On the choice of initial guesses for the Newton-Raphson algorithm

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Abstract

The initialization of equation-based differential-algebraic system models, and more in general the solution of many engineering and scientific problems, require the solution of systems of nonlinear equations. Newton-Raphson’s method is widely used for this purpose; it is very efficient in the computation of the solution if the initial guess is close enough to it, but it can fail otherwise. In this paper, several criteria and an algorithm are introduced to analyze the influence of the initial guess on the evolution of Newton-Raphson’s algorithm, and to identify which initial guesses need to be improved in case of convergence failure. In particular, indicators based on first and second derivatives of the residual function are introduced, whose values allow to assess how much the initial guess of each variable can be responsible for the convergence failure. The use of the criteria and algorithm, which are based on rigorously proven results, is successfully demonstrated in two exemplary test cases.

Keywords: Newton-Raphson’s algorithm, Convergence, Nonlinear equations, Equation-based modelling.

Declarations of interest: none.

1. Introduction

1.1. Goal of the paper

Newton-Raphson’s (NR) algorithm and its variants have been used for over 250 years to solve implicit nonlinear equations. The algorithm is iterative and...
the convergence to the desired solution crucially depends on the choice of the initial guess for the unknowns of the problem. Once the result of the iterations is close enough to the solution, under mild regularity conditions and under the assumption of non-singular Jacobian, the algorithm converges to the solution in a superlinear fashion.

In general, it may not be easy or practical to obtain an initial guess close enough to the solution to ensure that the asymptotic convergence result is obtained after a moderate number of iterations. In fact, if the initial guess is sufficiently far from the sought-after solution, NR’s algorithm may not converge at all to it.

Many theorems have been proven in the past, originated from the classical result by Kantorovich [8], which provide sufficient conditions for the convergence of NR’s method to a solution, see e.g. [7, 1] and references therein. Although such results are very powerful, they cannot be used to answer the following two practical questions, that very often arise when using NR’s method to solve real life problems:

- For which variables is it actually necessary to provide a good initial guess?
- In case of convergence failure starting from a certain initial guess, how should one improve it to eventually achieve convergence to the desired solution?

The aim of this paper is to answer these two questions based on rigorous results or, where necessary, on heuristic criteria based on rigorous results.

1.2. Background

The introduction of Equation-based, Object-Oriented modelling Languages and Tools (EOOLTs), such as Modelica [9, 6] or gPROMS [2], started in the mid 90’s of the last century, has made the need of good answers to the above-mentioned questions compelling.

These modelling languages allow to build complex system models, described by differential-algebraic equations, which can potentially span multiple physical domains, such as mechanical, electrical, thermal, thermal-hydraulic, chemical, etc. The system models are obtained by assembling equation-based component models in a modular way, possibly taking them from libraries of well-tested and validated reusable component models developed by third-parties.

The simulation of such models requires finding a consistent initial solution for their DAEs [11]. Such solution can be obtained by adding a set of initial equations to the DAEs, often resulting in very large sets of nonlinear equations. The tools which handle these models are agnostic, in the sense that they are not limited to a specific physical domain or to a pre-specified set of models, for which some heuristic criterion to provide initial guesses for the initialization problem can be found and embedded in the software. To the contrary, the users of such tools have complete freedom to combine equation-based models from multiple reusable libraries, together with other models and initial conditions that they write themselves in the form of equations with arbitrary structure.
Thanks to the high-level, modular approach to modelling of EOOLTs, building complex system models using these tools is relatively straightforward; unfortunately, the solution of the corresponding initialization problems often turns out to be a critical task. In most cases, the model equations are nonlinear, the nonlinear solvers often fail, and the end user is left to struggle with very low-level error messages and log files to analyze, in order to understand how to eventually succeed in the solution process. In many cases, this issue is the main limiting factor in the adoption of EOOLTs in a certain application domain.

There are some strategies to avoid this kind of problems. When dealing with a complex interconnected modular system, one can first try to solve the initialization problem for each of its component separately, applying suitable system boundaries, and then collect the found solutions to get the initial guesses for the solution of the system-wide initialization process. However, this process is quite convoluted, and it requires the a-priori knowledge of consistent system boundaries for the involved sub-systems.

Another well-known strategy to make the selection of initial guesses less cumbersome (among other things) is tearing \[4\], whereby a certain subset of tearing variables is chosen, so that all other variables can be explicitly computed from them following a certain sequence of assignments. In this case, it is only necessary to provide initial guesses for the tearing variables, since guesses of all the other unknowns are automatically computed by the sequence of assignments during the first iteration of NR’s algorithm. However, the choice of those initial guesses is still critical and can lead to convergence failure.

In some cases, a homotopy-based approach can help finding the initial solution of the system by first solving a simplified problem, and then transforming the simplified problem into the actual one by means of a homotopy transformation, using a continuation solver, see e.g. \[13\] and references therein. However, also in this case, unless the simplified model is linear, solving the initial simplified problem also requires the use of an iterative, NR-type solver, which is prone to failure if not initialized correctly.

1.3. Contents of the paper

Given this scenario, there is a definite need of general criteria to guide the choice of the initial guess values to solve generic systems of nonlinear equations, coming from physical system modelling problems of arbitrary nature, by means of NR solvers. To the authors’ best knowledge, this general problem is not addressed as such in the published literature. The goal of this paper is thus to provide such criteria, based as much as possible on rigorous results and, where necessary, on some heuristic assumptions.

The paper is structured as follows. In Section 2 several new theorems are stated, which provide the rigorous groundwork for the remainder of the paper. In Section 3 the relevance of these theorems with respect to the two questions stated in Section 1.1 is discussed, leading to the formulation of several criteria and of an algorithm, aimed at the effective choice of initial guesses for NR’s algorithm. In Section 4 those criteria and algorithm are successfully demonstrated.
on two exemplary physical modelling problems. Finally, Section 5 concludes the paper.

2. Method

Consider the equation

\[ f(x) = 0, \]

where \( x \in \mathbb{R}^m \) and \( f : \mathbb{R}^m \to \mathbb{R}^m \) is a vector function which is continuously differentiable in an open neighbourhood \( D \) of the solution \( \bar{x} \), \( f(\bar{x}) = 0 \). Denote the Jacobian matrix of function \( f(x) \) with respect to \( x \) as \( f_x(x) \). Assume the vector of the unknowns \( x \) is suitably ordered, so that it can be split into two sub-vectors \( w \in \mathbb{R}^q \) and \( z \in \mathbb{R}^{m-q} \)

\[
x = \begin{bmatrix} w \\ z \end{bmatrix},
\]

\( w \) being the smallest possible sub-set of \( x \) such that

\[ f_x(x) = J(w), \]

i.e., the Jacobian matrix of \( f(x) \) depends only on \( w \) and not on \( z \), and therefore the function \( f(x) \) depends only linearly on \( z \). Assume the equations in (1) are ordered so that \( f(x) \) can be split into two vector functions \( n(x) \) and \( l(x) \), \( n : \mathbb{R}^m \to \mathbb{R}^p \), \( l : \mathbb{R}^m \to \mathbb{R}^{m-p} \)

\[
f(x) = \begin{bmatrix} n(x) \\ l(x) \end{bmatrix},
\]

where \( n(x) \) contains the non-linear equation residuals and \( l(x) \) contains the linear equation residuals.

The solution \( \bar{x} \) can be computed iteratively by NR’s algorithm, which requires to solve the following linear equation at each iteration \( j \)

\[
f_x(x_{j-1})(x_j - x_{j-1}) = -f(x_{j-1}), \quad j = 1, 2, \ldots
\]

starting from a given initial guess \( x_0 \).

**Theorem 1.** If the Jacobian \( f_x(\bar{x}) \) is non-singular in the solution \( \bar{x} \) and Lipschitz-continuous in a neighbourhood of \( \bar{x} \), for all \( x_0 \) sufficiently close to \( x \) the sequence \( \{x_j\} \) of the solutions of (5) converges not less than quadratically to \( \bar{x} \).

**Proof.** This is a well-known result, see e.g. [10]. [4]

**Theorem 2.** If Equation (1) is linear and \( f_x \) is non-singular, then NR’s algorithm converges in one step, irrespective of the chosen initial guess \( x_0 \).

**Proof.** If Equation (1) is linear, \( f(x) = Jx + b \), where \( J = f_x \) is a constant \( m \times m \) matrix and \( b = f(0) \). The first iteration of (5) becomes

\[
J(x_1 - x_0) = -(Jx_0 + b)
\]

whose solution \( x_1 \) is the solution of \( Jx + b = 0 \). [4]
Theorem 3. If NR’s algorithm is initialized with a first guess

\[ x_0 = \begin{bmatrix} w_0 \\ z_0 \end{bmatrix}, \]  

(7)

the values of the approximated solution \( x_j \) at each step \( j > 0 \) only depend on the guess values \( w_0 \) of the variables affecting the Jacobian, regardless of the choice of \( z_0 \).

