Continuation and Gauss-Newton techniques

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Abstract

This paper reviews various Gauss-Newton-type iteration schemes for application on continuation problems. The successful implementation of one of these schemes is demonstrated within the continuation code COLCON.

1 Introduction

The modelling of most physical systems leads to nonlinear computational problems that include a number of physical parameters. Then, very often one is interested in the behaviour of the solution under variation of selected parameters. The standard way to attack such problems numerically is by means of so-called continuation methods.

Treating real life applications in this context, not only highly nonlinear problems must be solved but also very complex algorithmic structures and a huge amount of data output must be handled. Therefore, an important task of numerical analysis is to select robust and reliable numerical procedures and of scientific computing to design and implement procedures which treat the given problem as far as possible automatically and give an instrument for managing the generated data.

A common method for solving continuation problems depending on a single parameter is, starting with a given solution, to compute an approximate solution by going along the tangent with a certain stepsize (predictor) and then to iterate back to the solution branch by some method for solving

nonlinear equations (corrector).

The purpose of the present paper is to show in a general setting that the Gauss-Newton method as corrector has some advantages compared with other methods in the sense that it does not introduce any additional nonlinearity, see section 2. In section 3, we discuss some aspects when specializing these methods in the context of boundary value problems for ordinary differential equations. We then give some details on a corresponding implementation of a general purpose code reflecting the requirements of scientific computing, compare section 4. Finally, we report on some numerical examples and discuss applicablility and limitations of the implemented code in section 5.

2 Tangent continuation and Gauss-Newton method

Let a nonlinear problem of the form

$$F(z) = 0 \tag{1}$$

be given with

$$F{:}\,\Omega \subseteq Z \to Y \tag{2}$$

where Z and Y are Hilbert spaces. Further, we assume that in a neighborhood U of a solution z^* of (1) the function F is Fréchet differentiable and its Fréchet derivative $DF(z) \in L(Z,Y)$, $z \in U$ is a bounded linear Fredholm operator with

$$\dim\ker DF(z) = 1\,, \qquad DF(z)Z = Y\,. \tag{3}$$

In particular, this means that $DF(z)$ is a Fredholm operator of index 1. Then, the solution z^* locally extends to a smooth one-dimensional manifold of solutions of (1). This would be true if Z and Y were only Banach spaces, cp. Fink and Rheinboldt (1983), but in Hilbert spaces we can now define, at least in U, the Moore-Penrose pseudoinverse and the Gauss-Newton method.

In the special case of (3), we define the Moore-Penrose pseudoinverse $DF(z)^+$ of $DF(z)$ to be the unique linear operator in $L(Y,Z)$ with

$$DF(z)\,DF(z)^+ = id_Y \tag{4}$$

and, if $t(z)$ spans $\ker DF(z)$ with $\|t(z)\|_Z = 1$,

$$\langle DF(z)^+ y, t(z)\rangle_Z = 0 \quad \forall\, y \in Y\,. \tag{5}$$

See e.g. Ben-Israel and Greville (1974) for details and the general case.

With this, we can now locally define the Gauss-Newton method by

$$\begin{aligned} \Delta z^k &= -DF(z^k)^+ F(z^k)\,, \\ z^{k+1} &= z^k + \Delta z^k\,, \end{aligned} \qquad k = 0,1,\ldots, \quad z^0 \text{ given.} \tag{6}$$

Its convergence properties are described by the following theorem.

