5 iterations were *damped* GN steps) with 27 trajectory evaluations. The computing time was about 1.2 sec. The solution obtained was

$$y_1(0) = 1.8521 \qquad T = 9.6133 \qquad \mu_1 = 0.99$$
$$y_2(0) = 1.2053 \qquad\qquad\quad \mu_2 = 2 \cdot 10^{-12}.$$

The graph of the solution trajectory is presented in Fig. 1. As can be seen from the Floquet multipliers, the periodic orbit is stable. The essential difficulty in this example is the determination of T. It may be worth mentioning that, due to the stability of the orbit, a few revolutions in the (y_1, y_2)-plane already lead to the stable orbit. So methods especially designed for *stable* orbits (such as [11] might be preferable. These methods, however, require one to know the stability in advance!

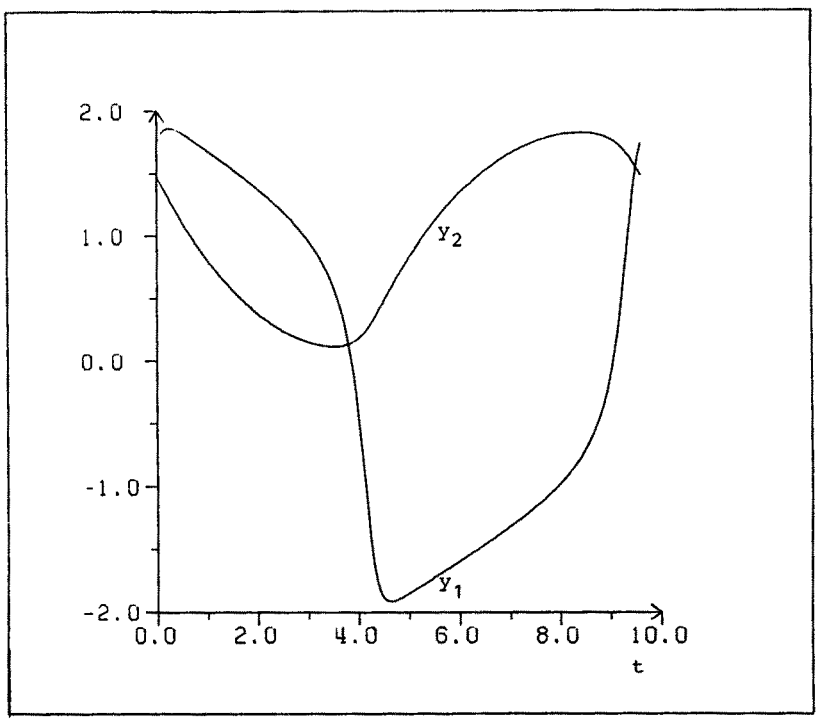

Fig. 1. Solution trajectories for example 3.1.

3.2. *Heated flow problem* ([11], [10]).

This model is obtained by a reduction of a system of Navier-Stokes and heat transfer equations describing the flow in a layer of liquid heated from below. The ODEs are (in terms of Cartesian coordinates)

$$\begin{aligned} x' &= -\sigma(x-y) \\ y' &= x(r-z)-y \\ z' &= xy-bz \end{aligned} \tag{3.2}$$

As in [10], the parameter set $\sigma = 1.6$, $b = 4$ was chosen. In order to test the code for an unstable orbit, the value $r = 153.083$ was taken from [10], Table II. Initial guesses were $(x_1^0, T^0) = (0, -28, 140, 0.95)$. The remaining guesses were once more obtained from the associated IVP solution.

The code PERIOD required 12 GN iterations (including 7 damped GN iterations) and 35 trajectory evaluations. The computing time was about 1.5 sec. The solution obtained was

$$\begin{aligned} x(0) &= -0.87890\,D-3 & \mu_1 &= 1.00 \\ y(0) &= -0.27732\,D+2 & \mu_2 &= 11.6 \\ z(0) &= 0.14188\,D+3 & \mu_3 &= 2D-10. \\ T &= 0.94664 \end{aligned}$$

A plot of the solution orbit in space is given in Fig. 2.

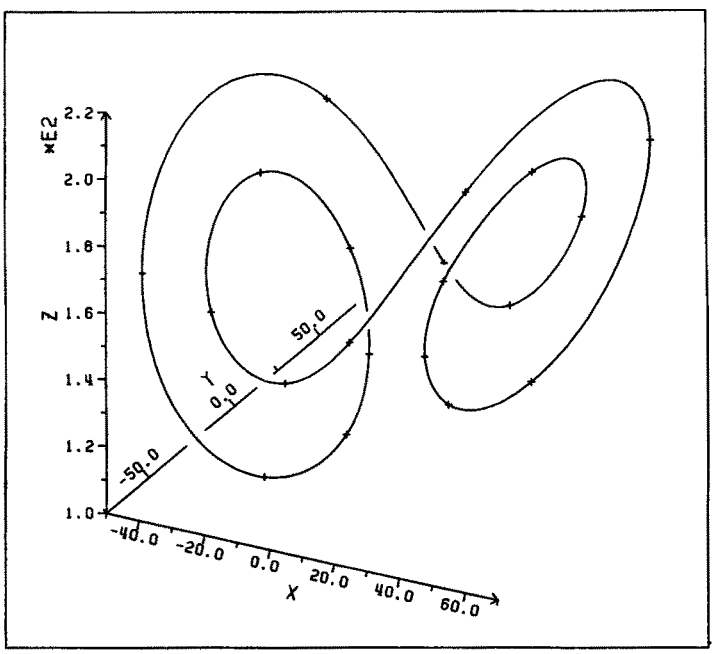

Fig. 2. Solution orbit of example 3.2 in 3 space dimensions.

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