Proof. Equation (3) implies that the Jacobian matrix \( f_x \) can be partitioned as follows

\[ f_x(x) = \begin{bmatrix} f_w(w) & f_z \end{bmatrix}, \]

(8)

where \( f_z \) is a constant matrix. Therefore, the nonlinear function \( f \) can be rewritten as

\[ f \left( \begin{bmatrix} w \\ z \end{bmatrix} \right) = g(w) + f_z z. \]

(9)

The first iteration of NR’s algorithm (5) yields

\[ \begin{bmatrix} f_w(w_0) & f_z \end{bmatrix} \begin{bmatrix} w_1 - w_0 \\ z_1 - z_0 \end{bmatrix} = -f \left( \begin{bmatrix} w_0 \\ z_0 \end{bmatrix} \right), \]

(10)

which can be expanded into

\[ f_w(w_0)(w_1 - w_0) + f_z(z_1 - z_0) = -g(w_0) - f_z z_0. \]

(11)

Now the two terms \(-f_z z_0\) on the left and right-hand side cancel out, yielding

\[ f_w(w_0)(w_1 - w_0) + f_z z_1 = -g(w_0), \]

(12)

whose solution

\[ x_1 = \begin{bmatrix} w_1 \\ z_1 \end{bmatrix}, \]

(13)

which is the result of the first iteration, does not depend on the initial guess \( z_0 \). Hence, the values of the subsequent iterations \( x_2, x_3, \ldots \) also do not depend on \( z_0 \). \( \square \)

Theorem 4. The residuals of the linear equations in system (1) after the first iteration of NR’s algorithm are zero, i.e., \( l(x_1) = 0 \), regardless of the initial guess values \( x_0 \).

Proof. The Jacobian matrix of function (1) can be partitioned as follows:

\[ f_x(x) = \begin{bmatrix} n_w(w) & n_z \\ l_w & l_z \end{bmatrix}, \]

(14)

where the Jacobians \( n_z, l_w, \) and \( l_z \) are constant matrices. The linear equations residuals \( l(x) \) can then be formulated as

\[ l(x) = l_w w + l_z z + l(0) \]

(15)
The first iteration of NR’s algorithm reads
\[
\begin{bmatrix} n_w(w_0) & n_z \\ l_w & l_z \end{bmatrix} \begin{bmatrix} w_1 - w_0 \\ z_1 - z_0 \end{bmatrix} = - \begin{bmatrix} n(x_0) \\ l(x_0) \end{bmatrix}.
\] (16)

By expanding and rearranging the last rows of Equation (16), and by taking into account Equation (15) with \( x = x_0 \), one gets
\[
l_w w_1 + l_z z_1 = l_w w_0 + l_z z_0 - l(x_0) = -l(0).
\] (17)

Hence,
\[
l(x_1) = l_w w_1 + l_z z_1 + l(0) = -l(0) + l(0) = 0.
\] (18)

**Definition 1.** Consider the NR algorithm (15). Assume that each component \( i \) of the function \( f(x) \), denoted as \( f_i(x) \), is twice continuously differentiable in an open neighbourhood \( \mathcal{O} \) containing the initial guess \( x_0 \) and the result of the first iteration \( x_1 \). Denote the Jacobian matrix of \( f_i(x) \) with respect to \( x \) as \( f'_i(x) \) and the Hessian matrix as \( f''_i(x) \). By means of a Taylor series expansion, one can write
\[
f_i(x_1) = f_i(x_0) + f'_i(x_0)(x_1 - x_0) + \frac{1}{2}(x_1 - x_0)' f''_i(x_0)(x_1 - x_0) + h^i(x_1 - x_0),
\] (19)
which implicitly defines the third-order residual functions \( h^i(\cdot) \).

**Definition 2.** With reference to NR’s iteration (15), define the \( i \)-th nonlinear residual at iteration point \( x_{k-1} \) as
\[
r^i(x_{k-1}) = f^i(x_{k-1}) + f_z^i(z_k - z_{k-1})
\] (20)

**Definition 3.** Define the coefficients \( \alpha_i > 0, \ i = 1, \cdots, m \), such that
\[
|h^i(x_1 - x_0)| = \alpha_i |r^i(x_0)|
\] (21)
and let
\[
\alpha = \max(\alpha_i).
\] (22)

**Definition 4.** Define the curvature factor \( \Gamma_{ijk} \) of the \( i \)-th nonlinear equation with respect to variables \( w_j, w_k \) after the first iteration as
\[
\Gamma_{ijk} = \left| \frac{1}{2} \frac{\partial^2 g^i(w_0)}{\partial w_j \partial w_k} \frac{w_{1,k} - w_{0,k}}{r^i(x_0)} \frac{w_{1,j} - w_{0,j}}{r^i(x_0)} \right|, \quad i = 1, \ldots, p, \quad j, k = 1, \ldots, q.
\] (23)

**Theorem 5.** Given a constant \( \beta > 0 \), a sufficient condition for the property
\[
|f^i(x_1)| \leq (\alpha + \beta) |r^i(x_0)| \quad \forall i
\] (24)
to hold is that
\[
\sum_{jk} \Gamma_{ijk} \leq \beta \quad i = 1, \cdots, p.
\] (25)
\textbf{Proof.} Equation (5) for the first iteration reads

\[ f_x(x_0)(x_1 - x_0) = -f(x_0) \quad (26) \]

Computing \( f^i(x_1) \) with Equation (19) and plugging in Equation (26), one obtains

\[ f^i(x_1) = \frac{1}{2} \sum_{jk} \frac{\partial^2 f^i(x_0)}{\partial x_j \partial x_k} (x_{1,j} - x_{0,j})(x_{1,k} - x_{0,k}) + h^i(x_1 - x_0) \quad (27) \]

Regarding the linear equations \((i = p + 1, \ldots, m)\), according to Theorem 2 \( f^i(x_1) = 0 \). Hence, condition (24) is always satisfied for all \( \alpha > 0, \beta > 0 \) and for any value of \( r^i(x_0) \), including zero. As concerns the nonlinear equations \((i = 1, \ldots, p)\), recalling (8), (21), (22), (23), and observing that the higher-order residual \( h(x_1 - x_0) \) can only depend on the \( w \) variables, the following chain of inequalities holds:

\[
|f^i(x_1)| \leq \left| \frac{1}{2} \sum_{jk} \frac{\partial^2 f^i(x_0)}{\partial x_j \partial x_k} (x_{1,j} - x_{0,j})(x_{1,k} - x_{0,k}) + h^i(x_1 - x_0) \right| \quad (28)
\]

\[
\leq \left| \frac{1}{2} \sum_{jk} \frac{\partial^2 g^i(w_0)}{\partial w_j \partial w_k} (w_{1,j} - w_{0,j})(w_{1,k} - w_{0,k}) + h^i(w_1 - w_0) \right| \quad (29)
\]

\[
\leq \left| \frac{1}{2} \sum_{jk} \frac{\partial^2 g^i(w_0)}{\partial w_j \partial w_k} (w_{1,j} - w_{0,j})(w_{1,k} - w_{0,k}) + h^i(w_1 - w_0) \right| + |h^i(w_1 - w_0)| \quad (30)
\]

\[
\leq \left| \frac{1}{2} \sum_{jk} \frac{\partial^2 g^i(w_0)}{\partial w_j \partial w_k} (w_{1,j} - w_{0,j})(w_{1,k} - w_{0,k}) + h^i(w_1 - w_0) \right| + \alpha_i |r^i(x_0)| \quad (31)
\]

\[
\leq \sum_{jk} \Gamma_{ijk} |r^i(x_0)| + \alpha_i |r^i(x_0)| \quad (32)
\]

\[
\leq \beta |r^i(x_0)| + \alpha |r^i(x_0)| \quad (33)
\]

\[
\leq (\alpha + \beta) |r^i(x_0)| \quad (34)
\]

\[ \square \]

\textbf{Remark 1.} \( r^i(\bar{x}) = r^i(\bar{w}) = f^i(\bar{x}) = 0 \)

\textbf{Remark 2.} \textit{If the Jacobian} \( J(x) \) \textit{is non-singular, then} \( (w_{1,k} - w_{0,k}) = 0 \) \quad \forall k \iff \ f(x_1) = 0 \).

\textbf{Remark 3.} \textit{The coefficients} \( \alpha_i \) \textit{of the nonlinear equations, showing up in The-}
orem can be computed from Equations (5), (19), and (21), yielding

\[ \alpha_i = \frac{f_i(x_1) - \frac{1}{2}(x_1 - x_0)' f_{xx}^i(x_0)(x_1 - x_0)}{r^i(x_0)} \]  

(35)

\[ = \frac{f_i(x_1) - \frac{1}{2}(w_1 - w_0)' f_{ww}^i(w_0)(w_1 - w_0)}{r^i(x_0)} \]  

(36)

Remark 4. \( \alpha_i = 0 \) for \( i = p + 1, \ldots, m \), since the Taylor expansion of linear equations obviously lacks all terms of order greater than one.

