DOE/ER/25026--26

DE89 009584

REPORT NO. UIUCDCS-R-89-1505

DIFFERENTIAL ALGEBRAIC EQUATIONS, INDICES, AND INTEGRAL ALGEBRAIC EQUATIONS

by

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April 1989

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Supported in part by the U.S. Department of Energy under grant DOE DEFG02-87ER25026, and by NSF under grant DMS 87-03226.

1 Introduction

A general DAE takes the form

$$f(y', y, t) = 0 \tag{1}$$

where f and y are in R^n. The differential index, di, of the system is the minimum integer, m, such that the system of equations (1) and

$$\frac{df(y', y, t)}{dt} = 0$$

$$\cdots$$

$$\frac{d^m f(y', y, t)}{dt^m} = 0$$

can be solved for $y' = y'(y)$. A formal reduction technique to derive this system of equations, called the underlying ODE, is given in [2]. Hairer et al [1] define what we will call the perturbation index, pi, as the smallest value of the integer m such that the difference between the solution of (1) and the solution of the perturbed equation

$$f(z', z, t) = e(t) \tag{2}$$

can be bounded by an expression of the form

$$\max \|z(t) - y(t)\| \leq K(\max(\|e(t)\|) + \max(\|\dot{e}(t)\|) + \cdots + \max(\|e^{(m-1)}\|). \tag{3}$$

The perturbation index is clearly an important factor in the numerical solution of a DAE since it will play a major role in determining the impact of roundoff errors. It is clear that one can expect errors of the order of ϵ/h^{pi} because the method will be performing a numerical differentiation on roundoff errors assumed to be order of ϵ. However, the differential index determines some major characteristics of the underlying structure of the DAE: it determines, for example, the number of manifolds on which the solution is constrained to lie – it is the number of sets of algebraic relations developed in the index reduction process shown in [2]. We will show that for general systems, $pi = di + 1$ unless the DAE satisfies some special conditions that, unfortunately, are difficult to describe in terms of the original DAE. One important form occurs when the equation is linear in y' and the components containing y' are total differentials, that is, if

$$f(y', y, t) \equiv a_y(y, t)y' + b(y, t) = 0. \tag{4}$$

DAEs which can be written in this form will be said to have integral form. In this case, $pi = di$. (It is noted on page 6 of [1] that this condition is sufficient for the index 1 case.)

To simplify expressions we will consider the autonomous form independent of t. This does not reduce generality. Eq. (4) can be written as

$$a(y) = a(y_0) - \int_0^t b(y(s), s)ds \tag{5}$$

which is a particular case of the *integral algebraic equation*, IAE,

$$a(y) = a(y_0) + \int_0^t k(t, s, y(s))ds, \tag{6}$$

which itself is a special case of the general IAE

$$a(y) = a(y_0) + \int_0^t K(y(t), y(s))ds. \tag{7}$$

These display a very similar behavior to DAEs and will be discussed later.

2 The Relationship Between the Indices

We will restrict ourselves to problem formulations for which both indices are well defined. It is always possible to restate a problem in a form in which the formal definitions do not apply. For example, consider the problem

$$y^2 = 0$$

It has no perturbation index since we cannot get a bound of the form of (3) for any m. If we apply the index reduction technique, the first differentiation yields $yy' = 0$ which has two solutions, $y' = 0$ implying that its index is one, and $y = 0$, implying that its index is two, so it's differential index could be said to be one or two.

The main result of this section is $di \leq pi \leq di + 1$.

As defined in [1], the perturbation index can not be less than one. To allow for pi to be zero, we will modify the definition as follows. Define

$$E(t) = \int_0^t e(\tau)d\tau \tag{8}$$

The perturbation index is the minimum integer, m, such that the difference in the solutions of (1) and (2) satisfies a bound of the form

$$\max \|z(t) - y(t)\| \leq K[\max(\|E(t)\| + \sum_{j=0}^{m-1} \max(\|e^{(j)}(t)\|)]. \tag{9}$$

