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Discretization of implicit ODEs for singular root-finding problems

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Abstract

This paper addresses the use of dynamical system theory to tackle singular root-finding problems. The use of continuous-time methods leads to implicit differential systems when applied to singular nonlinear equations. The analysis is based on a taxonomy of singularities and uses previous stability results proved in the context of quasilinear implicit ODEs. The proposed approach provides a framework for the systematic formulation of quadratically convergent iterations to singular roots. The scope of the work includes also the introduction of discrete-time analysis techniques for singular problems which are based on continuous-time stability and numerical stability. Some numerical experiments illustrate the applicability of the proposed techniques. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The qualitative relations between discrete and continuous time dynamical systems have been extensively addressed in the last decades. In particular, the discrete dynamics resulting from the numerical integration of ODEs have motivated much of this research: see [41] and references therein. Within the so-called *dynamical systems approach to numerical analysis*, the iteration obtained from the numerical integration of an ODE may be studied as a discrete dynamical system, parameterized by

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the constants of the integration method. This provides a framework for studying the inheritance of different qualitative properties.

Following this approach, the present paper analyzes different discretizations of continuous-time models for singular root-finding and optimization problems. These singular problems arise, for example, in the presence of bifurcation points in continuation methods, as discussed in Section 1.1. The role of singularities can be properly framed, in the continuous-time context, within the theory of implicit ODEs, which in turn are closely related to differential-algebraic equations or DAEs [4,18]. The use of continuous models also allows one to perform a discretization adapted to the specific features of the problem under consideration. In this direction, the purpose of the present work is two-fold: from a general point of view, we aim to elaborate on the use of discrete-time analysis techniques for singular problems, based on continuous-time stability and numerical stability. Our second goal is to introduce a systematic methodology for the formulation of quadratically convergent iterations for singular root-finding problems.

The document is structured as follows: the rest of this section presents some background on singular root-finding problems, continuous-time methods and singular ODEs. Section 2 summarizes some results from [36] concerning singularities of the continuous-time analog of Newton's method. The main results of the present paper are then discussed in Section 3, where a discretization study is carried out following a taxonomy of singular problems which classifies them into *weak* and *strong* ones. Finally, concluding remarks are compiled in Section 4.

1.1. Singular root-finding problems

Let us consider the problem of locating a zero x^* of $f \in C^l(\mathbb{R}^n, \mathbb{R}^n)$, $l \geqslant 4$, where the Jacobian matrix $J \in C^{l-1}(\mathbb{R}^n, \mathbb{R}^{n\times n})$ ($\mathbb{R}^{n\times n}$ being the set of all $n \times n$ real matrices) is singular, that is, such that $J(x^*)$ is a noninvertible matrix. These problems arise, for example, in the presence of bifurcation points in continuation methods [1,45].

The classical Newton iteration, widely used as a corrector in PC methods for the above-mentioned continuation problem, is defined by the linearly implicit (or quasilinear) difference equation

$$-J(x^{(k)})(x^{(k+1)} - x^{(k)}) = f(x^{(k)}) \tag{1}$$

and becomes ill-conditioned, or even undefined, around such singular solutions. The simplest singular case is characterized by the transversality condition

$$(\det J)'(x^*)v \neq 0 \quad \text{for } v \in \operatorname{Ker} J(x^*) - \{0\}, \tag{2}$$

which has three major implications. First, the Jacobian matrix $J(x)$ is singular on a hypersurface $\Psi \ni x^*$. As will be discussed in Section 1.3, this hypersurface typically includes impasse points which introduce specific difficulties in both continuous and discrete time. Also, it is easily proved (see [27]) that condition (2) implies that $\dim \operatorname{Ker} J(x^*) = 1$. This indicates that the transversality hypothesis is a minimal degeneracy assumption, since in this case the Jacobian matrix is rank-deficient by one. Finally, as proved by Keller [21], singular equilibria satisfying (2) are isolated, which is not always the case in general singular problems.

Under conditions equivalent to the transversality hypothesis (2), a result of linear convergence from a cone-shaped region with vertex in the root was proved by Reddien [30]. This work was later improved by several authors (see [8,10,16,17,21,23] and references therein), and then extended to other numerical methods for singular problems [9,11,22,24]. Some of these papers present acceleration schemes to improve the rate of convergence at singular roots [22,23]. As an example, the iteration

$$y^{(k)} = x^{(k)} - J^{-1}(x^{(k)})f(x^{(k)}), \tag{3a}$$

$$z^{(k)} = y^{(k)} - J^{-1}(y^{(k)})f(y^{(k)}), \tag{3b}$$

$$x^{(k+1)} = z^{(k)} - 2J^{-1}(z^{(k)})f(z^{(k)}), \tag{3c}$$

reported in [23], yields quadratic convergence to certain singular roots.

The present work discusses a different approach to this issue, based on the fact that the loss of quadratic convergence in the classical Newton method may be seen as the result of a (in a certain sense) defective transformation of spectra at singular solutions. In this direction, iterations (1) and (3) may be respectively seen as an Euler and a 3-stage explicit Runge–Kutta integration of the continuous Newton method presented below. This topic is introduced in Section 1.2, and extensively discussed in Sections 2 and 3.

1.2. Continuous-time methods

The use of continuous-time systems to solve nonlinear equations may be traced back to Davidenko [7]. These techniques have been later developed through the introduction of different analogs of root-finding algorithms [2,15,26,34,35,42,43,46,47], using ODE and DAE formulations [3,19,37,38], in the context of homotopy techniques [14,20], and as trajectory methods (see [12] for a survey). Difficulties related to the presence of singularities are usually better addressed in the continuous-time setting. These models are often oriented to global problems, although the present paper is focused on local convergence issues. A unique continuous system may lead to different iterative techniques, including accelerated versions of basic methods, through the use of different integration schemes. The convergence analysis of these iterations is then shifted to a stability study of the continuous system and the discretization method. Damped methods may also be derived from continuous-time models using variable-stepsize integrators: these techniques are however beyond the scope of the present work, which essentially requires the use of fixed-stepsize integration schemes to guarantee quadratic convergence.

