Regularization of Index-1 Differential-Algebraic Equations with Rank-Deficient Constraints

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Abstract—in this paper, we present a regularization for semiexplicit index-1 differential-algebraic equations with rank-deficient or singular constraints. We consider those problems for which the solution is well defined through the singularity. We give convergence results for the regularization applied to linear DAEs, and present some numerical experiments which illustrate its effectiveness.

Keywords—Differential-algebraic equations, Regularization, Singularity, Rank-deficient.

1. INTRODUCTION

In this paper, we consider semiexplicit differential-algebraic equations (DAE)

\[ \dot{x} = f(x, y), \]
\[ 0 = g(x, y). \]

The DAE (1.1) is index-1 [1], if \( \frac{\partial g}{\partial y} \) is nonsingular. These types of systems arise, for example, in circuit analysis, chemical process simulation, power systems, and many other applications.

Problems with rank-deficient or singular constraints can exhibit a number of different solution behaviors. For example, if the constraints are rank-deficient (i.e., if \( g_y \) is rank-deficient) but constant-rank, the problems can be higher-index [1] or the solution may fail to exist at all, or there may be a well-defined solution. If the constraints become singular at a single point, the solution may bifurcate at that point, there may be an impasse where the solution does not exist.

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beyond the singular point, or the solution may be well defined through the singularity. In this paper, we are interested in problems for which the solution is well defined through the singularity and the problem is essentially index-1.

In Section 2, we introduce a regularization for rank-deficient or singular index-1 problems. The regularization is motivated by trust-region methods from numerical optimization and is related to some regularizations proposed for higher-index systems in [2]. In Section 3, we define more precisely for linear DAEs the class of problems which the regularization is designed to handle, and give convergence results. In Section 4, we present some numerical experiments which illustrate the effectiveness of the regularization for linear and nonlinear DAEs.

Regularizations for DAEs of index-1 have been studied in [3–6]. However, to our knowledge, these regularizations are not applicable if the system is rank deficient or singular.

Much work has appeared on regularizations for higher-index DAEs. See, for example, [6–8] which deal with problems in which there are no singularities. A regularization for Euler-Lagrange equations which is based on the augmented Lagrangian method from numerical optimization is proposed in [9–12]. An extension which is applicable for singular systems is given in [13].

A regularization for Euler-Lagrange systems is proposed in [14,15] which deals with singularities by first identifying them via Gaussian elimination and then adding to the vanishing and linearly independent constraints of their third derivatives. An alternative scheme for singular higher-index DAEs is a global coordinate mapping strategy, which reduces a differential-algebraic system to a singular ordinary differential equation system [16].

2. INDEX-1 REGULARIZATION

In this section, we will derive a regularization of (1.1) which is appropriate for singular problems. Beginning with the regularization

\[
\begin{align*}
    \dot{x'} &= f(x, y), \\
    0 &= g(x, y + h\dot{y'}),
\end{align*}
\]

for index-1 problems without singularities, expanding \( g \) in Taylor's series yields

\[
\begin{align*}
    \dot{x'} &= f(x, y), \\
    h\dot{g_y}y' &= -g(x, y).
\end{align*}
\]

We note that when \( g_y \) is nonsingular \( y' \) is in a Newton direction, and when \( g_y \) is singular it is not possible to solve for \( y' \) in (2.2).

Now observe that the constraint in (2.1) is equivalent to the optimization problem

\[
\min_{y'} \frac{1}{2} \|g(x, y) + h\dot{g_y}y'\|_2^2.
\]

Adding a trust-region constraint to deal with the singularity, we obtain the model optimization problem

\[
\min_{y'} \frac{1}{2} \|g(x, y) + h\dot{g_y}y'\|_2^2, \quad \text{subject to } \frac{1}{2} \|\dot{y'}\|_2^2 \leq \delta.
\]

The Lagrangian function for this optimization problem is given by

\[
L = \frac{1}{2} \|g(x, y) + h\dot{g_y}y'\|_2^2 + \left( \frac{1}{2} \|\dot{y'}\|_2^2 - 1 \right),
\]

where \( \varepsilon = h/\delta \). Letting \( \nabla_{y'} L = 0 \), we obtain an ODE for \( y' \),

\[
(h\dot{g_y}^T + \varepsilon I)y' = -g_y^T g,
\]
which together with the ODE in (2.1a), yields the regularized system

\[ x' = f(x, y), \tag{2.5a} \]
\[ (hg_y^T g_y + \epsilon I) y' = -g_y^T g. \tag{2.5b} \]

When \( \epsilon = 0 \) and \( g_y \) are nonsingular, (2.5b) is equivalent to (2.2b). At points \((x^*, y^*)\) where \( g_y \) is singular, then \( g_y^T \) of (2.5b) becomes rank-deficient. We handle this problem by perturbing \( g_y \) at the singular point to obtain

\[ x' = f(x, y), \tag{2.6a} \]
\[ (hg_y^T g_y + \epsilon_1 I) y' = - (g_y^T + \epsilon_2 I) g. \tag{2.6b} \]

Later we will see how to choose \( \epsilon_1 \) and \( \epsilon_2 \) (in the linear case we can choose \( \epsilon_2 = 0 \)), although it will be understood throughout that \( h, \epsilon_1, \) and \( \epsilon_2 \) are all nonnegative.