We first show that $pi \geq di$. This follows directly from an examination of the index reduction process in [2]. The first step consists of selecting a maximum subset of equations (2) that are independent in z' and eliminating the derivatives from the remaining equations to get non differential ("algebraic") relations. This does not change the index but yields a set of algebraic equations, $g_{1,j}(z, e) = e_j$, whose right-hand sides, e_j, are a subset of all the e. Furthermore, the e_j that appear on the right-hand sides do not appear in the left-hand sides. Subsequent steps of the process differentiate the algebraic equations and then repeat the above process. The m-th step of the process yields a similar algebraic subsystem which contains $e_j^{(m-1)}$ on the right-hand side, but these terms do not also appear on the left-hand sides. The process can be continued until $m = di + 1$, at which time there are no further algebraic equations (this being equivalent to the definition of the differential index). Hence, when $m = di$ we obtain a subsystem of algebraic equations

$$g_{di,j}(z, \{e, \dot{e}, \cdots, e^{(di-1)}\}) = e_j^{(di-1)} \tag{10}$$

where j selects a non-null subset of the original equations and the components of $e^{(di-1)}$ that appear on the right-hand side do not appear in the left-hand side. When the same process is applied to the original system (1) we get the algebraic relations

$$g_{di,j}(y, 0) = 0. \tag{11}$$

Subtracting (11) from (10) for a choice of $e(t)$ such that the right-hand side of (10) is of order one and all e terms on the left-hand side are arbitrarily small, we find that

$$\|z - y\| \geq \|e^{(di-1)}\| / \|\partial g_m / \partial y\| \tag{12}$$

Hence, $pi \geq di$.

Now we show that $pi \leq di + 1$. After the di-th differentiation, we have the underlying ODE

$$z' = f(z, \{e, \dot{e}, \cdots, e^{(di)}\}).$$

Subtracting

$$y' = f(y, 0)$$

from this we easily obtain

$$\max \|z(t) - y(t)\| \leq K(\|z(0) - y(0)\| + \max(\|e(t)\|) + \max(\|\dot{e}(t)\|) + \cdots + \max(\|e^{(di)}\|).$$

thus showing that $pi \leq di + 1$.

3 Integral Form DAEs

The main result of this section is that $pi = di$ if the DAE has integral form. Since the DAE has integral form, it can be written by eq. (4) as

$$\frac{da(y)}{dt} + b(y) = 0 \tag{13}$$

The corresponding perturbed equations are

$$\frac{da(z)}{dt} + b(z) = e(t) \tag{14}$$

Writing $\dot{E}(t) = e(t)$ we have

$$\frac{d}{dt}[a(z) - E(t)] + b(z) = 0. \tag{15}$$

Hence

$$\frac{d}{dt}[a(z) - a(y) - E(t)] + b(z) - b(y) = 0. \tag{16}$$

If $di = 0$ then a_y is nonsingular and for small enough $E(t)$ there exists a function $\delta(t) = O(E(t))$ such that $a(y + \delta(t)) = a(y) + E(t)$. Substituting in (16) we get

$$\frac{d}{dt}[a(z) - a(y + \delta(t))] = -b(z) + b(y) = B[y + \delta(t) - z - \delta(t)] \tag{17}$$

where B is bounded. Eq. (17) immediately yields

$$\|z - y\| \leq K_1(\|z(0) - y(0)\| + \|\delta\|) \leq K(\|z(0) - y(0)\| + \|E\|) \tag{18}$$

where the norms are the max norms over the interval unless indicated otherwise. Hence the perturbation index is zero.

If $di \neq 0$ then a_y is singular. If $Q_1(y)$ is the maximum dimension, full rank matrix for which $Q_1(y)a_y$ is null, then the first step of the index reduction process in [2] yields the algebraic equations

$$Q_1(z)dE/dt - Q_1(z)b(z) \equiv g_1(z, e) = 0 \tag{19}$$

plus a subset of eqs (15). If di is non zero, (19) is a non-empty set. The next step in the index reduction process is to differentiate (19) to get

$$\frac{d}{dt}g_1(z, e) = 0, \tag{20}$$

then select a maximum number of rows of (20) linearly independent in z' of (14) and of themselves, and eliminate z' from the remaining rows of (20) by forming

$$Q_{21}(z, e)(a_y z' + b(z) - e) + Q_{22}(z, e)\frac{d}{dt}g_1(z, e) \equiv g_2(z, e, \dot{e}) = 0. \tag{21}$$

