SOLVING NONLINEAR SYSTEMS OF EQUATIONS VIA SPECTRAL RESIDUAL METHODS: STEPSIZE SELECTION AND APPLICATIONS

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Abstract. Spectral residual methods are derivative-free and low-cost per iteration procedures for solving nonlinear systems of equations. They are generally coupled with a nonmonotone line search strategy and compare well with Newton-based methods for large nonlinear systems and sequences of nonlinear systems. The residual vector is used as the search direction and choosing the steplength has a crucial impact on the performance. In this work we address both theoretically and experimentally the steplength selection and provide results on a real application such as a rolling contact problem.

Keywords. Nonlinear systems of equations, spectral gradient methods, steplength selection, approximate norm descent methods

1. Introduction. This work addresses the solution of the nonlinear system of equations

\[ F(x) = 0, \]

with \( F : \mathbb{R}^n \to \mathbb{R}^n \) continuously differentiable, by means of spectral residual methods. Spectral residual methods were introduced in [25] and starting from the proposal in [26] consist of iterative procedures for solving (1.1) without the use of derivative information. Given the iterate \( x_k \), these methods use the residual vectors \( \pm F(x_k) \) in a systematic way and select the step \( x_{k+1} - x_k \) along either the direction \((-\beta_k F(x_k))\) or \((\beta_k F(x_k))\) with \( \beta_k \) being a nonzero steplength inspired by the Barzilai and Borwein method for the unconstrained minimization problem \( \min_{x \in \mathbb{R}^n} f(x) \). Similarly to the Barzilai and Borwein method for unconstrained optimization, \( \|F\| \) does not decrease monotonically along iterations and its effectiveness heavily relies on the steplength \( \beta_k \) used.

Spectral residual methods have received a large attention since they are low-cost per iteration and require a low memory storage being matrix free, see e.g. [21, 25–27, 31, 34, 35, 41]. They belong to the class of Quasi-Newton methods which are particularly attractive when the Jacobian matrix of \( F \) is not available analytically or its computation is not relatively easy. Quasi-Newton methods showed to be effective both in the solution of large nonlinear systems and in the solution of sequences of medium-size nonlinear systems as those arising in applications where sequences are generated by model refinement procedures, see e.g. [5,21,25,26,31,41].

It is well known that the performance of the Barzilai and Borwein method does not depend on the decrease of the objective function at each iteration but relies on the relationship between the steplengths used and the eigenvalues of the average Hessian matrix of \( f \) [3,15,36]. Based on such feature, several strategies for steplength selection have been proposed to enhance the performance of the method, see e.g., [8,10,12,15,16]. On the other hand, to our knowledge, an analogous study of the relationship between the steplengths originated by spectral methods and the eigenvalues of the average Jacobian matrix of \( F \) has not been carried out, and the impact of the choice of the steplengths on the convergence history has not been investigated in details. The aim of this paper is to analyze the properties of the spectral residual steplengths and study how they affect the performance of the methods. This aim is addressed both from a theoretical and experimental point of view.

The main contributions of this work are: the theoretical analysis of the steplengths proposed in the literature and of their impact on the norm of \( F \) also with respect to the nonmonotone

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behaviour imposed by globalization strategies; the analysis of the performance of spectral methods with various rule for updating the steplengths. Rules based on adaptive strategies that suitably combine small and large steplengths result by far more effective than rules based on static choices of $\beta_k$ and, inspired by the steplength rules proposed in the literature for unconstrained minimization problems, we propose and extensively test adaptive steplength strategies. Numerical experience is conducted on sequences of nonlinear systems arising from rolling contact models which play a central role in many important applications, such as rolling bearings and wheel-rail interaction [23,24]. Solving these models gives rise to sequences which consist of a large number of medium-size nonlinear systems and represent a relevant benchmark test set for the purpose of this work.

The paper is organized as follows. Section 2 introduces spectral residual methods. In Section 3 and 4 we provide a theoretical analysis of the steplengths including their impact on the behaviour of $\|F_k\|$ and on a standard nonmonotone linesearch. In Section 5 we introduce the spectral residual method used in our tests and provide a theoretical investigation. The experimental part is developed in Section 6 where we describe several strategies for selecting the steplength, introduce our test set and discuss the numerical results obtained. Some conclusions are presented in Section 7.

1.1. Notations. The symbol $\|\cdot\|$ denotes the Euclidean norm, $I$ denotes the identity matrix, $J$ denotes the Jacobian matrix of $F$. Given a symmetric matrix $M$, $\{\lambda_i(M)\}_{i=1}^n$ denotes the set of eigenvalues of $M$, $\lambda_{\text{min}}(M)$ and $\lambda_{\text{max}}(M)$ denote the minimum and maximum eigenvalue of $M$ respectively, and $\{v_i\}_{i=1}^n$ denotes a set of associated orthonormal eigenvectors. Given a sequence of vectors $\{x_k\}$, for any function $f$ we let $f_k = f(x_k)$.

2. Preliminaries. In the seminal paper [2] Barzilai and Borwein proposed a gradient method for the unconstrained minimization

$$
\min_{x \in \mathbb{R}^n} f(x),
$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is a given differentiable function. Given an initial guess $x_0 \in \mathbb{R}^n$, the Barzilai-Borwein (BB) iteration is defined by

$$
x_{k+1} = x_k - \alpha_k \nabla f_k,
$$

where $\alpha_k$ is a positive steplength inspired by Quasi-Newton methods for unconstrained optimization [11]. In Quasi-Newton methods, the step $p_k = x_{k+1} - x_k$ solves the linear system

$$
B_k p_k = -\nabla f_k,
$$

and $B_k$, $k \geq 1$, satisfies the secant equation, i.e.,

$$
B_k p_{k-1} = z_{k-1}, \quad p_{k-1} = x_k - x_{k-1}, \quad z_{k-1} = \nabla f_k - \nabla f_{k-1}.
$$

Letting $B_k = \alpha^{-1} I$ and imposing condition (2.4), Barzilai and Borwein derived two steplengths which are the least-square solutions of the following problems:

$$
\alpha_{k,1} = \arg\min_{\alpha} \|\alpha^{-1} p_{k-1} - z_{k-1}\|^2_2 = \frac{p_{k-1}^T p_{k-1}}{p_{k-1}^T z_{k-1}},
$$

$$
\alpha_{k,2} = \arg\min_{\alpha} \|p_{k-1} - \alpha z_{k-1}\|^2_2 = \frac{p_{k-1}^T z_{k-1}}{z_{k-1}^T z_{k-1}}.
$$

The second least-squares formulation is obtained from the first by symmetry. The steplength $\alpha_k$ in (2.2) is set to be positive, bounded away from zero and not too large, i.e., $\alpha_k \in [\alpha_{\text{min}}, \alpha_{\text{max}}]$ for some positive $\alpha_{\text{min}}, \alpha_{\text{max}}$; to this end, one of the two scalars $\alpha_{k,1}, \alpha_{k,2}$ is used and the thresholds $\alpha_{\text{min}}, \alpha_{\text{max}}$ are applied to it, see e.g., [12,13].

Choosing $B_k = \alpha^{-1} I$ yields a low-cost iteration while the use of the steplengths $\alpha_{k,1}, \alpha_{k,2}$ yields a considerable improvement in the performance with respect to the classical steepest descent
method \cite{2,15}. The BB method is commonly employed in the solution of large unconstrained optimization problems \cite{21} and the behaviour of the sequence \{f(x_k)\} is typically nonmonotone, possibly severely nonmonotone, in both the cases of quadratic and general nonlinear functions \(f\). The performance of the BB method depends on the relationship between the steplength \(\alpha_k\) and the eigenvalues of the average Hessian matrix \(\int_0^1 \nabla^2 f(x_{k-1} + t p_{k-1}) dt\); hence this approach is also denoted as spectral method and an extensive investigation on steplength’s selection has been carried on \cite{8,10,12,15,16}.

The extension of this approach to the solution of nonlinear systems of equations \cite{15} was firstly proposed by La Cruz and Raydan in \cite{25}. Here we summarize such a proposal and the issues that were inherited by subsequent procedures falling into such framework and designed for both general nonlinear systems \cite{21,25–27,31,34,41} and for monotone nonlinear systems \cite{1,29,30,32,40,44}. Instead of applying the spectral method to the merit function

\[ f(x) = \|F(x)\|^2, \] (2.7)

the BB approach is specialized to the Newton equation yielding the so-called spectral residual method. Thus, let \(p_–\) satisfy the linear system

\[ B_k p_– = -F_k, \] (2.8)

and let \(B_k = \beta^{-1}I\) satisfy the secant equation

\[ B_k p_{k-1} = y_{k-1}, \quad p_{k-1} = x_k - x_{k-1}, \quad y_{k-1} = F_k - F_{k-1}. \]

Reasoning as in BB method, two steplengths are derived:

\[ \beta_{k,1} = \frac{p_{k-1}^T p_{k-1}}{p_{k-1}^T y_{k-1}}, \] (2.9)

\[ \beta_{k,2} = \frac{p_{k-1}^T y_{k-1}}{y_{k-1}^T y_{k-1}}. \] (2.10)

These scalars may be positive, negative or even null; moreover \(\beta_{k,1}\) is not well defined if \(p_{k-1}^T y_{k-1} = 0\) and \(\beta_{k,2}\) is not well defined if \(y_{k-1} = 0\). In practice, the steplength \(\beta_k\) is chosen equal either to \(\beta_{k,1}\) or to \(\beta_{k,2}\) as long as it results to be bounded away from zero and \(|\beta_k|\) is not too large, i.e., \(|\beta_k| \in [\beta_{\text{min}}, \beta_{\text{max}}]\) for some positive \(\beta_{\text{min}}, \beta_{\text{max}}\). The step resulting from (2.8) turns to be of the form \(p_- = -\beta_k F_k\). But, once \(\beta_k\) is fixed, the \(k\)th iteration of the spectral residual method employs the residual directions \(\pm F_k\) in a systematic way and tests both the steps

\[ p_- = -\beta_k F_k \quad \text{and} \quad p_+ = +\beta_k F_k, \]

for acceptance using a suitable linesearch strategy. The use of both directions \(\pm F_k\) is motivated by the fact that, contrary to \((-\alpha_k \nabla f_k), \alpha_k > 0\), in (2.2), \((-\beta_k F_k)\) is not necessarily a descent direction for (2.7) at \(x_k\); the value \(\nabla f_k^T (-\beta_k F_k) = -2\beta_k F_k^T J_k F_k\) could be positive, negative or null. On the other hand, if \(F_k^T J_k F_k \neq 0\), trivially either \((-\beta_k F_k)\) or \(\beta_k F_k\) is a descent direction for \(f\).

Analogously to the spectral method, the spectral residual method is characterized by a nonmonotone behaviour of \{\(\|F_k\|\}\) and is implemented using nonmonotone line search strategies. The adaptation of the spectral method to nonlinear systems is low-cost per iteration since the computation of \(\beta_{k,1}\) and \(\beta_{k,2}\) is inexpensive and the memory storage is low, and turned out to be effective in the solution of medium and large nonlinear systems, see e.g., \cite{21,25,27,34,41}.

Unlike the context of BB method for unconstrained optimization, to our knowledge a systematic analysis of the stepsizes \(\beta_{k,1}\) and \(\beta_{k,2}\) in the context of the solution of nonlinear systems and their impact on convergence history has not been carried out. The steplength \(\beta_{k,1}\) has been used in most of the works on this subject \cite{25,27,31,34}. On the other hand, in \cite{21} it was observed experimentally that alternating \(\beta_{k,1}\) and \(\beta_{k,2}\) along iterations was beneficial for the performance
and in [41] it was observed experimentally that using $\beta_{k,2}$ performed better in terms of robustness with respect to using $\beta_{k,1}$.

In the next two sections we will analyze the two steplengths $\beta_{k,1}$ and $\beta_{k,2}$ and provide: their expression in terms of the spectrum of average matrices associated to the Jacobian matrix of $F$; their mutual relationship; their impact on the behaviour of $\|F_k\|$ and on a standard nonmonotone linesearch.

The matrices involved in our analysis are the following. Given a square matrix $A$, we let $A_S = \frac{1}{2}(A + A^T)$ be the symmetric part of $A$, $G_{k-1}$ be the average matrix associated to the Jacobian $J$ of $F$ around $x_{k-1}$

$$G_{k-1} \overset{\text{def}}{=} \int_0^1 J(x_{k-1} + t p_{k-1}) dt,$$  \hspace{1cm} (2.11)

and $(G_S)_{k-1}$ be the average matrix associated to the symmetric part $J_S$ of $J$ around $x_{k-1}$

$$(G_S)_{k-1} \overset{\text{def}}{=} \int_0^1 J_S(x_{k-1} + t p_{k-1}) dt.$$  \hspace{1cm} (2.12)

Moreover, given a symmetric matrix $M$ and a nonzero vector $p$, we employ the Rayleigh quotient defined as

$$q(M, p) = \frac{p^T M p}{p^T p},$$  \hspace{1cm} (2.13)

and the following property [18, Theorem 8.1-2]

$$\lambda_{\min}(M) \leq q(M, p) \leq \lambda_{\max}(M).$$  \hspace{1cm} (2.14)

3. Analysis of the steplengths $\beta_{k,1}$ and $\beta_{k,2}$. We analyze the stepsizes $\beta_{k,1}$ and $\beta_{k,2}$ given in (2.9) and (2.10) making the following assumptions.

