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The Grand Four.

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Abstract

This paper gives a concise synopsis and some new insights concerning four affine invariant globalizations of the local Newton method. The invariance classes include: affine covariance, affine contravariance, affine conjugacy, and affine similarity. In view of algorithmic robustness, each of these classes of algorithms is particularly suitable for some corresponding problem class.

Contents

Introduction

In 1972, in his thesis, the author constructed a first algorithm of the kind later called *affine invariant* Newton methods (see [4]). Already with this first algorithm, hard problems (mostly from NASA) could be solved that could not be solved by the standard techniques in use then. Early on, Georg Bock joined this algorithmic line, see the series of papers [1, 2, 3] starting from 1981. Next, in 1979, the author [5] extended his approach to continuation methods and formalized it. On this basis, the author wrote a first research monograph on the topic and distributed it among colleagues who used it in their lectures. However, in 1993, his PhD student A. Hohmann [12] introduced so-called *affine contravariant* Newton methods, at the same time renaming *affine invariant* to *affine covariant* Newton methods. Once the door had been opened, two further invariance classes were introduced: *affine conjugacy* by the author and M. Weiser [11]) and *affine similarity* by the author himself. With these now *four* affine invariance classes at hand, the author again started to write a research monograph [6] that appeared in 2004. Today, this book contains most of the present state of the art about the topic.

The present article gives a concise survey on affine invariant Newton algorithms from the pure point of view of the ("grand") four invariance classes. For reasons of clarity, the presentation is mainly restricted to the simplest case of *exact* Newton methods. The aim is to deepen structural insight and, as will turn out, gain certain new algorithmic tools that are not included in the monograph [6]. In Section 1, affine covariance is treated, which involves iterative *natural monotonicity* and affine covariant computational estimates of *Kantorovich quantities* as a theoretical basis for some adaptive trust region strategy. In addition, continuation methods with local Newton methods as correctors are treated. In Section 2, affine contravariance is worked out. It merely requires iterative monotonicity of *nonlinear residual norms* and allows for computational estimates of the affine contravariant counterparts of the Kantorovich quantities, again as a theoretical basis for an adaptive trust region strategy. Here, an inexact Newton method with GMRES as inner iteration is inserted. Next, in Section 3, the case of nonlinear elliptic PDEs is treated in the framework of affine conjugate Newton methods, requiring functional monotonicity and corresponding Kantorovich quantities as well as their computational estimates. Finally, Section 4 deals with affine similar Newton methods, often called *pseudo-continuation methods*, which apply to steady state problems. Special attention is paid to those problems that originate from time dependent problems with implicit conservation properties: they cause singular Jacobians, so that standard Newton methods are bound to fail. In this class of algorithms, a rather recent update beyond [6] is presented.

1 Affine covariance: error oriented approach

Let $F(x) = 0$ with $F : D \subset \mathbb{R}^n \to \mathbb{R}^n$ denote a system of n nonlinear equations. For ease of presentation, we here focus on the finite-dimensional case. The extension to Banach spaces is for most cases straightforward. In the affine covariant approach, the underlying idea is that the problem at hand is equivalent to any problem out of the class

$$G(x) := AF(x) = 0 \quad \text{where} \quad A \in GL(n) \; . \tag{1}$$

Obviously, the choice of the nonsingular matrix A does not affect the *local* Newton iteration

$$x^{k+1} = x^k + \Delta x^k \; , \quad k = 0, 1, \dots \; , \tag{2}$$

defined by the *ordinary* Newton corrections Δx^k via

$$AF'(x^k)\Delta x^k = -AF(x^k) \; . \tag{3}$$

1.1 Global Newton method

Based on the principle of affine covariance, the so-called *Newton path* $\overline{x}(\lambda)$ may be obtained by intersection of all level sets

$$G(x|A) := \{z \in D | \; \|AF(z)\|_2 \leq \|AF(x)\|_2\} \; .$$

to yield

$$\overline{G}(x) := \bigcap_{A \in GL(n)} G(x|A) = \{\overline{x} | \; F(\overline{x}(\lambda)) = (1-\lambda)F(x^0) \; , \lambda \in [0,1]\} \; . \tag{4}$$

By construction, the Newton path is an affine covariant mathematical object, which starts at an initial guess $x^0 = \overline{x}(0)$ and ends at some solution point $x^* = \overline{x}(1)$. It may also end at a point where the Jacobian is singular, from where there is no possible continuation of the Newton path. An efficient algorithm should, of course, take this possible occurrence into account. In view of globalization, the property

$$\dot{\overline{x}}(0) = \Delta x^0 \; ,$$

i.e. the Newton direction is just the tangent direction at the Newton path. Hence, the direction of the Newton correction is right, but the iterative step may be "too large". This geometrical insight directly leads to the construction of the *global* Newton method

$$x^{k+1} = x^k + \lambda_k \Delta x^k \; , \quad 0 < \lambda_k \leq 1, \quad k = 0, 1, \dots \; . \tag{5}$$

The values of the selected damping factors λ_k will depend on the choice of the matrix A in the general monotonicity test

$$\|AF(x^{k+1})\| \leq \|AF(x^k)\| \; . \tag{6}$$

Note that this class of tests includes the standard test in terms of the nonlinear residual

$$\|F(x^{k+1})\| \leq \|F(x^k)\| \tag{7}$$

which is typically found in classical textbooks. A comparative analysis of the class (6) of tests (as given in [4]) reveals that the worst case damping factors look like

$$\lambda_k \sim 1/\mathrm{cond}(AF'(x^k)) \; . \tag{8}$$

This means that the above monotonicity test (7) may be of little help in global Newton methods for problems with ill-conditioned Jacobian.