In this context, the continuous Newton method is paradigmatic [34,35,42]. This method is defined by the linearly implicit differential equation [4,36]

$$-J(x)\dot{x} = f(x). \tag{4}$$

Regular roots of f (points where $f(x^*) = 0$ and $J(x^*)$ is invertible) lead to asymptotically stable equilibria of (4), their linearization having a unique (index-1) eigenvalue $\lambda = -1$. Euler discretization with stepsize $h = 1$ leads to the classical Newton method (1), and the semisimple eigenvalue of the continuous system yields a semisimple null eigenvalue in the discrete setting. Quadratic convergence to regular roots follows from this fact, the behavior being substantially different at singular solutions.

1.3. Singular ODEs

The continuous Newton method (4) may be framed within the general context of *linearly implicit* (or *quasilinear*) ordinary differential equations [27–29,33,36,40]:

$$A(x)\dot{x} = f(x), \tag{5}$$

where $A \in C^k(\mathbb{R}^n, \mathbb{R}^{n\times n})$, and $f \in C^l(\mathbb{R}^n, \mathbb{R}^n)$, with $k, l \geqslant 1$. The continuous Newton system is a particular case of (5), with $A = -J$.

System (5) may be trivially reduced to the explicit ODE

$$\dot{x} = A(x)^{-1} f(x) \equiv h(x), \tag{6}$$

around points where $A(x)$ is regular. If, on the contrary, $A(x)$ has constant rank $r < n$ on a neighborhood of a singular point x^*, the equation can be often reduced to a regular system in the theory of differential-algebraic equations (DAEs) [4,18].

The attention in this work is restricted to cases in which $A(x)$ is singular on a hypersurface Ψ, with $x^* \in \Psi$. This occurs if x^* is a *noncritical singular point* [27], that is, if the condition $(\det A)'(x^*) \neq 0$ is satisfied. Singular points will be assumed to be noncritical in this paper, system (5) being in this case a singular index-0 DAE [36]. In this situation, it follows that $\dim \operatorname{Ker} A(x^*) = 1$ [27]. This case can be reformulated, using an additional variable, as the singular index-1 semiexplicit DAE [32,36]

$$\dot{x} = y,$$
$$0 = A(x)y - f(x).$$

This enlargement is often oriented to the numerical treatment of the system [18]. It is worth mentioning that, conversely, singular semiexplicit index-1 DAEs can be reduced to quasilinear form on the solution manifold, under generic assumptions [32]. Singularities of DAEs also arise in power systems, magnetohydrodynamics, and nonlinear circuits: in this framework, different qualitative properties have been studied in [32,39,44].

The main taxonomy of singular points in noncritical quasilinear equations (5) classifies them into *algebraic singularities*, where $f(x^*) \notin \operatorname{Rg} A(x^*)$, and *geometric singularities*, satisfying $f(x^*) \in \operatorname{Rg} A(x^*)$ [28,29]. Algebraic singularities typically behave as *impasse points* [5,6,27], where trajectories collapse in finite time with infinite speed. This phenomenon was heuristically observed in the continuous Newton method [26] while, at the same time, it was being characterized in the linearly implicit setting [27].

On the other hand, singular equilibria (where $f(x^*) = 0$ and $A(x^*)$ is noninvertible) are geometric singularities, the local behavior around them being substantially different from that of impasse points. The qualitative behavior of quasilinear problems around singular roots has been analyzed in [36], and the main results are surveyed in Section 2. These results underly the discretization study carried out in Section 3.

2. Singularities of the continuous Newton method

The main stability results for singular zeros of the continuous Newton method are summarized in this section (see [31,34–36]). These results are structured according to a taxonomy which classifies geometric singularities (and, in particular, singular equilibria) into *weak* and *strong* ones.

A noncritical geometric singular point x^* is said to be a *weak singularity* if there exists a singular neighborhood $U^{x^*} \cap \Psi$ of x^* entirely formed by geometric singularities. Geometric singular points which fail to satisfy this condition will be termed *strong singularities*, being accumulation points of the set of algebraic singularities. With the notation $g(x) = \operatorname{Adj} A(x) f(x)$, $\omega(x) = \det A(x)$, weak singular points may be equivalently defined as singularities around which there exists a neighborhood U^{x^*} where $\omega(x) = 0 \Rightarrow g(x) = 0$ [36].

Weak singular points are important since $h(x) = A(x)^{-1} f(x) = g(x)/\omega(x)$ may be extended as a C^{m-1} vector field, with $m = \min\{k, l\}$, on a whole neighborhood of x^* (including singular points) if this is a noncritical weak singularity [34]. Hence, weak singular problems may be studied using classical linearization tools, and allow one to structure the singularity analysis. They represent a first step in this analysis, and provide some hints for the study of the more general strong case.

2.1. Weak singular roots

It is well known that the classical Newton method may still be applied to singular one-dimensional problems, displaying a 1/2 eigenvalue at singular roots where $f''(x^*) \neq 0$. Quadratic convergence is recovered using the modified iteration $x^{(k+1)} = x^{(k)} - 2f(x^{(k)})/f'(x^{(k)})$. The extension of this behavior to multidimensional problems falls within the setting of weak singularities. The continuous-time case is summarized here, whereas the corresponding discretization study is carried out in Section 3.1.

Weak singular zeros yield asymptotically stable equilibria of the continuous Newton method, under the transversality assumption (2) [36]:

Theorem 1. *Let x^* be a weak singular zero of the continuous Newton method for $f \in C^4(\mathbb{R}^n, \mathbb{R}^n)$, satisfying the transversality hypothesis* (2). *The linearization of the Newton field $F(x) = -J(x)^{-1} f(x)$ at x^* has eigenvalues $-1/2$ (simple, with eigenspace* $\operatorname{Ker} J(x^*)$), *and (if $n \geqslant 2$) -1, with index* 1. *Therefore, this equilibrium is asymptotically stable.*

This result is proved in [36] through the analysis of certain matrix equations and, in particular, using a singular version of Lyapunov's equation. The weak case provides counterexamples to the usual assumption that the domain of convergence of Newton's method, when applied to singular roots, should always exclude other singularities [16,17]. A simple example of this behavior is given by the continuous Newton method when applied to the fold $f(x_1, x_2) = (x_1^2, x_2)$, which yields the linear system $F(x_1, x_2) = (-x_1/2, -x_2)$.