Remark 5. Assuming the system of equations comes from a physical modelling problem, both the unknowns \( w \) and the residuals \( f_i(x) \) are in general dimensional quantities. However, the curvature factors defined in turn out to be dimensionless. This is a very nice property, which also implies that the values of those factors are invariant with respect to a change of measurement unit or, in other words, that they are insensitive to the specific choice of units taken for the modelling activity. In particular, the fact that a certain \( \alpha_i \) or a certain \( \Gamma_{ijk} \) are smaller or larger than one does not depend on the scaling of the problem, but only on the intrinsic non-linearity of the \( i \)-th equation with respect to variables \( (w_j, w_k) \).

Theorem 6. Given a problem and an initial guess \( w_0 \) for the nonlinear variables, the values of \( r^i(x_0) \), \( \alpha_i \), and \( \Gamma_{ijk} \) are invariant with respect to the choice of the initial guess \( z_0 \) for the linear variables.

Proof. The first NR iteration can be expanded as

\[ f(x_0) + f_w(w_0)(w_1 - w_0) + f_z(z_1 - z_0) = 0, \]  

(37)

which implies

\[ r^i(x_0) = f^i(x_0) + f_z^i(z_1 - z_0) = -f_w^i(w_0)(w_1 - w_0). \]  

(38)

Hence, from Equation (36), \( \alpha_i \) can be computed as

\[ \alpha_i = \frac{f_i(x_1) - \frac{1}{2}(w_1 - w_0)' f_{ww}^i(w_0)(w_1 - w_0)}{f_w^i(w_0)(w_1 - w_0)} \].  

(39)

According to Theorem 3, \( x_1 \) and \( w_1 \) do not depend on \( z_0 \), therefore also \( \alpha_i \) doesn’t. Taking into account Equation (38) again, it is apparent from Equation (23) that \( \Gamma_{ijk} \) also does not depend on \( z_0 \).

Theorem 7. The sensitivity of the solution \( x_1 \) after the first NR iteration, with respect to changes in the initial guess \( x_0 \), can be computed as:

\[ \frac{\partial x_1}{\partial x_0} = S, \]  

(40)
where

\[ H_i = f_{ww}(w_0)(w_1 - w_0) \]  

(41)

\[ H = \begin{bmatrix} H_1 \\ H_2 \\ \vdots \\ H_p \end{bmatrix} \]  

(42)

\[ S = - \left[ f_x(w_0) \right]^{-1} \begin{bmatrix} H_p \times q & 0_{p \times (m-q)} \\ 0_{(m-p) \times q} & 0_{(m-p) \times (m-q)} \end{bmatrix}. \]  

(43)

**Proof.** The first NR iteration, Equation (5) with \( j = 1 \), reads

\[ f_x(x_0)(x_1 - x_0) = -f(x_0) \]  

(44)

By differentiating the \( i \)-th row with respect to \( x_0 \), one obtains the following \( 1 \times m \) matrix equation

\[ f_{xx}^i(x_0)(x_1 - x_0) + f_x^i(x_0) \frac{\partial(x_1 - x_0)}{\partial x_0} = -f_x^i(x_0), \]  

(45)

where \( f_{xx}^i \) and \( f_x^i \) are the Jacobian and Hessian matrices of the \( i \)-th equation residual function. By stacking the \( m \) row vectors corresponding to each equation in (I) and recalling that all the derivatives of function \( f(x) \) only depend on \( w \), one obtains the following matrix equation with \( m \times m \) terms

\[ H + f_x(w_0) \frac{\partial(x_1 - x_0)}{\partial x_0} = -f_x(w_0), \]  

(46)

where

\[ H_i = f_{xx}^i(x_0)(x_1 - x_0) \]  

(47)

\[ H = \begin{bmatrix} H_1 \\ H_2 \\ \vdots \\ H_m \end{bmatrix} \]  

(48)

which can be solved for the sensitivity matrix by left-multiplying each term in equation (46) by the inverse Jacobian \([f_x(w_0)]^{-1}\), yielding

\[ \frac{\partial}{\partial x_0}(x_1 - x_0) = -[f_x(w_0)]^{-1}H - I_{m \times m}. \]  

(49)

Considering that

\[ \frac{\partial(x_1 - x_0)}{\partial x_0} = \frac{\partial x_1}{\partial x_0} - I_{m \times m}, \]  

(50)

equation (49) can be reduced to

\[ \frac{\partial x_1}{\partial x_0} = -[f_x(w_0)]^{-1}H. \]  

(51)
Since the first derivatives of \( f(x) \) only depend on the first \( p \) elements of vector \( x \) (i.e., the \( w \) vector), the last \( m - q \) rows and columns of \( f_i \) are zero. Hence, the last \( m - q \) columns of each \( H_i \) are zero, and so are the last \( m - q \) columns of the stacked matrix \( H \). Furthermore, when computing the matrix product inside (47), the last \( m - q \) terms of the \( x_1 - x_0 \) vector, i.e., \( z_1 - z_0 \), always get multiplied by zero second derivatives, so they can be skipped. Finally, since the last \( m - p \) equation residuals are linear, their Hessians are zero, so the last \( m - p \) row vectors \( H_i \) are also zero.

Hence, it is possible to compute matrix \( H \) more efficiently by skipping all those elements that do not contribute to the final result, yielding

\[
\tilde{H}_i = f_{ww}(w_0)(w_1 - w_0), \quad i = 1, \ldots, p \quad (52)
\]

\[
\tilde{H} = \begin{bmatrix} H_1 \\ H_2 \\ \vdots \\ H_p \end{bmatrix} \quad (53)
\]

\[
H = \begin{bmatrix} \tilde{H}_{p \times q} & 0_{p \times (m-q)} \\ 0_{(m-p) \times q} & 0_{(m-p) \times (m-q)} \end{bmatrix} \quad (54)
\]

**Remark 6.** When computing the sensitivity (40) at the solution \( x_0 = \bar{x} \), since \( x_1 = x_0 = \bar{x} \), it follows that \( H = 0 \), so the sensitivity \( S \) turns out to be zero.

This means that if an initial guess equal to the solution plus an infinitesimally small perturbation \( x_0 = \bar{x} + \delta x \) is chosen, the solution \( x_1 \) after the first NR iteration is not affected at all. This is consistent with the fact that \( f(x) \) can be approximated as a linear function in a small neighbourhood of the solution \( \bar{x} \), so that Theorem 2 guarantees that the first NR iteration converges to the solution \( \bar{x} \) in just one iteration, irrespective of the initial guess.

If the initial guess \( x_0 \) is close enough to the solution \( \bar{x} \) that the function \( f(x) \) is still approximately linear in a neighbourhood containing \( x_0 \) and \( \bar{x} \), then the same behaviour is preserved.

As \( x_0 \) is taken farther away from the solution \( \bar{x} \), nonlinear effects kick in, accounted for by matrix \( S \), which can be then considered an indicator of how far the initial guess is from the sweet spot of NR convergence.

Indeed, according to Equations (41)-(43), matrix \( S \) becomes larger as the initial guesses of the nonlinear variables \( w_0 \) get farther away from \( \bar{w} \), increasing \( (w_1 - w_0) \), and also depending on how large the corresponding second derivatives in the Hessians \( f_{ww}^i \) are. On the other hand, the fact that the initial value of the linear variables \( z_0 \) gets farther from \( \bar{z} \) is completely irrelevant, since \( (z_1 - z_0) \) does not enter in the computation of \( S \) at all. This is also consistent with Theorem 3.

**Remark 7.** The last \( m - q \) columns of matrix \( S \) are zero; this means that the sensitivity of the increment \( x_1 - x_0 \) with respect to \( z_0 \) is nil; this is also consistent
with Theorem 3. However, the sensitivity of $z_1 - z_0$ with respect to $w_0$ can in general be non-zero. Hence, matrix $S$ has the following structure:

$$S = \begin{bmatrix} S_{ww} & 0_{q \times (m-q)} \\ S_{zw} & 0_{(m-q) \times (m-q)} \end{bmatrix}$$ (55)

**Remark 8.** Assuming that the system of equations (1) comes from a physical modelling problem, the dimension of a generic element $s_{j,k}$ of matrix $S$ is the dimension of $x_j$ divided by the dimension of $x_k$. Hence, while the diagonal elements of $S$ are non-dimensional, the off-diagonal elements in general are not. This means that the off-diagonal terms of $S$ are in general not invariant with respect to a change of units in the formulation of the physical problem. It also means that the fact that one such element is much smaller or much greater than one doesn’t have any particular meaning, since its actual value depends on the choice of units of the problem, which is arbitrary, and is not invariant with respect to the scaling of the problem.

**Definition 5.** The weighted sensitivity matrix $\Sigma$ is defined as

$$W = \text{diag}(w_{1,1} - w_{0,1}, w_{1,2} - w_{0,2}, \ldots, w_{1,q} - w_{0,q})$$ (56)

$$\Sigma = W^{-1} S_{ww} W$$ (57)

**Remark 9.** Matrix $\Sigma$ is well-defined only if $W$ is invertible, i.e., if all the nonlinear variable increments after the first NR iteration ($w_{1,j} - w_{0,j}$) are non-zero. In the unlikely event that some of the variable increments are zero, this requirement can be easily enforced without loss of generality by adding a small perturbation to the corresponding initial guess.