Natural monotonicity test. The above undesirable occurrence (8) motivates the choice $A = F'(x^k)^{-1}$, which leads to the so-called *natural* monotonicity test

$$\|\overline{\Delta x}^{k+1}\| \leq \|\Delta x^k\|, \tag{9}$$

where $\overline{\Delta x}^{k+1}$ denotes the *simplified* Newton correction defined via

$$F'(x^k)\overline{\Delta x}^{k+1} = -F(x^{k+1}) \; . \tag{10}$$

Observe that the linear system (10) uses the same matrix as in (3), but a different right hand side. By construction, it is also independent of any choice the matrix A. Experience shows that, in most and especially in challenging cases of boundary value problems for ordinary and partial differential equations, this natural monotonicity test is much more efficient than the standard test (7).

Affine covariant Lipschitz condition. Following the paper [9] by the author and G. Heindl , let us introduce some Lipschitz constant $\omega \geq 0$ via

$$\|F'(x)^{-1}\left(F'(\bar{x}) - F'(x)\right)(\bar{x} - x)\| \leq \omega\|\bar{x} - x\|^2 \; . \tag{11}$$

Note that this kind of condition is independent of the choice of the matrix A as can be seen from

$$G'(x)^{-1}\left(G'(\bar{x}) - G'(x)\right)(\bar{x} - x) = F'(x)^{-1}A^{-1}A\left(F'(\bar{x}) - F'(x)\right)(\bar{x} - x)$$

In passing we note that with this choice of Lipschitz condition, the traditional convergence theorems for *local* Newton methods, such as the ones by L. Kantorovich [13] or by I. Mysovskikh[16], can be shown by proofs much simpler than usual. Here, however, we are interested in the convergence analysis for *global* Newton methods, which will follow next.

Affine covariant convergence analysis. For the global Newton algorithm we need to study the local convergence of the natural level functions, which is obtained as

$$\|\,\overline{\Delta x}^{k+1}(\lambda)\| \leq \left(1 - \lambda + 1/2\;\lambda^2 h_k\right)\|\Delta x^k\| \; , \quad h_k := \|\Delta x^k\|\omega \; , \tag{12}$$

in terms of the quantity h_k, which we call *Kantorovich quantity* in view of the original paper [13]. For the optimal choice of damping factor we obtain

$$\lambda_k^{\text{opt}} = \min\left(1, \frac{1}{h_k}\right) . \tag{13}$$

Clearly, whenever $h_k < 1$, then $\lambda_k^{\text{opt}} = 1$, i.e. we are in the local contraction domain of the ordinary Newton method. Whenever $h_k > 1$, then the damping factor depends on the computationally known ordinary Newton correction and the unknown Lipschitz constant ω. Hence, this result seems to be useful only for theoretical purposes.

Affine covariant adaptive trust region strategy. In 1979, the author introduced the notion of computational estimates (see [5])

$$[h_k] \leq h_k , \tag{14}$$

which are lower bounds for Kantorovich quantities. Insertion of these bounds into (13) supplies an adaptive trust region strategy defined by

$$[\lambda_k^{\text{opt}}] := \min\left(1, \frac{1}{[h_k]}\right) .$$

The geometric situation can be seen in Fig. 1.

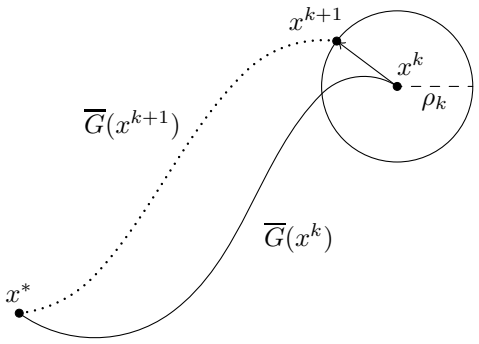

Figure 1: **Geometrical interpretation:** Newton path $\overline{G}(x^k)$ and Newton step with locally optimal damping factor λ_k^{opt}. Note that $\|x^{k+1} - x^k\| = \rho_k$, the radius of the local Kantorovich ball, which is the adaptive trust region.

The relation (14) induces that

$$[\lambda_k^{\text{opt}}] \geq \lambda_k^{\text{opt}} ,$$

which means that the suggested algorithmic damping factors may be too large. As a consequence, any damping strategy will have to be realized in two parts,

a prediction strategy and a correction strategy.

Prediction strategy. In 1975, the author had made a first suggestion. This has been slightly improved in [6] to yield

$$[\omega_k] := \frac{\| \overline{\Delta x}^k - \Delta x^k \|}{\lambda_{k-1} \|\Delta x^{k-1}\| \|\overline{\Delta x}^k\|} \leq \omega_k \ .$$

For Newton step $k > 0$, the idea is to pick some $\lambda_k = [\lambda_k^{\rm opt}]$ for $[h_k] = \|\Delta x^k\|[\omega_k]$. For $k = 0$, an ad hoc value must be determined. If, for the selected value λ_k, the natural monotonicity test fails, then a corrected value should be chosen as to be shown next.