The process continues until, after di differentiations, g_{di+1} is a null system. The underlying ODE is given by subsets of equations (15), (20), and so on, having the form

$$\frac{d}{dt}[a(z) - E(t)] + b(z) = 0 \tag{22}$$

$$\frac{d}{dt}g_i(z, e, \dot{e}, \cdots, e^{(i-1)}) = 0, \qquad i = 1, \cdots, di. \tag{23}$$

This system is an index zero DAE which has integral form, so the difference between its solution and y (which satisfies the same equations with $E = e = \cdots = e^{(di-1)} = 0$) satisfies

$$||z - y|| \leq K(||y(0) - z(0)|| + ||E|| + ||e + ||\dot{e}|| + \cdots + ||e^{(di-1)}||). \tag{24}$$

Hence the perturbation index $pi \doteq di$.

4 When is $pi = di + 1$?

The previous section shows that integral form equations have $pi = di$ so we only have to examine non-integral form equations. For index 0 problems, the answer is all such equations have $pi = di+1$. We will prove this by selecting a perturbation $e(t)$ such that $E(t)$ is arbitrarily small but the solution of the DAE is changed by greater than order $||E||$. Let $f(y', y) = 0$ be an index zero DAE and consider the solution of $f(z', z) = e$. We treat two cases below, equations non-linear in the derivatives and equations linear in the derivatives.

First suppose that f is nonlinear in z' (in which case it does not have integral form). Consequently somewhere along the solution $y(t)$, $(\partial^p y/\partial y^p)/p! = d_p$ is nonzero for some $p > 1$. (If all such partials are zero along the solution, the equation is either linear in the neighborhood of the solution, or has a singularity at the solution. We restrict our discussion to nonsingular problems.) Let q be the smallest such value of p and suppose $d_q \neq 0$ in an interval I of length L.

If q is even, chose $e(t)$ to be a square wave with magnitude $\pm\delta$ and period L/N for N cycles in the interval I and zero elsewhere. Over each cycle, the direction of the vector $e(t)$ will be constant so that $E(nL/N) = 0$ for all integer n, but the vector direction can change from cycle to cycle. For small enough δ, the perturbation to y' is $f_{y'}^{-1}[\pm\delta - d_q(f_{y'}^{-1}\delta)^q]$ plus higher order terms in δ and $1/N$, so is independent of N to the first approximation. The effect of this change on y over the interval I is of order $f_{y'}^{-1}d_q(f_{y'}^{-1}\delta)^q$. Since the value of $\|E\| = \| \int_0^t e(\tau)d\tau\|$ is bounded by $\delta/2N$ which can be arbitrarily small, any bound on the perturbation to the solution due to e must involve $\|e\|$, so the perturbation index is one.

If, on the other hand, q is odd, choose the magnitude of e in I to alternate between the 2δ for an interval of length $L/3N$ and $-\delta$ for an interval of length $2L/3N$. Again, keep the vector direction of e constant over each cycle. The value of $\|E\|$ is bounded by $2\delta/3N$ so is arbitrarily small, while the perturbation to y' is $f_{y'}^{-1}[2\delta - d_q(2f_{y'}^{-1}\delta)^q]$ plus higher order terms in one direction and $-f_{y'}^{-1}[\delta - d_q(f_{y'}^{-1}\delta)^q]$ in the other direction. If N is large enough, the value of d_q will not change appreciably over each cycle of length L/N so the total effect of the perturbation on y in one cycle will be of order $(2^q - 1)f_{y'}^{-1}d_q(f_{y'}^{-1}\delta)^q L/N$. Hence the effect over the interval I will be of order $(2^q - 1)f_{y'}^{-1}d_q(f_{y'}^{-1}\delta)^q$, so once again the perturbation index is one.