**Remark 10.** Each element $\sigma_{j,k}$ of matrix $\Sigma$ has the dimensions of $s_{j,k}$, multiplied by the dimension of $w_j$ and divided by the dimension of $w_j$, hence, considering Remark 8 it is dimensionless. This implies that the values of matrix $\Sigma$ are independent of the choice of units in the original problem (1) and, more in general, to the scaling of the variables and residuals of the problem.

3. Discussion

The theorems stated in the previous section can be used to formulate four criteria and one algorithm for the selection of the initial guess values $x_0$ for NR’s algorithm.

The well-know Theorem 1 implies that if the initial guess $x_0$ is close enough to the sought solution $\bar{x}$, NR’s algorithm converges quickly to the exact solution; however, it does not provide any indication on how close the initial guesses $x_0$ must be to the solution $\bar{x}$ for this outcome to take place.

Theorem 2 indicates that in case function $f(x)$ is fully linear, NR’s algorithm always converges in one step, no matter what the initial guess $x_0$ is. This is an interesting limit case, but it hardly has any practical importance, since
NR algorithms are normally employed to solve systems that include nonlinear equations.

Theorem 3, instead, is of much greater practical importance when dealing with systems of mixed linear and nonlinear equations, a case often encountered in applications, as it states that the value of $x_1$ after one iteration will be the same regardless of the initial guess of the linear variables $z_0$. Hence, taking care of providing initial guess values for $z$ is a complete waste of time; one should rather invest time and effort in providing good initial guesses $w_0$ for the nonlinear variables $w$ that actually influence the Jacobian.

This consideration is valid assuming that a direct method, e.g. LU decomposition) is used to solve the linear system; in case an iterative method is used, the initial guess of the linear part could play a role in determining the number of iterations of the linear solver, and thus the performance of NR’s algorithm. However, the typical size of the problems addressed by this paper does not usually exceed the tens of thousands size, and the structure of the problems is usually characterized by a high degree of sparsity, with only a handful of variables showing up in each equation. Therefore, direct solvers can be employed, possibly using sparse algorithms such as KLU \[5\] if $p$ exceeds a few tens of equations, with satisfactory performance, see e.g.\[3\], making the statement above valid in practical applications.

Based on these considerations, the following first Criterion can then be formulated:

**Criterion 1.** When choosing the initial guesses $x_0$ for NR’s algorithm, provide good initial guesses for the variables $w$ that influence the Jacobian. The other variables $z$, that only appear linearly in the system of equations, can be given a trivial initial guess $z_0 = 0$, without affecting the convergence of NR’s algorithm.

If the initial guess $x_0$ is close enough to the solution $\bar{x}$, the convergence of the sequence $x_p$ is fast; as a consequence, every component $f_i(x_p)$ becomes much smaller than the previous one at each iteration $p$, starting from the first one. A good initial guess $x_0$ could then be identified as fulfilling the following property:

$$
|f_i(x_1)| \ll |f_i(x_0)| \quad i = 1, \cdots m.
$$

However, if one wants to exploit the invariance of the NR iterations with respect to the initial guess of the linear variables $z_0$ and thus apply Criterion 1, the trivial initial guess $z_0 = 0$ may be quite far from the solution $\bar{z}$, possibly causing $f_i(x_0)$ to become quite large. Thus, in general, a large reduction of the residuals at the first iteration is not a reliable indicator of the algorithm being near to convergence, but rather an effect of the reduction of the residuals of the linear terms in the equations, due to the large value of the increment $(z_1 - z_0)$ after the first iteration.

A better indication of closeness to convergence can then be obtained by deducting from $f_i(x_0)$ the effect of the linear variables increment $(z_1 - z_0)$, hence using the nonlinear residuals $r_i(x_0)$ as defined in Equation 20 in place...
of $f^i(x_0)$. The following condition is then sought:

$$|f^i(x_1)| \ll |r^i(x_0)| \quad \forall i,$$

(59)

which has the nice property of not depending on the choice of $z_0$ thanks to Theorem 6 and thus to be fully consistent with Criterion 1.

Note that condition (59) still only has heuristic value, as it is possible to build counter-examples where this property holds, but then subsequent iterations do not converge to any solution. However, in most practical cases, if condition (59) is fulfilled, it is quite unlikely that convergence is not eventually achieved.

Conversely, if convergence to the solution is not achieved and condition (59) is not satisfied for some $i$, a possible explanation for the convergence failure is that at least one of the initial guesses $w_0$ is not close enough to the solution, and as a consequence the curvature of the hyper-surfaces $y = f(x)$ causes the increment $(w_1 - w_0)$ to go astray, blowing up the nonlinear residual after the first iteration. Theorems 5 and 7 then allow to formulate heuristic criteria to understand which components of the vector of initial guesses $w_0$ are to blame for this, and should then be improved to eventually achieve convergence.

The sufficient condition of Theorem 5 to obtain property (59) requires

$$\alpha + \beta \ll 1$$

(60)

to hold. If $\alpha_i > 1$ for some $i$, then the sufficient condition is violated. In this case, the problem is that across the first iteration of NR’s algorithm, the third-order residual $h^i(w_1 - w_0)$ of the Taylor expansion plays a major role, which obviously contradicts the requirement that all iterations should take place in a neighbourhood of the solution, where the functions $f^i(x)$ are well approximated by linear ones, ensuring fast convergence. Hence, the initial values of the nonlinear variables appearing in $f^i(x)$ are not good enough, and should be improved. Unfortunately, it is not possible in this case to discriminate among the role played by each individual nonlinear variable, in case more than one is involved in the $i$-th equation.

In case $\alpha \ll 1$, then the sufficient condition is satisfied if also $\beta \ll 1$, which can only be achieved if $\Gamma_{ijk} \ll 1, \forall i, j, k$. If a certain $\Gamma_{ijk} > 1$, this causes the violation of the sufficient condition, which is due to the fact that poor initial guesses of the $j$-th and $k$-th nonlinear variables in vector $w_0$ cause the first iteration of NR’s algorithm to span an interval where the curvature of the corresponding hyper-surfaces in $y = f^i(x)$ is large enough to potentially cause convergence problems.

Note that a violation of the sufficient (but not necessary!) condition of Theorem 5 does not necessarily mean that the residuals $f^i(x_s)$ will not get smaller with increasing $s$, nor that NR’s algorithm will not eventually converge. However, in case of convergence failure of NR’s algorithm, Theorem 5 can provide useful indications about which components of initial guesses in $w_0$ are likely to be responsible for the failed convergence.

One important remark is due at this point: in case the initial guess $w_0$ is sufficiently far from the solution $\bar{x}$, it may happen that vector $x_1$ of the
unknowns after the first iteration does not belong to the domain of definition of the residual function \( f(x) \), preventing the computation of \( f(x_1) \) and thus the computation of the \( \alpha_i \) factors.

In order to still obtain useful information about the variables potentially causing the convergence failure because of high-order terms in the Taylor expansion, one can compute a damped first NR iteration \( x_1^* \) such that

\[
x_1^* - x_0 = \lambda(x_1 - x_0), \quad 0 < \lambda \leq 1
\]

or, equivalently

\[
f_2(x_0)(x_1^* - x_0) = -\lambda f(x_0).
\]

By taking a small enough value of \( \lambda \), one can get \( x_1^* \) arbitrarily close to the initial guess \( x_0 \), hence within the domain of definition of \( f(x) \), assuming that \( x_0 \) is an interior point of that domain. One can then exploit the Taylor expansion

\[
f^i(x_1^*) = f^i(x_0) + f^i_2(x_0)(x_1^* - x_0) + \frac{1}{2} f^i_3(x_0)(x_1^* - x_0) + h^i(x_1^* - x_0)
\]

to compute \( h^i(x_1^* - x_0) \). Is it then possible to re-define \( \alpha_i \) as

\[
|h^i(x_1^* - x_0)| = \alpha_i \lambda^3 |r^i(x_0)|,
\]

where \( \lambda^3 \) accounts for the fact that the term \( h^i(x_1^* - x_0) \) shrinks as \( \lambda^3 \) asymptotically as \( \lambda \to 0 \), thus making definition \( \lambda^3 \) asymptotically invariant as \( \lambda \to 0 \).

By combining the previous three equations, one can compute the new \( \alpha_i \) as:

\[
\alpha_i = \frac{f^i(x_1^*) - (1 - \lambda)f(x_0) - \frac{1}{2} (x_1^* - x_0) f^i_2(x_0)(x_1^* - x_0)}{\lambda^3 r^i(x_0)}
\]

\[
\alpha_i = \frac{f^i(x_1^*) - (1 - \lambda)f(x_0) - \frac{1}{2} (w_1^* - w_0) f^i_3(x_0)(w_1^* - w_0)}{\lambda^3 r^i(x_0)}.
\]

One should then reduce \( \lambda \) until \( x_1^* \) is close enough to the solution to allow computing \( f(x_1) \), then use Equation (66) to compute the \( \alpha_i \) factors.