**Assumption 3.1.** The scalars $\beta_{k,1}$ and $\beta_{k,2}$ are well defined and nonzero.

**Assumption 3.2.** Given $x$ and $p$, $F$ is continuously differentiable in an open convex set $D \subset \mathbb{R}^n$ containing $x + tp$ with $t \in [0, 1]$.

We note that Assumption 3.1 holds whenever $p_{k-1}^T y_{k-1} \neq 0$.

In the following lemma we analyze the mutual relationship between the stepsizes $\beta_{k,1}$ and $\beta_{k,2}$ and give their characterization in terms of suitable Rayleigh quotients for the average matrices in (2.11) and (2.12). We use repeatedly the property

$$p^T A p = p^T A_S p,$$  \hspace{1cm} (3.1)

which holds for any square matrices $A$, $A_S = \frac{1}{2}(A + A^T)$, and any vector $p$ of suitable dimension.

**Lemma 3.3.** Let Assumption 3.1 hold and Assumption 3.2 hold with $x = x_{k-1}$, $p = p_{k-1} = \pm \beta_{k-1} F_{k-1}$. The steplengths $\beta_{k,1}$, $\beta_{k,2}$ are such that:

P1) they have the same sign and $|\beta_{k,2}| \leq |\beta_{k,1}|$;

P2) either it holds $\beta_{k,1} \leq \beta_{k,2} < 0$ or $0 < \beta_{k,2} \leq \beta_{k,1}$;

P3) they take the form

$$\beta_{k,1} = \frac{1}{q(G_S)_{k-1, p_{k-1}}} = \frac{1}{q(G_S)_{k-1, F_{k-1}}},$$  \hspace{1cm} (3.2)

and

$$\beta_{k,2} = \frac{q((G_S)_{k-1, p_{k-1}})}{q(G^T_{k-1} G_{k-1}, p_{k-1})} = \frac{q((G_S)_{k-1, F_{k-1}})}{q(G^T_{k-1} G_{k-1}, F_{k-1})},$$  \hspace{1cm} (3.3)

with $q(\cdot, \cdot)$ being the Rayleigh quotient in (2.13), $G_{k-1}$ and $(G_S)_{k-1}$ being the matrices in (2.11) and (2.12), respectively.
Proof. By (2.9) and (2.10), we can write

\[ \beta_{k,2} = \frac{p_{k-1}^T p_{k-1}}{p_{k-1}^T y_{k-1} y_{k-1} (p_{k-1}^T p_{k-1})} \]

\[ = \beta_{k,1} \frac{\|p_{k-1}\|^2 \|y_{k-1}\|^2 \cos^2 \varphi_{k-1}}{\|p_{k-1}\|^2 \|y_{k-1}\|^2} \]

\[ = \beta_{k,1} \cos^2 \varphi_{k-1}, \] \hspace{1cm} (3.4)

where \( \varphi_{k-1} \) is the angle between \( p_{k-1} \) and \( y_{k-1} \), and P1) follows.

Property P2) follows as well since \( \beta_{k,2} \neq 0 \) by Assumption 3.1.

As for property P3), by the Mean Value Theorem [11, Lemma 4.1.9] and (2.11) we have

\[ y_{k-1} = F_k - F_{k-1} = \int_0^1 J(x_{k-1} + tp_{k-1})p_{k-1} \, dt = G_{k-1}p_{k-1}. \]

Then using (3.1) and (2.13), \( \beta_{k,1} \) takes the form

\[ \beta_{k,1} = \frac{p_{k-1}^T p_{k-1}}{p_{k-1}^T G_{k-1}p_{k-1}} = \frac{p_{k-1}^T p_{k-1}}{p_{k-1}^T (G_k)_{k-1}p_{k-1}} = \frac{1}{q((G_k)_{k-1}, p_{k-1})}, \]

while \( \beta_{k,2} \) takes the form

\[ \beta_{k,2} = \frac{p_{k-1}^T G_{k-1}p_{k-1}}{p_{k-1}^T (G_k)_{k-1}p_{k-1}} = \frac{q((G_k)_{k-1}, p_{k-1})}{q((G_k)_{k-1}, p_{k-1})}. \]

The rightmost equalities in (3.2) and (3.3) easily follow using the form of the step \( p_{k-1} = \pm \beta_{k,1} F_{k-1} \).

The above characterization P3) allows to derive bounds on the stepsizes \( \beta_{k,1} \) and \( \beta_{k,2} \) diversifying cases according to the spectral properties of the Jacobian matrix and the average matrices in (2.11) and (2.12). The relationship between \( \beta_{k,1} \) and the spectral information of the symmetric part of average matrix (2.11) was observed in [25-26-34] but the following results are not contained in such references.

**Lemma 3.4.** Let Assumption 3.1 hold and Assumption 3.2 hold with \( x = x_{k-1}, p = p_{k-1} \). Then, the steplengths \( \beta_{k,1} \) and \( \beta_{k,2} \) are such that:

(i) If the Jacobian \( J \) is symmetric and positive definite on the line segment in between \( x_{k-1} \) and \( x_{k-1} + p_{k-1} \) then \( \beta_{k,1} \) and \( \beta_{k,2} \) are positive and

\[ \frac{1}{\lambda_{\max}(G_{k-1})} \leq \beta_{k,2} \leq \beta_{k,1} \leq \frac{1}{\lambda_{\min}(G_{k-1})}; \] \hspace{1cm} (3.5)

(ii) if \( (G_k)_{k-1} \) in (2.12) is positive definite, then \( \beta_{k,1} \) and \( \beta_{k,2} \) are positive and

\[ \max \left\{ \frac{1}{\lambda_{\max}((G_k)_{k-1})}, \beta_{k,2} \right\} \leq \beta_{k,1} \leq \frac{1}{\lambda_{\min}((G_k)_{k-1})}, \] \hspace{1cm} (3.6)

\[ \frac{\lambda_{\min}((G_k)_{k-1})}{\lambda_{\max}(G_{k-1}^T G_{k-1})} \leq \beta_{k,2} \leq \min \left\{ \frac{\lambda_{\max}((G_k)_{k-1})}{\lambda_{\min}(G_{k-1}^T G_{k-1})}, \beta_{k,1} \right\}; \]

(iii) if \( (G_k)_{k-1} \) in (2.12) is indefinite and \( G_{k-1} \) in (2.11) is nonsingular, then

(iii.1) \( \beta_{k,1} \) satisfies either

\[ \beta_{k,1} \leq \min \left\{ \frac{1}{\lambda_{\min}((G_k)_{k-1})}, \beta_{k,2} \right\} \text{ or } \beta_{k,1} \geq \max \left\{ \frac{1}{\lambda_{\max}((G_k)_{k-1})}, \beta_{k,2} \right\}; \] \hspace{1cm} (3.8)
(iii.2) $\beta_{k,2}$ satisfies either
\[
0 < \beta_{k,2} \leq \min \left\{ \frac{\lambda_{\max}((G_S)_{k-1})}{\lambda_{\min}(G_{k-1}^T G_{k-1})}, \beta_{k,1} \right\},
\]

or
\[
\max \left\{ \frac{\lambda_{\min}((G_S)_{k-1})}{\lambda_{\max}(G_{k-1}^T G_{k-1})}, \beta_{k,1} \right\} \leq \beta_{k,2} < 0.
\]

**Proof.** Consider properties P1), P2) and P3) from Lemma 3.3

(i) Steplengths $\beta_{k,1}$ and $\beta_{k,2}$ are positive due to (3.2), (3.3). The rightmost inequality of (3.5) follows from (3.2) and (2.14). The remaining part of (3.5) is proved observing that (3.3) yields
\[
\beta_{k,2} = \frac{p_{k-1}^T G_{k-1}^{1/2} G_{k-1}^{1/2} p_{k-1}}{p_{k-1}^T G_{k-1}^{1/2} G_{k-1}^{1/2} p_{k-1}} = \frac{1}{q(G_{k-1}, G_{k-1}^{1/2} G_{k-1}^{1/2} p_{k-1})},
\]

and using P2) and (2.14).

(ii) Using (3.2), (2.14) and P2) we get positivity of $\beta_{k,1}$ and (3.6). Consequently, $\beta_{k,2}$ is positive by property P1), and bounds (3.7) can be derived using (3.3), (2.14) and item P2) of Lemma 3.3

(iii) If $(G_S)_{k-1}$ is indefinite then its extreme eigenvalues have opposite sign, i.e., $\lambda_{\min}((G_S)_{k-1}) < 0$ and $\lambda_{\max}((G_S)_{k-1}) > 0$. Hence, (3.2), (2.14) and P2) give (3.8). Moreover, since $G_{k-1}^T G_{k-1}$ is symmetric and positive definite, we can use, as before, P1) and (2.14) and get (3.9) and (3.10).

\[\square\]

**Remark 3.5.** Lemma 3.4 easily extends to the case where matrices are negative definite.

Item (ii) of Lemma 3.4 includes the case where $F$ is strictly monotone, i.e., $(F(x) - F(y))^T(x - y) > 0$ for any $x, y \in \mathbb{R}^n$ with $x \neq y$, see e.g. [14].

4. On the impact of the steplength $\beta_k$ on $\|F_{k+1}\|$. In this section we investigate how the choice of the steplength $\beta_k$ may affect $\|F_{k+1}\|$ in a spectral residual method. Results are first derived using a generic $\beta_k$ and discussed thereafter with respect to the choice of either $\beta_{k,1}$ or $\beta_{k,2}$.

The first result concerns the case where $J$ is symmetric and analyzes the residual vector $F_{k+1}$ componentwise. It heavily relies on the existence of a set of orthonormal eigenvectors for the average matrix $G_k$.

**Lemma 4.1.** Suppose that Assumption 3.2 holds with $x = x_k$ and $p = p_k$ and that the Jacobian $J$ is symmetric. Let $p_k = p_+ = -\beta_k F_k \neq 0$, $x_{k+1} = x_k + p_k$, $\{\lambda_i(G_k)\}_{i=1}^n$ be the eigenvalues of matrix $G_k$ in (2.17) and $\{v_i\}_{i=1}^n$ be a set of associated orthonormal eigenvectors. Let $F_k$ and $F_{k+1}$ be expressed as
\[
F_k = \sum_{i=1}^n \mu_k^i v_i, \quad F_{k+1} = \sum_{i=1}^n \mu_{k+1}^i v_i,
\]
where $\mu_k^i, \mu_{k+1}^i, i = 1, \ldots, n$, are scalars. Then
\[
F_{k+1} = (I - \beta_k G_k) F_k, \quad \mu_{k+1}^i = \mu_k^i (1 - \beta_k \lambda_i(G_k)), \quad i = 1, \ldots, n.
\]

Moreover, it holds:
(a) if $\beta_k \lambda_i(G_k) = 1$, then $|\mu_{k+1}^i| = 0$;
(b) if $0 < \beta_k \lambda_i(G_k) < 2$, then $|\mu_{k+1}^i| < |\mu_k^i|$; otherwise $|\mu_{k+1}^i| \geq |\mu_k^i|$.
Proof. The Mean Value Theorem [11, Lemma 4.1.9] gives
\[ F_{k+1} = F_k + \int_0^1 J(x_k + tp_k)p_k \, dt, \]
and \( p_k = -\beta_k F_k \) and (2.11) yield (4.1). Moreover, since \( \{v_i\}_{i=1}^n \) are orthonormal we have for \( i = 1, \ldots, n \)
\[
\mu_{i,k+1} = (v_i)^T F_{k+1} = (v_i)^T (I - \beta_k G_k) F_k = \mu_i^k (1 - \beta_k \lambda_i(G_k)),
\]
i.e., equation [4.2]. Consequently, Item (a) follows trivially; Item (b) follows noting that \( |1 - \beta_k \lambda_i(G_k)| < 1 \) if and only if \( 0 < \beta_k \lambda_i(G_k) < 2 \). \( \square \)

Remark 4.2. Lemma [4.4] trivially extends to the case where \( p_k = p_+ = \beta_k F_k \).

If the nonlinear system [11] represents the first-order optimality condition of the optimization problem (2.1) where \( f(x) = \frac{1}{2} x' Ax - b' x \) is quadratic and \( A \) is symmetric and positive definite, then the previous lemma reduces to well known results on the behaviour of the gradient method in terms of the spectrum of the Hessian matrix \( A \), see [36]. In fact, the nonlinear residual is \( F(x) = Ax - b \) and its Jacobian is constant \( J(x) = A, \forall x \). Then the following strict relationship between \( F_k \) and the \( i \)th eigenvalue \( \lambda_i(A) \) of the Jacobian holds throughout the iterations
\[
\mu_{i,k+1} = \mu_i^k (1 - \beta_k \lambda_i(A)) = \mu_0^i \prod_{j=0}^{k} (1 - \beta_j \lambda_i(A)),
\]
where \( \mu_{i,k+1} \) and \( \mu_i^k \), \( i = 1, \ldots, n \), are the eigencomponents of \( F_{k+1} \) and \( F_k \) respectively, with respect to the eigendecomposition of \( A \). As a consequence, a small steplength \( \beta \), i.e., close to \( 1/\lambda_{\text{max}}(A) \), can significantly reduce the values \( |\mu_{i,k+1}| \) corresponding to large eigenvalues \( \lambda_i(A) \) while a small reduction is expected for the scalars \( |\mu_{i+1}^k| \) corresponding to small eigenvalues \( \lambda_i(A) \). On the contrary, a large steplength \( \beta \), i.e., close to \( 1/\lambda_{\text{min}}(A) \), can significantly reduce the values \( |\mu_{i+1}^k| \) corresponding to small eigenvalues \( \lambda_i(A) \) while tends to increase the scalar \( |\mu_{i+1}^k| \) corresponding to large eigenvalues \( \lambda_i(A) \). This offers some intuition for choosing the steplenghts by alternating in a balanced way small and large steplenghts in order to reduce the eigencomponents, see e.g., [12, p. 178].