Correction strategy. In 1983, H. G. Bock [2] suggested

$$[h_k] := [\omega_k]\|\Delta x^k\| := \frac{2\|\overline{\Delta x}^{k+1}(\lambda) - (1-\lambda)\|\Delta x^k\|}{\lambda^2 \|\Delta x^k\|}\Big|_{\lambda=\lambda_k} \ .$$

All terms in this expression are computationally available, as soon as the natural monotonicity test had failed (or otherwise been evaluated). This combined prediction/correction strategy works efficiently even in rather challenging problems, in most cases already without the necessity of a correction step.

Codes. The here presented algorithm is realized in the code NLEQ-ERR, which is publicly available, see the software page in [6]. It is suitable for moderate size nonlinear systems. For large scale, but still finite dimensional systems, the inexact Newton codes GIANT-GBIT (GIANT: Global Inexact Affine invariant Newton Techniques) with inner iteration by some "good Broyden method" GBIT for linear systems with general non-symmetric matrix is applied (see [8] by the author together with R. Freund and A. Walter).

1.2 Discrete continuation by local Newton methods

A different globalization exploits more specific properties of the nonlinear mapping under consideration. Rather than just solving $F(x) = 0$, we now solve the problem family

$$F(x, \lambda) = 0 \ , \quad \lambda \in [\lambda_0, \lambda^*] \tag{15}$$

in terms of the embedding parameter λ. Numerically, this means to solve a sequence of problems

$$F(x, \lambda_\nu) = 0 \ , \quad \lambda_{\nu+1} = \lambda_\nu + \Delta\lambda_\nu \ , \tag{16}$$

a process often called discrete continuation or numerical pathfollowing. Of course, in this approach, the control of the stepsizes $\Delta\lambda_\nu$ is crucial.

Newton continuation methods. The principle here is to construct a sequence of problems (16) such that the ordinary Newton method converges locally in each continuation step. Geometrically speaking, we construct some known *prediction path* $\widehat{x}(\lambda)$ substituting the unknown solution path $\overline{x}(\lambda)$. Following the classification from [5], we define the *order* p of a continuation method by

$$\|\widehat{x}(\lambda) - \overline{x}(\lambda)\| \leq \eta_p \, \Delta\lambda^p, \quad p > 0 \, . \tag{17}$$

The associated convergence analysis (see [6, Section 5]) leads to a feasible stepsize bound

$$\Delta\lambda_\nu \leq \Delta\lambda_{\max} := \left(\frac{2}{\omega\eta_p}\right)^{\frac{1}{p}} \, , \tag{18}$$

where ω represents some affine covariant Lipschitz constant. In the spirit of the preceding Section 1.1, we replace the unknown theoretical quantities by available computational estimates $[\cdot]$ so that computational estimates

$$[\Delta\lambda_{\max}] := \left(\frac{2}{[\omega][\eta_p]}\right)^{\frac{1}{p}}$$

arise as a basis for an adaptive stepsize strategy. The quantities $[\omega] \leq \omega$ and $[\eta_p] \leq \eta_p$ are easily obtained in the course of the algorithm. Due to the relation $[\Delta\lambda_{\max}] \geq \Delta\lambda_{\max}$ again a prediction and a correction strategy for the stepsizes is needed.

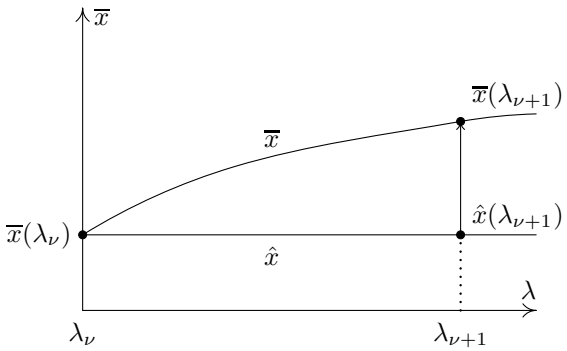

Figure 2: Classical continuation method ($p = 1$).

Classical continuation method. In the most popular approach, the prediction path is defined by just keeping the "old" solution as the initial guess for the next local Newton iteration:

$$\widehat{x}(\lambda) = \overline{x}(\lambda_\nu), \quad \lambda \geq \lambda_\nu \, .$$

This approach is geometrically represented in Fig. 2 from [5, 6].

Tangent continuation method. Another also popular choice is to continue along the local tangent direction so that

$$\widehat{x}(\lambda) = \overline{x}(\lambda_\nu) + (\lambda - \lambda_\nu)\, \dot{\overline{x}}(\lambda_\nu)\ , \quad \lambda \geq \lambda_\nu\ ,$$

wherein

$$F_x\Big(\overline{x}(\lambda_\nu),\, \lambda_\nu\Big)\, \dot{\overline{x}}(\lambda_\nu) = -F_\lambda\Big(\overline{x}(\lambda_\nu),\, \lambda_\nu\Big)\ .$$

The geometrical interpretation is given in Fig. 3, again from [5, 6].

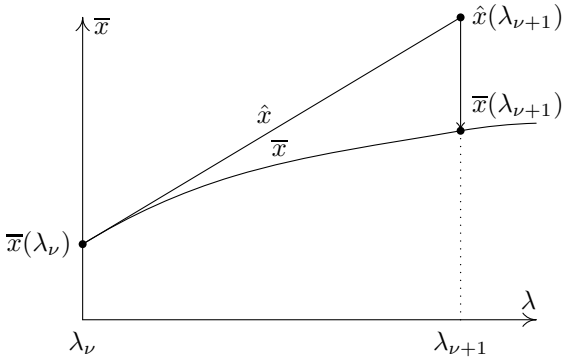

Figure 3: Tangent continuation method ($p = 2$).