Summing up, the idea is that the larger values of \( \alpha_i \) and/or \( \Gamma_{ijk} \) point to the initial guesses which are more likely to be the cause of the convergence failure. Moreover, the signs of the increments \( (w_1 - w_0) \) also provide indication whether the initial guesses should be increased or reduced, though they do not give any reliable information about the required magnitude of such change.

All of these results can be summarized in the following Criterion.

**Criterion 2.** In case of failure of NR’s algorithm to converge to the desired solution \( \bar{x} \) starting from the initial guess \( w_0 \), improve the initial guess of the variables \( w \) that appear in nonlinear equations with \( \alpha_i > 1 \), as well as the initial guess of those variables \( w \) corresponding to the indeces \( j \) and \( k \) of the curvature factors \( \Gamma_{ijk} > 1 \), computed after the first iteration of NR’s algorithm. The initial guesses should be increased or decreased according to the sign of their increment after the first NR iteration.
This criterion implicitly assumes that if the initial guess of the \( j \)-th nonlinear variable \( w_{0.j} \) is far enough from the solution \( \bar{w}_{j} \), this will affect the corresponding \( \alpha_{i} \) and \( \Gamma_{ijk} \) indicators and only them, so that they can be used backwards to pinpoint the critical initial guesses. Unfortunately, this is not necessarily the case: it is possible that a significant error on \( w_{0.j} \) has an influence on \( w_{1.k}, k \neq j \), and thus on the \( \alpha_{i} \) and \( \Gamma_{ijk} \) indicators pertaining to the \( k \)-th nonlinear variable, leading to the potentially incorrect diagnosis that the initial guess \( w_{0.k} \) is wrong too and needs to be improved. In other words, an error on the initial guess of the \( j \)-th nonlinear variable could spill over to the indicators of other variables, leading to false positives of Criterion 2.

One way to spot this potential spill-over effect and be alerted about possible false positives of Criterion 2 is to look at the off-diagonal elements of the scaled sensitivity matrix \( \Sigma \) introduced in Definition 5, to check if and by how much an error on the initial guess of the \( j \)-th nonlinear variable can have an influence on the \( k \)-th nonlinear variable after the first iteration.

The interpretation of matrix \( \Sigma \) is straightforward: the value of each element \( \sigma_{jk} \) indicates the ratio between the (small) percentage change of the initial guess of the \( k \)-th variable and the percentage change of the \( j \)-th variable after one iteration. The percent changes are computed on the basis of the actual variable increments.

Matrix \( \Sigma \) can also be directly used to provide information about the initial guesses \( w_{0.j} \) which are most likely the cause of NR’s algorithm failure. If the initial guess \( w_{0} \) is close enough to the solution \( \bar{x} \) that the function \( f(x) \) is approximately linear in a neighbourhood containing both, then Theorems 1 and 2 suggest that the solution \( w_{1} \) after one iteration will be much closer to the solution \( \bar{x} \) than \( w_{0} \). Therefore, a small change in \( w_{0.j} \) will cause a much smaller change in \( w_{1.j} \), which means \( |\sigma_{jj}| \ll 1 \). It is also expected that off-diagonal elements of the scaled sensitivity matrix will be small. Conversely, an element \( |\sigma_{jk}| > 1 \) indicates that a small change on the initial guess \( w_{0.k} \) has an effect of larger magnitude on the result of the first iteration \( w_{0.j} \), which is incompatible with \( w_{0.j} \) being close enough to the solution to be in the sweet spot of superlinear convergence. Hence, \( w_{0.k} \) should be improved by increasing or decreasing it, depending on the sign of the corresponding variable increment after the first NR iteration.

From this point of view, the elements \( \sigma_{jk} \) provide second-order information which is somewhat related, but at the same time complementary, to the second-order information provided by the \( \Gamma_{ijk} \) indicators. The only major shortcoming of \( \Sigma \) is that it relies exclusively on local first- and second-order information about function \( f(x) \) and has no provision to take into account third- or higher-order effects, contrary to the \( \alpha_{i} \) indicators of Criterion 2.

One could then formulate the following alternative criterion that only uses information from the \( \Sigma \) matrix.

**Criterion 3.** In case of failure of NR’s algorithm to converge to the desired solution \( \bar{x} \) starting from the initial guess \( w_{0} \), improve the initial guess of the variables \( w \) whose indeces correspond to the indeces \( k \) of the elements \( |\sigma_{jk}| > 1 \).
of matrix $\Sigma$, computed after the first iteration of NR’s algorithm. The initial guesses should be increased or decreased according to the sign of their increment after the first NR iteration.

The other most important use of the $\Sigma$ matrix, as already anticipated, is to detect the spill-over effect of the errors on the initial guess of the $k$-th nonlinear variable on some other $j$-th nonlinear variables after the first iteration, which is indicated by a large value of $|\sigma_{jk}|$. This information can be combined with the information provided by the $\alpha_j$ and $\Gamma_{ijk}$ factors to detect potential false positives of Criterion 2, leading to the following criterion:

**Criterion 4.** If Criterion 2 indicates that the initial guesses of two nonlinear variables $w_{0,j}$ and $w_{0,k}$ should be improved, but $|\sigma_{jk}| > 1$ while $|\sigma_{kj}| \ll 1$, then it is possible that the error in $w_{0,k}$ spills over to $w_{1,j}$, causing a false positive on $w_{0,j}$. One should then first try to improve $w_{0,k}$, and only consider improving $w_{0,j}$ if the indication of Criterion 2 on this variable persists once condition $|\sigma_{jk}| \ll 1$ has become true.

It is then possible to formulate a heuristic algorithm to address the failures of NR’s algorithm, by combining Criteria 2 and 4. The first part of the algorithm (Steps 1–7) only takes $\alpha_i$ into account, and is meant to bring the initial guess $w_0$ within a region where second-order-based indicators provide meaningful information for diagnostics. The second part (Steps 8–13) makes use of that information, encoded in the $\Gamma_{ijk}$ and $\sigma_{jk}$ indicators, to eventually achieve convergence.

**Algorithm 1.** In case of failure of NR’s algorithm to converge to the desired solution $\bar{x}$ starting from the initial guess $w_0$, $z_0 = 0$:

1. Let $\lambda = 1$
2. Compute the first damped NR iteration \( (62) \), then compute the $\alpha_i$ coefficients \( (66) \) and the $\Sigma$ matrix. If some $\alpha_i$ cannot be computed because $x^*_1$ falls outside the domain of definition of $f(x)$, then reduce $\lambda$ and repeat Step 2.
3. Identify the sub-set $A_1$ of the nonlinear variables $w$ appearing in all the $i$-th equations such that $\alpha_i > 1$, ranking them based on the actual values of $\alpha_i$.
4. Identify the sub-set $A_2 \subseteq A_1$ of variables $w_j$ such that $|\sigma_{jk}| > 1$ and $|\sigma_{kj}| \ll 1$
5. Let $A = A_1 - A_2$. If $A = \emptyset$ then go to Step 8.
6. Improve the initial guesses of the variables $w_j \in A$, by increasing or decreasing them based on the sign of the increment $(w_{1,j}^* - w_{0,j})$.
7. Run NR’s algorithm starting from the improved initial guess $w_0$; in case of success then stop, otherwise go to Step 1.
8. Compute the first NR iteration \( (20) \) from the current initial guess, then compute the curvature factors $\Gamma_{ijk}$ and the $\Sigma$ matrix.
9. Identify the sub-set $C_1$ of the nonlinear variables $w$ corresponding to indeces $j$ and $k$ of the factors $\Gamma_{ijk} > 1$ and $|\sigma_{jk}|$, ranking them based on the actual values of $\Gamma_{ijk}$ and $|\sigma_{jk}|$.

10. Identify the sub-set $C_2 \subseteq C_1$ of variables $w_j$ such that $|\sigma_{jk}| > 1$ and $|\sigma_{kj}| \ll 1$.

11. Let $C = C_1 - C_2$.

12. Improve the initial guesses of all variables $w_j \in C$, starting from the ones with higher values of $\Gamma$ and $|\sigma|$, by increasing or decreasing them, according to the sign of the increments $w_{1,j} - w_{0,j}$.

13. Run NR’s algorithm starting from the improved initial guess $w_0$; in case of convergence, stop, otherwise go to Step 8.

Note that Algorithm 1 is not meant to be run directly by a computer and achieve convergence automatically; it is rather a procedure to be followed by a human operator, which needs to apply expert judgement when evaluating the ranking of the $\Gamma_{ijk}$ and $|\sigma_{jk}|$ values, when deciding how many variables in subsets $A$ and $C$ to improve at each iteration of Steps 6 and 12 and, last but not least, when deciding how to improve the initial guesses within the same steps.

In fact, even the choice of 1 as the threshold of attention for $\alpha_i$, $\Gamma_{ijk}$, and $|\sigma_{jk}|$ is somewhat arbitrary: in case of convergence problems, one should try to reduce the values of those indicators, starting from the larger ones, until convergence is achieved. In some cases, even values of 1.5 or 2 could still be acceptable to achieve convergence, while in other cases it may be necessary to reduce them below 0.5 or even more.