3. CONVERGENCE

In this section, we will consider convergence of the regularized system (2.6) for linear problems of the form (1.1),

\[ x' = A(t)x + B(t)y + q(t), \quad x(0) = x_0, \tag{3.1a} \]
\[ 0 = C(t)x + D(t)y + r(t). \tag{3.1b} \]

We will consider two cases; first, when the null space of \( g_y \) is constant and second, when it is not constant.

We will require the following lemma.

**Lemma 1.** Let \( D \) be an \( m \times m \) matrix of rank \( r \). Let \( v_1, \ldots, v_{m-r} \) be an orthonormal basis for \( \mathcal{N}(D) \), the nullspace of \( D \). Then \( \exists U \), an orthogonal matrix and \( v_{m-r+1}, \ldots, v_m \) s.t. \( v_1, \ldots, v_m \) is an orthonormal basis for \( \mathbb{R}^m \) and s.t. \( U^T DV \) is the singular value decomposition (SVD) of \( D \).

**Proof.** Let \( v_1, \ldots, v_{m-r}, w_{m-r+1}, \ldots, w_m \) be an orthonormal basis for \( \mathbb{R}^m \). Then \( Dw_{m-r+1}, \ldots, Dw_m \) spans at most a \( r \)-dimensional subspace of \( \mathbb{R}^m \). Let \( u_1, \ldots, u_{m-r} \) be orthonormal such that \( u_i^T Dw_k = 0 \), \( i = 1, 2, \ldots, m-r, k = m-r+1, \ldots, m \), and let \( u_1, \ldots, u_{m-r}, x_{m-r+1}, \ldots, x_m \) be an orthonormal basis for \( \mathbb{R}^m \). Then

\[ \hat{D}_1 \equiv U_1^T DV_1 \equiv \begin{bmatrix} u_1^T \\ \vdots \\ u_{m-r}^T \\ x_{m-r+1}^T \\ \vdots \\ x_m^T \end{bmatrix} D [v_1, \ldots, v_{m-r}, w_{m-r+1}, \ldots, w_m] = \begin{bmatrix} 0 & 0 \\ 0 & D_1 \end{bmatrix}. \]

Since \( D = U_1 \hat{D}_1 V_1^T \), rank \( D = \text{rank } \hat{D}_1 \), and the nullity \( D = \text{nullity } \hat{D}_1 = m - r + \text{nullity } D_1 \), which implies that the nullity \( D_1 = 0 \). Additionally, \( D^T D = V_1 \hat{D}_1^T \hat{D}_1 V_1^T \) which implies that \( D \) and \( \hat{D}_1 \) have the same singular values. Now apply the algorithm of [17] to \( D_1 \) to complete the proof.

A more general result which implies Lemma 1 has recently appeared [18]. We have included our proof because it is simple and uses a different approach.

We are interested in problems for which the solution is well defined and the problem is essentially an index-1 DAE (i.e., if we were to remove the redundant constraints, the resulting problem would be index-1). Hence, we make the following definition.
DEFINITION 3.1. Consider the linear semiexplicit DAE (3.1). The problem will be called a rank-deficient index-1 DAE if the following holds.

1. \( \mathcal{N}(D) \) is constant, where \( \mathcal{N}(D) \) is the null space of \( D \).
2. \( \mathcal{N}(D) \subset \mathcal{N}(B) \).
3. The redundant constraints are consistent, that is, if \( D = U \begin{pmatrix} \Sigma & 0 \\ 0 & 0 \end{pmatrix} V^T \), where \( V \) and \( U \) are obtained by Lemma 1, then \( U^T C = \begin{pmatrix} C \\ 0 \end{pmatrix} \) and \( U^T r = \begin{pmatrix} r \end{pmatrix} \).
4. The reduced problem is index-1. The reduced problem is the problem which remains after the redundant constraints have been eliminated and is given by (3.5).

We will also assume that \( V(t) \) is smooth.