In the second case we suppose that f is linear in y' but not of integral form, so the DAE can be written as $A(y)y' + b(y) = 0$ where $A(y) \neq a_y$ for any a. Hence we have

$$A(y+r)r' + [A(y+r) - A(y)]y' + (b(y+r) - b(y)) = e(t) \tag{25}$$

where $r = z - y$. As a DAE in r ($y(t)$ is a given function), this has integral form only if the original DAE does. Viewing y as a given function of t, this equation has form

$$A(r,t)r' = e(t) + B(r,t)r. \tag{26}$$

Equation (26) has an integral form iff $\oint A(r,t)dr = 0$ for all closed paths in the r-plane with t fixed, hence we know that this integral is non-zero for some paths. For any two orthogonal vectors p and q and point r_0 in r-space, let $P(r_0, p, q)$ be the plane containing r_0, p, and q. Define $c(t, r_0, p, q)$ to be a vector whose i-th component is the curl, in $P(r_0, p, q)$, of the projection of the i-th row of $A(r,t)$ into $P(r_0, p, q)$. If the equation does not have integral form, c is non zero for some values of its arguments in a neighborhood of $r_0 = 0$ (since a closed path can be approximated arbitrarily closely by the union of a number of closed paths in such planes). Choose $p(t)$ and $q(t)$ such that c is non zero for some interval in t, say, $[0, L]$. For small enough L, c can be represented as a constant plus a small perturbation over the interval. For a closed path in the plane P (we drop the arguments when they are obvious), we have

$$\oint A(r,t)dr = \int c(t,r,p,q)dv = c(t,r_0,p,q)V(path) + O(\|\bar{r} - r_0\|^3) \tag{27}$$

where the second integral is over the area in P bounded by the path, $V(path) = \int dv$ is the area contained within the path, r_0 is a point to be chosen inside this area, and $\bar{r}$ is the most distant point on the path from r_0.

We first give an outline of the essential idea of the proof, then fill in the details. Start by integrating (26) w.r.t. t to get

$$\int A(r,t)dr = \int e(t)dt + \int B(r,t)rdt. \tag{28}$$

We select a value of $e(t)$ which is approximately periodic with very small period, $2T$, and whose integral is zero over a full period. We are going to make T arbitrarily small. Hence, if $\dot{E}(t) = e(t), E(0) = 0$ then $E = O(Te)$. We want to choose this value so that r in (26) changes by more than $O(E)$ over an interval. Note that if we integrate over $N = o(1/T)$ periods of e, the interval has length of $o(1)$ as $T \to 0$, so it is arbitrarily small. Choose e to be composed of two parts: the first part, over $[0, T]$, corresponds to a closed path in a plane P in r-space. From (27) we know that this leads to a non-zero left-hand side of (28) for suitable choice of P. Since we are starting from a zero error r at $t = 0$, the last term in (28) can be kept very small, so we conclude that $\int_0^T e(t)dt = E(T)$ is $O(V(path))$ while $r(T) - r(0) = 0$. We now set $e(t) = -E(T)/T$ over the interval $(T, 2T)$ so that $E(2T) = 0$. From (26) we see that $r' = O(E(T)/T)$, hence $r(2T) = O(E(T))$. We now repeat this over $N = o(1/T)$ cycles to get $r(2NT) = O(NE(T))$ which cannot be expressed as $O(E)$. The details, given below, select the paths and the relative orders of components so that the neglected terms are of higher order.

For the first half of the period we choose the path for r to be a circle in P of radius δ center r_0. Hence, $V(path) = \pi\delta^2$. From, (27) and (28) we have

$$E(T) = O(\delta^2) + O(T(r_0 + \delta) + \delta^3) \tag{29}$$

as long as c is non zero. For the second half of the period we have $e = -E(T)/T$ so we have from (28)

$$r(2T) = -A(r_0, 0)^{-1}E(T) + O(rT). \tag{30}$$

Hence, after N periods, we get

$$r(2NT) = -NA(r_0, 0)^{-1}E(T) + O(rT) + o(NE(T)), \tag{31}$$

which cannot be expressed as $O(\|E\|)$. Hence $pi = 1$.

For higher index cases, we can have pi = di even without integral form. If we start with two independent DAEs, one of integral form with $pi_1 = di_1$ and the other with non integral form with $pi_2 = di_2 + 1$ and we have $di_1 > di_2$, the indices for the union of the two systems will have $pi = di = di_1$ although the combined system will not have integral form. For example, the DAE

$$(x')^2 = 1$$

$$y = 1$$

has differential index one (because of the second equation) and perturbation index one because of both equations.