Theorem 1

Let $F:\Omega \to Y$, $F \in C^1(\Omega)$ for some convex subset $\Omega \subseteq Z$ such that the Fréchet derivative DF of F satisfies (3) for all $z \in \Omega$. Then, under the assumptions

$$\|\Delta z^0\|_Z \leq \alpha_o, \qquad z^0 \in \Omega \tag{7a}$$

$$\|DF(z_1)^+[DF(z_2) - DF(z_3)]\|_Z \leq \omega_o \|z_2 - z_3\|_Z \tag{7b}$$

$$\text{for any } z_1, z_2, z_3 \in \Omega,\ z_2 - z_3 \in \text{range}\, DF(z_1)^+$$

$$h_o = \frac{1}{2}\alpha_o\omega_o < 1 \tag{7c}$$

$$S(z^0, r) = \left\{ z \in Z \;\middle|\; \|z - z^0\|_Z \leq r \right\} \subset \Omega \tag{7d}$$

$$\text{for } r = \frac{\alpha_o}{1 - h_o}\,,$$

iteration (6) remains in $S(z^0, r)$ and converges to some z^* with

$$F(z^*) = 0$$

on the solution manifold. The rate of convergence is quadratic, i.e.

$$\|z^{k+2} - z^{k+1}\|_Z \leq \frac{\omega_o}{2}\|z^{k+1} - z^k\|_Z^2\,.$$

The proof is a straightforward consequence of theorem 4 in Deuflhard and Heindl (1979).

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Note that the same result holds if we consider multiparameter problems, i.e. where $\dim \ker DF(z) = p \geq 1$. But the investigation and implementation of continuation methods for the case $p > 1$ are just beginning. See Allgower and Schmidt (1985) and Rheinboldt (1988) for first results.

Further, we want to stress that quadratic convergence can be obtained by replacing $DF(z)^+$ by any generalized pseudoinverse $DF(z)^-$ satisfying

$$DF(z)^-\, DF(z)\, DF(z)^- = DF(z)^-\,, \tag{8}$$

see e.g. Ortega and Rheinboldt (1970). But in general, we only need some iterative method as corrector in a continuation process which converges to a nearby solution z^* in the manifold given by (1). Often, this is done by extending (1) by a single appropriately chosen equation

$$N(z) = 0\,, \qquad N:\Omega \subseteq Z \to I\!R \tag{9}$$

such that (1) together with (9) forms a nonlinear problem whose overall Fréchet derivative now shall be invertible thus allowing us to replace the Gauss-Newton method for (1) by Newton's method for (1) together with (9).

We now discuss briefly how we can get a theoretically backed stepsize control on the basis of tangent continuation as predictor and Gauss-Newton method as corrector. The main idea is taken from Deuflhard, Fiedler and Kunkel (1987a).

Let z_0 be a given solution of (1). To advance along the one-dimensional solution branch, we linearize the problem thus proceeding along the tangent $t(z_0)$ with a stepsize s which gives the predictor value

$$z^0 = z_0 + st(z_0)\,. \tag{10}$$

With this value, we can start iteration (6). Note that in our notation a possible function $N(z)$ would be

$$\|z - z_0\|_Z^2 - s^2 = 0. \tag{11}$$

This extension is suggested by Keller (1977) as $N_2(z,s)$ and known as pseudoarclength normalization.

Clearly, we want to choose s as large as possible. But on the other hand, we also want the Gauss-Newton method to converge. This leads to

Theorem 2

Consider the continuation process (10) with the iteration scheme (6). In addition to the assumptions of theorem 1, let

$$\|DF(z_5)^+[DF(z_4) - DF(z_0)]t(z_0)\|_Z \le \omega_t s_1 \|t(z_0)\|_Z^2 \tag{12}$$

for any

$$z_4 = z_0 + s_1 t(z_0)\,, \quad z_5 = z_0 + s_2 t(z_0)\,, \quad 0 \le s_1, s_2 \le s$$

such that $z_4, z_5 \in \Omega$ and z_0 is a solution of (1). Then the iteration (6) converges to a solution z^* of (1) for any starting point z^0 from (10) with

$$s < s_{\max} = 2\left(\frac{1}{\omega_o \omega_t}\right)^{1/2}. \tag{13}$$

For a proof, see Deuflhard, Fiedler and Kunkel (1987a).