THEOREM 3.1. Consider the rank-deficient index-1 DAE (3.1). If \( x, q, r, \) and their derivatives are bounded then solutions \( \hat{x} \) to the regularization

\[
\begin{align*}
\hat{x}' &= A(t)\hat{x} + B(t)\hat{y} + q(t), \\
\hat{y}' &= -D^T(t)(C(t)\hat{x} + D(t)\hat{y} + r(t)), \\
\hat{x}(0) &= x_0, \quad \hat{y}(0) = y_0,
\end{align*}
\]

where \( \epsilon_1 = o(h) \), converge to the solutions \( x \) of (3.1) for any \( t > 0 \), as \( h \to 0 \). Specifically, \( \| x - \hat{x} \|_2 = O(h) \), as \( h \to 0 \). We remark that under our assumptions, there is no guarantee that \( \hat{y} \) converges to \( y \). However, the "nonredundant" portion of \( y \) can be recovered from \( \hat{x} \) using the SVD.

PROOF. For convenience we drop the notation of the dependence on \( t \). Let \( D = U\Sigma V^T = U \begin{pmatrix} \Sigma & 0 \\ 0 & 0 \end{pmatrix} V^T \) be the SVD of \( D \) where \( V \) and \( U \) are obtained via Lemma 1. Then \( V \) can be written (by simple permutation) as \( V = (V_{m, r} V_{m, m-r}) \), where the columns of \( V_{m, m-r} \) are an orthonormal basis for \( \mathcal{N}(D) \). By the constant nullspace assumption and Lemma 1,

\[
V_{m, m-r} = 0. \tag{3.3}
\]

Multiplying (3.1a) by \( U^T \) yields

\[
0 = U^T Cx + \begin{pmatrix} \tilde{\Sigma} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \end{pmatrix} + U^T r, \tag{3.4}
\]

where \( z \equiv (\hat{x}_1 \hat{x}_2) = V^T y \). Thus, since \( \mathcal{N}(D) \subset \mathcal{N}(B) \), (3.1) is equivalent to

\[
\begin{align*}
x' &= A x + \tilde{B} z_1 + q, \\
z_1 &= -\tilde{\Sigma}^{-1} (\tilde{C} x + r),
\end{align*}
\]

where \( \tilde{B} = BV_{m, r} \).

On the other hand, multiplying (3.2b) by \( V^T \) gives

\[
(h\Sigma^2 + \epsilon_1 I) V^T \hat{y}' = -\Sigma (U^T C x + \Sigma \hat{x} + U^T r), \tag{3.6}
\]

where \( \hat{z} = V^T \hat{y} \). Now

\[
V^T \hat{y}' = \hat{x}' - (V^T)' V \hat{x}. \tag{3.7}
\]

From (3.3) it follows that

\[
(V^T)' V = \begin{pmatrix} \hat{V}_{11} & \hat{V}_{12} \\ 0 & 0 \end{pmatrix}. \tag{3.8}
\]

Differentiating the identity \( V^T V = I \) yields

\[
(V^T)' V + V^T V' = 0. \tag{3.9}
\]
Thus, using (3.3), (3.8), and (3.9),
\[ \hat{V}_{12} = - (V_{11}^T V_{12} + V_{21}^T V_{22}) = 0. \] (3.10)

From (3.7), (3.8), and (3.10), it follows that
\[ V^T \dot{y}' = \begin{pmatrix} \dot{z}_1 \\ \dot{z}_2 \end{pmatrix} - \begin{pmatrix} \hat{V}_{11} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{z}_1 \\ \dot{z}_2 \end{pmatrix}. \] (3.11)

Then (3.6) is equivalent to
\[
(\epsilon_1 \hat{\Sigma}^2 + \epsilon_1 I) \begin{pmatrix} \dot{z}_1' \\ \dot{z}_2' \end{pmatrix} = - \hat{\Sigma} \left( \hat{C} \dot{x} + \hat{\Sigma} \dot{y}_1 + \hat{r} \right), \]
\[ \epsilon_1 \dot{z}_2 = 0. \] (3.12a)

Recall that \( \dot{z}_2 \) contributes only to the redundant portion of \( y \) and is therefore unnecessary.
Let

\[ P(t) = (h\Sigma^2 + \epsilon_1 I)^{-1} \Sigma^2 - \hat{V}_{11}, \]  \hspace{1cm} (3.13a)

\[ Q(t) = (h\Sigma^2 + \epsilon_1 I)^{-1} \hat{E} \hat{C}, \]  \hspace{1cm} (3.13b)

\[ R(t) = (h\Sigma^2 + \epsilon_1 I)^{-1} \hat{E} \hat{r}, \]  \hspace{1cm} (3.13c)

and let \( W(t) \) be the fundamental matrix for the matrix differential equation

\[ W'(t) + P(t)W(t) = 0, \quad W(0) = I. \]  \hspace{1cm} (3.14)