On the other hand, if \( F \) is a general nonlinear mapping then \( G_k \) changes at each iteration and Lemma [4.1] suggests the expected change of \( F \) from iteration \( k \) to iteration \( k+1 \) and the following guidelines. The first guideline concerns the case where \( J \) is positive definite. A nonmonotone behaviour of the sequence \( \{||F_k||\} \) is expected. By Item (i) of Lemma [4.4] both \( \beta_{k,1} \) or \( \beta_{k,2} \) are positive and \( \beta_k \lambda_i(G_k) \) lies in the interval \( \left[ \frac{\lambda_i(G_k)}{\lambda_{\text{max}}(G_{k-1})}, \frac{\lambda_i(G_k)}{\lambda_{\text{min}}(G_{k-1})} \right] \) for \( i = 1, \ldots, n \). Assuming without loss of generality that the eigenvalues are numbered in nondecreasing order, by standard arguments on perturbation theory for the eigenvalues it holds
\[
|\lambda_i(G_k) - \lambda_i(G_{k-1})| \leq ||G_k - G_{k-1}||,
\]
i.e., \( \lambda_i(G_k) - \lambda_i(G_{k-1}) \) lies in the interval \( \left[ \frac{\lambda_i(G_k)}{\lambda_{\text{max}}(G_{k-1})}, \frac{\lambda_i(G_k)}{\lambda_{\text{min}}(G_{k-1})} \right] \) for \( i = 1, \ldots, n \).\[18\] Theorem 8.1-6. Thus, if the Jacobian is Lipschitz continuous in an open convex set containing \( x_{k-1} + tp_{k-1} \) and \( x_k + tp_k \) with constant \( L_J > 0 \), it follows
\[
||G_k - G_{k-1}|| \leq \frac{L_J}{2} \left( ||p_{k-1}|| + ||p_k|| \right).
\]
Hence, if \( ||p_{k-1}|| \) and/or \( ||p_k|| \) are large, by Item (b) no decrease of \( \mu_{i,k+1}^k \) may occur. On the contrary, for small values of \( ||p_{k-1}|| \) and \( ||p_k|| \), as occurs if \( \{x_k\} \) is convergent, \( G_k \) undergoes small
changes with respect to $G_{k-1}$ and the behaviour of $\mu'_{k+1}$ shows similarities with the case where $J$ is constant. Thus, a small steplength $\beta_k$ close to $1/\lambda_{\max}(G_{k-1})$ can significantly reduce the scalars $|\mu'_{k+1}|$ corresponding to large eigenvalues $\lambda_i(G_k)$, while a small reduction is expected for the values $|\mu'_{k+1}|$ corresponding to small eigenvalues $\lambda_i(G_k)$. A large steplength $\beta_k$ close to $1/\lambda_{\min}(G_{k-1})$ can significantly reduce the scalars $|\mu'_{k+1}|$ corresponding to small eigenvalues $\lambda_i(G_k)$ while tends to increase the eigencomponents $|\mu_{k+1}|$ corresponding to large eigenvalues $\lambda_i(G_k)$. As for the case of a constant Jacobian, these features suggest to choose the steplengths by alternating in a balanced way small and large steplengths in order to reduce the eigencomponents.

The second guideline concerns the case where $J$ is indefinite and $\lambda_{\min}(G_k) < 0 < \lambda_{\max}(G_k)$. If $\beta_k > 0$, from Item (b) it follows that $|\mu'_{k+1}|$ corresponding to positive $\lambda_i(G_k)$ are smaller than $|\mu_k|$ if $\beta_k\lambda_i(G_k)$ is small enough while all $|\mu'_{k+1}|$ corresponding to negative eigenvalues increase with respect to $|\mu_k|$ and the amplification depends on the magnitude of $\beta_k\lambda_i(G_k)$. If $\beta_k < 0$ similar conclusions hold. In general, a nonmonotone behaviour of the sequence $\{\|F_k\|\}$ is expected but a possibly large increase of $\|F_{k+1}\|$ with respect to $\|F_k\|$ does not occur if $\{||\beta_k\lambda_i(G_k)||\}_{i=1,...,n}$ are small or of moderate size. Since a small value of $\{||\beta_k\lambda_i(G_k)||\}_{i=1,...,n}$ might be induced by a small value of $|\beta_k|$, the use of $\beta_{k,2}$ might be advisable taking into account that $|\beta_{k,2}| \leq |\beta_{k,1}|$ and $\beta_{k,1}$ can arbitrarily grow in the indefinite case (see Lemma 3.4).

4.1. On the impact of the steplength $\beta_k$ in the approximate norm descent line-search. In this section we embed the spectral residual method in a general globalization scheme based on the so-called approximate norm descent condition [28]

$$\|F_{k+1}\| \leq (1 + \eta_k)\|F_k\|, \quad (4.3)$$

where $\{\eta_k\}$ is a positive sequence satisfying

$$\sum_{k=0}^{\infty} \eta_k < \eta < \infty. \quad (4.4)$$

Intuitively, large values of $\eta_k$ allow a highly nonmonotone behaviour of $\|F_k\|$ while small values of $\eta_k$ promote the decrease of $\|F\|$. Several linesearch strategies in the literature fall in this scheme [19][28][31][34]. The main idea is that, given $x_k$, the steps take the form

$$p_- = -\gamma_k\beta_k F_k \quad \text{or} \quad p_+ = +\gamma_k\beta_k F_k \quad (4.5)$$

where the sign $\pm$ and $\gamma_k \in (0, 1]$ are selected so that (4.3) is satisfied. The scalar $\gamma_k$ can be computed using a backtracking process. Enforcing condition (4.3) ensures the convergence of the sequence $\{\|F_k\|\}$ [28] Lemma 2.4.

We now analyse the properties of $\|F_{k+1}\|$ as a function of the stepsize $\gamma_k\beta_k$ and determine conditions on $\gamma_k\beta_k$ which enforce (4.3). First of all we observe that by the Mean Value Theorem [11] Lemma 4.1.9 and (4.5) we have

$$F_{k+1} = (I \pm \gamma_k\beta_k G_k)F_k. \quad (4.6)$$

Using this equation we can write

$$\|F_{k+1}\|^2 = \|F_k\|^2 + 2\gamma_k\beta_k F_k^T (G_S)k F_k + \gamma_k^2\beta_k^2 F_k^T G_k^2 G_k F_k, \quad (4.7)$$

and analyze the fulfillment of either the decrease of $\|F\|$ or (4.3) as given below.

Theorem 4.3. Suppose that Assumption [3.2] holds and Assumption [3.2] holds with $x = x_k$ and $p = p_k$. Suppose $F_k^T J_k F_k \neq 0$ and $F_k^T G_k F_k \neq 0$ with $G_k$ given in (2.11). Let $\Delta = q((G_S)k, F_k)^2 + (\eta_k^2 + 2\eta_k)q(G_k^2 G_k, F_k)$, then

1. If $x_{k+1} = x_k + p_k$, $p_k = p = -\gamma_k\beta_k F_k$, $\gamma_k \in (0, 1]$, we have that $\|F_{k+1}\| < \|F_k\|$ when

$$\beta_k q((G_S)k, F_k) > 0 \quad \text{and} \quad \gamma_k |\beta_k| < \frac{2 q((G_S)k, F_k)}{q(G_k^2 G_k, F_k)}. \quad (4.8)$$
Condition 4.3 is satisfied when
\[
\frac{q((G_S)_k, F_k) - \sqrt{\Delta}}{q(G_k^T G_k, F_k)} \leq \gamma_k \beta_k \leq \frac{q((G_S)_k, F_k) + \sqrt{\Delta}}{q(G_k^T G_k, F_k)}.
\] (4.9)

(2) If \(x_{k+1} = x_k + p_k, p_k = p_+ = \gamma_k \beta_k F_k\), \(\gamma_k \in (0, 1]\), we have that \(\|F_{k+1}\| < \|F_k\|\) when
\[
\beta_k q((G_S)_k, F_k) < 0 \quad \text{and} \quad \gamma_k |\beta_k| < \frac{2 |q((G_S)_k, F_k)|}{q(G_k^T G_k, F_k)}
\] (4.10)

Condition 4.3 is satisfied when
\[
\frac{-q((G_S)_k, F_k) - \sqrt{\Delta}}{q(G_k^T G_k, F_k)} \leq \gamma_k \beta_k \leq \frac{-q((G_S)_k, F_k) + \sqrt{\Delta}}{q(G_k^T G_k, F_k)}.
\] (4.11)

**Proof.** Concerning Item (1), using (4.6) we get
\[
\|F_{k+1}\|^2 = \|(I - \gamma_k \beta_k G_k)F_k\|^2
= \left(1 - 2\gamma_k \beta_k \frac{F_k^T (G_S)_k F_k}{\|F_k\|^2} + \gamma_k^2 \beta_k^2 \frac{F_k^T G_k^T G_k F_k}{\|F_k\|^2}\right) \|F_k\|^2
= \left(1 - 2\gamma_k \beta_k q((G_S)_k, F_k) + \gamma_k^2 \beta_k^2 q(G_k^T G_k, F_k)\right) \|F_k\|^2.
\]
Noting that by assumption \(q((G_S)_k, F_k) \neq 0\) and \(q(G_k^T G_k, F_k) > 0\), \(\|F_{k+1}\| < \|F_k\|\) holds if
\[
\beta_k q((G_S)_k, F_k) > 0 \quad \text{and} \quad -2\gamma_k \beta_k q((G_S)_k, F_k) + \gamma_k^2 \beta_k^2 q(G_k^T G_k, F_k) < 0,
\]
and these conditions can be rewritten as in (4.8). Condition (4.9) follows trivially.

Item (2) follows analogously. From (4.6) and imposing and \(\|F_{k+1}\| < \|F_k\|\) we get the condition
\[
\beta_k q((G_S)_k, F_k) < 0 \quad \text{and} \quad 2\gamma_k \beta_k q((G_S)_k, F_k) + \gamma_k^2 \beta_k^2 q(G_k^T G_k, F_k) < 0
\]
which is equivalent to (4.10). Condition (4.11) follows trivially. \(\square\)

We remark that, due to the form of \(G_k\) and \((G_S)_k\), conditions (4.8)–(4.11) are implicit in \(\gamma_k \beta_k\). The above theorem supports testing the two steps (4.5) systematically because of the following fact. At \(k\)-th iteration, \(\beta_k, q(J_k, F_k)\) and \(q(J_k^T J_k, F_k)\) are given and by continuity of the Jacobian, the Rayleigh quotients \(q((G_S)_k, F_k)\) and \(q(G_k^T G_k, F_k)\) tend to \(q(J_k, F_k)\) and \(q(J_k^T J_k, F_k)\) respectively as \(\gamma_k\) tends to zero. Hence, if \(\gamma_k\) is sufficiently small then
\[
\frac{q(J_k, F_k) - \epsilon}{q(J_k^T J_k, F_k) + \epsilon} \leq \frac{q((G_S)_k, F_k)}{q(G_k^T G_k, F_k)} \leq \frac{q(J_k, F_k) + \epsilon}{q(J_k^T J_k, F_k) - \epsilon},
\]
and if \(0 < \epsilon < \frac{1}{2} \min\{q(J_k, F_k), q(J_k^T J_k, F_k)\}\) then \(\frac{q((G_S)_k, F_k)}{q(G_k^T G_k, F_k)}\) has the same sign as \(\frac{q(J_k, F_k)}{q(J_k^T J_k, F_k)}\). Consequently, for \(\gamma_k\) sufficiently small, either condition (4.8) or (4.10) is fulfilled. Analogous considerations can be made for conditions (4.9) and (4.11).

As a final comment, the previous theorem suggests that a small \(|\beta_k|\) promotes the fulfillment of conditions (4.8) and (4.10) or (4.9) and (4.11). Again, by Lemma 3.4 the use of \(\beta_{k,2}\) may be advisable taking into account that \(|\beta_{k,2}| \leq |\beta_{k,1}|\) and that \(\beta_{k,1}\) can arbitrarily grow in the indefinite case; taking the steplength equal to \(\beta_{k,1}\) may cause a large number of backtracks and an erratic behaviour of \(\{|\|F_k\||\}\) as long as \(\eta_k\) is sufficiently large.
5. A spectral residual approximate norm descent method. In this section we describe a spectral residual algorithm which implements a line-search along \( \pm F_k \) and enforces the approximate norm descent condition \((4.3)\). We also discuss the convergence properties of the method and provide sufficient conditions for the convergence of the sequence \( \{ \| F_k \| \} \) to zero.

The Projected Approximate Norm Descent (PAND) algorithm was developed in [34] for solving convexly constrained nonlinear systems. Among its variants proposed in [31, 34] and based on Quasi-Newton methods, we consider the spectral residual implementation for unconstrained nonlinear systems which is the focus of this work and denote it as Spectral Residual Approximate Norm Descent (SRAND) method.