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On the basis of this upper bound for the possible continuation stepsizes, one can obtain a steplength control by replacing the unknown global quantities ω_o and ω_t by accessible local estimates. For nonlinear problems, this must be done in a predictor-corrector manner. Following Deuflhard, Fiedler and Kunkel (1987a), a possible predictor stepsize after a successful continuation step with stepsize s_{old} is given by

$$s_{\text{pred}} = \sqrt{\frac{\theta_{\max}}{\theta_0} \frac{\|\Delta z^0\|_Z}{\|z^0 - z^*\|_Z} \frac{|c_*|^2}{|c_0|^3}}\; s_{\text{old}} \tag{14}$$

where

$$c_* = \langle t(z^*), t(z^0)\rangle_Z \,, \quad c_0 := \langle t(z_0), t(z^0)\rangle_Z \tag{15}$$

describe the curvature of the solution manifold and

$$\theta_k = \frac{\|\overline{\Delta z}^{k+1}\|_Z}{\|\Delta z^k\|_Z} \,, \quad \overline{\Delta z}^{k+1} = -DF(z^k)^+ F(z^{k+1}) \tag{16}$$

measures the speed of convergence of the Gauss-Newton method. Furthermore, $\theta_{\max} \leq 1$ is a fixed chosen safety factor.

If the convergence behaviour of the Gauss-Newton method turns out to be too poor, i.e. $\theta_k > \theta_{\max}$, the continuation stepsize is reduced by

$$s_{\text{corr}} = \sqrt{\frac{\theta_{\max}}{\theta_k}}\, s_{\text{pred}} \tag{17}$$

also obtained from (13) but with updated estimates for ω_o and ω_t.

Consider now the application of Newton's method on the inflated system (1) and (9). As it will turn out, this approach will in general increase the nonlinearity of the original problem. First, recall that a class of generalized inverses satisfying (8) is generated by inflating the Fréchet derivative DF by any linear functional $l\colon Z \to I\!R$ with $l(t(z)) = \alpha(z) \neq 0$. Under this assumption, the resulting system is invertible and we find

$$\begin{pmatrix} DF(z) \\ l \end{pmatrix}^{-1} = \left(DF(z)^- \,,\, v(z) \right) \tag{18}$$

where $v(z) = \alpha(z)^{-1} t(z)$. Note that for the special choice of the functional $l(\,\cdot\,) = \langle t(z),\, \cdot\,\rangle_Z$ this construction reduces to the definition of the Moore-Penrose pseudoinverse, cf. (4), (5).

For the application of Newton's method to the inflated system (1) and (9), the linear functional l from (18) has to be identified with the Fréchet derivative $DN(z)$ of $N(z)$. This implies that the Newton correction is of the form

$$\Delta z = -DF(z)^- F(z) - v(z) N(z) \,. \tag{19}$$

From the above condition (3) it follows that this correction can also be represented in the alternative form

$$\Delta z = \Delta z^+ + \beta t(z) \tag{20}$$

where $\Delta z^+ = -DF(z)^+ F(z)$, and the scalar unknown β is determined by

$$l(\Delta z) = l(\Delta z^+) + \beta l(t(z)) = -N(z) \,. \tag{21}$$

This relation together with a standard estimation similar to Winkler (1988) yields the bounds

$$\|\Delta z^+\|_Z \leq \|\Delta z\|_Z \leq \left(1 + \frac{\|l\|_{I\!R \leftarrow Z}}{|\alpha(z)|}\right) \|\Delta z^+\|_Z + \frac{|N(z)|}{|\alpha(z)|} \,. \tag{22}$$

Note that this type of estimate can be used to compare the behaviour of a large class of corrector methods with the Gauss-Newton method. In particular, this applies for methods which keep a selected solution component fixed during the corrector iteration.