The solution of (3.12a) can be written as

\[ \hat{z}_1 = W(t)\hat{z}_1(0) - \int_0^t W(t)W^{-1}(s)Q(s)\hat{z}(s) \, ds - \int_0^t W(t)W^{-1}(s)R(s) \, ds. \]  \hspace{1cm} (3.15)

Thus, (3.2a) is equivalent to

\[ \hat{x}' = A\hat{x} + B\hat{z}_1 + q, \]  \hspace{1cm} (3.16)
Figure 3. Numerical approximation of $x$ (left) and $y$ (right) computed via our regularization with DASSL for Example 4.1. Top: $h = 10^{-2}$, $\epsilon_1 = \epsilon_2 = 10^{-8}$. Bottom: $h = 10^{-2}$, $\epsilon_1 = \epsilon_2 = 10^{-10}$.

together with (3.15) and (3.12b). Rewrite (3.5a) as

$$x' = Ax - B \int_0^t W(t) W^{-1}(s) Q(s) x(s) \, ds$$

$$+ B \left[ \int_0^t W(t) W^{-1}(s) Q(s) x(s) \, ds - \bar{\Sigma}^{-1} \tilde{C} x \right] - \tilde{B} \Sigma^{-1} \tilde{f} + q.$$  \hspace{1cm} (3.17)

Subtracting (3.16) from (3.17) gives

$$e' = Ae - B \int_0^t W(t) W^{-1}(s) Q(s) e(s) \, ds$$

$$+ B \left[ \int_0^t W(t) W^{-1}(s) Q(s) x(s) \, ds - \bar{\Sigma}^{-1} \tilde{C} x \right]$$

$$+ \tilde{B} \left[ \int_0^t W(t) W^{-1}(s) R(s) \, ds - \bar{\Sigma}^{-1} \tilde{f} \right] - \tilde{B} W(t) \hat{z}_1(0),$$  \hspace{1cm} (3.18)
where $e = x - \dot{x}$. For $h$ sufficiently small, $P(u)$ can be approximated by $(1/h)I$ on $0 \leq u \leq t$ and thus $W(t)W^{-1}(s) \approx e^{-(1/h)(t-s)}I$. An application of Watson's lemma for the asymptotic expansion of integrals [19] yields

$$- \int_0^t W(t)W^{-1}(s)Q(s)e(s) \, ds = -\Sigma^{-1}\bar{C}e(t) + O(h)e', \quad (3.19a)$$

$$\int_0^t W(t)W^{-1}(s)Q(s)x(s) \, ds - \Sigma^{-1}\bar{C}x = O(h)x', \quad (3.19b)$$

$$\int_0^t W(t)W^{-1}(s)R(s) \, ds - \Sigma^{-1}r = O(h). \quad (3.19c)$$

Thus, (3.18) can be rewritten as

$$e' = [A - B\Sigma^{-1}\bar{C} + O(h)]e + O(h), \quad (3.20)$$

with $e(0) = 0$. Thus, $e(t) \to 0$ as $h \to 0$. \hfill $\blacksquare$
Figure 5. Numerical approximation of \( z_1 \) (upper left), \( z_2 \) (upper right), \( y_1 \) (lower left), and \( y_2 \) (lower right) computed via our regularization with DASSL for Example 4.3 with \( p = 1, q = 2, h = 10^{-4}, \epsilon_1 = \epsilon_2 = 10^{-6} \).

A different proof could be obtained by using the transformation method in [20] for singularly perturbed linear homogeneous initial value problems.

REMARK. The same analysis can now be used to show that

\[ z_1 - \hat{z}_1 = O(h). \]  

We now wish to consider the case that \( \mathcal{N}(D) \) is constant, except at one point \( t_0 \) where its rank decreases. The class of problems is defined by the following.

DEFINITION 3.2. Consider the linear semiexplicit DAE (3.1). Assume the following.

1. \( \Sigma \) is nonsingular except at \( t^* \).
2. \( B\Sigma^{-1}C \) is continuous for all \( t \).
3. \( B\Sigma^{-1}r \) is continuous for all \( t \).
Then (3.1) has a solution for \( x \) near the singularity, and we will call the problem a kinematically-singular index-1 DAE.

A linear DAE (3.1) will be called a rank-deficient kinematically-singular index-1 DAE if after eliminating any redundant constraints as in Definition 3.1, the reduced problem is a kinematically-singular index-1 DAE.