Polynomial extrapolation method. In 1985, H. G. Bock [3] extended the above continuation methods towards polynomial extrapolation, for details see also [6, p.241]. With standard polynomial extrapolation, one obtains $p = 1$, while Hermite extrapolation yields $p = 2$. Both approaches are affine covariant by construction.

Example. Space shuttle problem (NASA). In this example, the parameter λ represents the maximum temperature of the space shuttle shield. The effect of the various affine covariant Newton algorithms can be illustrated by an optimal control problem concerning a space shuttle from NASA, see Table 1.

In passing we note that NASA had wanted (in vain) to reduce the maximum heating temperature of the shield of the shuttle from $2850°F$ to $2000°F$. This has for the first time been achieved in [10] by the author together with J. Pesch and P. Rentrop using a simple modification of the tangent continuation method. The finally achievable temperature of $1700°F$ has been computed by H. G. Bock in [1] - showing that below that temperature an optimal solution no longer exists.

htb

Continuation method	*Newton method*	*work*
classical	residual monotonicity (NASA)	failure
classical	natural monotonicity, empirical damping	~ 340
classical	natural monotonicity, adaptive trust region	114
tangent	natural monotonicity, adaptive trust region	18

Table 1: **Space Shuttle problem:** Fixed continuation step from $\lambda = 0.0085$ to $\lambda = 0.0080$. Comparison of different Newton and continuation methods counted in numbers of trajectories needed in a multiple shooting algorithm. The Gauss-Newton continuation iteration to be given below would result in a further computational speed-up by a factor of at least 2.

Gauss-Newton continuation methods. This most sophisticated continuation method has been worked out in the paper [7] by the author, B. Fiedler and P. Kunkel. Here the equation (15) is understood as an *underdetermined* system of equations for the extended variable $y = (x, \lambda) \in \mathbb{R}^{n+1}$, i.e.

$$F(y) = 0 \; . \tag{19}$$

Linearization leads to the underdetermined system

$$\delta y \in \mathcal{L} := \{\delta y | F'(y)\delta y + F(y) = 0\} \; .$$

Note that any such solution δy is defined in affine covariant terms. A special role is played by the (normalized) tangent $t(y) \in \mathbb{R}^{n+1}$, a basis for the null space of the Jacobian, i.e.

$$F'(y)t(y) = 0 \; .$$

With these definitions, a prediction path in $\mathbb{R}^{n+1}$ can be determined as

$$\widehat{y}(s) = \overline{y}_\nu + st(\overline{y}_\nu), \quad s > 0 \; . \tag{20}$$

As local correction a Gauss-Newton iteration is conveniently applied via

$$\Delta y := -F'(\widehat{y})^+ F(\widehat{y}) \;\; \perp t(\widehat{y}) \; .$$

Note that Δy is the "shortest" solution in the subspace $\mathcal{L}$. In local combination with a special quasi-Newton method, this quasi-Gauss-Newton iteration can be restricted to some hyperplane $H \perp t(\widehat{y})$ and thus be simply interpreted as quasi-Newton iteration in H. The geometric situation is depicted in Fig. 4. Following

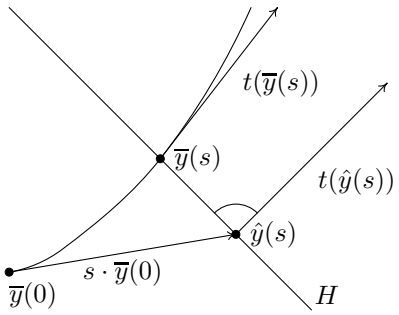

Figure 4: Discrete tangent continuation in $y = (x, \lambda)$.

the same line of thoughts as before, an adaptive trust region strategy based on computational estimates for theoretical quantities can be derived, details are left to the original paper [7] or the monograph [6, Section 5.2].

Code. The algorithm as described here is realized in the code ALCON, which is publicly available, see also the software page in [6]. By construction, this algorithm has no problem around turning points. Moreover, it includes an extension to bifurcation analysis.

2 Affine contravariance: residual approach

In most textbooks, global Newton methods are presented with the iterative standard monotonicity test (7) in terms of the nonlinear residual norm $\|F(x)\|$. However, as pointed out in the thesis of A. Hohmann [12], there is some arbitrariness in the domain space of F so that the problem $F(x) = 0$ is equivalent to the class of problems

$$G(y) := F(Bx) = 0 \quad \text{where} \quad y = Bx,\ B \in GL(n)\ . \tag{21}$$

Note that $G'(y) = F'(x)B$. Obviously, the choice of the nonsingular matrix B affects the *local* Newton iteration in a *contravariant* form (which gives the name)

$$y^0 = Bx^0,\ \ y^{k+1} = y^k + \Delta y^k \ \ \leftrightarrow \ \ Bx^{k+1} = Bx^k + B\Delta x^k\ ,\ \ k = 0, 1, \dots\ , \tag{22}$$

defined by the *ordinary* Newton corrections Δx^k via

$$F'(x^k)\Delta x^k = -F(x^k) \ \ \leftrightarrow \ \ G'(y^k)\Delta y^k = -G(y^k)\ . \tag{23}$$

Affine contravariant Lipschitz condition. In our context, we define some affine contravariant Lipschitz constant ω [12] by

$$\| \left(F'(\bar{x}) - F'(x)\right) BB^{-1}(\bar{x} - x)\| \leq \omega \|F'(x)BB^{-1}(\bar{x} - x)\|^2 \ . \tag{24}$$

Note that this ω is independent of the choice of the matrix B. With this type of Lipschitz condition, local convergence in the spirit of the theorem of I. Mysovskikh can again be proven, here in terms of the residuals only, which excludes questions of uniqueness of the solution.