Given the current iterate \( x_k \), a new iterate \( x_{k+1} \) is computed as \( x_{k+1} = x_k + p_k \) with \( p_k \) given by either \( -\gamma_k \beta_k F_k \) or \( +\gamma_k \beta_k F_k \), \( \gamma_k \in (0,1] \). The main phases of SRAND are as follows. First, the scalar \( \beta_k \) is chosen to that \( |\beta_k| \in [\beta_{min}, \beta_{max}] \). Second, the scalar \( \gamma_k \in (0,1] \) is fixed using a backtracking strategy so that either the linesearch condition

\[
\| F(x_k + p_k) \| \leq (1 - \rho (1 + \gamma_k)) \| F_k \|, \tag{5.1}
\]

holds or the linesearch condition

\[
\| F(x_k + p_k) \| \leq (1 + \eta_k - \rho \gamma_k) \| F_k \|, \tag{5.2}
\]

holds where \( \rho \in (0,1) \) is quite small [11,34] and \( \{ \eta_k \} \) is a positive sequence satisfying \((4.4)\).

The linesearch conditions \((5.1)\) and \((5.2)\) are derivative-free; the first condition imposes at each iteration a sufficient decrease in \( \| F \| \) which can be accomplished for suitable values of \( \pm \gamma_k \beta_k F_k \) as long as \( F_k^T J_k F_k \neq 0 \), and is crucial for establishing results on the convergence of \( \{ \| F_k \| \} \) to zero. On the other hand, the second condition allows for an increase of \( \| F \| \) depending on the magnitude of \( \eta_k \). Trivially \((5.1)\) implies \((5.2)\) and both imply the approximate norm descent condition \((4.3)\).

The formal description of the SRAND method is reported in Algorithm 5.1 where we deliberately do not specify the form of the stepsize \( \beta_k \). Termination of Step 2 is guaranteed by Theorem 4.3. The theoretical properties of SRAND given in [34] Theorem 4.2 and Theorem 4.3 are summarized in the following theorem.

**Theorem 5.1.** Let the positive sequence \( \{ \eta_k \} \) satisfy \((4.4)\) and let \( \{ x_k \} \) be the sequence generated by the SRAND algorithm. Then

1. the sequence \( \{ x_k \} \) is convergent and consequently the sequence \( \{ \| F_k \| \} \) is convergent;
2. the sequence \( \{ \gamma_k \| F_k \| \} \) is convergent and such that \( \lim_{k \to \infty} \gamma_k \| F_k \| = 0 \);
3. if \((5.1)\) is satisfied for infinitely many \( k \), then \( \lim_{k \to \infty} \| F_k \| = 0 \).

The above results hold for any choice of the steplength \( \beta_k \) and Item 3 identifies one occurrence where the SRAND algorithm solves problem \((1.1)\), i.e., \( \{ \| F_k \| \} \) converges to zero. In this section we complete the theoretical analysis of the SRAND algorithm by providing sufficient conditions that ensures that the sequence \( \{ \| F_k \| \} \) converges to zero.

We start by recalling a simple result.

**Lemma 5.2.** Suppose that Assumption 3.4 holds. Then for \( p_k = \pm \gamma_k \beta_k F_k \), it holds

\[
\| F_{k+1} \|^2 = \left( 1 \pm 2 \gamma_k \beta_k q((G_k)_{k+1}) F_k \right) \| F_k \|^2 \left( 1 + \int_0^1 (F(x_k + p_k) - F(x_k))^T J(x_k + p_k) F_k \ dt \right) \| F_k \|^2. \tag{5.3}
\]

**Proof.** Assume that \( p_k = -\gamma_k \beta_k F_k \). Then,

\[
\| F_{k+1} \|^2 = \| F_k \|^2 + 2 \int_0^1 (F(x_k + p_k)^T J(x_k + p_k) p_k \ dt \]
\[
= \| F_k \|^2 - 2 \gamma_k \beta_k \int_0^1 (F(x_k + p_k)^T J(x_k + p_k) F_k \ dt \]
\[
= \| F_k \|^2 - 2 \gamma_k \beta_k \int_0^1 (F(x_k + p_k)^T J(x_k + p_k) F_k \ dt \]
\[
\pm 2 \gamma_k \beta_k \int_0^1 (F(x_k)^T J(x_k + p_k) F_k \ dt \]
\[
= \| F_k \|^2 - 2 \gamma_k \beta_k F_k^T G_k F_k - 2 \gamma_k \beta_k \int_0^1 (F(x_k + p_k) - F(x_k))^T J(x_k + p_k) F_k \ dt, \]

that gives \((5.3)\) using \((3.1)\) and \((2.13)\). The case \( p_k = +\gamma_k \beta_k F_k \) is analogous. \( \square \)
Algorithm 5.1: The SRAND algorithm

Given \( x_0 \in \mathbb{R}^n \), \( 0 < \beta_{\text{min}} < \beta_{\text{max}} \), \( \beta_0 \in [\beta_{\text{min}}, \beta_{\text{max}}] \), \( \rho, \sigma \in (0, 1) \), a positive sequence \( \{\eta_k\} \) satisfying (4.4).

If \( \|F_0\| = 0 \) stop.
For \( k = 0, 1, 2, \ldots \) do
1. Set \( \gamma = 1 \).
2. Repeat
   2.1 Set \( p_\gamma = -\gamma \beta_k F_k \) and \( p_\beta = \gamma \beta_k F_k \).
   2.2 If \( p_\gamma \) satisfies (5.1), set \( p_k = p_\gamma \) and go to Step 3.
   2.3 If \( p_\beta \) satisfies (5.1), set \( p_k = p_\beta \) and go to Step 3.
   2.4 If \( p_\beta \) satisfies (5.2), set \( p_k = p_\beta \) and go to Step 3.
   2.5 If \( p_\beta \) satisfies (5.2), set \( p_k = p_\beta \) and go to Step 3.
   2.6 Otherwise set \( \gamma = \sigma \gamma \).
3. Set \( \gamma_k = \gamma, x_{k+1} = x_k + p_k \).
4. If \( \|F_{k+1}\| = 0 \) stop.
5. Choose \( \beta_{k+1} \) such that \( |\beta_{k+1}| \in [\beta_{\text{min}}, \beta_{\text{max}}] \).

Under specific assumptions on the Jacobian \( J \), the following two theorems give conditions that ensures \( F(x^*) = 0 \) where \( x^* \) is the limit point of \( \{x_k\} \): Theorem 5.3 concerns the cases when \( J_S(x^*) \) is positive (negative) definite and when \( J \) is symmetric too, Theorem 5.4 regards the case when \( J_S(x^*) \) is indefinite.

**Theorem 5.3.** Suppose that \( F \) is continuously differentiable on \( \mathbb{R}^n \). Let the positive sequence \( \{\eta_k\} \) satisfy (4.4) and let \( \{x_k\} \) be the sequence generated by the SRAND algorithm. Moreover assume that \( J_S(x^*) \) is positive definite at the limit point \( x^* \) of \( \{x_k\} \). Letting \( \sigma_{\text{max}}(J(x^*)) \) be the largest singular value of \( J(x^*) \), if eventually

\[
\nu \geq \beta_k > \left( 1 + \epsilon \right) \sigma_{\text{max}}(J(x^*)) \tag{5.4a}
\]

and

\[
\beta_k q((G_S)_k, F_k) > \frac{3}{2} \rho, \tag{5.4b}
\]

with \( \rho \in (0, 1) \) as in (5.1) and (5.2) and for some \( \epsilon \in (0, 1) \) and \( \nu > 0 \), then \( F(x^*) = 0 \). If \( \beta_k \) is either \( \beta_{k,1} \) or \( \beta_{k,2} \), only condition (5.4b) has to be satisfied to get \( F(x^*) = 0 \). Moreover, for some \( \omega_1, \omega_2 \in (0, 1) \), sufficient conditions for (5.4b) to hold are

1. if \( \beta_k = \beta_{k,1} \) for \( k \) large enough:

\[
\kappa(J_S(x^*)) < \frac{2\omega_1}{3\rho}, \tag{5.5}
\]

2. if \( \beta_k = \beta_{k,2} \) for \( k \) large enough:

\[
\kappa(J_S(x^*)) < \omega_2 \sqrt{\frac{2}{3\rho}}, \tag{5.6}
\]

3. if \( J \) is symmetric and \( \beta_k \) is either \( \beta_{k,1} \) or \( \beta_{k,2} \) for \( k \) large enough:

\[
\kappa(J(x^*)) < \frac{2\omega_1}{3\rho}, \tag{5.7}
\]

where \( \kappa(\cdot) \) is the 2-norm condition number.

**Proof.** Since \( J_S(x^*) \) is assumed to be positive definite, continuity implies that there exists a scalar \( \xi > 0 \) sufficiently small such that, for all \( y \in B(x^*, \xi) = \{ x \in \mathbb{R}^n : \| x - x^* \| \leq \xi \} \), \( J_S(y) \) is positive definite and

\[
\lambda_{\text{min}}(J_S(y)) \geq (1 - \epsilon)\lambda_{\text{min}}(J_S(x^*)), \quad \lambda_{\text{max}}(J_S(y)) \leq (1 + \epsilon)\lambda_{\text{max}}(J_S(x^*)), \tag{5.8}
\]
with $\epsilon \in (0, 1)$. Moreover, the convergence of the sequence $\{x_k\}$ implies that $x_{k-1} + tp_{k-1}$ and $x_k + tp_k$ both belong to $\mathcal{B}(x^*, \xi)$ for large enough $k$ and all $t \in [0, 1]$. As a consequence, reducing $\xi$ if necessary, we deduce that, for $k$ sufficiently large,
\[
\begin{align*}
\min \{\lambda_{\min}((G_S)_k), \lambda_{\min}((G_S)_{k-1})\} & \geq (1 - \epsilon)\lambda_{\min}(J_S(x^*)), \\
\max \{\lambda_{\max}((G_S)_k), \lambda_{\max}((G_S)_{k-1})\} & \leq (1 + \epsilon)\lambda_{\max}(J_S(x^*)).
\end{align*}
\]
and by (2.14),
\[
q((G_S)_k, F_k) \in [\lambda_{\min}((G_S)_k), \lambda_{\max}((G_S)_k)] \subseteq [(1 - \epsilon)\lambda_{\min}(J_S(x^*)), (1 + \epsilon)\lambda_{\max}(J_S(x^*))].
\]
Finally, again by continuity, reducing $\xi > 0$ if necessary, for all $y \in \mathcal{B}(x^*, \xi)$ it holds
\[
\sigma_{\max}(J(y)) \leq (1 + \epsilon)\sigma_{\max}(J(x^*)), \quad \sigma_{\max}(G_k) \leq (1 + \epsilon)\sigma_{\max}(J(x^*)).
\]

Now, we consider (5.3) and $p_k = -\gamma_k \beta_k F_k$. From the Mean Value Theorem [11] Lemma 4.1.9, we have that
\[
\int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k \, dt = \int_0^1 \left( \int_0^1 (J(x_k + \xi tp_k) tp_k \, d\xi \right) J(x_k + tp_k) F_k \, dt,
\]
$\xi \in [0, 1]$. Again, for $k$ sufficiently large, $x_k + \xi tp_k \in \mathcal{B}(x^*, \xi)$ for $t, \xi \in [0, 1]$. Thus, $p_k = -\gamma_k \beta_k F_k$ and (5.10) imply
\[
\int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k \, dt \leq \int_0^1 t \gamma \beta_k \max_{z \in \mathcal{B}(x^*, \xi)} ||J(z)||^2 ||F_k||^2 \, dt
\]
\[
= \frac{1}{2} \gamma \beta_k \max_{z \in \mathcal{B}(x^*, \xi)} \sigma_{\max}(J(z))^2 ||F_k||^2
\]
\[
\leq \frac{1}{2} \gamma \beta_k (1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2 ||F_k||^2.
\]
Combining this expression with (5.3), we have that for $k$ sufficiently large
\[
\|F_{k+1}\|^2 \leq \left( 1 - 2\gamma \beta_k q((G_S)_k, F_k) + \frac{2 \gamma \beta_k}{\|F_k\|^2} \int_0^1 (F(x_k + p_k) - F(x_k))^T J(x_k + tp_k) F_k \, dt \right) \|F_k\|^2
\]
\[
\leq (1 - 2\gamma \beta_k q((G_S)_k, F_k) + \gamma \beta_k^2 (1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2) \|F_k\|^2.
\]
Thus, for $k$ sufficiently large, the linesearch condition (5.2) is satisfied if
\[
1 - 2\gamma \beta_k q((G_S)_k, F_k) + \gamma \beta_k^2 (1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2 \leq (1 - \rho \gamma)^2,
\]
which is equivalent to
\[
\delta_2 \gamma^2 + 2\delta_1 \gamma \triangleq (1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2 \beta_k^2 - \rho^2 \gamma^2 + 2(\rho - \beta_k q((G_S)_k, F_k)) \gamma \leq 0.
\]
Clearly (5.4a) implies that $(1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2 \beta_k^2 - \rho^2 \gamma^2 \geq \delta_2 > 0$. Moreover, if eventually (5.4b) holds then $\delta_1 < 0$ and (5.12) is satisfied whenever $\gamma \leq \gamma^* = -\delta_1/\delta_2$. Now, $\gamma^*$ is uniformly bounded below since $-\delta_1 \geq 1/2 \rho$, i.e., $\gamma^* \geq \frac{\delta_1}{\delta_2} \geq \frac{\delta_1}{\delta_2} \geq \gamma \triangleq \rho/(1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2 \rho^2$. Then, the mechanism of Step 3.6 of the SRAND algorithm guarantees that, for $k$ sufficiently large, the loop in Step 2 terminates with $\gamma_k \geq \min \{1, \sigma \gamma \}$, and $\gamma$ independent of $k$. As a consequence, $\liminf_{k \to \infty} \gamma_k > 0$ and by Item 2. in Theorem 5.1 we have that $F(x^*) = 0$.