DEFINITION 3.3. A linear DAE (3.1) will be called a rank-deficient kinematically-singular index-1 DAE with a singularity of multiplicity \( m \) if near \( t = t^* \):

1. \( \sigma_i(t) = k_i |t - t^*|^{m_i} + O(|t - t^*|^{m_i+1}) \), \( i = 1, 2, \ldots, s \).
2. \( m = m_1 \geq m_2 \geq m_3 \geq \cdots \geq m_s > 0 \).
3. \( \sigma_i(t^*) > 0 \), \( i = s + 1, \ldots, r \).
4. The elements \( \tilde{c}_{ij} \) of \( \tilde{C} \) satisfy \( \tilde{c}_{ij}(t) = O((t - t^*)^{n_i}) \), \( n_i \geq 0 \), \( i = 1, 2, \ldots, s \), \( j = 1, 2, \ldots, r \).
5. The elements \( \tilde{f}_i(t) \) of \( \tilde{f} \) satisfy \( \tilde{f}_i(t) = O((t - t^*)^{n_i}) \), \( n_i \geq 0 \), \( i = 1, 2, \ldots, s \).
6. The elements \( \tilde{b}_{ij}(t) \) of \( \tilde{B} \) satisfy \( \tilde{b}_{ij}(t) = O((t - t^*)^{l}) \), \( l = \max_i \leq s (0, m - (m/m_i)m_i) \), \( i, j = 1, 2, \ldots, r \).

We remark that assumptions (4)-(6) guarantee that (2) and (3) of Definition 3.1 will be satisfied.
Figure 7. Numerical approximation of $z_1$ (upper left), $z_2$ (upper right), $y_1$ (lower left), and $y_2$ (lower right) computed via our regularization with DASSL for Example 4.3 with $p = 1$, $q = 2$, $h = 10^{-4}$, $\epsilon_1 = \epsilon_2 = 10^{-10}$.

Also, note that $l = \max_{1 \leq i \leq s}(0, m/m_i(m_i - n_i))$ and $m/m_i \geq 1$. If $D$ is already in SVD form ($U = V = I$) then condition (6) simplifies to the following.

6'. The elements $\tilde{b}_{ij}(t)$ of $\tilde{B}$ satisfy $\tilde{b}_{ij}(t) = O((t - t^*)^{l_j})$, $l_j = \max(0, m_j - n_j)$, $i = 1, 2, \ldots, r$, $j = 1, 2, \ldots, s$.

THEOREM 3.2. Consider the rank-deficient kinematically-singular index-1 DAE (3.1). Then for any $T > 0$, the solution $\dot{x}$ to the regularized system (3.2) converges to the solution $x$ of (3.1) as $h \to 0$, i.e., $\|x - \dot{x}\| = O(h)$ as $h \to 0$. Herein we consider the transformed systems outlined in Theorem 3.1.

PROOF. Fix $T \geq t^* \gg 0$ (the case $T < t^*$ is proved by Theorem 3.1). Henceforth, let $\sigma_1(t) \leq \sigma_i(t)$, $i = 2, 3, \ldots, r$, and $\sigma_{s+1}(t) \leq \sigma_i(t)$, $i = s + 2, \ldots, r$ in a neighborhood of $t^*$. Let

$$h \leq \min_{\min(0, t^*-1/4), t^*+1/4} \left( \frac{10\sigma_{s+1}(t)}{k} \right)^{1/m}, \quad \epsilon_1 = \frac{k^2}{100} h^{2m+1};$$

(3.22)

where $k = \max_{1 \leq i \leq s} k_i$, $T_L = t^* - h$, $T_U = t^* + h$, $T^i_L = t^* - h^{m/m_i}$, and $T^i_U = t^* + h^{m/m_i}$. 
Figure 8. Numerical approximation of \( x_1 \) (upper left), \( x_2 \) (upper right), \( y_1 \) (lower left), and \( y_2 \) (lower right) computed via our regularization with DASSL for Example 4.3 with \( p = 1, q = 4, h = 10^{-4}, \epsilon_1 = \epsilon_2 = 10^{-10} \).

\( i = 1, 2, \ldots, s \). On the interval \( 0 < t \leq T_L \), we can apply Theorem 3.1 since at \( t = T_L \), \( P(T_L) \approx (1/h)I \).