2.2. Strong singular roots

In the more general strong case, the existence of a cone-shaped region which is positively invariant and convergent to the root is proved in [31,36]:

Theorem 2. *Let x^* be a strong singular zero of the continuous Newton method for $f \in C^4(\mathbb{R}^n, \mathbb{R}^n)$, satisfying the transversality hypothesis* (2). *There exists a cone-shaped region*

$$\mathscr{W}_{\theta,\rho} = \{x \in \mathbb{R}^n \colon \|P_X(x - x^*)\| \leqslant \theta \|P_N(x - x^*)\|,\ \|x - x^*\| \leqslant \rho\}, \tag{7}$$

where $N = \operatorname{Ker} J(x^*)$, $\mathbb{R}^n = N \oplus X$, *and* P_X (*resp.* P_N) *denotes a projection onto* X (*resp.* N) *along* N (*resp.* X), *which is positively invariant and convergent to* x^*. *Taking* $X = T_{x^*}\Psi$, $\hat{x} = x - x^*$, $z = P_N(\hat{x})$, $y = P_X(\hat{x})$, *the Newton field* F *may be described on* $\mathscr{W}_{\theta,\rho}$ *as*

$$P_N F(z,y) = -\frac{z}{2} + \beta\left(\frac{yy}{z}\right) + \gamma(zz) + O(\|y\|\,\|z\|) + o(\|\hat{x}\|^2), \tag{8a}$$

$$P_X F(z,y) = -y + \delta(yz) + O(\|y\|^2) + o(\|\hat{x}\|^2), \tag{8b}$$

where β, γ *and* δ *represent*, *with abuse of notation*

$$\beta\left(\frac{yy}{z}\right) = \frac{\operatorname{Adj} J(x^*) f''(x^*) yy}{2(\det J)'(x^*) z}, \tag{9}$$

$$\gamma(zz) = \frac{\operatorname{Adj} J(x^*) f'''(x^*) zzz}{12(\det J)'(x^*) z}, \tag{10}$$

$$\delta(yz) = P_X \frac{(\operatorname{Adj} J)'(x^*) z f''(x^*) yz}{2(\det J)'(x^*) z}. \tag{11}$$

This result represents a continuous-time analog of Reddien's theorem describing the behavior of the classical Newton method at singular roots [30]. Theorem 2 is proved in [36] using a Lyapunov–Schmidt decomposition and standard ODE results. It is worth mentioning that the values $-1/2$ and -1 in the leading terms of (8) correspond to the eigenvalues of the linearization in the above-mentioned weak case.

3. Discretization issues

It is well known that the classical Newton iteration is quadratically convergent when applied to regular problems. Newton's method is obtained after Euler's discretization of the continuous method (4) with stepsize one, and this quadratic behavior may be seen as the result of the transformation of the continuous spectrum $\sigma = \{-1\}$ through the mapping $\lambda \to 1 + \lambda$. In this section we address this issue for singular problems, in which quadratic convergence is lost, through the use of other Explicit Runge–Kutta (ERK) discretizations. In the weak case, a spectral study is sufficient to design quadratically convergent iterations, whereas in strong problems a study of invariance is also needed.

Our study is founded on the following result, based on the concept of Q-order of convergence [25]:

Proposition 1. *Let* x^* *be a fixed point of* $G \in C^2(\mathbb{R}^n, \mathbb{R}^n)$, *the spectral radius* $\mathrm{r}(G'(x^*))$ *satisfying* $0 < \mathrm{r}(G'(x^*)) < 1$. *Then* x^* *is an attractor for* G *with linear convergence*. *If*, *on the other hand*, *it is* $G'(x^*) = 0$, *then the convergence is* (*at least*) *quadratic*.

For later use, note that the assumption $\mathrm{r}(G'(x^*)) = 0$ does not necessarily imply $G'(x^*) = 0$: the condition that the (unique) null eigenvalue has index-1 is also needed to guarantee the vanishing of $G'(x^*)$.

3.1. Weak problems: spectral conditions

Theorem 1 in Section 2.1 reduces the study of weak problems to an explicit setting and, therefore, allows for the use of classical tools in the analysis of such singularities. Concerning discretization issues, in explicit systems, as well as in linearly implicit problems around weak singularities, the existence of a vector field describing the dynamics makes it possible to perform the convergence study through the spectral transform associated with the discretization process. The basic result in this direction is the following [13, Theorem 4.4.3]:

Proposition 2. *Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of a square matrix A. If $p(\mu)$ is a scalar polynomial, then $p(\lambda_1), \ldots, p(\lambda_n)$ are the eigenvalues of $p(A)$.*

It is immediate to check that an eigenvector of A is also an eigenvector of $p(A)$. This result may be applied, in particular, to cases in which the polynomial p results from the application of a numerical integration scheme. Let us consider an s-stage ERK method

$$x^{(k+1)} = x^{(k)} + h\sum_{i=1}^{s} b_i F(\tilde{x}^i) \tag{12}$$

with stage values $\tilde{x}^i$ given by

$$\tilde{x}^1 = x^{(k)}, \qquad \tilde{x}^i = x^{(k)} + h\sum_{j=1}^{i-1} a_{ij} F(\tilde{x}^j), \quad 1 < i \leqslant s. \tag{13}$$

This method defines a parameterized iteration of the form $x^{(k+1)} = G(x^{(k)}, b_i, a_{ij}, h)$. F being the Newton field, our purpose is to characterize the convergence properties of such iterations around a singular equilibrium x^*, depending on the coefficients b_i and a_{ij}. These properties are closely linked to the spectral features of $G'(x^*)$, which can be recursively expressed in terms of $F'(x^*)$:

$$G'(x^*) = I_n + h\sum_{i=1}^{s} b_i F'(x^*) \left.\frac{\mathrm{d}\tilde{x}^i}{\mathrm{d}x^{(k)}}\right|_{x^*},$$

$$\left.\frac{\mathrm{d}\tilde{x}^i}{\mathrm{d}x^{(k)}}\right|_{x^*} = I_n + h\sum_{j=1}^{i-1} a_{ij} F'(x^*) \left.\frac{\mathrm{d}\tilde{x}^j}{\mathrm{d}x^{(k)}}\right|_{x^*}, \tag{14}$$

where $\tilde{x}^i = x^*$ since x^* is an equilibrium point. This allows us to express $G'(x^*)$ as a polynomial on $F'(x^*)$ of degree s:

$$G'(x^*) = I_n + \sum_{i=1}^{s} d_i (hF'(x^*))^i. \tag{15}$$

In this polynomial, the coefficient d_i has the generic form

$$\sum_{m=i}^{s} b_m a_{mj_{i-1}} a_{j_{i-1}j_{i-2}} \dots a_{j_2 j_1}, \tag{16}$$