Affine contravariant convergence analysis. In order to analyze the convergence properties of the global Newton method

$$x^{k+1} = x^k + \lambda_k \Delta x^k, \quad 0 < \lambda_k \leq 1, \quad k = 0, 1, \ldots$$

we may conveniently use the above Lipschitz constant to obtain

$$\|F(x^{k+1}(\lambda))\| \leq \left(1 - \lambda + 1/2 \ \lambda^2 h_k\right) \|F(x^k)\| \ , \quad h_k := \|F(x^k)\|\omega \ , \tag{25}$$

which defines the residual counterpart h_k for the Kantorovich quantity. In this framework, the optimal damping factor arises as

$$\lambda_k^{\text{opt}} = \min\left(1, \frac{1}{h_k}\right) \ . \tag{26}$$

The above value of the damping factor supplies the theoretical basis for some *global* convergence theorem - unlike the situation in the affine covariant case.

Affine contravariant adaptive trust region strategy. Proceeding as in Section 1.1, we may equally identify computational estimates $[h_k]$ to be evaluated in the course of the algorithm. Thus, we again arrive at some adaptive trust region strategy, both in the form of a prediction and a correction strategy.

Prediction strategy. As a slight modification from [12], the one suggested in [6, Section 3.2] seems to be the most simple one:

$$[h_k] := \frac{\|F(x^k(\lambda))\|}{\|F(x^{k-1})\|}[h_{k-1}] \leq h_k \ . \tag{27}$$

This estimate is easily available in the course of the global Newton iteration and defines

$$[\lambda_k^{\text{opt}}] := \min\left(1, \frac{1}{[h_k]}\right) \leq \lambda_k^{\text{opt}} \ .$$

Correction strategy. Once the residual monotonicity test has been performed, the information for a further computational estimate is available as

$$[h_k] := \frac{2\|F(x^{k+1}) - (1-\lambda)F(x^k)\|}{\lambda^2 \|F(x^k)\|}\Big|_{\lambda=\lambda_k} \leq h_k \ . \tag{28}$$

If the test failed, the above value could be used to define some better damping factor.

Inexact Newton-GMRES method. The main reason for A. Hohmann to introduce the affine contravariant Newton method in his thesis [12] had been that he wanted to construct an adaptive *inexact* Newton method with inner iteration by GMRES, the most robust and popular linear iterative solver for general unsymmetric matrix. In this solver, the exact linear system (23) is replaced by the *inner* iteration

$$F'(x^k)\delta x_i^k = -F(x^k) + r_i^k, \quad i = 0, 1, \ldots, i^* \quad \text{with} \quad \delta x_0^k = 0, r_0^k = F(x^k)$$

and the exact Newton iteration by the *outer* iteration

$$x_i^{k+1} = x^k + \lambda_k \delta x_i^k \ .$$

The index i^* is determined by the threshold criterion

$$\frac{\|r_i^k\|}{\|F(x^k)\|} \leq \eta^k \ . \tag{29}$$

Affine contravariant convergence analysis and trust region strategy. A careful affine contravariant convergence analysis in [12, 6] shows that the theoretically optimal damping factors and their computational estimates arise as

$$\lambda_k^{\text{opt}} = \min\left(1, \frac{1}{(1+\eta_k)h_k}\right), \quad [\lambda_k^{\text{opt}}] = \min\left(1, \frac{1}{(1+\eta_k)[h_k]}\right) \geq \lambda_k^{\text{opt}} \ .$$

Since in GMRES the property $\eta_{k+1} \leq \eta_k$ holds, a criterion of the kind

$$\eta_k \leq \overline{\eta} \ , \quad \text{for} \quad k \geq k^*$$

can be easily realized in (29), which means that the number of inner iterations can be conveniently controlled. Details of the associated prediction/correction strategies are omitted here.

Codes. The above combined prediction/correction strategy for the exact Newton method is realized in the public domain code NLEQ-RES for moderate size systems. The presented affine contravariant prediction/correction strategy for the inexact Newton method is realized in the code GIANT-GMRES, see the software page in the monograph [6].

Comparative numerical results. In order to compare the affine covariant and contravariant algorithms (as realized in NLEQ-ERR and NLEQ-RES), let us demonstrate their performance for a set of general partial differential equations as given in [6, Section 8.2.1]. The set consists of the four examples:

- an artificial test problem atp1 of dimension $n = 961$,
- two driven cavity problems (dcp1000, dcp5000), one for laminar flow (with $Re = 1000, n = 1922$), one for turbulent flow (with $Re = 5000, n = 7983$),

- a supersonic transport problem sst2 of dimension $n = 10404$.

In all cases, *exact* Newton methods were realized, using direct solvers for the moderate size discretized systems. The results are presented in Table 2. The parameter ITMAX means termination after more than 75 Newton iterations, while λ-fail indicates termination due to 'too small' damping factor $\lambda_k < 10^{-4}$. The code NLEQ-RES/L represents some (left) preconditioned version of NLEQ-RES, where the preconditioner is obtained from an ILU-decomposition with pentadiagonal structure. It should be mentioned that this preconditioner will change from step to step, so that the norms $\|C_L(x)F(x)\|$ in the monotonicity test (7) as well as the above prediction strategy (27) and the correction strategy (28) must be handled with care. Intuitively speaking, the algorithm behind NLEQ-RES/L is half-way between NLEQ-RES and NLEQ-ERR.