5 Algebraic Integral Equations

We will consider the IAE (6). If $A = a_y$ is such that $\|A^{-1}\| < \infty$ and k is smooth, it is easy to show that this equation has a unique solution using a Picard iteration to define a new iterate for the solution $y(t)$ on the left-hand side in terms of the previous iterate inserted on the right-hand side of (6). In this case, we will call the system an index zero system. The solution of such systems can be approximated using quadrature. For example, if we have computed $\{y_i, i = 1, \cdots, n-1\}$ we can computed y_n by

$$a(y_n) = a(y_0) + \sum_{i=0}^{n} \omega_i k(t_n, t_i, y_i) \tag{32}$$

where the $\{\omega_i\}$ are suitable weights. For small enough ω_n, this will have a solution, and for close enough mesh spacing, ω_n will be small enough. (Of course, this may not be the best approach to a computational approximation.) Note that a similar situation holds for (7) if $A = a_y - \int_0^t K_1(y(t), y(s))ds$ has a bounded inverse, where K_1 is the partial derivative of $K(y(t), y(s))$ with respect to its first argument.

If A is singular, then there is no guarantee that there is a solution, since the system has a structure similar to that of DAEs of index greater than zero. Below we will give an "index reduction procedure" similar to that in [2] for DAEs which, if it terminates, determines the "index" of the IAE and ensures that there is a solution if the initial values lie on the constraint manifolds implied by the IAE. We will consider the IAE (6) only, (7) follows in a similar manner.

We first rewrite (6) as

$$a(y) + w_1 = a_0 \equiv a(y_0) \tag{33}$$

$$w_1 = -\int_0^t k(t, s, y(s))ds. \tag{34}$$

We will also be interested in the perturbed problem

$$a(z) + x_1 = a_0 + E \tag{35}$$

$$x_1 = -\int_0^t k(t, s, z(s))ds. \tag{36}$$

We will deal with eqs. (35) and (36) for z and x_1. The solution for y and w_1 will follow by setting $E = 0$. Following the approach used in [2] we assume that the components of z are ordered so that the first r_1 columns of a_y are linearly independent, where r_1 is the rank of a_y. We set $z = [z_1^T, v_1^T]^T$ where the dimension of z_1 is r_1. Hence, (35) can be solved, in principle, for z_1 to get

$$z_1 = z_1(v_1, x_1, E). \tag{37}$$

This uses r_1 rows of (35). The remaining rows provide a set of $n - r_1$ constraints on x_1, namely

$$g_1(x_1, E) = 0. \tag{38}$$

Note that neither z_1 nor x_1 can appear in equation (38), or the rank of a_y would be larger than r_1, contrary to the definition of z_1. We now differentiate (38) w.r.t. t and substitute (36) to get

$$g_{1,1}[-k(t,t,z(t)) - \int_0^t k_t(t,s,z(s))ds)] + g_{1,2}\dot{E} = 0 \tag{39}$$

where $g_{i,j}$ is the partial of g_i w.r.t. its j-th argument and k_t is the partial of k with respect to its first argument. We will rewrite (39) using (37) as

$$g_{1,1}x_2 + g_{1,2}\dot{E} = g_{1,1}k(t,t,[z_1^T(v_1,x_1,E), v_1^T]^T) \equiv a_2(v_1, x_1, E) \tag{40}$$

and

$$x_2 = -\int_0^t k_t(t,s,z(s))ds. \tag{41}$$

If $a_{2,1} = \partial a_2/\partial v_1$ in (40) is non singular, we can solve (40) for v_1 to get

$$z_2 \equiv v_1 = z_2(x_1, x_2, E, \dot{E}). \tag{42}$$

In this case, we will define the index of the IAE to be one. Note that equations (36), (37), (41), and (42) form a standard Volterra integral equation for z_1, z_2, x_1, and x_2.