where the sum is extended over all combinations of $i-1$ sub-indices $j_1, \dots, j_{i-1}$ such that $0 < j_1 < j_2 < \dots < j_{i-1} < m$. For instance, in a 3-stage method the coefficients d_i are

$$d_1 = b_1 + b_2 + b_3, \tag{17a}$$

$$d_2 = b_2 a_{21} + b_3 a_{31} + b_3 a_{32}, \tag{17b}$$

$$d_3 = b_3 a_{32} a_{21}. \tag{17c}$$

Following Proposition 2, the spectrum of $G'(x^*)$ may be obtained from the eigenvalues λ_i of $F'(x^*)$ through the polynomial transformation

$$p(\lambda_i) = 1 + \sum_{j=1}^{s} d_j (h\lambda_i)^j. \tag{18}$$

Note that the eigenvalues of the Newton field at a noncritical weak equilibrium are $-1/2$ and, in dimension greater than one, -1. The goal of this study is then the derivation of conditions on the coefficients b_i, a_{ij} allowing for the application of Proposition 1, yielding linearly or quadratically convergent iterations to singular zeros. Note that the freedom in the selection of these coefficients makes it possible to normalize the study fixing $h = 1$, which simplifies the analysis when compared with the alternative of choosing the coefficients b_i according to the consistency condition $\sum_{i=1}^{s} b_i = 1$.

Linear convergence is guaranteed under the conditions $|p(-1/2)| < 1$, $|p(-1)| < 1$. If any of these values is nonnull, the convergence will be strictly linear. In a 1-stage ERK method, described by the iteration

$$x^{(k+1)} = x^{(k)} + b_1 F(x^{(k)}), \tag{19}$$

where the presence of the coefficient b_1 is due to the normalization $h = 1$, the spectral transformation has the form

$$p(\lambda_i) = 1 + b_1 \lambda_i. \tag{20}$$

The particular case $b_1 = 1$ yields the classical Newton iteration, and maps the eigenvalues $-1/2$, -1, into $1/2$, 0, respectively. This is responsible for the linear convergence of Newton's method to weak singular roots. In one-dimensional problems, in which the unique eigenvalue of the continuous method is $-1/2$, the selection $b_1 = 2$ yields a null eigenvalue in the discrete system. This fact leads to a quadratically convergent iteration, as indicated in Section 2.1. In dimensions greater than one, on the other hand, it is not possible to obtain a quadratically convergent iteration using 1-stage methods. In the sequel, the problem dimension will be assumed greater than one and, therefore, multistage ERK methods will be needed to achieve quadratic techniques.

From Proposition 1 and the fact that the eigenvalues $-1/2$ and -1 of the continuous Newton method have index-1, it follows that a necessary and sufficient condition to achieve (at least) quadratic convergence of an ERK discretization to noncritical weak singular zeros is that

$0 = p(-1/2) = p(-1)$. This is equivalent to the requirement that the polynomial $p(\lambda_i)$ has $(2\lambda_i + 1)$ and $(\lambda_i + 1)$ as divisors, namely, that its factorization is of the form

$$p(\lambda_i) = (2\lambda_i + 1)(\lambda_i + 1)q(\lambda_i). \tag{21}$$

This yields certain conditions on the coefficients b_i, a_{ij} which will be termed *spectral conditions* for quadratic convergence. Note that, as indicated above, at least two stages are needed in an ERK method to obtain a factorization of form (21).

In the particular case of a 2-stage ERK method, polynomial (18) reads as

$$p(\lambda_i) = b_2 a_{21} \lambda_i^2 + (b_1 + b_2)\lambda_i + 1, \tag{22}$$

and must be equal to $(2\lambda_i + 1)(\lambda_i + 1) = 2\lambda_i^2 + 3\lambda_i + 1$. This yields the following spectral conditions:

$$b_2 a_{21} = 2, \tag{23a}$$

$$b_1 + b_2 = 3. \tag{23b}$$

For instance, the combinations $b_1 = 1$, $b_2 = 2$, $a_{21} = 1$ and $b_1 = 2$, $b_2 = 1$, $a_{21} = 2$ satisfy the above-mentioned conditions. As a sample, the former yields the following quadratically convergent iteration to weak singular roots:

$$x^{(k+1)} = x^{(k)} + F(x^{(k)}) + 2F(x^{(k)} + F(x^{(k)})). \tag{24}$$

In the 3-stage case, the reasoning is analogous, taking into account the fact that in (21) there is an additional factor $(c\lambda_i + 1)$ with arbitrary c. The polynomial

$$p(\lambda_i) = b_3 a_{32} a_{21} \lambda_i^3 + (b_2 a_{21} + b_3 a_{31} + b_3 a_{32})\lambda_i^2 + (b_1 + b_2 + b_3)\lambda_i + 1 \tag{25}$$

now has the form

$$p(\lambda_i) = 2c\lambda_i^3 + (2 + 3c)\lambda_i^2 + (3 + c)\lambda_i + 1, \tag{26}$$

which yields, after some simple computations, the spectral conditions

$$2(b_1 + b_2 + b_3) - b_3 a_{32} a_{21} = 6, \tag{27a}$$

$$3(b_1 + b_2 + b_3) - (b_2 a_{21} + b_3 a_{31} + b_3 a_{32}) = 7. \tag{27b}$$

The parameter set $b_1 = b_2 = a_{21} = a_{31} = a_{32} = 1$, $b_3 = 2$, which characterizes the iteration (3) proposed in [23], verifies, in particular, these conditions.

The above study may be summarized in the following result:

Theorem 3. *Let x^* be a weak singular zero of the continuous Newton method for $f \in C^4(\mathbb{R}^n, \mathbb{R}^n)$, satisfying the transversality hypothesis* (2). *An ERK discretization of the continuous Newton method, with stepsize $h = 1$, yields a (at least) quadratically convergent iteration to x^* if and only if the coefficients of the method verify the spectral conditions given by the factorization* (21). *In particular, for* 2- *and* 3-*stage methods, such conditions are given by* (23) *and* (27), *respectively.*

The same reasoning may be applied to non-transversal or critical weak singular zeros at which the Newton field is well-defined, as illustrated below (see [34]).