Name	NLEQ-RES	NLEQ-RES/L	NLEQ-ERR
atp1	4 (0)	4 (0)	4 (0)
dcp1000	ITMAX	10 (5)	8 (4)
dcp5000	ITMAX	ITMAX	11 (7)
sst2	λ-fail	12 (11)	13 (8)

Table 2: Performance of various global exact Newton codes: adaptive trust region control via residual norm (NLEQ-RES), (left) preconditioned residual norm (NLEQ-RES/L), and error norm (NLEQ-ERR).

Examination of the above table shows:

- The easy problem atp1 is solved by all three versions, it even converges for the local Newton method with the prescribed initial guess.
- The code NLEQ-ERR clearly outperforms the other versions.
- Preconditioning in the residual version does indeed help, but not in the most difficult problem.

Though based on few examples only, the overall picture obtained from this small set has also been experienced in a larger class of problems.

Remark 1. The reader may be puzzled to learn that this residual based Newton method is successful in the cases, where damping factors are expected to show the behavior

$$\lambda_k \sim 1/\mathrm{cond}(F'(x^k)) \ ,$$

as indicated in (8). However, the whole affine contravariant approach only worked, since A. Hohmann changed the mapping F by reformulating the boundary value problems, where possible, as *Fredholm integral equations of the* 2*nd kind*, see [12, Section 5.2]. In the discretization of this operator formulation, the Jacobian is no longer ill-conditioned.

Remark 2. In his popular textbook [14], Tim Kelley reports satisfactory algorithmic performance based on nonlinear residual criteria. It may be worth mentioning that he has two key examples: (a) a 2D convection-diffusion equation, see [14, (6.21), p. 108], in a mild ($C = 20$) and a more challenging version ($C = 100$); for the mild version already a local Newton method converges, while the more challenging version requires a global strategy, at best with *preconditioning*, in agreement with our results in Table 2; (b) the Chandrasekhar H-equation, [14, (5.21), p.87], which is a *Fredholm integral equation of the* 2*nd kind*, in agreement with Remark 1 above.

3 Affine conjugacy: convex optimization

Assume that we have a strictly monotone functional

$$f(x) = \min, \quad f : D \subset X \to \mathbb{R} \, . \tag{30}$$

to be minimized over some Banach space X. In order to find some inner minimum, we have to solve the nonlinear system (in function space: differential equations)

$$F(x) = f'(x)^T = 0, \quad x \in D \subset X \, .$$

For the global Newton method, we have as usual

$$x^{k+1} = x^k + \lambda_k \Delta x^k, \quad 0 < \lambda_k \leq 1, \quad k = 0, 1, \dots \, ,$$

where

$$F'(x^k)\Delta x^k = -F(x^k) \, , \quad \text{here with} \quad F'(x) = f''(x) \quad \text{symmetric positive} \, .$$

In this context it is natural to require functional monotonicity, i.e.

$$f(x^{k+1}) \leq f(x^k) \, .$$

Following invariance considerations of [11, 6], we see that problem (30) is equivalent to the whole class of problems

$$g(y) = \min, \quad y = Bx, \quad B \quad \text{injective} \, . \tag{31}$$

As a consequence, we would get

$$G(y) = B^* F(Bx) = 0 \, , \quad G'(y) = B^* F'(x) B \, ,$$

where B^* denotes the adjoint of B. Observe that the transformation from $F'(x)$ to $G'(y)$ is affine conjugate (which gives the name).

Affine conjugate Lipschitz condition. Under the assumption that the functional f is *strictly* convex all $G'(y)^{1/2}$ exist. So we are able to define the Lipschitz condition

$$\|G'(y)^{-1/2}\left(G'(\overline{y})-G'(y)\right)(\overline{y}-y)\| \le \omega\|G'(y)^{1/2}(\overline{y}-y)\|^2 \ ,$$

which, cancelling the transformation B, is equivalent to

$$\|F'(x)^{-1/2}\left(F'(\overline{x})-F'(x)\right)(\overline{x}-x)\| \le \omega\|F'(x)^{1/2}(\overline{x}-x)\|^2 \ . \tag{32}$$

As in the preceding sections, the thus defined Lipschitz constant ω is invariant under any such transformation.

Affine conjugate convergence analysis. Under mild assumptions on D we obtain the upper bound [11]

$$f(x^k+\lambda\Delta x^k) \le f(x^k) - t_k(\lambda)\epsilon_k \ , \tag{33}$$

where

$$t_k(\lambda) = \lambda - \frac{1}{2}\lambda^2 - \frac{1}{6}\lambda^3 h_k$$

in terms of the affine conjugate quantities

$$h_k = \|F'(x^k)^{1/2}\Delta x^k\|\omega \ , \quad \epsilon_k = \langle \Delta x^k, F'(x^k)\Delta x^k\rangle = \|F'(x^k)^{1/2}\Delta x^k\|_2^2 \ .$$

Observe that, by mere invariance considerations, the local energy product and thus the function spaces H^1 and $W^{1,p}$ for $1<p<\infty$ appear naturally. The optimal damping factor comes out to be

$$\lambda_k^{\text{opt}} = \frac{2}{1+\sqrt{1+2h_k}} \le 1 \ . \tag{34}$$

With these estimates, a global convergence theory is possible. However, as in the preceding sections, the damping factors are of theoretical value only, since the quantity ω is unknown.