We now show that when $\beta_k$ is either $\beta_{k,1}$ or $\beta_{k,2}$ for $k$ sufficiently large, then only condition (5.4b) has to be satisfied to get $F(x^*) = 0$.

Let $\beta_k = \beta_{k,1}$. Using Item (ii) in Lemma 3.4 and (5.6), we have that $\beta_k$ is positive and satisfies
\[
\frac{1}{(1 + \epsilon)\lambda_{\max}(J_S(x^*))} \leq \beta_k \leq \frac{1}{(1 - \epsilon)\lambda_{\min}(J_S(x^*))}.
\]
By definition of \( J_S \), \( \|J_S(x^*)\| \leq \|J(x^*)\| \), hence \( \lambda_{\max}(J_S(x^*)) \leq \sigma_{\max}(J(x^*)) \). Therefore (5.4a) is satisfied being \( \rho \in (0, 1) \) and setting \( \nu = 1/(1 - \epsilon)\lambda_{\min}(J_S(x^*)) \).

Let \( \beta_k = \beta_{k,2} \). Since \( \beta_{k,2} \leq \beta_{k,1} \), the upper bound in (5.4a) is guaranteed from the discussion above. Moreover from (5.11) and again from \( \beta_{k,2} \leq \beta_{k,1} \), the linesearch condition (5.2) is satisfied if

\[
\delta_2 \gamma^2 + 2 \delta_1 \gamma \overset{\text{def}}{=} \left( (1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2 \beta_{1,k}^2 - \rho^2 \right) \gamma^2 + 2 \left( \rho - \beta_{2,k} q((G_S)_k, F_k) \right) \gamma \leq 0. \tag{5.14}
\]

Following the previous considerations on \( \beta_{k,1} \), \( \delta_2 \) is positive. Further, using (5.4b) and repeating the arguments above on the scalar \( \gamma \) satisfying (5.14), the loop in Step 2 terminates with \( \gamma_k \geq \min\{1, \sigma \gamma\} \), and \( \bar{\gamma} \) independent of \( k \).

To conclude, as for Item 1., if \( \beta_{k,1} \) is used eventually then (3.6) and (5.9) give \( \beta_k q((G_S)_k, F_k) \geq \frac{\omega}{\kappa(J_S(x^*))} \) and trivially (5.5) implies (5.4b) for all \( k \) sufficiently large.

As for Item 2., if \( \beta_{k,2} \) is used eventually then (3.7), (5.10) and (5.9) give \( \beta_k q((G_S)_k, F_k) \geq \frac{\omega}{\kappa(J_S(x^*))} \) with \( \omega = \frac{(1 + \epsilon)\|J_S(x^*)\|}{1 + \epsilon \|J(x^*)\|^2} \) and (5.6) implies (5.4b) for all \( k \) sufficiently large.

Concerning Item 3., (5.4b) reads \( \beta_k q(G_k, F_k) > \frac{3}{2} \rho \), and by Lemma 3.4 \( \beta_{k,1} \) and \( \beta_{k,2} \) are positive and

\[
\beta_{k,1} \geq \beta_{k,2} \geq \frac{1}{\sigma_{\max}(G_{k-1})} \geq \frac{1}{(1 + \epsilon)\sigma_{\max}(J(x^*))}. \tag{5.15b}
\]

Thus, by (5.9) it follows \( \beta_k q(G_k, F_k) \geq \frac{\omega}{\kappa(J(x^*))} \) and trivially (5.7) implies (5.4b) for all \( k \) sufficiently large. \( \square \)

We remark that analogous conditions to (5.4) can be derived for the case when \( J_S(x^*) \) is negative definite.

**Theorem 5.4.** Suppose that \( F \) is continuously differentiable on \( \mathbb{R}^n \). Let the positive sequence \( \{\eta_k\} \) satisfy (4.4) and let \( \{x_k\} \) be the sequence generated by the Barzilai-Borwein algorithm. Moreover assume that \( J_S(x^*) \) is indefinite and \( J(x^*) \) is nonsingular at the limit point \( x^* \) of \( \{x_k\} \). If eventually

\[
\nu \geq |\beta_k| > \frac{\rho}{(1 + \epsilon)\sigma_{\max}(J(x^*))} \tag{5.15a}
\]

and

\[
|\beta_k q((G_S)_k, F_k)| > \frac{3}{2} \rho, \tag{5.15b}
\]

with \( \rho \in (0, 1) \) as in (5.11) and (5.2) and for some \( \epsilon \in (0, 1) \) and \( \nu > 0 \), then \( F(x^*) = 0 \).

**Proof.** We observe that for \( k \) sufficiently large, the inequalities (5.8)–5.9 hold for some \( \epsilon \in (0, 1) \). Moreover, considering \( p_k = \pm \gamma \beta_k F_k \) and proceeding as in the proof of Theorem 5.3 we get that for \( k \) sufficiently large the following inequality holds

\[
\|F_{k+1}\|^2 \leq (1 \pm 2 \gamma \beta_k q((G_S)_k, F_k) + \gamma \beta_k^2 (1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2) \|F_k\|^2.
\]

Therefore the linesearch condition (5.2) is satisfied if

\[
\delta_2 \gamma^2 + 2 \delta_1 \gamma \overset{\text{def}}{=} \left( (1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2 \beta_k^2 - \rho^2 \right) \gamma^2 + 2 \left( \rho \pm \beta_k q((G_S)_k, F_k) \right) \gamma \leq 0. \tag{5.16}
\]

Clearly (5.15a) implies that \( (1 + \epsilon)^2 \sigma_{\max}(J(x^*))^2 \beta_k^2 - \rho^2 \gamma^2 + 2 \left( \rho \pm \beta_k q((G_S)_k, F_k) \right) \gamma \leq 0. \) (5.16)

We now show that (5.15b) implies that \( \delta_1 > 0 \) so that we conclude that \( F(x^*) = 0 \) as in the proof of Theorem 5.3.

Let us analyse the case \( \beta_k q((G_S)_k, F_k) < 0 \) and consider the step \( p_k = \gamma_k \beta_k F_k \). Then condition (5.15b) means that \( -\beta_k q((G_S)_k, F_k) \geq \frac{3}{2} \rho \), that is \( \delta_1 = \rho + \beta_k q((G_S)_k, F_k) < -\frac{1}{2} \rho < 0 \). The case \( \beta_k q((G_S)_k, F_k) > 0 \) is analogous considering the step \( p_k = -\gamma_k \beta_k F_k \). Now, repeating the arguments in Theorem 5.3 we conclude that \( \liminf_{k \to \infty} \gamma_k > 0 \). \( \square \)

### 6. Numerical experiments

In view of our theoretical analysis and guidelines on steplength selection given in Section 4, we attempt to tailor Barzilai and Borwein rules for unconstrained optimization to spectral residual methods. In this section we discuss several steplength rules for
spectral residual methods and perform their experimental analysis using the SRAN algorithm described in Algorithm 5.1. Our test set consists of sequences of nonlinear systems arising in the solution of rail-wheel contact models and is described in details in Section 6.2.

SRAN was implemented in Matlab (MATLAB R2019b) and the experiments were carried out on a Intel Core i7-9700K CPU @ 3.60GHz x 8, 16 GB RAM, 64-bit.

6.1. Steplength rules. We now present six rules for the choice of the steplength in spectral residual methods that were used in our experiments. Besides the straightforward choice of one of the two steplengths \( \beta_{k,1}, \beta_{k,2} \), along all iterations, we consider adaptive strategies that suitably combine them and parallel those used for quadratic and nonlinear optimization problems. Below, given a scalar \( \beta \), \( T(\beta) \) is the thresholding rule which projects \( |\beta| \) onto \( I_\beta \equiv [\beta_{\min}, \beta_{\max}] \)

$$T(\beta) = \min \left\{ \beta_{\max}, \max \left\{ \beta_{\min}, |\beta| \right\} \right\}.$$  (6.1)

BB1 rule. By \[21,25,27,34\], at each iteration let

$$\beta_k = \begin{cases} \beta_{k,1} & \text{if } |\beta_{k,1}| \in I_\beta \\
T(\beta_{k,1}) & \text{otherwise} \end{cases}$$  (6.2)

BB2 rule. At each iteration let

$$\beta_k = \begin{cases} \beta_{k,2} & \text{if } |\beta_{k,2}| \in I_\beta \\
T(\beta_{k,2}) & \text{otherwise} \end{cases}$$  (6.3)

ALT rule. Following \[8,21\], at each iteration let us alternate between \( \beta_{k,1} \) and \( \beta_{k,2} \):

$$\beta_k^{\text{ALT}} = \begin{cases} \beta_{k,1} & \text{for } k \text{ odd} \\
\beta_{k,2} & \text{otherwise} \end{cases}$$  (6.4)

$$\beta_k = \begin{cases} \beta_k^{\text{ALT}} & \text{if } |\beta_k^{\text{ALT}}| \in I_\beta \\
\beta_{k,1} & \text{if } k \text{ even, } |\beta_{k,1}| \in I_\beta, |\beta_{k,2}| \notin I_\beta \\
\beta_{k,2} & \text{if } k \text{ odd, } |\beta_{k,2}| \in I_\beta, |\beta_{k,1}| \notin I_\beta \\
T(\beta_k^{\text{ALT}}) & \text{otherwise} \end{cases}$$  (6.5)

ABB rule. Following \[45\] and ABB rule in \[16\], we define the Adaptive Barzilai-Borwein (ABB) rule as follows. Given \( \tau \in (0,1) \), let

$$\beta_k^{\text{ABB}}(\xi_1, \xi_2) = \begin{cases} \xi_2 & \text{if } \frac{\xi_2}{\xi_1} < \tau \\
\xi_1 & \text{otherwise} \end{cases}$$  (6.6)

for some given \( \xi_1, \xi_2 \). Then

$$\beta_k = \begin{cases} \beta_k^{\text{ABB}}(\beta_{k,1}, \beta_{k,2}) & \text{if } |\beta_{k,1}|, |\beta_{k,2}| \in I_\beta \\
\beta_{k,1} & \text{if } |\beta_{k,1}| \in I_\beta, |\beta_{k,2}| \notin I_\beta \\
\beta_{k,2} & \text{if } |\beta_{k,2}| \in I_\beta, |\beta_{k,1}| \notin I_\beta \\
\beta_k^{\text{ABB}}(T(\beta_{k,1}), T(\beta_{k,2})) & \text{otherwise} \end{cases}$$  (6.7)

Observe that a large value of \( \tau \) promotes the use of \( \beta_{k,2} \) with respect to \( \beta_{k,1} \). The rule allows to switch between the steplengths \( \beta_{k,1} \) and \( \beta_{k,2} \) and was originally motivated by the behaviour of the Barzilai and Borwein method applied to convex and quadratic minimization problem (see \[16,45\] and our discussion below Lemma 4.1).
**ABBm rule.** This rule elaborates the ABBminmin rule given in [16], taking into account that \( \beta_{k,2} \) may be negative along iterations. Let \( m \) be a nonnegative integer, and

\[
\beta_{k,2} = \begin{cases} 
\beta_{k,2} & \text{if } |\beta_{k,2}| \in I_{\beta} \\
T(\beta_{k,2}) & \text{otherwise}
\end{cases}
\]

(6.8)

\[
j^* = \arg\min\{|\beta_{j,2}| : j = \max\{1, k - m\}, \ldots, k\}.
\]

Given \( \tau \in (0, 1) \), we fix \( \beta_k \) as follows

\[
\beta_k^{\text{ABBm}}(\xi_1, \xi_2) = \begin{cases} 
\beta_{j^*, 2} & \text{if } \frac{\xi_2}{\xi_1} < \tau \\
\xi_1 & \text{otherwise}
\end{cases}
\]

(6.9)

\[
\beta_k = \begin{cases} 
\beta_k^{\text{ABBm}}(\beta_{k,1}, \beta_{k,2}) & \text{if } |\beta_{k,1}|, |\beta_{k,2}| \in I_{\beta} \\
\beta_{k,1} & \text{if } |\beta_{k,1}| \in I_{\beta}, |\beta_{k,2}| \notin I_{\beta} \\
\beta_{k,2} & \text{if } |\beta_{k,2}| \in I_{\beta}, |\beta_{k,1}| \notin I_{\beta} \\
\beta_k^{\text{ABBm}}(T(\beta_{k,1}), T(\beta_{k,2})) & \text{otherwise}
\end{cases}
\]

(6.10)

Again, a large value of \( \tau \) promotes the use of a step from BB2 rule instead of \( \beta_{k,1} \). In case \( |\beta_{k,1}|, |\beta_{k,2}| \in I_{\beta} \) and \( \frac{\beta_{k,2}}{\beta_{k,1}} < \tau \), the smallest absolute value \( \beta_{j^*, 2} \) over the last \( m + 1 \) iterations is selected; taking into account that \( \beta_{j,2} \) for \( j = \max\{1, k - m\}, \ldots, k \) can be negative, the rationale for selecting \( \beta_{j^*, 2} \) in (6.9) is to mitigate the nonmonotone behavior of the objective function [16]. Consequently, smaller steplengths are expected using the ABBm rule than using the ABB rule.