Example 1. Let us consider the function $f(x_1,x_2)=(x_1^2x_2, x_1^4+x_2^2)$, which has a unique zero at the origin. The Jacobian matrix is

$$J(x_1,x_2)=\begin{pmatrix} 2x_1x_2 & x_1^2 \\ 4x_1^3 & 2x_2 \end{pmatrix}, \tag{28}$$

its determinant being

$$\omega(x_1,x_2)=\det J(x_1,x_2)=4x_1(x_2^2-x_1^4). \tag{29}$$

The singular set is formed by the x_2 axis and the two parabolas $x_2=\pm x_1^2$. On the other hand, it is also easy to check that

$$g(x_1,x_2)=-\mathrm{Adj}\,J(x_1,x_2)f(x_1,x_2)=(-x_1^2(x_2^2-x_1^4), -2x_1x_2(x_2^2-x_1^4)). \tag{30}$$

Hence, $\omega(x_1,x_2)=0 \Rightarrow g(x_1,x_2)=0$. Therefore, the whole singular set is formed by weak singularities, which are noncritical except at the origin. The Newton field may be analytically defined on the whole plane $\mathbb{R}^2$, with $(0,0)$ the only possible exception. In fact, the Newton field is defined at every point of $\mathbb{R}^2$, and is given by

$$F(x_1,x_2)=(-x_1/4, -x_2/2). \tag{31}$$

This expression shows that the origin is a critical weak zero which admits an extension of the vector field. This zero leads to a globally asymptotically stable equilibrium whose eigenvalues are $-1/4$ and $-1/2$.

An ERK discretization yielding quadratically convergent iterations for this kind of roots must have a factorization of (18) of the form $p(\lambda_i)=(4\lambda_i+1)(2\lambda_i+1)q(\lambda_i)$. In the case of a 2-stage method, this is equivalent to

$$b_2a_{21}=8, \tag{32a}$$

$$b_1+b_2=6. \tag{32b}$$

Note, finally, that a taxonomy of the eigenvalues which may be displayed by the Newton field at different singular roots, allows for the design of quadratic iterations for several types of zeros. In particular, a 3-stage discretization having a factorization (21) of the form $(4\lambda+1)(2\lambda+1)(\lambda+1)$, leads to a quadratically convergent iteration to regular roots, noncritical weak singular roots and critical weak singular roots such as the one above.

3.2. Strong problems: invariance

Strong singular roots raise new and interesting stability issues in the context of singular ODEs and differential-algebraic equations [32,36]. Directional convergence may be proved in certain problems, the key aspect of this behavior being the existence of cone-shaped regions which are (positively) invariant for the dynamics. This avoids the evolution towards impasse points close to the solution, which would result in big jumps after discretization.

These phenomena also pose challenging problems in the discrete setting. The spectral conditions presented in Section 3.1 are no longer sufficient to guarantee quadratic convergence to strong roots.

It is also necessary to preserve the invariance of the above-mentioned regions or, more precisely, the existence of invariant regions also in the discrete context. To achieve this, certain *invariance conditions* must be added to the previously discussed spectral ones.

Let us first consider some cases in which the discrete dynamics may be proved linearly convergent to a strong root from certain regions. The following result is a discrete analog of [36, Theorem 4]:

Lemma 1. *Let N and X be vector subspaces with dimensions 1 and $n-1$, respectively, such that $\mathbb{R}^n = N \oplus X$, and let $z = P_N(x)$, $y = P_X(x)$ be the projections associated with this direct sum. Consider the iteration*

$$z^{(k+1)} = \alpha z^{(k)} + O\left(\frac{\|y^{(k)}\|^2}{\|z^{(k)}\|}\right) + O(\|x^{(k)}\|^2) \tag{33a}$$

$$y^{(k+1)} = By^{(k)} + O(\|x^{(k)}\|^2), \tag{33b}$$

where $\alpha \in \mathbb{R}$ and B is a linear operator $X \to X$. If $\mathrm{r}(B) < |\alpha| < 1$, then there exist $\theta, \rho > 0$ such that the set $\mathscr{W}_{\theta,\rho} = \{x \in \mathbb{R}^n \colon \|P_X(x)\| \leqslant \theta \|P_N(x)\|, \|x\| \leqslant \rho\}$ is positively invariant and linearly convergent to the origin.

Proof. The invariance of the region $\mathscr{W}_{\theta,\rho}$ follows from the fact that $O(\|y^{(k)}\|^2/\|z^{(k)}\|)$ may be rewritten as $\theta^2 O(\|z^{(k)}\|)$ on this region. Reducing ρ and θ if necessary, it is possible to take $\varepsilon > 0$ small enough so that, in a certain norm, it is

$$\|By^{(k)}\| \leqslant (\mathrm{r}(B) + \varepsilon)\|y^{(k)}\|, \tag{34}$$

$$\|z^{(k+1)}\| \geqslant (|\alpha| - \varepsilon)\|z^{(k)}\|, \tag{35}$$

$$\frac{\mathrm{r}(B) + \varepsilon}{|\alpha| - \varepsilon} = C < 1. \tag{36}$$

From the definition of $\mathscr{W}_{\theta,\rho}$, it is possible to bound the term $O(\|x^{(k)}\|^2)$ in (33b) by an expression of the form $\gamma\|z^{(k)}\|^2$. Reducing additionally $\rho(\theta)$ to guarantee that

$$\frac{\gamma\rho}{(|\alpha| - \varepsilon)(1-\theta)(1-C)} \leqslant \theta, \tag{37}$$

we get

$$\frac{\|y^{(k+1)}\|}{\|z^{(k+1)}\|} \leqslant \frac{(\mathrm{r}(B)+\varepsilon)\|y^{(k)}\| + \gamma\|z^{(k)}\|^2}{(|\alpha| - \varepsilon)\|z^{(k)}\|} \leqslant C\theta + \frac{\gamma\rho}{(|\alpha| - \varepsilon)(1-\theta)} \leqslant \theta. \tag{38}$$

Finally, linear convergence follows immediately from the contractivity of z and y. $\square$