From this point of view, different classes of problems, e.g., depending on the physical domain(s) involved, may require different strategies, that a human operator would learn by experience, and that could possibly be coded later into an actual computer-run algorithm. Developing these strategies goes beyond the scope of this paper, which only provides Algorithm 1 as a general operational guideline.

In particular, within the context of equation-based modelling, Algorithm 1 could be used as a basis to design a convenient user interface, which takes care of computing all the required indicators, to rank them in descending order, and to update them when the user inputs new improved guess values. The detailed design of such an interface is also beyond the scope of this paper.

4. Example cases

In this section, the practical usefulness and feasibility of the criteria and algorithm presented in the previous section are demonstrated in two example cases, one from the field of thermo-fluid systems, the other from electrical circuit theory.

4.1. Thermo-hydraulic system example

Consider a system comprising a heat exchanger, that absorbs heat from an environment at fixed temperature $T_a$. The working fluid, with specific heat capacity $c$, comes from a source at fixed pressure and temperature $p_s$, $T_s$. 
The fluid first flows through a shut-off valve, which is normally open and thus has a very large flow coefficient \( k_p \), corresponding to a small pressure drop, then flows through the heat exchanger, which has a certain pressure drop depending on the coefficient \( k_h \), and finally flows through a control valve with flow coefficient \( k_v \), that discharges at a fixed pressure \( p_d \). The heat duty \( Q \) depends on area \( A \) of the heat transfer surface, on the specific heat transfer coefficient \( \gamma \) that follows a power law depending on the flow rate \( w \), and on the difference between the environment temperature and the fluid average temperature.

The system is described by the following equations

\[
0 = f - k_p \sqrt{p_s - p_i} \quad (67)
\]
\[
0 = p_i - p_o - k_h f^2 \quad (68)
\]
\[
0 = f - k_v \sqrt{p_o - p_d} \quad (69)
\]
\[
0 = Q - fc(T_o - T_s) \quad (70)
\]
\[
0 = Q - \gamma A \left( T_a - \frac{T_s + T_o}{2} \right) \quad (71)
\]
\[
0 = \gamma - \gamma_0 \left( \frac{f}{f_0} \right)^\nu \quad (72)
\]

The goal of the problem is to find the value of the valve flow coefficient \( k_v \) that delivers a certain required heat duty \( Q \). Hence, \( p_s, p_d, k_p, k_h, c, f_0, \gamma_0, \nu, T_s, T_o, Q, A \) are known parameters, while \( x = w = [f \quad k_v \quad T_o \quad \gamma \quad p_o \quad p_i]^T \).

Taking \( p_s = 2.201, p_d = 1, k_p = \sqrt{1000}, k_h = 0.2, c = 1, f_0 = 1, \gamma_0 = 1, \nu = 0.8, T_s = 0, T_o = 6, Q = 4, A = 1 \), the system has an exact solution \( f = 1, k_v = 1, T_o = 4, \gamma = 1, p_o = 2, p_i = 2.2 \).

In this example, all variables affect the Jacobian, but they do not do so with the same intensity. The most strongly nonlinear equation is the first one (67), due to the very large flow coefficient \( k_p \), which leads to a very small pressure drop \( p_s - p_i \), the first equation residual is much more sensitive to errors in the initial guess of its nonlinear variable \( p_i \) than all the other ones. In fact, an error of 1% on the initial guess of \( p_i \) can have dramatic consequences on the convergence of NR’s algorithm, while all other variables can tolerate an initial guess with errors of 20 – 30% without substantially hampering the convergence.

It is expected that the criteria proposed in the previous section allow to get to the same conclusions automatically, without the need of any such expert insight on the mathematical properties of the system.

Table 1 reports the initial guesses \( w_0 \), the number of NR iterations, and all the relevant \( \alpha_i, \Gamma_{ijk}, \) and \( \Sigma \) indicators, corresponding to different choices of \( w_0 \). The NR algorithm is stopped when the absolute value of the largest increment after the last iteration is less than \( 10^{-12} \).

Since values of the indicators much smaller than unity are not relevant to the analysis, results are displayed with two decimal digits only, two avoid cluttering the presented results with irrelevant detail. Note that the residuals of the second, fourth, and fifth equations are second-degree polynomials, hence \( \alpha_2 = \alpha_4 = \alpha_5 = 0 \) irrespective of the chosen initial guess.
Table 1: Convergence analysis of heat exchanger test

| Var    | #1       | #2       | #3       | #4       | #5       | #6       |
|--------|----------|----------|----------|----------|----------|----------|
| $f$    | 0.99999  | 0.99999  | 0.99999  | 0.99999  | 0.99999  | 3.00     |
| $k_x$  | 0.99999  | 0.99999  | 0.99999  | 0.99999  | 0.99999  | 0.99999  |
| $T_b$  | 3.99996  | 3.996    | 3.6      | 3.6      | 3.996    | 3.996    |
| $\gamma$ | 0.99999 | 0.99999  | 0.99999  | 0.99999  | 0.99999  | 0.99999  |
| $p_0$  | 19.9998  | 1.998    | 1.8      | 1.8      | 1.998    | 1.998    |
| $p_1$  | 21.9998  | 2.198    | 2.178    | 1.98     | 2.151    | 2.198    |
| $N_{iter}$ | 3   | 5       | –       | –       | –       | –        |
| $\lambda$ | 1.00 | 1.00     | 0.49     | 0.49     | 0.49     | 0.70     |
| $\sigma_1$ | 0.00 | 0.27     | 0.68     | 1.33     | 0.90     | 0.18     |
| $\sigma_3$ | 0.00 | 0.00     | 0.00     | 0.06     | 0.00     | 0.051    |
| $\sigma_6$ | 0.00 | 0.00     | 0.00     | 0.00     | 0.00     | 0.029    |
| $\Gamma_{166}$ | 0.01 | 0.22     | 0.39     | 0.46     | 0.42     | 0.18     |
| $\Gamma_{211}$ | 0.00 | 0.00     | 0.11     | 0.01     | 0.51     | 0.58     |
| $\Gamma_{335}$ | 0.00 | 0.00     | 0.01     | 0.06     | 0.08     |          |
| $\Gamma_{355}$ | 0.00 | 0.00     | 0.02     | 0.26     | 0.06     |          |
| $\Gamma_{413}$ | 0.00 | 0.00     | 0.00     | 0.03     | 0.03     |          |
| $\Gamma_{534}$ | 0.00 | 0.00     | 0.01     | 0.05     | 0.05     | 0.67     |
| $\Gamma_{611}$ | 0.00 | 0.00     | 0.00     | 0.05     | 0.05     | 0.07     |

$$
\Sigma_1 = \begin{bmatrix}
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.01 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\end{bmatrix}
$$

$$
\Sigma_2 = \begin{bmatrix}
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\end{bmatrix}
$$

$$
\Sigma_3 = \begin{bmatrix}
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\end{bmatrix}
$$

$$
\Sigma_4 = \begin{bmatrix}
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\end{bmatrix}
$$

$$
\Sigma_5 = \begin{bmatrix}
-0.03 & 0.00 & 0.00 & 0.04 & 0.00 & 0.00 \\
-0.02 & -0.15 & -0.00 & 0.07 & 0.09 & 0.51 \\
-0.09 & 0.00 & -0.11 & -0.04 & 0.00 & 0.00 \\
-0.04 & 0.00 & 0.00 & 0.03 & 0.00 & 0.00 \\
-0.01 & 0.00 & 0.00 & 0.01 & 0.00 & -0.31 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -0.86 \\
\end{bmatrix}
$$

$$
\Sigma_6 = \begin{bmatrix}
-0.12 & 0.00 & -0.01 & 0.00 & 0.00 & 0.00 \\
-2.10 & -0.49 & -0.06 & 0.00 & 0.00 & -0.87 \\
-1.02 & 0.00 & 0.56 & -0.04 & 0.00 & 0.00 \\
-1.00 & 0.00 & 0.58 & -0.02 & 0.00 & 0.00 \\
-2.21 & 0.00 & -0.03 & 0.00 & 0.00 & 0.00 \\
-0.30 & 0.00 & -0.03 & 0.00 & 0.00 & -0.54 \\
\end{bmatrix}
$$
In Case #1, an initial guess very close to the solution is chosen, with a relative error of $-10^{-5}$ on the six nonlinear unknowns. NR’s algorithm converges in just three iterations. As expected, the values of $\alpha_i$ and $\Gamma_{ijk}$ and $\sigma_{jk}$ are all below 0.02, indicating an excellent initial guess.

In Case #2, an initial guess with a $-0.1\%$ error is chosen for the six nonlinear unknowns. NR’s algorithm converges in 5 iterations. The maximum $\alpha_i$ is $\alpha_1 = 0.27$, indicating that higher-order terms play some role in the first equation, while the maximum $\Gamma_{ijk}$ is $\Gamma_{166} = 0.22$, hence $\alpha = 0.27$ and $\beta = 0.22$. In this case, the sufficient condition of Theorem 5 applies with $\alpha + \beta = 0.49$, which guarantees a reduction of the nonlinear residual after the first iteration with respect to the nonlinear residual computed with the initial guess of a factor about 2 or more, which is consistent with the relatively fast convergence of the algorithm.