Of special interest are functionals l of the form

$$l(\,\cdot\,) = \langle \hat{t},\, \cdot\, \rangle_Z \tag{23}$$

where $\hat{t}$ is some approximate tangent direction. Compare also with $N_3(z,s)$ in Keller (1977) where the special choice $\hat{t} = t(z_0)$ is suggested. Note that the functionals (23) include in particular inflation functions of the type (11) where

$$l(\,\cdot\,) = 2\langle z - z_0,\, \cdot\, \rangle_Z\,.$$

For simplicity in the following, we assume that $\hat{t}$ is in the plane spanned by Δz^+ and $t(z)$ and that $\hat{t}$ is of unit norm. If this is not the case a priori, we can without loss of generality project $\hat{t}$ into this plane and normalize $\|\hat{t}\|_Z = 1$ by a simple scaling of the inflation function $N(z)$. Finally, let $l(t(z)) = \alpha(z) = \cos\varphi > 0$ where $\varphi = \varphi(z)$ is the angle between $\hat{t}$ and $t(z)$.

Exploiting now the orthogonality of Δz^+ and $t(z)$ in equation (21) yields

$$l(\Delta z) = \sin\varphi \|\Delta z^+\|_Z + \beta \cos\varphi = -N(z)$$

giving the estimate

$$\|\Delta z^+\|_Z \le \|\Delta z\|_Z \le \frac{\|\Delta z^+\|_Z + |N(z)|}{\cos\varphi}\,. \tag{24}$$

Note that this estimate can not be improved as in the special case $N(z) = 0$ the right hand estimate holds with equality, i.e.

$$\|\Delta z\|_Z = \frac{\|\Delta z^+\|_Z}{\cos\varphi}\,.$$

Now assume that the quantities $\alpha_o^+ = \alpha_o$, $\omega_o^+ = \omega_o$, and $\omega_t^+ = \omega_t$ which describe the nonlinearity in the above theorems are chosen to be optimal. If we now substitute the estimate (24) into corresponding theorems, we deduce that the optimal estimates must be replaced by larger values

$$\alpha_o \ge \frac{\alpha_o^+}{\cos\overline{\varphi}}\,, \quad \omega_o \ge \frac{\omega_o^+}{\cos\overline{\varphi}}\,, \quad \omega_t \ge \frac{\omega_t^+}{\cos\overline{\varphi}}\,, \quad \overline{\varphi} = \sup_{z\in\Omega} \varphi(z)\,.$$

This in turn leads to a reduction of the maximal possible continuation steplength $s_{\max}^+ = s_{\max}$ from (13) to

$$s_{\max} = s_{\max}^+ \cos\overline{\varphi}\,. \tag{25}$$

Comparing these considerations with the numerical comparison in Deuflhard, Fiedler and Kunkel (1987b) for the procedure of Deuflhard (1984) shows a better performance of the Gauss-Newton iteration when turning from a generalized inverse to the Moore-Penrose pseudoinverse.

Summarizing, we have shown that in the above sense the classical Gauss-Newton method with Moore-Penrose pseudoinverse is best suited for solving problem (1). In connection with a continuation method, one can now expect that it will allow larger stepsizes thus improving at least the efficiency of the continuation procedure.

3 Boundary value problems

The general continuation procedure of section 2 now can be used in principle for all problems of the form (1). This is clear if the Hilbert spaces are finite dimensional, that is (1) is a finite system of nonlinear equations. In the infinite dimensional case, however, we must discretize (1) to obtain a problem which is treatable on a computer. In this section, we want to concentrate on a scalar m-th order differential equation with a single parameter

$$\begin{aligned} \mathcal{L}(y,\tau) \equiv y^{(m)} - f(x, y, y', \ldots, y^{(m-1)}; \tau) = 0 \,, \\ a < x < b \,, \qquad \tau \in I\!R \end{aligned} \tag{26a}$$

together with m boundary conditions

$$\mathcal{B}_j(y,\tau) \equiv g_j(\boldsymbol{y}(\xi_j);\tau) = 0 \,, \qquad a \le \xi_j \le b \,, \quad 1 \le j \le m \tag{26b}$$

where

$$\boldsymbol{y}(x) = (y(x), y'(x), \ldots, y^{(m-1)}(x))^T$$

denotes the state vector of the corresponding first-order system. As appropriate Hilbert spaces, we choose