We used the term "index" without qualifying it as a differential or a perturbation index. It is clear for the index zero and one cases defined above, the difference between z and y (the solution with $E \equiv 0$) can be bounded by $L\|E\|$ (index zero) or $L(\|E\| + \|\dot{E}\|)$ (index one). Furthermore, (42) shows that, in the index one case, z does depend on $\dot{E}$ since $\partial z_2/\partial \dot{E} = [a_{2,1}]^{-1}g_{1,2}$ and $g_{1,2}$ is non null. Hence, with the same definition of perturbation index as for DAEs, we find that the perturbation index and the index defined above are identical for index zero and one systems. The same is true for the higher index systems to be defined below.

If $a_{2,1}$ in (40) is singular, we can not solve it for v_1. Let the rank of $a_{2,1}$ be r_2. Continuing as before set $v_1 = [z_2^T, v_2^T]^T$, where the dimension of z_2 is r_2. Assume that the variables have been ordered so that the first r_2 columns of $a_{2,1}$ are linearly independent. Then (40) can be solved for z_2 to get

$$z_2 = z_2(v_2, x_1, x_2, E, \dot{E}) \tag{43}$$

with the remaining rows reducing to

$$g_2(x_1, x_2, E, \dot{E}) = 0. \tag{44}$$

As before, we differentiate (44) w.r.t. t and substitute (41) and (36) in it to get

$$g_{2,1}x_2 + g_{2,2}x_3 + g_{2,3}\dot{E} + g_{2,4}\ddot{E} = g_{2,1}k(t,t,z(t)) + g_{2,2}k_t(t,t,z(t)) \equiv a_3(v_2, x_1, x_2, E, \dot{E}) \tag{45}$$

where

$$x_3 = -\int_0^t k_{tt}(t,s,z(t))ds. \tag{46}$$

The process is now clear. If $\partial a_{m+1}/\partial v_m$ is non singular, we can solve the equation equivalent to (45) for $z_{m+1} \equiv v_m$ to get a system of equations for z_i and x_i, $i = 1, \cdots, m+1$ which are a Volterra integral equation. We will then define the index of the original IAE to be m. It requires m differentiations to reduce it to a regular integral equation, just as an index m DAE requires m differentiations to reduce it to an ODE. In the differentiation process, the perturbation E will be differentiated m times, so, if the perturbation index is defined similarly to the index perturbation index for DAEs, the perturbation index will also be m. (Note that the perturbation introduced in IAEs is E, whereas the perturbation introduced in DAEs is $e = \dot{E}$.)

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DOE F 1332.16 (10-84)
(Formerly RA-427)

OMB Approval
No. 1910-1400

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1. Report No. UIUCDCS-R-89-1505

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3. Recipient's Accession No.

4. Title and Subtitle
DIFFERENTIAL ALGEBRAIC EQUATIONS, INDICES, AND INTEGRAL ALGEBRAIC EQUATIONS

5. Report Date April 1989

6.

7. Author(s)
C. W. Gear

8. Performing Organization Rept. No. R-89-1505

9. Performing Organization Name and Address
Department of Computer Science UIUC
1304 W. Springfield Avenue
Urbana, IL 61801

10. Project/Task/Work Unit No.

11. Contract/Grant No.
DOE DEFG0287ER25026
NSF DMS87-03226

12. Sponsoring Organization Name and Address
Department of Energy
Argonne, IL

National Science Foundation
Washington, DC

13. Type of Report & Period Covered Technical

14.

15. Supplementary Notes

16. Abstracts

In a recent report, Hairer et al [1] define the index of Differential Algebraic Equations (DAEs) by considering the effect of perturbations of the equations on the solutions. This index is called the perturbation index, pi. An earlier form of index used by a number of authors is determined by the number of differentiations of the DAEs that are required to generate an ordinary differential equation (ODE) satisfied by the solution. We will call this the differential index, di. Hairer et al give an example whose differential index is one and perturbation index is two and other examples where they are identical. We will show that $di \le pi \le di + 1$ and that di = pi if the derivative components of the DAE are total differentials. This means that the differential components have a first integral. The integrals are a special case of a new type of integral equation we will call Integral Algebraic Equations (IAEs).

17. Key Words and Document Analysis. 17a. Descriptors

17b. Identifiers/Open-Ended Terms

17c. COSATI Field/Group

18. Availability Statement
unlimited

19. Security Class (This Report) UNCLASSIFIED

20. Security Class (This Page UNCLASSIFIED

21. No. of Pages 15

22. Price