**DABBm rule.** Following [7,6], a dynamic threshold \( \tau_k \in (0, 1) \) can be used in place of the prefixed threshold \( \tau \) in (6.9). Given \( \beta_{k,2} \) and \( j^* \) in (6.8), we propose the rule defined as

\[
\beta_k^{\text{DABBm}}(\xi_1, \xi_2) = \begin{cases} 
\beta_{j^*, 2} & \text{if } \frac{\xi_2}{\xi_1} < \tau_k \\
\xi_1 & \text{otherwise}
\end{cases}
\]

(6.11)

\[
\beta_k = \begin{cases} 
\beta_k^{\text{DABBm}}(\beta_{k,1}, \beta_{k,2}) & \text{if } |\beta_{k,1}|, |\beta_{k,2}| \in I_{\beta} \\
\beta_{k,1} & \text{if } |\beta_{k,1}| \in I_{\beta}, |\beta_{k,2}| \notin I_{\beta} \\
\beta_{k,2} & \text{if } |\beta_{k,2}| \in I_{\beta}, |\beta_{k,1}| \notin I_{\beta} \\
\beta_k^{\text{DABBm}}(T(\beta_{k,1}), T(\beta_{k,2})) & \text{otherwise}
\end{cases}
\]

(6.12)

with the dynamic threshold set as

\[
\tau_k = \min \left\{ \tau, \|F_k\|^{1/(2+b_i^2)} \right\},
\]

(6.13)

\[
b_i = \max\{b_j : j = \max\{1, k - w\}, \ldots, k\}.
\]

(6.14)

Here \( \tau \in (0, 1) \) is an upper bound on the value of \( \tau_k \), \( w \) is a nonnegative integer and \( b_j \) denotes the number of backtracks performed at iteration \( j \) (see Step 2 of Algorithm [5.1]). If \( \|F_k\| \) is getting small and the number of performed backtracks in the last \( w + 1 \) iterations is small, then (6.13) promotes the use of steplength from BB1 rule, i.e., larger steplengths which can speed convergence to a zero of \( F \). On the other hand, when the number of backtracks performed along previous iterations is large and \( \tau \) is large, the use of the smaller steplength from BB2 rule is encouraged.

We conclude the discussion on steplength selection, noting that conditions (5.4) and (5.15) for the convergence of \( \{x_k\} \) to a zero of \( F \) apply to all our rules.

The rules and parameters used in our experiments are summarized in Table [6.1].
6.2. Problem set: nonlinear systems arising from rolling contact models. Rolling contact is a fundamental issue in mechanical engineering and plays a central role in many important applications such as rolling bearings and wheel-rail interaction [23, 24]. In order to perform simulations of complex mechanical systems with a good tradeoff between accuracy and efficiency, three working hypotheses are usually made in modelling rolling contact: non-conformal contact, i.e., the typical dimensions of the contact area are negligible if compared to the curvature radii of the contact body surfaces; planar contact, i.e., the contact area is contained in a plane; half-space contact, i.e., locally, the contact bodies are viewed as three-dimensional half-spaces [23, 24]. In this framework, we focus on the Kalker’s rolling contact model which represents a relevant and general model in contact mechanics.

The solution of Kalker’s rolling contact model can be performed using different approaches. The approach in [42, 43] calls for the solution of constrained optimization problems while the so-called CONTACT algorithm [24] gives rise to sequences of nonlinear systems. Our problem set derives from the application of CONTACT algorithm, here we describe in which phase of the Kalker’s model solution they arise and give some of their features. We refer to Appendix A for a sketch of Kalker’s model, its discretization, and the Kalker’s CONTACT algorithm.

Kalker’s CONTACT algorithm determines the normal pressure, the tangential pressure, the contact area, the adhesion area and the sliding area in the contact between two elastic bodies and relies on the elastic decoupling between the normal contact problem and the tangential contact problem. Such problems are solved separately: first the normal problem is solved via the so-called NORM algorithm, second the tangential problem is solved via the so-called TANG algorithm. Algorithms NORM and TANG are expected to identify the elements in the contact area and in the adhesion-sliding areas, respectively. These algorithms are applied sequentially and repeatedly until the values of the computed pressures undergo a sufficiently small change that suggests their reliable approximation; in general, a few repetitions of NORM and TANG algorithms are required. Each repetition of NORM algorithm calls for the solution of a sequence of linear systems while each repetition of TANG algorithm calls for the solution of a sequence of linear and nonlinear systems. Computationally, the major bottleneck is the numerical solution of the sequence of nonlinear systems generated in the TANG phase. Importantly, each CONTACT iteration requires few repetitions of TANG algorithm but the CONTACT algorithm is performed for several time instances *.

Our tests were made on wheel-rail contact in railway systems. The benchmark vehicle is a driverless subway vehicle, designed by Hitachi Rail on MLA platform (Light Automatic Metro). The vehicle is a fixed-length train composed of four carbodies and five bogies (four motorized and one, the third, trailer), see Figure 6.1. The multibody model has been realized in the Simpack Rail environment [39]. We considered a train route of length 400 m including a typical railway curved track characterized by three significant parts: two straight lines (from 0 m to 70 m and from 233 m to 400 m), the curve (from 116 m to 186 m) and two cycloids (from 70 m to 116 m and from

| Rule | $\beta_k$ in (6.2) |
|------|------------------|
| BB1  | $\beta_k$ in (6.3) |
| ALT  | $\beta_k$ in (6.4), (6.5) |
| ABB01| $\beta_k$ in (6.6), (6.7) with $\tau = 0.1$ |
| ABB08| $\beta_k$ in (6.6), (6.7) with $\tau = 0.8$ |
| ABBm01| $\beta_k$ in (6.8), (6.10) with $\tau = 0.1, m = 5$ |
| ABBm08| $\beta_k$ in (6.8), (6.10) with $\tau = 0.8, m = 5$ |
| DABBm| $\beta_k$ in (6.8), (6.11), (6.14) with $\tau = 0.8, m = 5, w = 20$ |

*In Appendix A see: (A.1) for the form of normal contact problem and tangential contact problem, (A.5) for the form of the nonlinear systems to be solved, Figure A.2 for the flow of Kalker’s CONTACT algorithm.
186 m to 233 m) which smoothly connect the straight lines and the curve in terms of curvature radius. The radius of the curve is 500 m. In this analysis, we focused on the contact between the first vehicle wheel and the rail; since the vehicle length is equal to 45.7 m, at the beginning of the dynamic simulation the considered wheel starts in the position 45.7 m along the track. We performed a simulation in an interval of 10 seconds using 500 time steps, which amounts to 500 calls to CONTACT algorithm, for train speeds with magnitude $v$ taking the values: $v = 10 \text{ m/s}$ and $v = 16 \text{ m/s}$. Accordingly, during the whole simulation the considered wheel travels along the track a distance equal to 100 m and 160 m, respectively. The traveling velocities considered give a realistic lateral acceleration along the curve according to the current regulation in force in the railway field.

**Fig. 6.1.** Multibody model of the benchmark vehicle.

Two sets of experiments were performed. First, we solved a large number of sequences of nonlinear systems arising from wheel-rail contact in railway systems by the eight SRAND variants based on the rules in Table 6.1. Second, we compared experimentally the best performing SRAND variant and a standard Newton trust-region when embedded in the CONTACT algorithm.

The set of test problems used in the first part of the experiments was generated implementing the CONTACT algorithm in Matlab and using a standard trust-region Newton method‡ for solving the arising nonlinear systems. Afterwards, a representative subset of the nonlinear systems was selected to form our problem set. Specifically, six sequences of nonlinear systems generated by the CONTACT algorithm and corresponding to six consecutive time instances for each track section (straight line, cycloid and curve) and for each velocity were selected. Such sequences are representative of the systems arising throughout the whole simulation and allow a fair analysis of SRAND on nonlinear systems from a real application. Table 6.2 summarizes the features of the sequences: magnitude of the train velocity $v$, section of the route, time instances, number of nonlinear systems in the sequence, dimension $n$ of the systems (proportional to the number of mesh nodes in the potential contact area). A typical feature of the contact model is that $n$ increases as the velocity increases and when the train curves along the route (i.e., the track curvature increases). The total number of systems associated to $v = 10 \text{ m/s}$ and $v = 16 \text{ m/s}$ is 121 and 153 respectively.

| $v$(m/s) | Track Section | Time Instances | Number of Systems | $n$  |
|---------|----------------|----------------|-------------------|-----|
| 10      | Straight line  | 100-105        | 10                | 156 |
|         | Cycloid        | 300-305        | 56                | 897 |
|         | Curve          | 450-455        | 55                | 1394|
| 16      | Straight line  | 50-55          | 8                 | 156 |
|         | Cycloid        | 150-155        | 63                | 1120|
|         | Curve          | 350-355        | 82                | 1394|

Table 6.2
Sequences of nonlinear systems forming the first problem set.

### 6.3. Numerical results
In this section we present the performance of SRAND algorithm. The results presented concern the solution of the sequences of nonlinear systems summarized in

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†The data that support the findings of this study are available from the corresponding author upon reasonable request.
‡The code in [33] was applied using the default setting and dropping bound constraints on the unknown.
Table 6.2 and a comparison between the best performing SRAND variant and a standard Newton trust-region method when embedded in the CONTACT algorithm. SRAND algorithm was implemented as described in Section 6.1 and with parameters

$$\beta_{\text{min}} = 10^{-10}, \beta_{\text{max}} = 10^{10}, \rho = 10^{-4}, \sigma = 0.5, \eta_k = 0.99^k(100 + \|F_0\|^2) \forall k \geq 0,$$

see [34]. The null vector $x_0 = 0$ was chosen as initial guess. A maximum number of iterations and $F$-evaluations equal to $10^5$ was imposed and a maximum number of backtracks equal to 40 was allowed at each iteration. The procedure was declared successful when

$$\|F_k\| \leq 10^{-6}.$$  

(6.15)

A failure was declared either because the assigned maximum number of iterations or $F$-evaluations or backtracks is reached, or because $\|F\|$ was not reduced for 50 consecutive iterations.

We now compare the performance of all the variants of SRAND method in the solution of the sequences of nonlinear systems in Table 6.2. Further, in light of the theoretical investigation presented in this work, we analyze in details the results obtained with BB1 and BB2 rule and support the use of rules that switch between the two steplengths.

Figure 6.2 shows the performance profiles [13] in terms of $F$-evaluations employed by the SRAND variants for solving the sequence of systems generated both with $v = 10\, m/s$ (121 systems) (upper) and with $v = 16\, m/s$ (153 systems) (lower) and highlights that the choice of the steplength is crucial for both efficiency and robustness. The complete results are reported in Appendix B. We start observing that BB2 rule outperformed BB1 rule; in fact the latter shows the worst behaviour both in terms of efficiency and in terms of number of systems solved. Alternating $\beta_{k,1}$ and $\beta_{k,2}$ in ALT rule without taking into account the magnitude of the two scalars improves performance over BB1 rule but is not competitive with BB2 rule. On the other hand, the variants of SRAND using adaptive strategies are the most robust, i.e., they solve the largest number of problems, and efficient. Specifically, comparing ABB, ABBm and DABBm rules, the most effective steplength selections are ABBm and DABBm. Using ABBm01 rule, 98.3% (2 failures) and 96.1% (6 failures) out of the total number of systems were solved successfully for $v = 10\, m/s$ and $v = 16\, m/s$ respectively; using ABBm08 rule, 98.3% (2 failures) and 96.7% (5 failures) of the total number of systems were solved successfully with $v = 10\, m/s$ and $v = 16\, m/s$ respectively; using the dynamic selection DABBm, the largest number of systems was solved successfully, i.e., 99.2% (1 failure) and 98% (3 failures) out the total number of systems with $v = 10\, m/s$ and $v = 16\, m/s$ respectively. Overall, ABBm08 rule gives rise to the most efficient algorithm for both velocity values and the profile related to BB2 rule is within a factor 2 of it in roughly the 80% and the 70% of the runs for $v = 10\, m/s$ and $v = 16\, m/s$, respectively.

Let us now focus on the performance SRAND coupled with BB1 and BB2 rules. As a representative run of our numerical experience reported in Appendix B we consider the nonlinear system arising with $v = 16\, m/s$, at time $t = 150$, iteration 2 of the CONTACT algorithm and iteration 2 of the TANG algorithm (system 150_2,2 in Table B.3). In the upper part of Figure 6.3 we display $\|F\|$ along iterations and the number of $F$-evaluations performed. We note that using the stepsize $\beta_{k,1}$ causes a highly nonmonotone behavior of $\|F\|$ and such behaviour is not productive for convergence; using BB1 rule 276 iterations and 476 $F$-evaluations are performed while using BB2 rule 163 iterations and 228 $F$-evaluations are required. The distinguishing feature of these runs is the high number of backtracks performed using $\beta_{k,1}$ at some iterations, as reported at the bottom part of the figure where the number of backtracks versus iterations is reported for both SRAND variants. This behaviour is in accordance with the analysis in Section 4.1 since $\beta_{k,1}$ can be arbitrarily larger than $\beta_{k,2}$ in the indefinite case, the need to perform a large number of backtracks to enforce approximate norm decrease is likely to occur in case $\beta_{k,1}$ is taken as the initial steplength. Such observation supports the use of $\beta_{k,2}$; the benefit from using shorter steps is further shown by the performance of ABBm over ABB, the former tends to take shorter steps than the latter by exploiting the iteration history and results to be more effective.