From (3.18), it follows that for \( t \in (T_L, T_U) \),

\[
e' = Ae - \int_{T_L}^{t} \tilde{B}(t)W(t)W^{-1}(s)Q(s)e(s)\,ds + \int_{T_L}^{t} \tilde{B}(t)W(t)W^{-1}(s)Q(s)x(s)\,ds - \tilde{B}(t)\Sigma^{-1}(t)\bar{C}(t)x(t) + \int_{T_L}^{t} \tilde{B}(t)W(t)W^{-1}(s)R(s)\,ds - \tilde{B}(t)\Sigma^{-1}(t)\bar{F}(t) - \tilde{B}W(t)\xi_1(T_L).
\]

(3.23)

From (3.13a), the diagonal elements \( p_{ii}(t) \) of \( P(t) \) satisfy

\[
p_{ii}(t) = \frac{\sigma_i^2}{h\sigma_i^2 + \epsilon_1} - \hat{\sigma}_i > -\max|\hat{\sigma}_i(t)| + O(h).
\]

(3.24)
The off-diagonal elements \( p_{ij}(t) \) of \( P(t) \) are bounded by

\[
|p_{ij}(t)| < \max_{i,j} |\hat{p}_{ij}(t)| + O(h). \tag{3.25}
\]

The Gershgorin Circle Theorem [17] implies that the real part of all the eigenvalues of \(-P(t)\) is bounded by a positive constant. Thus, elements of \( W(t)W^{-1}(s) \) which represent the solution of (3.14) with \( W(s) = I \) are bounded on \([T_L, T_U]\).

The elements \( \hat{q}_{ij} \) of \( \hat{Q} \equiv \hat{B}(t)W(t)W^{-1}(s)Q(s) \) have the form

\[
\hat{q}_{ij} = \sum_{l=1}^{r} \left( \frac{\sigma_l}{h \sigma_l^2 + \epsilon_1} \hat{a}_{lj} + O(h) \right) \sum_{k=1}^{r} \hat{b}_{lk} w_{kl}, \tag{3.26}
\]

where \( w_{kl} \) are the elements of \( W(t)W^{-1}(s) \). If \( \hat{Q}^l \) is the matrix whose entries are
Figure 10. Numerical approximation of $x_1$ (upper left), $x_2$ (upper right), $y_1$ (lower left), and $y_2$ (lower right) computed via our regularization with DASSL for Example 4.3 with $p = 1$, $q = 4$, $h = 10^{-4}$, $\epsilon_1 = \epsilon_2 = 10^{-14}$.

\[ q_{ij} = \frac{\sigma_i}{h^2} \sum_{k=1}^{r} b_{ik} w_{kl} + O(h) \]  \hspace{1cm} (3.27)

then $\hat{Q} = \sum_{i=1}^{r} \hat{Q}^i$. Similarly, the elements $\hat{r}_i$ and $\hat{r}_i^l$ of $\hat{R} = \hat{B}(t)W(t)W^{-1}(s)R(s)$ and $\hat{R}^l$, respectively, have the form

\[ \hat{r}_i = \sum_{l=1}^{r} \left[ \left( \frac{\sigma_l}{h^2} + \epsilon_1 \right) \sum_{k=1}^{r} b_{ik} w_{kl} \right] + O(h) \]  \hspace{1cm} (3.28)

and

\[ \hat{r}_i^l = \left[ \frac{\sigma_l}{h^2} + \epsilon_1 \right] \sum_{k=1}^{r} b_{ik} w_{kl}, \]  \hspace{1cm} (3.29)

where $\hat{R} = \sum_{i=1}^{r} \hat{R}^l$. 
Substituting (3.26) and (3.28) into (3.23) yields

\[
e' = Ae - \sum_{l=1}^{r} \int_{T_L}^{t} \dot{Q}^l(s)e(s) \, ds \\
+ \sum_{l=1}^{r} \int_{T_L}^{t} \dot{Q}^l(s)x(s) \, ds - \bar{B}(t)\bar{\Sigma}^{-1}(t)\bar{C}(t)x(t) \\
+ \sum_{l=1}^{s} \int_{T_L}^{t} \dot{P}^l(s) \, ds - \bar{B}(t)\bar{\Sigma}^{-1}(t)\bar{P}(t) - \bar{B}(t)W(t)W^{-1}(T_L)W(T_L)\bar{1}(T_L).
\]

We first consider the matrices \(\dot{Q}^l, l = s + 1, \ldots, r\). Then from (3.22a), (4), and (6) of Definition 3.3 and boundedness of \(w_{ij}\), it follows that

\[
|\dot{q}^l_{ij}| < \frac{C}{h}, \quad l = s + 1, \ldots, r.
\]
Figure 12. Numerical approximation of $z$ (left) and $y$ (right) computed via our regularization with the modification $\text{sgn}(g_y)e_2$ and with DASSL for Example 4.4 with $h = 10^{-7}$, $\epsilon_1 = \epsilon_2 = 10^{-9}$.

Figure 13. Numerical approximation of $x$ (left) and $y$ (right) computed via our regularization with the modification $\text{sgn}(g_y)e_2$ and with DASSL for Example 4.5 with $h = 10^{-8}$, $\epsilon_1 = \epsilon_2 = 10^{-10}$.

