Index concepts for differential-algebraic equations

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Abstract

We discuss several of different index concepts for differential-algebraic equation (differentiation, strangeness, tractability, geometric, perturbation, and structural index) and analyze their relationship.

1 Introduction

Differential-algebraic equations (DAEs) present today the state-of-the-art in mathematical modeling of dynamical systems in almost all areas of science and engineering. Modeling is done in a modularized way by combining standardized sub-models in a hierarchically built network. The topic is well-studied from an analytic, numerical and control theoretical point of view, and several monographs are available that cover different aspects of the subject [1, 2, 9, 14, 15, 16, 21, 28, 29, 34].

The mathematical model can usually be written in the form

$$F(t, x, \dot{x}) = 0, \tag{1}$$

where $\dot{x}$ denotes the (typically time) derivative of x. Denoting by $C^k(\mathbb{I}, \mathbb{R}^n)$ the set of k times continuously differentiable functions from $\mathbb{I} = [\underline{t}, \overline{t}] \subset \mathbb{R}$ to $\mathbb{R}^n$, one usually assumes that $F \in C^0(\mathbb{I} \times \mathbb{D}_x \times \mathbb{D}_{\dot{x}}, \mathbb{R}^m)$ is sufficiently smooth, and that $\mathbb{D}_x, \mathbb{D}_{\dot{x}} \subseteq \mathbb{R}^n$ are open sets. The model equations are usually completed with initial conditions

$$x(\underline{t}) = \underline{x},\ \ \underline{t} \in \mathbb{I}. \tag{2}$$

Linear DAEs

$$E\dot{x} - Ax - f = 0, \tag{3}$$

with $E, A \in C^0(\mathbb{I}, \mathbb{R}^{m,n})$, $f \in C^0(\mathbb{I}, \mathbb{R}^m)$ often arise after linearization along trajectories, see [4], with constant coefficients in the case of linearization around an equilibrium solution. DAE models are also studied in the case when x is infinite-dimensional, see e. g. [7, 37] but here we only discuss the finite dimensional case.

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Studying the literature for DAEs, one quickly realizes an almost babylonian confusion in the notation, in the solution concepts, in the numerical simulation techniques and in control and optimization methods. These differences partially result from the fact that the subject was developed by different groups in mathematics, computer science and engineering. Another reason is that it is almost impossible to treat automatically generated DAE models directly with standard numerical methods, since the solution of a DAEs may depend on derivatives of the model equations or input functions and since the algebraic equations restrict the dynamics of the system to certain manifolds, some of which are only implicitly contained in the model. This has the effect that numerical methods may have a loss in convergence order, are hard to initialize, or fail to preserve the underlying constraints and thus yield physically meaningless results, see e.g. [2, 21] for illustrative examples. Furthermore, inconsistent initial conditions or violated smoothness requirements can give rise to distributional or other classes of solutions [8, 21, 27, 35] as well as multiple solutions [21]. Here we only discuss *classical solutions*, $x \in C^1(\mathbb{I}, \mathbb{C}^n)$ that satisfy (1) pointwise.

Different approaches of classifying the difficulties that arise in DAEs have lead to different so-called *index* concepts, where the index is a 'measure of difficulty' in the analytical or numerical treatment of the DAE. In this contribution the major index concepts will be surveyed and put in perspective with each other as far as this is possible. For a detailed analysis and a comparison of various index concepts with the differentiation index, see [5, 12, 14, 21, 22, 24, 31]. Since most index concepts are only defined for uniquely solvable square systems with $m = n$, here only this case is studied, see [21] for the general case.

2 Index concepts for DAEs

The starting point for all index concepts are the linear systems with constant coefficients. In this case the smoothness requirements can be determined from the Kronecker canonical form [11] of the matrix pair (E, A) under equivalence transformations $E_2 = PE_1Q$, $A_2 = PA_1Q$, with invertible matrices P, Q, see e. g. [21]. The size of the largest Kronecker block associated with an infinite eigenvalue of (E, A) is called *Kronecker index* and it defines the smoothness requirements for the inhomogeneity f. For the linear variable coefficient case, it was first tried to define a Kronecker index, see [13]. However, it was soon realized that this is not a reasonable concept [5, 17], since for the variable coefficient case the equivalence transformation is $E_2 = PE_1Q$, $A_2 = PA_1Q - PE_1\dot{Q}$, and it locally does not reduce to the classical equivalence for matrix pencils. Canonical forms under this equivalence transformation have been derived in [17] and existence and uniqueness of solutions of DAEs has been characterized via global equivalence transformations and differentiations.