We conclude our experimental analysis using a spectral residual method in the CONTACT algorithm. To this purpose, we compare two implementations of CONTACT algorithm which differ...
only in the nonlinear solver for the nonlinear systems arising in the TANG algorithm. The first implementation (CONTACT-NTR) uses a standard Newton trust-region method and the second one (CONTACT-DABBm) uses DABBm which turned out to be the more robust Srand version in the analysis above (see Figure 6.2). As a standard Newton trust-region method, we used the Matlab code proposed in [33]; default parameters were used and bound constraints on the unknown were dropped using the setting indicated in the code. The Jacobian matrix of $F$ was approximated by finite differences.

As a preliminary issue, we observe that the Jacobian matrices of $F$ are dense through the iterations; thus they cannot be formed as a low computational cost by finite difference procedures for sparse matrices [7]. We also observed in the experiments that the Jacobian matrices are nonsymmetric, do not have dominant diagonals and they are not close to diagonal matrices. For example, let us consider the Jacobian matrix of the system corresponding to speed $v = 16 m/s,$
curve track section, instant $t = 355$, iteration 2 of the CONTACT and iteration 4 of the TANG algorithm (355,2,4 in Table B.6). It has dimension $292 \times 292$ and, evaluated at the final iterate computed using ABBm08 rule, 96.18% of its elements are nonzero. The structure of the Jacobian can be observed in Figure 6.4 where the absolute values of its elements are plotted in a logarithmic scale (the surface of the full matrix on the left and a plot of the row 146 on the right). This structure is observed along all the iterations of the nonlinear system solvers and is common to all sequences generated by the CONTACT algorithm.

Fig. 6.4. Jacobian matrix: surface of the full matrix and plot of the central row (base 10 logarithm of the absolute values).
In our implementation, CONTACT algorithm terminated when the relative error between two successive values of the computed pressures dropped below $10^{-4}$ or a maximum of 20 alternating cycles between NORM and TANG was reached. Both nonlinear solvers were run until the stopping rule \hyperlink{6.15}{(6.15)} is met. We ran CONTACT-NTR and CONTACT-DABBm over the whole track for both velocities, that is we considered the whole sequence of 500 time steps. CONTACT-NTR generated 3759 and 5353 nonlinear systems for $v = 10 \text{ m/s}$ and $v = 16 \text{ m/s}$, respectively and CONTACT-DABBm generated 4496 and 5494 nonlinear systems for the two velocities.

As a first remark, both procedures successfully solved the contact model described above and were reliable and accurate in the numerical simulation of wheel-rail interaction. Secondly, the use of the spectral residual method yields a gain in terms of time with respect to the use of a standard Newton method where finite difference approximation of Jacobian matrices is employed; this feature derives from the fact that spectral residual method is derivative-free and does not ask for the solution of linear systems. Figures \hyperlink{6.5}{6.5} and \hyperlink{6.6}{6.6} show the comparison of the two CONTACT implementations in terms of number of $F$-evaluations (excluding those needed to approximate the Jacobian matrices) and execution elapsed time. From the plots we observe that CONTACT-DABBm takes a larger number of $F$-evaluations than CONTACT-NTR but it is faster. Over the whole time interval, CONTACT-DABBm employs 1 hour, 19 mins and 2 hours, 28 mins to solve the generated nonlinear systems with $v = 10 \text{ m/s}$ and $v = 16 \text{ m/s}$, while CONTACT-NTR takes 7 hours and 49 mins and 12 hours and 41 mins, respectively.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{Fig65.pdf}
\caption{Comparison between CONTACT-DABBm and CONTACT-NTR, $v = 10 \text{ m/s}$: number of $F$-evaluations and elapsed time in seconds (logarithmic scale).}
\end{figure}

7. Conclusions. The numerical behaviour of spectral residual methods for nonlinear systems strictly depends on the choice of the spectral stepelength. Although most of the works on this subject make use of the stepsizes $\beta_{k,1}$, known results on the spectral gradient methods for unconstrained optimization suggest that a suitable combination of the stepsizes $\beta_{k,1}$ and $\beta_{k,2}$ could be of benefit for spectral residual methods as well. This work aims to contribute to this study by providing a first systematic analysis of the stepsizes $\beta_{k,1}$ and $\beta_{k,2}$. Moreover, practical guidelines for dynamic choices of the steplength are derived from new theoretical results in order to increase both the robustness and the efficiency of spectral residual methods. Such findings have been extensively tested and validated on sequences of nonlinear systems arising in the solution of a contact wheel-rail model.
Fig. 6.6. Comparison between CONTACT-DABBm and CONTACT-NTR, \( v = 16 \, \text{m/s} \): number of \( F \)-evaluations and elapsed time in seconds (logarithmic scale).

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Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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Appendix A. Kalker’s contact model and CONTACT algorithm.

We give an overview of the model and algorithm used to generate our set of nonlinear systems. Let bold letters represent vectors, the subscript \( T \) denote a vector with components in the tangential \( x-y \) contact place, the subscript \( N \) denote the component of a vector in the normal \( z \) contact direction. The contact problem between two elastic bodies \([23,24]\) determines the contact region \( C \) inside the potential contact area \( A_c \) (usually the interpenetration area between the wheel and rail contact surfaces), its subdivision into adhesion area \( H \) and slip area \( S \), and the tangential \( p_T \) and normal \( p_N \) pressures such that the following contact conditions are satisfied:

\[
\begin{aligned}
\text{normal problem} \quad & \text{in contact } C : & e = 0, & p_N \geq 0 \\
& \text{in exterior } E : & p_N = 0, & e > 0 \\
& C \cup E = A_c, & C \cap E = \emptyset \\
\text{tangential problem} \quad & \text{in adhesion } H : & \|s_T\| = 0, & \|p_T\| \leq g \\
& \text{in slip } S : & \|s_T\| \neq 0, & p_T = -g s_T / \|s_T\| \\
& S \cup H = C, & S \cap H = \emptyset
\end{aligned}
\]  

(A.1)

Above, \( e \) is the deformed distance between the two bodies and, by definition, it holds \( e = 0 \) and \( p_N \geq 0 \) in \( C \). Referring to Figure [A.1], the region \( E \) where \( e > 0 \) is called the exterior area and \( p_N = 0 \) therein. The potential contact area is such that \( A_c = C \cup E \). The contact area \( C \) is divided into the area of adhesion \( H \) where the tangential component \( s_T \) of the slip vanishes, and the area \( S \) of slip where \( s_T \) is nonzero. The slip \( s_T \) is the difference between the velocities of two
homologous points belonging to deformed wheel and rail surfaces inside the contact area and is a function of the pressures \( p_T \) and \( p_N \), \( q \) is the traction bound (Coulomb friction model [23, 24]). Overall, the first three equations in (A.1) model the normal contact problem (computation of \( p_N \) and of the shapes of the regions \( C \) and \( E \)), whereas the last three equations describe the tangential contact problem (computation of \( p_T \), of local slidings \( s_T \) and of the shapes of the regions \( H \) and \( S \)).

Let us consider the discretization of (A.1). Assuming that the contact patch is entirely contained in a plane, the region within which the potential contact area \( A_c \) can be located is easily discretized through a planar quadrilateral mesh, see Figure A.1. The coordinates of the center of each quadrilateral element are denoted \( x_I = (x_{I1}, x_{I2}, 0) \) where the capital index \( I \) identifies the specific element, say \( I = 1, \ldots, N_E \). Also, the standard indices \( i = 1, 2, 3 \), will indicate the vector components. For any element \( I \) and any generic vector \( w_I = (w_{I1}, w_{I2}, w_{I3}) \) associated to such mesh element, \( w_{I1}, w_{I2} \) are the components in the \( x-y \) contact plane and \( w_{I3} \) is the component in the normal contact direction \( z \). Namely, \( w_{I,T} = (w_{I1}, w_{I2}) \) and \( w_{I3} \) are the discrete counterparts of \( w_T \) and \( w_N \), respectively.

![Fig. A.1. Local representation of the discretized contact area.](image)

The discrete values of the elastic deformation \( u \) on the mesh nodes (i.e. the deformation of the elastic bodies in the contact area [23, 24]) are defined both at the current time instance \( t \) and at the previous time instance \( t' \):

\[
\begin{align*}
\mathbf{u}_I &= (u_{Ii}) \quad \text{at} \quad (x_I, t), \quad \mathbf{u}'_I &= (u'_{Ii}) \quad \text{at} \quad (x_I + v (t - t'), t'),
\end{align*}
\]

where \( v \) is the rolling velocity (i.e. the longitudinal velocity of the wheel) and \( I \) is an arbitrary mesh element). Analogously, for the contact pressures \( p \) it holds

\[
\begin{align*}
\mathbf{p}_J &= (p_{Jj}) \quad \text{at} \quad (x_J, t), \quad \mathbf{p}'_J &= (p'_{Jj}) \quad \text{at} \quad (x_J + v (t - t'), t'),
\end{align*}
\]

where \( J \) is an arbitrary mesh element. According to the Boundary Element Method Theory [23, 24], the discretized displacements \( u_I \) can now be written as a function of the discretized contact pressures \( p_J \) through the discretized version of the problem shape functions, that is

\[
u_I = \sum_{J=1}^{N_E} \sum_{j=1}^{3} A_{IjJj} p_{Jj}, \quad \text{with} \quad A_{IjJj} := B_{iJj} (x_I),
\]

and \( B_{iJj}(x_I) \) are the discrete shape functions of the problem describing the effect of a contact pressure \( p_J \) applied to the element \( J \) on displacement \( u_I \) of the node \( I \) (see [23, 24]). The shape function \( B_{iJj} \) usually depends on the problem geometry and the characteristics of the materials. An analogous expression can be derived for \( u'_I \). The elastic penetration \( e \) can be calculated at each node \( x_I \) as

\[
e_I = h_I + \sum_J A_{IJ3J3} p_{J3},
\]
where $h_I$ is the discretization of the (known) undeformed distance between the two bodies, see \[23,24\]. Similarly, the slip $s_T$ can be discretized by setting
\[
s_{I,T} = c_{I,T} + (u_{I,T} - u'_{I,T})/(t - t'),
\]  
(A.4)
where $c_{I,T}$ is the discretization of the (given) rigid creep, that is the difference between the velocities of two homologous points belonging to the undeformed wheel and rail surfaces inside the contact area and thought of as rigidly connected to the bodies.

We observe that both $u$ and $s_T$ depend linearly on the pressures $p$ and $p'$. Therefore, the discretization of equation $e = 0$ in the norm problem (A.1) yields a linear system in the discretized normal pressures $(p_{I3})$ while the discretization of the nonlinear equation
\[
p_T = -g s_T/\|s_T\|, 
\]  
in the tangential problem yields the nonlinear system
\[
s_{I,T} = -\|s_{I,T}\|p_{I,T}/g_I, \tag{A.5}
\]  
with $p_{I,T} = (p_{I1}, p_{I2})$ being the unknowns. When using the Coulomb-like friction model \[23,24\], the friction limit function takes the form $g_I = f_I p_{I3}$, where $f_I$ is a given constant friction value.

The flow of Kalker’s CONTACT algorithm is displayed in Figure A.2 \[23,24\]. At each time step of time integration, the inputs of the CONTACT algorithm are the potential contact area $A_c$ (usually the interpenetration area between wheel and rail surfaces), the rigid penetration $h$ and the rigid local sliding $c_T$ (inputs calculated, on turn, from the kinematic variables of the body: position and velocities of the gravity centers $G_1$, $G_2$, $V_{G1}$, $V_{G2}$, rotation matrices $R_1$, $R_2$ and angular velocities $\omega_1$, $\omega_2$) \[23,24\]. All these kinematic quantities are calculated at each time step by the ODE solver of the Simpack Rail multibody environment \[39\]. NORM algorithm solves the normal contact problem and returns the contact area $C$, the non-contact area $E$, the normal contact pressures $p_N$. Then, TANG algorithm returns the sliding area $S$, adhesion area $H$, the tangential contact pressures $p_T$ and local sliding $s_T$. Repetitions of NORM and TANG algorithms

\[\text{Fig. A.2. The architecture of the Kalker’s CONTACT algorithm.}\]

\[\text{§In the unlikely event } s_{I,T} = 0, \text{ the system in nonsmooth. We regularize (A.5) replacing the term } \sqrt{s_{I1}^2 + s_{I2}^2} \text{ with } \sqrt{s_{I1}^2 + s_{I2}^2 + \epsilon}, \text{ for some small positive } \epsilon.\]
Table B.1

| System | BB1 | BB2 | ALT | ABB | ABBm | DABBm |
|--------|-----|-----|-----|-----|------|-------|
| 101,1,2 | 69  | 59  | 74  | 75  | 59   | 71    |
| 101,2,2 | 382 | 148 | 248 | 295 | 205  | 198   |
| 103,1,2 | 37  | 31  | 35  | 37  | 30   | 37    |
| 103,2,2 | 37  | 31  | 35  | 37  | 30   | 37    |
| 104,1,2 | 36  | 36  | 37  | 36  | 38   | 36    |
| 104,2,2 | 36  | 36  | 37  | 36  | 38   | 36    |
| 105,1,2 | 39  | 38  | 39  | 39  | 38   | 39    |
| 105,2,2 | 40  | 37  | 39  | 40  | 38   | 40    |
| 105,2,3 | 74  | 73  | 86  | 75  | 70   | 67    |
| 105,2,3 | 74  | 73  | 86  | 75  | 70   | 67    |

Table B.1: Number of function evaluations performed by Srand variants in the solution of nonlinear systems arising from time 100 to time 105 and corresponding to a straight line with velocity 10 m/s. In the first column we indicate the time step, the CONTACT and the TANG iteration.