Theorem 4. *Let x^* be a strong singular zero of the continuous Newton method for $f \in C^4(\mathbb{R}^n, \mathbb{R}^n)$, satisfying the transversality hypothesis (2). Take $N = \operatorname{Ker} J(x^*)$, $X = T_{x^*}\Psi$. Consider the 1-stage discretization (with stepsize $h = 1$) $x^{(k+1)} = x^{(k)} + b_1 F(x^{(k)})$, and write $\hat{x} = x - x^*$. If $0 < b_1 < 4/3$, then there exists a region $\mathscr{W}_{\theta,\rho} = \{x \in \mathbb{R}^n \colon \|P_X(\hat{x})\| \leqslant \theta\|P_N(\hat{x})\|, \|\hat{x}\| \leqslant \rho\}$ which is positively invariant and linearly convergent to x^*.*

Proof. Consider expression (8) for the Newton field around a strong singular root. The 1-stage discretization indicated above yields an iteration of the form

$$z^{(k+1)} = \left(1 - \frac{b_1}{2}\right) z^{(k)} + \tilde{\beta}\left(\frac{y^{(k)}y^{(k)}}{z^{(k)}}\right) + \tilde{\gamma}(z^{(k)}z^{(k)}) + O(\|y^{(k)}\|\,\|z^{(k)}\|) + o(\|\hat{x}\|^2) \tag{39a}$$

$$y^{(k+1)} = (1 - b_1)y^{(k)} + \tilde{\delta}(y^{(k)}z^{(k)}) + O(\|y^{(k)}\|^2) + o(\|\hat{x}\|^2), \tag{39b}$$

where $\tilde{\beta} = b_1\beta$, etc. It is easy to check that $0 < b_1 < 4/3$ implies that $|1 - b_1| < |1 - b_1/2| < 1$. The result then follows from Lemma 1. □

The particular case $b_1 = 1$ yields the classical Newton iteration. The linear convergence of Newton's method to singular roots was proved by Reddien [30]. The greater generality of the result above guarantees that the stage values of certain multistage discretizations remain on the cone-shaped region in which expression (8) is valid.

The general invariance study of quadratically convergent iterations is an open problem. We discuss in the present work some particular illustrative results based on the following property:

Lemma 2. *Let N and X be vector subspaces as in Lemma* 1. *Consider the iteration*

$$z^{(k+1)} = \varphi(z^{(k)}z^{(k)}) + O(\|y^{(k)}\|\,\|z^{(k)}\|) + O(\|y^{(k)}\|^2) + o(\|x^{(k)}\|^2) \tag{40a}$$

$$y^{(k+1)} = O(\|y^{(k)}\|^2) + o(\|x^{(k)}\|^2) \tag{40b}$$

where φ is a bilinear operator $N \times N \to N$. If φ is nonnull, then there exist $\theta, \rho > 0$ such that the set $\mathscr{W}_{\theta,\rho} = \{x \in \mathbb{R}^n\colon \|P_X(x)\| \leqslant \theta\|P_N(x)\|,\ \|x\| \leqslant \rho\}$ is positively invariant and quadratically convergent to the origin.

Proof. Since N is one-dimensional and φ is nonnull, there exists a constant $c_0 > 0$ such that

$$\|\varphi(z^{(k)}z^{(k)})\| \geqslant c_0\|z^{(k)}\|^2. \tag{41}$$

Reducing sufficiently ρ and θ, it is then possible to take another constant $c_1 > 0$ such that

$$\|z^{(k+1)}\| \geqslant c_1\|z^{(k)}\|^2. \tag{42}$$

On the other hand, the term $O(\|y^{(k)}\|^2)$ in (40b) may be bounded by an expression of the form $c_2\|y^{(k)}\|^2$. Hence, we obtain

$$\frac{\|y^{(k+1)}\|}{\|z^{(k+1)}\|} \leqslant \frac{c_2\|y^{(k)}\|^2 + o(\|x^{(k)}\|^2)}{c_1\|z^{(k)}\|^2} \leqslant \frac{c_2}{c_1}\theta^2 + \frac{(1+\theta)^2 o(\|x^{(k)}\|^2)}{c_1\|x^{(k)}\|^2}. \tag{43}$$

Reducing θ and $\rho(\theta)$ so that

$$\frac{c_2}{c_1}\theta + \frac{(1+\theta)^2 o(\|x^{(k)}\|^2)}{\theta c_1\|x^{(k)}\|^2} \leqslant 1, \tag{44}$$

we get

$$\frac{\|y^{(k+1)}\|}{\|z^{(k+1)}\|} \leqslant \theta. \tag{45}$$

Strict quadratic convergence follows from the absence of linear terms in the iteration, together with the nonvanishing of φ. $\square$

Theorem 5. *Let x^* be a strong singular zero of the continuous Newton method for $f \in C^4(\mathbb{R}^n, \mathbb{R}^n)$, satisfying the transversality hypothesis* (2). *Take $N = \operatorname{Ker} J(x^*)$, $X = T_{x^*}\Psi$. Assume $f''(x^*)yz = 0$ and $\operatorname{Adj} J(x^*) f'''(x^*)zzz \neq 0$, for any $y \in X - \{0\}$ and any $z \in N - \{0\}$. Under these conditions, the* 2-*stage ERK discretization* (24), *defined by $b_1 = a_{21} = 1$, $b_2 = 2$, yields a quadratically convergent iteration to x^* from a certain positively invariant region $\mathscr{W}_{\theta,\rho} = \{x \in \mathbb{R}^n\colon \|P_X(x - x^*)\| \leqslant \theta \|P_N(x - x^*)\|,\ \|x - x^*\| \leqslant \rho\}$.*

Proof. The conditions imposed on f guarantee that $\gamma \neq 0$, $\delta = 0$ in (8). Let us then study the relations between the coefficients b_i, a_{ij} which make it possible to apply Lemma 2. To do so, note that the Newton field may be written, on a certain region $\mathscr{W}_{\theta,\rho}$, as

$$P_N F(z, y) = -\frac{z}{2} + \beta\left(\frac{yy}{z}\right) + \gamma(zz) + \text{h.o.t.} \tag{46a}$$

$$P_X F(z, y) = -y + \text{h.o.t.} \tag{46b}$$

where higher-order terms (h.o.t.) are those which do not influence the convergence of the iteration, in the terms defined by Lemma 2.