Bounds on the $q^l_{ij}$, $l = 1, 2, \ldots, s$ can be obtained by considering the three regions $[T_L, T_L^l]$, $[T_L^l, T_U^l]$, and $[T_U^l, T_U]$. For $t, s \in [T_L, T_L^l]$ or $t, s \in [T_U^l, T_U]$,

$$|q^l_{ij}| < C \frac{k_l}{h} \frac{|s - t^*|^m_l |s - t^*|^n_l |t - t^*|^l}{h} + O(h) < C \frac{|s - t^*|^n_l}{h} + O(h)$$

using (3.27) and (1), (2), (4), and (6) of Definition 3.3.

On $[T_L^l, T_U^l]$, we obtain

$$|q^l_{ij}| < C \frac{k_l}{h} \frac{|s - t^*|^m_l |s - t^*|^n_l |t - t^*|^l}{(k_l^2/100) h^{2m+1}} + O(h)$$

$$< C \frac{h^{(m/m_l)(n_l-m_l)-1}}{h} + O(h) < \frac{C}{h},$$

(3.32)
using (3.27) and (1), (2), (4), and (6) of Definition 3.3 and the fact that \( m / m_1 \geq 1 \). The same analysis with (5) replacing (4) from Definition 3.3 establishes

\[
|p_t| < \frac{C}{h}.
\]

Substituting estimates (3.31)–(3.34) into (3.30), and using bounds on \( \bar{B}_\Sigma^{-1}C_{x} \) and \( \bar{B}_\Sigma^{-1}F \) implied by (4)–(6) of Definition 3.3 yields

\[
\|e(t)\| \leq \|e(T_L)\| + C_0 \int_{T_L}^t \|e(s)\| ds + \frac{C_1}{h} \int_{T_L}^t \int_{T_L}^s \|e(u)\| du ds + O(h).
\]

Letting \( E(t) = \|e(t)\| \) and \( F(t) = \int_{T_L}^t E(u) du \), and using the Gronwall inequality we obtain from (3.35)

\[
E(T) \leq (E(T_L) + O(h)) e^{(C(T-T_L))/h}.
\]

Thus \( \|e(t)\| \leq C\|e(T_L)\| < Ch \) for all \( t \in [T_L, T_U] \), where \( C \) may depend on parameters in the problem such as \( s, r, k_i, i = 1, 2, \ldots, s, m_i, i = 1, 2, \ldots, s, \|x\| \), and \( \|A\| \) but not on \( h \). On the interval \( T \geq T_U \), the result follows from Theorem 3.1 and (3.36).

**Remark.** In the kinematically-singular case, \( z_1 \) may not exist at \( t^* \) while \( \dot{z}_1 \) does. However, the error in \( z_1 \) outside the interval around \( t^* \) can be shown to be \( O(h) \) using Theorem 3.1.

### 4. NUMERICAL EXPERIMENTS—SINGULAR LINEAR AND NONLINEAR DAEs

In this section, we present results of our regularization applied to several linear and nonlinear, singular DAEs. Several examples meet the conditions of Theorems 3.1 and 3.2, while the others show that the regularization performs well in more general settings. The DAE code DASSL [1] was used in all examples. Absolute and relative error tolerances were set to \( 10^{-6} \). The values of \( h, \epsilon_1, \) and \( \epsilon_2 \) are specified in each example. The finite-difference approximation to the Jacobian in DASSL was used in all cases. In none of the examples was DASSL able to compute the correct solution through the singularity without the regularization.

**Example 4.1.** Consider the linear DAE

\[
x' = ty, \quad -1 \leq t \leq 1,
\]

\[
0 = x - ty, \quad x(-1) = -1, \quad y(-1) = 1.
\]

In this example, the rank of \( D = -t \) is one except at \( t = 0 \) where the rank decreases to zero. Thus the problem is a rank-deficient kinematically-singular index-1 DAE with singularity of multiplicity 1. The rank of \( B(t) = t \) also decreases by one at the same point so this problem is covered by Theorem 3.2. We chose \( h = 10^{-4}, \epsilon_1 = \epsilon_2 = 10^{-k}, k = 6, 7, 8 \), which are less stringent than our proof of Theorem 3.2 required. Figures 1 and 2 show that our regularization accurately models the solution through the singularity. For \( \epsilon_1 = \epsilon_2 = 10^{-k}, k = 6, 7 \), the numerical solution experiences a small jump at the singularity. In Figures 1 and 2, we restricted the maximum absolute value of \( y \) and its numerical approximation so that the solution, away from the singularity, could be seen. Near the singularity, \( y \) becomes much larger (in terms of absolute value) than the numerical solution. However, this does not seem critical since we are not interested in accurately resolving the blow-up in \( y \). To show the dependence on \( h \) we also solved the problem with \( h = 10^{-2} \) and \( \epsilon_1 = \epsilon_2 = 10^{-k}, k = 6, 8, \) and 10. In Figures 2 and 3 it is seen that reducing \( \epsilon_1 \) and \( \epsilon_2 \) beyond a certain point does not lead to a more accurate solution, but that solution accuracy is limited by \( h \).