Affine conjugate trust region strategy. In order to derive an adaptive algorithm from the theoretical results above, we replace the Kantorovich quantities h_k by computational estimates $[h_k]$. As presented in [11], there are three possibilities to identify computational estimates. The least expensive one is the most unstable one against rounding errors, while the most expensive one, which reads

$$E_1(\lambda) := \langle \Delta x^k, \left(F'(x^k+\lambda\Delta x^k)-F'(x^k)\right)\Delta x^k\rangle \le \lambda h_k \epsilon_k \ ,$$

is best suited for computational evaluation. From this one obtains the Kantorovich estimate

$$[h_k] := \frac{|E_1(\lambda)|}{\lambda\epsilon_k} \le h_k \ .$$

For the optimal damping factor we obtain

$$[\lambda_k^{\rm opt}] = \frac{2}{1+\sqrt{1+2[h_k]}} \leq 1 \ ,$$

which is the basis for corresponding affine conjugate adaptive prediction and correction strategies (skipped here).

Codes. On the basis of this algorithmic derivation, the code NLEQ-OPT for moderate size nonlinear systems has been constructed, which is public domain, see the software page in [6]. For large scale, but still finite dimensional systems, the inexact Newton code GIANT-PCG with some PCG as inner iteration and for arbitrary preconditioner is available. Note that the linear iterative solver PCG is also affine conjugate. Other choices of inner iterations should be avoided! For general elliptic PDEs, the derivation scheme is extended to an inexact Newton method in function space. This leads to the adaptive multilevel FEM code NEWTON-KASKADE.

4 Affine similarity: steady state problems

This invariance class has been introduced as the most recent one by the author. The presentation here is an improvement over Section 6.4 in the monograph [6]. Assume you want to compute the steady state of a dynamical system

$$\dot{x} = F(x) = 0 \ . \tag{35}$$

Then, following the usual invariance considerations, this problem is equivalent to the whole class of problems (with $y = Bx$)

$$\dot{y} = B\dot{x} = BF(x) = BF(B^{-1}y) = 0, \quad , \tag{36}$$

where $B \in$ GL(n). Clearly, in this problem class, the domain and the image space of F are equivalent. Thus one obtains

$$G(y) = BF(B^{-1}y) = 0, \quad G'(y) = BF'(x)B^{-1} \ ,$$

which obviously is a similarity transform of the Jacobian (giving the name).

Fixed point iteration. The simplest affine similar scheme for the solution of the steady state problem certainly is the fixed point iteration

$$\Delta x^k = F(x^k), \quad x^{k+1} = x^k + \tau_k \Delta x^k \ , \tag{37}$$

which, in the field of numerical ODEs, is well-known as *explicit Euler discretization*. The parameter τ_k is just the local timestep. This scheme is known to work satisfactorily only in the *non-stiff* case.

Pseudo-transient continuation. For the *stiff* case, the following also affine similar scheme is quite popular (see, e.g., C.T. Kelley and D. Keyes [15])

$$(I - \tau_k F'(x^k))\Delta x^k = F(x^k) \ , \quad x^{k+1} = x^k + \tau_k \Delta x^k \ . \tag{38}$$

In the field of numerical ODEs, this scheme is known as the *linearly implicit Euler discretization*, applicable to *stiff* ODEs and *differential-algebraic* equations (DAEs). It looks like a linear combination of (37) with Newton's method. In fact, for $\tau_k \to \infty$ and nonsingular Jacobian, the scheme approaches Newton's method. In real life dynamical systems, however, the Jacobian is rarely nonsingular, as will be shown below.

Dynamical invariants. In the modelling of chemical dynamical systems, *mass conservation* occurs quite often, which can be written as

$$e^T x(t) = e^T x_0, \quad \text{where} \quad e^T = (1, \ldots, 1) \ . \tag{39}$$

Time differentiation of this relation leads to

$$e^T \dot{x} = e^T F(x(t)) \equiv 0 \ .$$

Differentiation with respect to x then yields

$$e^T F'(x) F(x) \equiv 0 \quad \text{for} \quad F(x) \neq 0 \ .$$

Summarizing, the Jacobian will be necessarily singular, whenever the dynamical system contains some (explicit or hidden) dynamical invariants. In this case, Newton methods will not work. Let

$$P^\perp = I - \frac{ee^T}{e^T e}$$

define the orthogonal projector characterizing the just shown property, then

$$P^\perp \dot{x} = P^\perp F(x) = 0 \quad \Rightarrow \quad P^\perp F'(x) = 0 \ .$$

Upon inserting the orthogonal operator into (38), the iterates can be seen to satisfy

$$P^\perp \Delta x^k = 0 \ .$$

Assuming $P^\perp x_0 = 0$, then all iterates can be seen to remain in the subspace

$$\mathcal{S} := \{u \mid P^\perp u = 0\} \ .$$

Affine similar Lipschitz conditions. As shown above, the dynamical system underlying the steady state problem (35) should be regarded as a DAE system. That is why (unlike [15]) we do not employ a first-order Lipschitz condition for $F(x)$, which is known to characterize the *non-stiff* case only. Recalling the above introduced subspace $\mathcal{S}$, the following two Lipschitz conditions appear to be useful:

- *first-order one-sided Lipschitz condition*

$$\frac{\langle u, F'(x)u\rangle}{\|u\|^2} \leq \nu < 0 \;, \quad \text{for} \quad u \in \mathcal{S} \;,$$

- *second-order Lipschitz condition*

$$\| \left(F'(x) - F'(\overline{x})\right)(x - \overline{x})\| \leq L_2 \|x - \overline{x}\|^2 \;.$$

Remark 3. Note that, for singular Jacobian, $\nu \geq 0$ would necessarily occur, unless the above argument u were restricted to the subspace $\mathcal{S}$.