The iteration resulting from the 2-stage ERK integration is given by

$$x^{(k+1)} = x^{(k)} + b_1 F(\tilde{x}^1) + b_2 F(\tilde{x}^2) \tag{47}$$

with stage values

$$\tilde{x}^1 = x^{(k)}, \quad \tilde{x}^2 = x^{(k)} + a_{21} F(x^{(k)}). \tag{48}$$

In particular, the point $\tilde{x}^2$ has the following projections:

$$P_N \tilde{x}^2 = z^{(k)} + a_{21}\left(-\frac{z^{(k)}}{2} + \beta\left(\frac{y^{(k)} y^{(k)}}{z^{(k)}}\right) + \gamma(z^{(k)} z^{(k)})\right) + \text{h.o.t.}, \tag{49a}$$

$$P_X \tilde{x}^2 = y^{(k)}(1 - a_{21}) + \text{h.o.t.} \tag{49b}$$

The condition $a_{21} = 1$, which following Lemma 1 implies that the stage value $\tilde{x}^2$ remains on $\mathscr{W}_{\theta,\rho}$, yields

$$P_N \tilde{x}^2 = \frac{z^{(k)}}{2} + \beta\left(\frac{y^{(k)} y^{(k)}}{z^{(k)}}\right) + \gamma(z^{(k)} z^{(k)}) + \text{h.o.t.}, \tag{50a}$$

$$P_X \tilde{x}^2 = \text{h.o.t.} \tag{50b}$$

and

$$P_N F(\tilde{x}^2) = -\frac{1}{2}\left(\frac{z^{(k)}}{2} + \beta\left(\frac{y^{(k)} y^{(k)}}{z^{(k)}}\right) + \gamma(z^{(k)} z^{(k)}) + \frac{1}{4}\gamma(z^{(k)} z^{(k)})\right) + \text{h.o.t.}$$

$$= -\frac{1}{4}z^{(k)} - \frac{1}{2}\beta\left(\frac{y^{(k)}y^{(k)}}{z^{(k)}}\right) - \frac{1}{4}\gamma(z^{(k)}z^{(k)}) + \text{h.o.t.} \tag{51a}$$

$$P_X F(\tilde{x}^2) = \text{h.o.t.} \tag{51b}$$

Hence, we may split $x^{(k+1)} = x^{(k)} + b_1 F(\tilde{x}^1) + b_2 F(\tilde{x}^2)$ as follows:

$$\begin{aligned} z^{(k+1)} &= P_N x^{(k)} + b_1 P_N F(\tilde{x}^1) + b_2 P_N F(\tilde{x}^2) \\ &= z^{(k)} + b_1\left(-\frac{z^{(k)}}{2} + \beta\left(\frac{y^{(k)}y^{(k)}}{z^{(k)}}\right) + \gamma(z^{(k)}z^{(k)})\right) \\ &\quad + b_2\left(-\frac{1}{4}z^{(k)} - \frac{1}{2}\beta\left(\frac{y^{(k)}y^{(k)}}{z^{(k)}}\right) - \frac{1}{4}\gamma(z^{(k)}z^{(k)})\right) + \text{h.o.t.} \\ &= \left(1 - \frac{b_1}{2} - \frac{b_2}{4}\right) z^{(k)} + \left(b_1 - \frac{b_2}{2}\right)\beta\left(\frac{y^{(k)}y^{(k)}}{z^{(k)}}\right) \\ &\quad + \left(b_1 - \frac{b_2}{4}\right)\gamma(z^{(k)}z^{(k)}) + \text{h.o.t.} \end{aligned} \tag{52a}$$

$$y^{(k+1)} = P_X x^{(k)} + b_1 P_X F(\tilde{x}^1) + b_2 P_X F(\tilde{x}^2) = (1 - b_1) y^{(k)} + \text{h.o.t.} \tag{52b}$$

The conditions $b_1 = 1,\ b_2 = 2$ guarantee that the coefficients of $z^{(k)}$ and β in $z^{(k+1)}$, as well as that of $y^{(k)}$ in $y^{(k+1)}$, are null. On the other hand, the coefficient of γ in $z^{(k+1)}$ does not vanish. This implies that the iteration above has the form indicated in Lemma 2, and quadratic convergence follows. □

The above reasoning is based on the simplifying symmetry hypothesis $f''(x^*)yz = 0$, which leads to $\delta(yz) = 0$: a general analysis should look for conditions yielding a bound for $\|\delta(yz)\|$ by $\|\gamma(zz)\|$. Note that, after imposing the condition $a_{21} = 1$ (which guarantees that the stage value $\tilde{x}^2$ remains on the cone), the values of b_1 and b_2 may also be obtained from the spectral conditions (23). Generally speaking, certain *invariance conditions* must be added to the spectral ones to guarantee quadratic convergence to singular roots from invariant regions. As an example, the 3-stage ERK method defined by $a_{ij} = 1,\ b_1 = b_2 = 1,\ b_3 = 2$, which defines the iteration (3), yields also quadratic convergence to strong singular roots [23].

Example 2. Let us consider the behavior of different discretizations of the continuous Newton method around the singular zero $(1, 0)$ of

$$f(x_1, x_2) = (x_1^2 - x_1^4, x_1^5 + x_2^2 + x_2^3 - 1). \tag{53}$$

The Jacobian matrix is

$$J(x_1, x_2) = \begin{pmatrix} 2x_1 - 4x_1^3 & 0 \\ 5x_1^4 & 2x_2 + 3x_2^2 \end{pmatrix}. \tag{54}$$

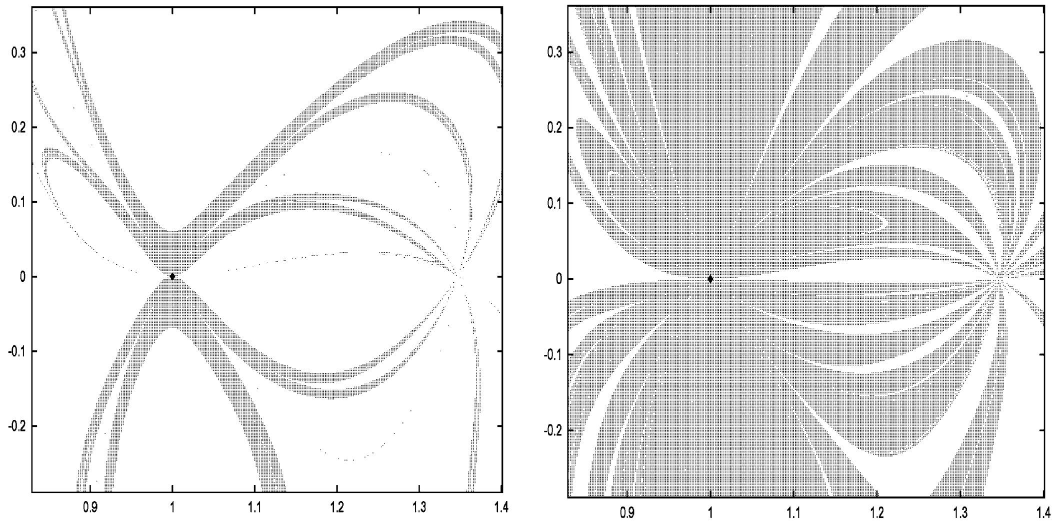

Fig. 1. Discretizations: (a) Euler: 6-step domain, (b) ERK-2: 3-step domain.