Appendix B. Complete results. In this section we collect the complete runs which gave rise to the performance profiles in Figure 6.2. Results concern two velocities \( v = 10 \text{ m/s} \) in Tables B.1-B.3 and \( v = 16 \text{ m/s} \) in Tables B.4-B.6 and the three different track sections (straight line in Tables B.1 and B.4, cycloid in Tables B.2 and B.5 and curve in Tables B.3 and B.6). Given a sequence of nonlinear systems, we label a single system from the sequence as Time,Citer,Titer specifying the instant time (Time), the CONTACT iteration (Citer) and the TANG iteration (Titer).

For each Srand variant applied to a system, we report the number of \( F \)-evaluations performed in case of convergence, or, in case of failure, the corresponding flag. We recall from Section 6.3 that a run is successful when \( \| F_k \| \leq 10^{-6} \). A failure is declared either because the assigned maximum number of iterations or \( F \)-evaluations or backtracks is reached, or because \( \| F \| \) was not reduced for 50 consecutive iterations. Such occurrences are denoted as \( F_{it}, F_{fe}, F_{bt}, F_{in} \), respectively.

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| Table 2. Results for each section of the staircase generated in the oculocochlear section of the brain with a duration of 10 m/s. |
|---------------------------------|
| Time (ks) | Results |
|---------------------------------|
| 0.12  | 0.18  |
| 0.24  | 0.30  |
| 0.42  | 0.48  |
| 0.60  | 0.66  |
| 0.78  | 0.84  |
| 0.96  | 1.02  |

Velocity 10 m/s - Cyclic
### Table B.3

Results for each system of the sequences generated in the curve segment of the train path with velocity $v = 10 \text{ m/s}$.

| System   | BB1 | BB2 | ALT | ABB | ABBm | velocity 10 m/s - curve | DABBm | System   | BB1 | BB2 | ALT | ABB | ABBm | DABBm |
|----------|-----|-----|-----|-----|------|-------------------------|-------|----------|-----|-----|-----|-----|------|-------|
| 450,1,2  | 386 | 210 | 246 | 251 | 293 | 293 | 211 | 284 | 453,1,3 | 402 | 319 | 457 | 427 | 405 | 409 | 255 | 316 |
| 450,1,3  | 623 | 204 | 303 | 285 | 281 | 268 | 1580 | 1627 | 453,1,4 | F_{fe} | F_{in} | 2705 | 656 | 1285 | 996 | 611 | 544 |
| 450,2,2  | 29520 | 492 | 457 | 475 | 416 | 458 | 320 | 471 | 453,2,2 | 596 | 356 | 379 | 593 | 409 | 362 | 329 | 355 |
| 450,2,3  | 12031 | 428 | 433 | 412 | 458 | 415 | 309 | 387 | 453,2,3 | F_{fe} | 739 | 872 | 1030 | 557 | 726 | F_{in} | 2018 | 1579 | 1535 | F_{in} |
| 450,3,2  | 13652 | 560 | 403 | 562 | 416 | 463 | 379 | 382 | 453,3,2 | 566 | 351 | 355 | 548 | 392 | 367 | 337 | 398 |
| 451,1,2  | 681 | 437 | 382 | 520 | 570 | 519 | 340 | 397 | 453,3,3 | F_{fe} | 558 | 598 | 796 | 617 | 612 | 536 | 568 |
| 451,1,3  | F_{in} | 1218 | 4314 | 999 | 1564 | 868 | 613 | 1501 | 453,4,3 | F_{in} | F_{in} | F_{in} | 2308 | F_{in} | 1487 | 1187 | 1607 |
| 451,2,1  | F_{in} | 3805 | 18920 | 1790 | F_{in} | 1305 | 1083 | 1334 | 454,1,2 | 147 | 153 | 165 | 139 | 153 | 137 | 138 | 150 |
| 451,2,2  | 324 | 274 | 329 | 264 | 264 | 263 | 210 | 250 | 454,1,3 | 207 | 175 | 206 | 229 | 192 | 194 | 154 | 175 |
| 451,2,3  | F_{in} | 1652 | 1046 | 859 | 1304 | 691 | 520 | 595 | 454,1,4 | 2367 | 276 | 293 | 286 | 332 | 283 | 252 | 314 |
| 451,2,4  | F_{fe} | 1573 | 1573 | 1260 | 1232 | F_{in} | 941 | 861 | 351 | 250 | 269 | 328 | 291 | 231 | 301 |
| 451,3,2  | 381 | 253 | 240 | 301 | 243 | 285 | 209 | 270 | 454,2,2 | 237 | 172 | 209 | 194 | 191 | 202 | 153 | 207 |
| 451,3,3  | F_{in} | 3141 | 2432 | 660 | 801 | 640 | 606 | 635 | 454,2,3 | 413 | 279 | 211 | 288 | 315 | 240 | 254 | 280 |
| 451,3,4  | F_{in} | F_{in} | F_{in} | F_{in} | 1042 | 956 | 888 | 570 | 363 | 209 | 256 | 307 | 262 | 227 | 261 |
| 451,4,2  | 358 | 296 | 321 | 279 | 295 | 268 | 213 | 263 | 454,3,4 | 239 | 204 | 204 | 183 | 198 | 183 | 157 | 183 |
| 451,4,3  | F_{in} | 2108 | 901 | 688 | 739 | 676 | 597 | 639 | 454,3,4 | 469 | 317 | 329 | 273 | 290 | 244 | 251 | 265 |
| 451,4,4  | F_{in} | F_{in} | F_{in} | F_{in} | 12872 | 1797 | 1093 | 821 | 454,3,4 | 450 | 302 | 231 | 277 | 297 | 254 | 229 | 270 |
| 452,1,2  | 66785 | 638 | 638 | 548 | 743 | 585 | 545 | 522 | 455,1,2 | 147 | 137 | 145 | 144 | 126 | 145 | 127 | 136 |
| 452,1,3  | 71198 | 701 | 725 | 535 | 789 | 489 | 552 | 508 | 455,1,3 | 212 | 184 | 203 | 219 | 166 | 226 | 166 | 196 |
| 452,2,1  | 45680 | 803 | 521 | 617 | 594 | 584 | 470 | 520 | 455,1,4 | 482 | 272 | 256 | 291 | 278 | 251 | 237 | 246 |
| 452,2,2  | 198 | 557 | 887 | 514 | 539 | 417 | 301 | 467 | 455,2,2 | 497 | 372 | 250 | 496 | 288 | 256 | 270 | 284 |
| 452,3,2  | 37979 | 608 | 714 | 474 | 672 | 456 | 425 | 454 | 455,3,2 | 563 | 393 | 473 | 441 | 340 | 436 | 357 | 348 |
| 452,4,2  | 40269 | 718 | 797 | 565 | 790 | 484 | 379 | 501 | 455,2,4 | F_{fe} | 840 | 5928 | 1544 | 929 | 1131 | 618 | 632 |
| 452,3,3  | 31280 | 433 | 451 | 438 | 517 | 345 | 405 | 354 | 455,3,2 | 341 | 270 | 268 | 391 | 392 | 302 | 238 | 282 |
| 452,3,4  | 41623 | 581 | 634 | 575 | 726 | 509 | 400 | 451 | 455,3,3 | 603 | 432 | 405 | 592 | 415 | 363 | 346 | 353 |
| 452,4,3  | 5592 | 477 | 658 | 572 | 570 | 457 | 407 | 470 | 455,3,4 | F_{fe} | 792 | 7505 | 1586 | 855 | 914 | 663 | 744 |
| 453,1,2  | 288 | 200 | 257 | 227 | 210 | 279 | 190 | 270 | 455,1,3 | 402 | 319 | 457 | 427 | 405 | 409 | 255 | 316 |
from time 50 to time 55 and corresponding to a straight line with velocity 16 m/s. In the first column we indicate the time step, the CONTACT and the TANG iteration.

| System  | BB1 | BB2 | ALT | ABB | ABBm | DABBm |
|---------|-----|-----|-----|-----|------|-------|
| 50_1,2 | 60  | 45  | 53  | 52  | 47   | 52    |
| 50_2,2 | 53  | 44  | 51  | 54  | 48   | 54    |
| 50_3,2 | 53  | 44  | 51  | 48  | 48   | 48    |
| 52_1,2 | 75  | 78  | 53  | 76  | 75   | 101   |
| 52_2,2 | 89  | 78  | 53  | 76  | 88   | 112   |
| 52_3,2 | 65  | 66  | 66  | 83  | 66   | 80    |
| 55_1,2 | 69  | 79  | 60  | 76  | 61   | 73    |
| 55_2,2 | 69  | 79  | 60  | 80  | 61   | 73    |
| 55_3,2 | 69  | 79  | 60  | 80  | 61   | 73    |

Table B.4

Number of function evaluations performed by the BARON variants in the solution of nonlinear systems arising from time 50 to time 55 and corresponding to a straight line with velocity 16 m/s. In the first column we indicate the time step, the CONTACT and the TANG iteration.
Table B.5

| System | BB1 | BB2 | ALT | ABB | ABBm | DABBm |
|--------|-----|-----|-----|-----|------|-------|
| \(150.1,2\) | 985 | 297 | 330 | 366 | 357 | 351 | 278 |
| \(150.1,3\) | 26886 | 569 | 512 | 612 | 555 | 487 | 419 |
| \(150.1,4\) | F_{fe} | 967 | 3163 | 653 | F_{in} | 550 | 604 |
| \(150.1,5\) | F_{fe} | 810 | 647 | 15.49 | 614 | 510 | 710 |
| \(150.2,2\) | 470 | 228 | 307 | 295 | 302 | 277 | 216 |
| \(150.2,3\) | 627 | 584 | 404 | 437 | 485 | 377 | 344 |
| \(150.2,4\) | 52573 | 585 | 479 | 491 | 7.39 | 438 | 391 |
| \(150.3,2\) | F_{fe} | 1304 | F_{in} | F_{in} | 1777 | 2707 | 1237 |
| \(150.3,3\) | F_{fe} | 2498 | F_{in} | F_{in} | 2300 | 1973 | 17.37 |
| \(150.3,4\) | F_{fe} | 6214 | F_{in} | F_{in} | 3097 | 2576 | F_{in} |
| \(150.4,2\) | F_{fe} | 1005 | 5095 | 841 | 905 | 664 | 605 |
| \(150.4,3\) | F_{fe} | 1114 | 5312 | 1421 | 1144 | 810 | 616 |
| \(150.4,4\) | F_{fe} | 1454 | 8154 | 1630 | 3755 | 1125 | 1399 |
| \(150.5,2\) | F_{fe} | 3590 | 13111 | 2610 | 1435 | 1231 | 864 |
| \(150.5,3\) | F_{fe} | 1387 | 12656 | 1333 | 3092 | 973 | 864 |
| \(150.5,4\) | F_{fe} | 3776 | 959 | 1983 | 2198 | 1077 | 949 |
| \(150.2,5\) | F_{fe} | 3013 | 9973 | 1867 | 3551 | 1409 | 870 |
| \(150.2,6\) | F_{fe} | 5005 | 18545 | 1831 | 3662 | 1635 | 1270 |
| \(150.2,7\) | F_{fe} | 7743 | 749 | 3893 | F_{in} | 939 | 803 |
| \(150.3,3\) | F_{fe} | 2293 | 9494 | 1383 | 1689 | 1089 | 809 |
| \(150.3,4\) | F_{fe} | 1235 | 7622 | 1416 | 1884 | 1075 | 856 |
| \(150.3,5\) | F_{fe} | 4085 | 24983 | 1853 | F_{in} | 1509 | 1147 |
| \(150.3,6\) | F_{fe} | 68856 | 822 | 1395 | 742 | 661 | 680 |
| \(150.3,7\) | F_{fe} | 682 | 4090 | 1153 | 1085 | 859 | 648 |
| \(150.2,8\) | F_{fe} | 20711 | 561 | 382 | 664 | 453 | 358 |
| \(150.2,9\) | F_{fe} | 75894 | 966 | 1098 | 522 | 898 | 639 |
| \(150.2,10\) | F_{fe} | 1146 | 4114 | 848 | 1152 | 744 | 558 |

Results for each system of the sequences generated in the cycloid section of the train track with velocity \(v = 16 \text{ m/s}\).
Results for each system of the sequences generated in the curve section of the train track with velocity 30 m/s.

| Time (s) | System | Curve | Velocity (m/s) |
|----------|--------|-------|----------------|
| 0.1      | A      | 0.20  | 30             |
| 0.2      | B      | 0.40  | 30             |
| 0.3      | C      | 0.60  | 30             |
| 0.4      | D      | 0.80  | 30             |
| 0.5      | E      | 1.00  | 30             |
| 0.6      | F      | 1.20  | 30             |
| 0.7      | G      | 1.40  | 30             |
| 0.8      | H      | 1.60  | 30             |
| 0.9      | I      | 1.80  | 30             |
| 1.0      | J      | 2.00  | 30             |

Note: The table above shows the results for each system at different times and velocities.
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