Affine similar convergence analysis. For both the analysis and the algorithmic realization, we may define the local one-sided Lipschitz constant

$$\hat{\nu}(\tau) := \frac{\langle \Delta x, F'(x)\Delta x\rangle}{\|\Delta x\|^2} \leq \nu < 0 \;. \tag{40}$$

Note that, if $\hat{\nu}(\tau) \geq 0$ appeared during the iteration, then the algorithm should be terminated.

We are now ready to address the main question, what kind of monotonicity test should be selected in the pseudo-continuation method. The following auxiliary result helps to decide this question:

$$\frac{d}{d\tau}\|F(x(\tau))\|^2\Big|_{\tau=0} = 2\langle F(x(\tau)), F'(x(\tau))\dot{x}\rangle\Big|_{\tau=0} = 2\hat{\nu}(0)\|F(x_0)\|^2 \;. \tag{41}$$

From this, it can be clearly seen that the *residual monotonicity test* can be applied. However, it will be successful only, if $\nu < 0$. In this case the residual norm will have some local timestep interval, where it decreases, i.e.

$$\|F(x(\tau))\| < \|F(x_0)\| \quad \text{for} \quad \tau \in [0, \tau^*] \;.$$

As for monotonicity in terms of corrections, the estimate

$$\|\Delta x\| \leq \frac{\|F(x_0)\|}{1 - \nu\tau} \;. \tag{42}$$

shows, why this is not a good idea.

With these preparations, the following theoretical result can be obtained:

$$\|F(x(\tau))\| \leq \Big(1 + \frac{1}{2}\frac{L_0 L_2 \tau^2}{1 - \nu\tau}\Big)\frac{\|F(x_0)\|}{1 - \nu\tau} \;, \tag{43}$$

where $L_0 = \|F(x_0)\|$ denotes the Peano constant. The above assumption $\nu < 0$ can be specified in more detail as

$$\nu + \Big(\frac{1}{2}L_0 L_2 - \nu^2\Big) \leq 0 \quad \Rightarrow \quad \|F(x(\tau))\| < \|F(x_0)\| \;.$$

Under this specification, the *optimal* timestep in (43) is achieved as

$$\tau_{\text{opt}} = \frac{|\nu|}{L_0 L_2 - \nu^2} \tag{44}$$

Affine similar trust region strategy. We now proceed as in the preceding sections and replace the unknown theoretical quantities by computationally available quantities $[\cdot]$ thus obtaining

$$[\tau_{\mathrm{opt}}] := \frac{[|\nu|]}{L_0[L_2] - [\nu]^2} \tag{45}$$

As for the one-sided Lipschitz constant, we may simply use definition (40) in the convenient form

$$[\nu]\tau := \hat{\nu}(\tau) = \frac{\langle \Delta x, \Delta x - F(x_0)\rangle}{\|\Delta x\|^2} \leq \nu\tau \ .$$

In view of the necessary condition (41), the algorithm should be terminated, as soon as $\hat{\nu} > 0$ occurs. For the other Lipschitz constant L_2 we may exploit

$$[L_2] := \frac{\|F(x(\tau)) - \Delta x\|}{\tau^2\|\Delta x\|^2} \leq L_2 \ . \tag{46}$$

These estimates can be easily obtained in the course of the iteration and inserted into (44) for the estimated optimal timestep.

A perhaps preferable choice would be obtained via the implicit reformulation

$$\tau_{\mathrm{opt}} = \frac{|\nu|(1 - \nu\tau_{\mathrm{opt}})}{L_0 L_2} \ ,$$

from which, using (42), we obtain

$$\|\Delta x(\tau_{\mathrm{opt}})\| L_2 \tau_{\mathrm{opt}} \leq \frac{L_0}{1 - \nu\tau_{\mathrm{opt}}} L_2 \frac{|\nu|(1 - \nu\tau_{\mathrm{opt}})}{L_0 L_2} = |\nu| \ .$$

From this relation, a computationally available optimal timestep would be the root of the scalar equation

$$g(\tau) = \|\Delta x(\tau)\|\tau - \frac{[|\nu|]}{[L_2]} = 0 \ . \tag{47}$$

In order to compute this root, one may construct the fixed point iteration

$$\tau^{k+1} = \tau^k \frac{[|\nu|]}{[L_2]\|\Delta x(\tau^k)\|\tau^k} \ . \tag{48}$$

The latter algorithmic tool has not been tried yet.

Conclusion

The present article on affine invariant Newton methods concisely surveys the contents of the author's book [6], yielding at the same time some new structural insight as well as a few new algorithmic details. In terms of robustness, the *affine covariant* Newton techniques appear to be well-suited for *discrete boundary value problems in ODEs and general PDEs*. The class of *affine contravariant* Newton methods fits particularly well to *Fredhom integral equations of the* 2*nd kind*. *Affine conjugacy* applies naturally to *elliptic PDEs*. Finally, for *steady state* problems in time dependent differential equations, the class of *affine similar* Newton methods seems to be appropriate. For this latter case, several new theoretical as well as algorithmic results beyond the book [6] are presented.

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