$$Z = W^m[a,b] \times I\!R \quad , \quad Y = W^0[a,b] \times I\!R^m \tag{27a}$$

with the scalar products

$$\begin{aligned} \langle (u_1,\tau_1),(u_2,\tau_2)\rangle_Z &= \langle u_1, u_2\rangle_m + \tau_1\tau_2 \,, \\ \langle (u_1,g_1),(u_2,g_2)\rangle_Y &= \langle u_1, u_2\rangle_0 + g_1^T g_2 \end{aligned} \tag{27b}$$

where $W^\nu[a,b]$, $0 \le \nu \le m$ denote the Sobolev spaces

$$W^\nu[a,b] = \{u \mid u^{(\nu)} \in L_2[a,b]\} \tag{28a}$$

equipped with the scalar products

$$\langle u, v\rangle_\nu = \sum_{l=0}^{\nu} \int_a^b u^{(l)}(s) v^{(l)}(s)\, ds \,. \tag{28b}$$

Note that the above problem can easily be generalized to mixed order systems depending on several parameters by just going over to appropriate product spaces.

Our next task is to discretize the given problem for its numerical treatment. This can be done in principle in various ways depending on the properties of the problem under consideration. In the context of a general purpose code for boundary value problems, a good choice seems to be k-stage collocation, $k \geq m$, with Gaussian points and representation of the discrete functions in the monomial Runge-Kutta basis. See Bader and Ascher (1987) and Bader and Kunkel (1989) for a more detailed description.

4 An implementation

Implementing a collocation code for the treatment of boundary value problems, one must select procedures and methods for the following parts
(1) discretization
(2) solution representation
(3) linear system solution
(4) error estimates and mesh selection
(5) nonlinear problem solution
with respect to the chosen problem class. For a general purpose continuation code, this was done in Bader and Kunkel (1989) and led to a code named COLCON.

Known alternative codes for the treatment of continuation and bifurcation problems for boundary value ordinary differential equations are for example AUTO of Doedel and Kernevez (1986) or BIFPACK of Seydel (1984). Compared with COLCON, these packages are intended to treat a wider class of problems. However, in the common range of applications, COLCON has proven to be more robust and reliable especially for highly nonlinear and stiff problems. This property is considered to be highly important in a scientific computing enviroment. See Bader and Kunkel (1989) for more details.

We now attach a brief description of the features of the code COLCON. The class of problems which can be treated by COLCON contains of systems of d nonlinear differential equations of orders m_ν, $1 \leq m_\nu \leq 4$, $1 \leq \nu \leq d$ of the form

$$y_\nu^{(m_\nu)} = f_\nu(x, \boldsymbol{y}; p)\,, \qquad a \leq x \leq b \tag{29}$$

where $\boldsymbol{y}$ is a vector

$$\boldsymbol{y} = (y_1, y_1', \ldots, y_1^{(m_1-1)}, y_2, \ldots, y_2^{(m_2-1)}, \ldots, y_d^{(m_d-1)})^T \tag{30}$$

of length $m^* = \sum_{\nu=1}^{d} m_\nu$ and p is a vector of parameters of length $npar$, subject to separated nonlinear side (or boundary) conditions

$$\begin{aligned} g_j(\boldsymbol{y}(\xi_j); p) = 0\,, \qquad & 1 \leq j \leq mside\,, \\ a \leq \xi_1 \leq \xi_2 \leq \cdots \leq \xi_{mside} \leq b\,. & \end{aligned} \tag{31}$$

The total number of unknowns is then $mstate = m^* + npar$. For the above equations to be a continuation problem in our sense, we must have $mstate = mside + 1$. In the case $mstate = mside$, COLCON contains a generalization of the code COLNEW (Bader and Ascher 1987) called COLPAR allowing a more efficient treatment of parameters. Note that dealing only with separated nonlinear boundary conditions is not really a restriction of the feasible problem class since general boundary conditions can easily be reformulated into the desired form by introducing additional parameters, see e.g. Ascher and Russell (1981).