**Example 4.2.** Consider the linear DAE

\[
x' = y, \quad -1 \leq t \leq 1,
\]

\[
0 = t^n(x - y), \quad x(-1) = -1, \quad y(-1) = -1, \quad n = 1, 2, 3.
\]
This example also has $D(t) = -t^n$ of constant rank except at $t = 0$. However, $B(t) = 1$ does not decrease rank at $t = 0$, but $D^{-1}C = 1$. Specifically we consider the case $n = 3$ with $\varepsilon_1 = \varepsilon_2 = 10^{-k}$, $k = 6, 8$. The results for both variables are shown in Figure 4.

**EXAMPLE 4.3.** Consider the linear DAE system

\[
\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}' = \begin{pmatrix} -5 & 4 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} 2 & -t^{q-p} \\ 2 & \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} 8 \\ 1 \end{pmatrix},
\]

\[
0 = \begin{pmatrix} 0 & 1 \\ t & 2t \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} y_1 + \begin{pmatrix} 0 & 1 \\ 0 & t \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix},
\]

with $x_1(-1) = 2$, $x_2(-1) = 2$. The matrix $D$ is full-rank except at $t = 0$ where the rank decreases to 1. The exact solution is given by $x_1 = 1 + e^{-6(1+t) + 6(t+1)e^{-6(1+t)}}$ and $x_2 = 2e^{-6(1+t) + 3(t+1)e^{-6(1+t)}}$ with $y_1 = -2x_1 - x_2$ and $y_2 = -t^{p-q}(x_1 + 2x_2)$.

We begin by considering the case $q = 2, p = 1$ with $h = 10^{-4}$, $\varepsilon_1 = \varepsilon_2 = 10^{-k}$, $k = 6, 8, 10$. The results are displayed in Figures 5–7. As in the previous examples, the error can be reduced by decreasing the size of $\varepsilon_1$ and $\varepsilon_2$. In the second case, $q = 4$ and $p = 1$. Now the singularity is much more severe, as seen in Figures 8–10. In this case, we used the same $h$ but $\varepsilon_1 = \varepsilon_2 = 10^{-k}$, $k = 10, 12, 14$. Note that the error is reduced as the numerical approximation to $y_2$ becomes more singular. The situation will become even more severe when $q$ is increased.

**EXAMPLE 4.4.** Consider the DAE [21]

\[
\frac{dx}{dt} = -1, 
0 = y^3 - x,
\]

with initial condition $(x(0), y(0)) = (1, 1)$. $(0, 0)$ is a singular point of this problem. The solution shown in the top of Figure 11 was computed using $h = 10^{-7}$ and $\varepsilon_1 = \varepsilon_2 = 10^{-9}$. In this case, the code handles the singularity correctly. Reducing $\varepsilon_2$ to $10^{-13}$ results in the solution seen in the bottom of Figure 11. Round-off in the term $g_1 + \varepsilon_2$ prevents the code from advancing past the singularity. Even more disturbing, if $y^3 - x$ is replaced by $x - y^3$ and with the values $\varepsilon_1 = \varepsilon_2 = 10^{-9}$, the solution for $y$ again gets stuck at 0. The latter shortcoming can be overcome by replacing the equation $g_1 + \varepsilon_2$ with $g_1 + \text{sgn}(g_1)\varepsilon_2$ (noting that in the scalar case $g_1 = g_1^\top$). Then, with the same values of $h$, $\varepsilon_1$, and $\varepsilon_2$, we obtain the solution shown in Figure 12. This example shows that care is needed when applying the regularization to nonlinear problems and points to a possible modification in the regularization strategy. Since our regularization models Newton's method, we would expect difficulty at $x = 0$ since $y = 0$ is a multiple root of $g$ in this case.

**EXAMPLE 4.5.** Consider [21]

\[
\frac{dx}{dt} = -y, 
0 = x - (y - 1)^3, 
\]

with initial condition $(x(0), y(0)) = (1, 2)$. $\frac{\partial g}{\partial y}$ is singular at $y = 1$. Figure 13 shows that the solution passes through the singular point with $h = 10^{-6}$, $\varepsilon_1 = \varepsilon_2 = 10^{-10}$. We note that $(-1, 0)$ is a stable equilibrium point of the DAE.

**REFERENCES**