The values $\alpha_1 = 0.27$ and $\Gamma_{166} = 0.22$ indicate that the only equation responsible for some non-negligible nonlinear behaviour in the NR iteration is the first one, and the responsible unknown variable is the sixth one, i.e. $p_i$. This is confirmed by matrix $\Sigma$, whose significantly non-zero values are only found in the sixth column, indicating the influence of the sixth nonlinear unknown on itself, as well as on the second and fifth one ($k_v$ and $p_o$).

In Case #3, an initial guess with a $-1\%$ error is chosen for the six nonlinear unknowns. NR’s algorithm fails after the first iteration, because the value of $p_i$ causes the argument of the square root in the first equation to become negative. Following Algorithm 1, there are no values $\alpha_i > 1$, so it is possible to jump at Step 8 and continue the analysis based on $\Gamma_{ijk}$ and $\Sigma$ only.

In this case, the subset $C_1$ only contains the sixth unknown $p_i$, while the set $C_2$ is empty, so $C = \{p_i\}$. Since the increment of $p_i$ in the first iteration is positive, one can try to improve the initial value of $p_i$ by increasing it, e.g. by halving the initial value of the term $p_s - p_i$ that appears under square root, which means $p_i = 2.1994$; this causes NR’s algorithm to converge in 4 iterations.

In Case #4, an initial guess with a $-10\%$ error is chosen for the six nonlinear unknowns. In this case, $\alpha_1 > 1$, so one should first try to improve the initial guess of the nonlinear variable affecting it, $p_i$, which should be increased. As in the previous case, one could find a value that halves $p_s - p_i$, i.e. $p_i = 2.0905$, which however still results in $\alpha_1 > 1$ and causes convergence failure. Further halving $p_s - p_i$ leads to Case #5, with $\alpha_1 < 1$, but still no convergence; the analysis of $\Gamma_{ijk}$ and $\Sigma$ clearly indicates that the sixth unknown is still to blame, and should be further increased. By repetitively halving $p_s - p_i$, the values of $\Gamma_{166}$ and of the sixth column of $\Sigma$ are progressively reduced, until convergence is achieved in 5 iterations when $p_i = 2.1976$.

Note how the criteria introduced in the previous section clearly indicate in this case that it is not necessary to change the initial guesses of the other five nonlinear unknowns in order to eventually reach convergence - this is due to the weaker nonlinearity of the equations involving them, which is reflected in the low values of the corresponding $\Gamma_{ijk}$ and $\sigma_{jk}$ factors.

Finally, in Case #6 the initial guess of all variables except the first is taken very close to the solution as in Case #2; however, it is assumed that the initial
guess of the first variable $f$ is wrong by a factor 3, due to some gross mistake. NR’s algorithm fails after the first iteration due to negative square root arguments. All values of $\alpha_i$ are much less than one, so one can jump directly to Step 8 of Algorithm 1.

At this point, although there are no curvature factors greater than one, the three largest curvature factors are $\Gamma_{211} = 0.58$ and $\Gamma_{534} = 0.67$, pointing to the first, third, and fourth unknown variables as potentially responsible for the convergence failure. Hence, $C_1 = \{f, T_0, \gamma\}$. However, the values of \(|\sigma_{31}|\) and \(|\sigma_{41}|\) are about one, while \(|\sigma_{13}|\) and \(|\sigma_{14}|\) are close to zero, hence $C_2 = \{T_0, \gamma\}$ and thus $C = \{f\}$. Since the increment of $f$ is negative after the first iteration, one should then reduce its initial guess value until getting convergence, which is exactly what is expected from the a-priori knowledge of the solution.

4.2. DC circuit example

Consider an electrical DC circuit, where the series connection of $N$ resistors and one diode is connected to an ideal voltage source, which provides a certain power $P$. The system is described by the following set of implicit equations:

\begin{align*}
i - i_s e^{v_d/v_t} - 1 &= 0 \quad (73) \\
v i - P &= 0 \quad (74) \\
v - \sum_{j=1}^{N} v_j - v_d &= 0 \quad (75) \\
v_j - R i &= 0 \quad (76)
\end{align*}

where $i_s, v_t, P, R$ are known parameters, $x = [i, v_d, v, v_1, v_2, \cdots, v_N]^T$, $w = [i, v_d, v]^T$, $z = [v_1, v_2, \cdots, v_N]^T$.

There are only three non-zero curvature factors for this problem, namely $\Gamma_{122}$, corresponding to $v_d$, and $\Gamma_{211} = \Gamma_{231}$, corresponding to $i$ and $v$.

Taking $i_s = 6.9144 \cdot 10^{-13}, v_t = 25 \cdot 10^{-3}, P = 10.7, R = 1, N = 10$, the system has an exact solution $\bar{i} = 1, \bar{v}_d = 0.7, \bar{v} = 10.7, \bar{v}_j = 1$.

According to Criterion 1 in order to ensure fast and reliable convergence, accurate initial guesses should be provided for the unknowns $w$, while $z_0$ can be safely taken to be zero, since other choice leads to exactly the same results after each iteration. In this specific case, this means that only 3 variables out of 13 require to be properly initialized. Some experiments confirmed that the results after the first iteration are not affected at all from the values of $z_0$.

Table 2 reports the initial guesses $w_0$, the number of NR iterations, and all the relevant $\alpha_i, \Gamma_{ijk}$, and $\Sigma$ indicators, corresponding to different choices of $w_0$.

Note that $\alpha_2 = 0$ in all cases; this is due to the fact that the residual of the second equation is a second-order polynomial, so obviously its Taylor expansion lacks terms above second order.

In Case #1, an initial guess very close to the solution is chosen, with a relative error of $-10^{-5}$ on the three nonlinear unknowns. NR’s algorithm converges
Table 2: Convergence analysis of the DC circuit test case

| Var | #1       | #2       | #3       | #4       | #5       |
|-----|----------|----------|----------|----------|----------|
| i   | 0.99999  | 0.99     | 0.9      | 0.8      | 0.25     |
| v   | 10.699893| 10.63    | 9.63     | 8.56     | 2.675    |
| v_d | 0.699993 | 0.693    | 0.63     | 0.56     | 0.693    |
| N_iter | 2       | 4        | 18       | –        | 7        |
| α_1 | 0.00     | 0.02     | 3.2 · 10^5 | 5.7 · 10^8 | 2.73     |
| Γ_{122} | 0.17     | 8.47     | 102.14   | 2.58     |
| Γ_{213} | 0.00     | 0.0025   | 0.03     | 0.01     | 1.87     |

\[
\Sigma_1 = \begin{bmatrix} 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 \end{bmatrix}, \quad \Sigma_2 = \begin{bmatrix} -0.01 & 0.01 & -0.01 \\ 0.00 & -0.32 & 0.00 \\ 0.00 & -0.01 & 0.00 \end{bmatrix}
\]
\[
\Sigma_3 = \begin{bmatrix} -0.07 & 3.05 & -0.07 \\ -0.01 & -14.99 & -0.01 \\ -0.05 & -2.30 & -0.05 \end{bmatrix}, \quad \Sigma_4 = \begin{bmatrix} -0.23 & -1934.46 & -0.23 \\ 0.01 & -158.10 & 0.01 \\ 0.02 & -85.09 & 0.02 \end{bmatrix}
\]
\[
\Sigma_5 = \begin{bmatrix} -3.80 & 0.00 & -3.80 \\ -5.16 & -1.86 & -5.16 \\ -3.70 & 0.00 & -3.70 \end{bmatrix}
\]

In just two iterations. As expected, the values of α_i and Γ_{ijk} and σ_{jk} are all below 0.01, indicating an excellent initial guess.

In Case #2, an initial guess with a −1% error is chosen for the three nonlinear unknowns. NR’s algorithm converges in 4 iterations. The maximum α_i is α_1 = 0.02, indicating that higher-order terms play a negligible role in the first equation, while the maximum Γ_{ijk} is Γ_{122} = 0.17, hence α = 0.02 and β = 0.17. In this case, the sufficient condition of Theorem 5 applies with α + β = 0.19, which guarantees a reduction of the nonlinear residual after the first iteration with respect to the nonlinear residual computed with the initial guess of a factor about 5, which is consistent with the very fast convergence of the algorithm. The values Γ_{122} = 0.17 and |σ_{22}| = 0.32 indicate that the second nonlinear unknown v_d is solely responsible for some non-negligible nonlinear behaviour in the first equation, which is however not large enough to cause problems. This is obviously due to the strongly exponential behaviour of the diode equation with respect to v_d.