The singular set Ψ is defined by the condition $\omega(x_1,x_2) = \det J(x_1,x_2) = 2x_1x_2(1 - 2x_1^2)(2 + 3x_2) = 0$, showing that the root located at (1,0) is singular. It is easy to check that all hypotheses in Theorems 2, 4 and 5 are satisfied. In particular, Theorem 2 predicts the existence of a locally cone-shaped invariant region for the continuous Newton method. This cone has vertical axis, since $\operatorname{Ker} J(1,0) = \{(0,v_2),\ v_2 \in \mathbb{R}\}$. Also, Theorems 4 and 5 state the existence of invariant cones for the classical Newton method (resulting after Euler's integration of the continuous method) and for the iteration defined by the ERK-2 scheme (24), characterized by the values $b_1 = a_{21} = 1,\ b_2 = 2$. In the former, linear convergence is expected from this cone-shaped region, whereas quadratic convergence is predicted for the latter.

Fig. 1 illustrates the different rates of convergence of both discretizations. Note first that the computational cost associated with one step of the 2-stage discretization (24) is equivalent to that of two steps of the classical Newton iteration, since this is obtained through a 1-stage (Euler) method. Fig. 1(a) displays the set of points which, after six or less iterations of the classical Newton method, are located within a 0.001-ball centered at the singular solution (1,0), using the d_∞ distance $d_\infty((x_1,x_2),(1,0)) = \max\{|x_1 - 1|, |x_2|\}$. Fig. 1(b) shows the corresponding picture for three or less iterations of the ERK-2 iteration (24). The improvement provided by the quadratic behavior of the latter is clear.

The irregular shape of both regions is due to the fact that the singular root at (1,0) is surrounded by impasse points $(x_1,0)$, $x_1 \neq 1$, which produce big jumps after fixed-step discretization.

As a final example, Tables 1 and 2 display the evolution of both iterations from the initial point $(1.05, 0.2)$. In both cases, the discrete dynamics evolve towards the singular equilibrium located at $(1,0)$. The third column of both tables displays the error evolution, computed as the d_∞ distance to this solution. Table 1 shows the evolution of the classical Newton method, obtained after Euler discretization of the continuous system. The linear rate along the vertical direction of the kernel (represented by the x_2 variable) is clearly displayed. On the contrary, in Table 2 the iteration presents a quadratic evolution towards the singular solution.

Table 1
Iteration from (1.05, 0.20), Euler discretization

x_1-coordinate	x_2-coordinate	Error
$x_1^{(0)} = 1.05$	$x_2^{(0)} = 0.20$	$e^{(0)} = 0.20$
$x_1^{(1)} = 1 + 5.34 \times 10^{-3}$	$x_2^{(1)} = 0.098$	$e^{(1)} = 0.098$
$x_1^{(2)} = 1 + 7.01 \times 10^{-5}$	$x_2^{(2)} = 0.051$	$e^{(2)} = 0.051$
$x_1^{(3)} = 1 + 1.22 \times 10^{-8}$	$x_2^{(3)} = 0.026$	$e^{(3)} = 0.026$
$x_1^{(4)} = 1 + \varepsilon \leqslant 10^{-14}$	$x_2^{(4)} = 0.013$	$e^{(4)} = 0.013$
$x_1^{(5)} = 1 + \varepsilon \leqslant 10^{-14}$	$x_2^{(5)} = 0.0066$	$e^{(5)} = 0.0066$
$x_1^{(6)} = 1 + \varepsilon \leqslant 10^{-14}$	$x_2^{(6)} = 0.0033$	$e^{(6)} = 0.0033$

Table 2
Iteration from (1.05, 0.20), ERK-2 discretization

x_1-coordinate	x_2-coordinate	Error
$x_1^{(0)} = 1.05$	$x_2^{(0)} = 0.20$	$e^{(0)} = 0.20$
$x_1^{(1)} = 1 - 5.20 \times 10^{-3}$	$x_2^{(1)} = 3.59 \times 10^{-3}$	$e^{(1)} = 5.20 \times 10^{-3}$
$x_1^{(2)} = 1 - 6.89 \times 10^{-5}$	$x_2^{(2)} = 3.23 \times 10^{-5}$	$e^{(2)} = 6.89 \times 10^{-5}$
$x_1^{(3)} = 1 - 1.19 \times 10^{-8}$	$x_2^{(3)} = 1.40 \times 10^{-8}$	$e^{(3)} = 1.40 \times 10^{-8}$

4. Concluding remarks

This paper shows the applicability of implicit ODEs in singular nonlinear equation solving and optimization problems. The link between these fields is given by the linearly implicit form of the continuous time analog of Newton's method.

Singular roots pose interesting stability issues in the continuous-time context of singular ODEs. These problems have been surveyed, under the noncritical assumption, following a taxonomy which classifies them into *weak* and *strong* ones. The weak case provides counterexamples to the usual assumption that the domain of convergence of Newton's method, when applied to singular roots, should always exclude other singularities. In these problems, the continuous-time context reduces the formulation of quadratically convergent iterations to a spectral study of ERK discretizations.

The presence of impasse points in the more general strong case involves directional stability results within the continuous-time framework. This motivates a study of invariance which complements the previous spectral analysis. The study leads to a systematic formulation of quadratically convergent iterations to singular roots from certain cone-shaped regions. Singular solutions generically satisfy the transversality hypothesis (2): hence, ERK-schemes such as the ones described by (3) or (24) might be appropriate when singular roots are expected and no additional information about the problem is available. Nevertheless, some examples suggest that the scope of the work potentially includes more general types of singularities, beyond the transversal ones here considered.

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