5 Numerical examples

In this section, we want to report on the performance of code COLCON for two selected problems exhibiting quite different solution characteristics. Besides that, COLCON has been successfully applied to many more continuation problems.

The following computations were performed on an IBM3090/180 in Fortran double precision. The number of collocation points per interval was four. Required accuracy was five digits for the solution and two digits for its derivative.

Example 1

We consider a forced nonlinear oscillator modelled by the differential equation

$$(\frac{\tau}{2\pi})^2 u'' + \frac{1}{25}(\frac{\tau}{2\pi})u' - \frac{1}{5}u + \frac{8}{15}u^3 = \frac{2}{5}\cos 2\pi x$$

together with the periodic boundary conditions

$$u(0) = u(1)\,, \quad u'(0) = u'(1)\,,$$

see e.g. Seydel (1984). To obtain a problem with separated boundary conditions, we introduce artificial parameters p_1 and p_2 and replace the above boundary conditions by

$$\begin{aligned} u(0) &= p_1\,, & u'(0) &= p_2\,, \\ u(1) &= p_1\,, & u'(1) &= p_2\,. \end{aligned}$$

The range for continuation is $\tau \in [0.06, 3]$. For decreasing τ, the solution profile becomes more and more complicated by building loops such that the mass point oscillates more and more often and rather irregularly during one period of incitation. In addition, sixteen turning points and the same number of bifurcation points must be passed in the above specified interval. Starting the computations at $\tau = 3$, COLCON needs 212 steps in 93.7 sec CPU-time to compute the whole solution branch.

Example 2

The steady state concentration and temperature profiles in a tubular reactor are modelled by

$$\frac{1}{\mathrm{Pe}_1} u_1'' = u_1' - \mathrm{Da} f(u) \,,$$
$$\frac{1}{\mathrm{Pe}_2} u_2'' = u_2' + \beta(u_2 - u_{2w}) - \mathrm{Da} B f(u) \,,$$

with the nonlinearity

$$f(u) = (1 - u_1) \exp\Big(\frac{u_2}{1 + u_2/\gamma}\Big)$$

describing an irreversible first-order reaction where u_1 denotes the relative concentration of a chemical species while u_2 denotes the temperature in the reactor. The set-up of this problem is completed by the boundary conditions

$$u_i'(0) - \mathrm{Pe}_i u_i(0) = 0 \,, \quad u_i'(1) = 0 \,, \quad i = 1, 2 \,,$$

and the following set of parameter values

$$\begin{aligned} \mathrm{Pe}_1 &= 320 \,, & \mathrm{Pe}_2 &= 100 \,, \\ \beta &= 0.72 \,, & u_{2w} &= -9.6 \,, \\ B &= 16.8 \,, & \gamma &= 16.9 \,. \end{aligned}$$

See Jensen and Ray (1981) for a detailed outline of this problem.

Continuation is done with respect to the so-called Damköhler number $\mathrm{Da} \in [0, 1]$ starting with $\mathrm{Da} = 0$. Varying the Damköhler number Da, a steep layer representing the reaction front builds up at the right boundary, detaches and moves to the left boundary where it finally disappears. See Bader and Kunkel (1989) for a plot of typical solution profiles. For this example, COLCON takes 253 steps and 104.8 sec CPU-time to complete the computations for the described branch.

The moving front requires a flexible adaptive mesh selection procedure to guarantee a good approximation of the differential operator near the solutions. In the current version of COLCON, the mesh is adapted during the corrector phase. As a consequence, several redistribution steps are necessary to adapt the discretization mesh to the new location of the front. In this situation, one would rather prefer a continuation method which would advance the mesh to the new location of the front as part of the prediction procedure.

Concluding this example, we mention that the strong nonlinearity of the reaction term as well as the stiffness together with the moving reaction

front turn out to make it to a challenging test example for any continuation code.

6 References

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