In Case #3, an initial guess with a −10% error is chosen for the three nonlinear unknowns. NR’s algorithm requires 18 iterations to converge. The large value α_1 = 3.2 · 10^5 clearly indicates that the cause of this difficult convergence is an error in the initial guess of only nonlinear variable appearing in the first equation, i.e., v_d, so, following Algorithm 1, one should try to improve the initial guess of that variable. Its positive increment suggests to increase it; in fact, increasing it by 0.05 to v_d = 0.68 reduces the number of iterations to 8, while increasing it by 0.10 to v_d = 0.73 reduces the number of iterations to 6. Note that it is not necessary to worry about the other initial guesses to substantially
improve the convergence performance.

In Case #4, an initial guess with a −20% error is chosen for the three nonlinear unknowns. NR’s algorithm fails at the second iteration because of badly conditioned Jacobian. The value of $\alpha_1$ reveals a huge contribution of the higher-order terms in the first equation - this is caused by the exponential in the first equation, which has a scaling factor $v_t = 0.025$, meaning that errors in $v_d$ significantly larger than the scaling factor have a dramatic impact on the behaviour of the equation residual. The result is a large overshoot of $w_{1,2} - w_{0,2}$ that brings $v_d$ so far away from the solution that the following iteration is not even possible to compute.

As in the previous case, the positive sign of the increment suggests to increase the initial guess of $v_d$, while the low values of $\alpha_2$, $\Gamma_{213}$, and $\sigma_{jk}, k \neq 2$, indicate that the initial guesses of $v$ and $i$ are close enough to the solution so as to not be a problem. An increase by 0.05 to $v_d = 0.61$ leads to convergence in 37 steps, with $\alpha_1 = 6.5 \cdot 10^{13}$ and $\Gamma_{122} = 21.85$; a further increase by 0.05 to $v_d = 0.66$ leads to convergence in 8 steps, with $\alpha_1 = 15.9$ and $\Gamma_{122} = 2.79$. Throughout these steps, all the indicators pertaining to the other two nonlinear variables remain well below unity.

In these first four cases, the information provided by the $\Sigma$ matrix is consistent with the information provided by $\alpha_i$ and $\Gamma_{ijk}$. More specifically, in the first two cases, where convergence is not critical, all elements of $\Sigma$ are smaller than one. In the third and fourth cases, where convergence is problematic or not achieved at all, the only column with numbers greater than one in magnitude is the second one, corresponding to variable $v_d$, which is the one whose initial guess actually needs to be fixed to improve the convergence.

In Case #5, the initial guess of $v_d$ has a small error of −1%, while the initial guess of the other two variables has a much larger error of −75%. NR’s algorithm converges in 7 steps, which is acceptable, but could be probably improved.

In this case, the information carried by Criterion 2 is misleading, because the values of $\alpha_1$, $\Gamma_{122}$, and $\Gamma_{213}$ apparently indicate that the initial guesses of all the three nonlinear unknowns should be improved. In fact, in this case we know a priori that the initial guess is quite good (only 1% off the solution), so we would expect to get an indication that $v$ and $i$ need an improvement of their start value (which we know to be badly off the mark), but not $v_d$. What happens in this case is that the initial guess of $v$ and $i$ causes a relatively small error in $v_d$ after one iteration, displacing it farther from the solution than the very good initial guess was. Due to the extremely nonlinear behaviour of the diode equation, this comparatively small error can nevertheless lead to values of the $\alpha_1$ and $\Gamma_{122}$ indicators which are larger than one.

In this case Criterion 4 provides the missing critical piece of information: $|\sigma_{21}| > 1$, while $|\sigma_{12}| \ll 1$. Similarly, $|\sigma_{23}| > 1$, while $|\sigma_{32}| \ll 1$. This means that an error in the initial guess of $v$ and $i$ has an influence on $v_d$ after the first iteration, but not the other way round. Criterion 4 as well as Algorithm 1 suggest in this case to provisionally remove $v_d$ from the set of initial guesses to improve, and only focus on $v$ and $i$. Given the positive increments of both variables, one can increase them, e.g., to 0.5 and 5, which reduces the number of
iterations to 6 but otherwise presents a similar situation, now with $|\sigma_{21}| = 1.26$, $|\sigma_{12}| = 0.0007$, $|\sigma_{23}| = 1.26$, $|\sigma_{32}| = 0.0007$. Then, one could further increase them, e.g., to 0.9 and 9, which leads to a further reduction of the number of iterations to 4 and brings all the indicators below unit magnitude.

5. Conclusion

In this paper, new theorems were presented concerning the choice of initial guess values for NR’s algorithm, when solving generic systems of nonlinear or mixed linear and nonlinear equations. Based on these theorems, four criteria and an algorithm were proposed to help choosing initial guess values for NR’s algorithm effectively.

Criterion 1, which is rigorous and only based on structural properties of the system of equations, suggests to only care about the initial guess of the subset of variables that influence the Jacobian of the nonlinear system; all other variables can be initially set to zero without any consequence on the convergence of NR’s algorithm.

Algorithm 1, which is based on heuristic criteria inspired by the theorems presented in Section 2, can be used in case of convergence failure of the NR solver, to identify those variables whose initial guesses are most likely the cause of the failure, and to suggest how to improve them to eventually achieve successful convergence of the iterative solution process.

Criterion 1 and Algorithm 1 were successfully demonstrated in two exemplary cases discussed in Section 4, an electrical circuit and a thermo-hydraulic system.

Algorithm 1 makes use of the non-dimensional indicators $\alpha_i$, $\Gamma_{ijk}$ and $\Sigma$, defined in Sections 2 and 3, which provide information about the second- and higher-order behaviour of the function residuals around the chosen initial guess, and thus require the first and second derivative of the equation residuals to be computed. The computation of these indicators require the Jacobian and Hessian matrices of the equation residuals; these can be computed analytically by symbolic differentiation, which is the standard approach taken by EOOLTs, or by numerical differentiation.

These indicators are invariant with respect to the scaling of the problem or, in other words, to the choice of measurement units of the involved variables, which is an important property for equations coming from physical system modelling.

In the context of EOOLTs, Criterion 1 can be used by developers of reusable model libraries, to identify which variables actually need good initial guesses, and thus to provide the proper infrastructure to do so, e.g. by providing ad-hoc parameters to be set by the end users. Algorithm 1 can instead be used by simulation tool developers, to provide meaningful diagnostic information in case of NR solver failures, guiding the end user towards the successful solution of the problem by means of a suitable graphical user interface.

The results of this paper are of course not limited to initialization problems in EOOLTs, but rather have a very broad applicability to any kind of problem.

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that requires the solution of implicit nonlinear (or mixed linear and nonlinear) systems of equations by means of NR’s algorithm.

6. Acknowledgements

The authors are grateful to colleagues Luca Bonaventura and Gianni Ferretti of Politecnico di Milano for their constructive comments on the first draft of the paper.

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

References

[1] I. K. Argyros and S. Hilout. Weaker conditions for the convergence of Newton’s method. *Journal of Complexity*, 28:364–387, 2012.

[2] P. I. Barton and C. C. Pantelides. The modeling of combined continuous and discrete processes. *AIChE Journal*, 40:966–979, 1994.

[3] W. Braun, F. Casella, and B. Bachmann. Solving large-scale Modelica models: new approaches and experimental results using OpenModelica. In *Proc. 12th International Modelica Conference*, pages 557–563, Prague, Czech Republic, May 15–17 2017.

[4] F. Cellier and E. Kofman. *Continuous System Simulation*. Springer-Verlag, 2006.

[5] T. A. Davis and E. P. Natarajan. Algorithm 907: KLU, a direct sparse solver for circuit simulation problems. *ACM Trans. Math. Softw.*, 37(3):36:1–36:17, Sept. 2010.

[6] P. Fritzson. *Principles of Object Oriented Modeling and Simulation with Modelica 3.3*. Wiley IEEE Press, 2014.

[7] A. Galantai. The theory of Newton’s method. *Journal of Computational and Applied Mathematics*, 124:25–44, 2000.

[8] L. V. Kantorovich and G. P. Akilov. *Functional Analysis in Normed Spaces*. Pergamon, Oxford, 1964.

[9] S. E. Mattsson, H. Elmqvist, and M. Otter. Physical system modeling with Modelica. *Control Engineering Practice*, 6(4):501–510, 1998.

[10] J. M. Ortega and W. C. Rheinboldt. *Iterative solution of nonlinear equations in several variables*. Academic Press, London and New York, 1970.

[11] C. Pantelides. The consistent initialization of differential-algebraic systems. *SIAM Journal on Scientific and Statistical Computing*, 9(2):213–231, 1988.
[12] M. Sielemann, F. Casella, and M. Otter. Robustness of declarative modeling languages: Improvements via probability-one homotopy. *Simulation Modelling Practice and Theory*, 38:38–57, 2013.

[13] M. Sielemann, F. Casella, M. Otter, C. Clauß, J. Eborn, S. E. Mattsson, and H. Olsson. Robust initialization of differential-algebraic equations using homotopy. In C. Clauss, editor, *Proceedings 8th International Modelica Conference*, pages 75–85, Dresden, Germany, Mar. 20–22 2011. Modelica Association.