Since the differentiation of computed quantities is usually difficult, it was suggested in [3] to differentiate first the original DAE (3) and then carry out equivalence transformations. For this we gather the original equation and its derivatives up to order ℓ into a so-called *derivative array*

$$F_\ell(t, x, \ldots, x^{(\ell+1)}) = \begin{bmatrix} F(t, x, \dot{x}) \\ \frac{d}{dt}F(t, x, \dot{x}) \\ \vdots \\ (\frac{d}{dt})^\ell F(t, x, \dot{x}) \end{bmatrix} \tag{4}$$

We require solvability of (4) in an open set and define the Jacobians

$$\begin{aligned} M_\ell(t, x, \dot{x}, \ldots, x^{(\ell+1)}) &= F_{\ell;\dot{x},\ldots,x^{(\ell+1)}}(t, x, \dot{x}, \ldots, x^{(\ell+1)}), \\ N_\ell(t, x, \dot{x}, \ldots, x^{(\ell+1)}) &= -(F_{\ell;x}(t, x, \dot{x}, \ldots, x^{(\ell+1)}), 0, \ldots, 0), \end{aligned}$$

which correspond to the derivative array in the linear case (3).

2.1 The differentiation index

The most common index definition is that of the *differentiation index*, see [5].

Definition 1 *Suppose that (1) is solvable. The smallest integer ν (if it exists) such that the solution x is uniquely defined by $F_\ell(t, x, \dot{x}, \ldots, x^{(\ell+1)}) = 0$ for all consistent initial values is called the* differentiation index *of (1).*

Over the years the definition of the differentiation index has been slightly modified to adjust from the linear to the nonlinear case [3, 5, 6] and to deal with slightly different smoothness assumptions. In the linear case it has been shown in [21] that the differentiation index ν is invariant under (global) equivalence transformations, and if it is well-defined, then there exists a smooth, pointwise nonsingular $R \in C(\mathbb{I}, \mathbb{C}^{(\nu+1)n,(\nu+1)n})$ such that $RM_\nu = \begin{bmatrix} I_n & 0 \\ 0 & H \end{bmatrix}$. Then from the derivative array $M_\nu(t)\dot{z}_\nu = N_\nu(t)z_\nu + g_\nu(t)$, where g_ν contains derivatives of f one obtains an ordinary differential equation (ODE)

$$\dot{x} = [\, I_n \;\; 0\,]R(t)M_\nu(t)\dot{z}_\nu = [\, I_n \;\; 0\,]R(t)N_\nu(t) \begin{bmatrix} I_n \\ 0 \end{bmatrix} x + [\, I_n \;\; 0\,]R(t)g_\nu(t),$$

which is called *underlying ODE*. Any solution of the DAE is also a solution of this ODE. This motivates the interpretation that the differentiation index is the number of differentiations needed to transform the DAE into an ODE.

2.2 The strangeness index

An index concept that is closely related to the differentiation index and extends to over- and under-determined systems is based on the following Hypothesis.

Hypothesis 1 *Consider the DAE (1) and suppose that there exist integers μ, a, and d such that the set $\mathbb{L}_\mu = \{z \in \mathbb{R}^{(\mu+2)n+1} \mid F_\mu(z) = 0\}$ associated with F is nonempty and such that for every point $z_0 = (t_0, x_0, \dot{x}_0, \ldots, x_0^{(\mu+1)}) \in \mathbb{L}_\mu$, there exists a (sufficiently small) neighborhood in which the following properties hold:*

1. *We have* $\operatorname{rank} M_\mu(z) = (\mu+1)n - a$ *on* $\mathbb{L}_\mu$ *such that there exists a smooth matrix function* Z_2 *of size* $(\mu+1)n \times a$ *and pointwise maximal rank, satisfying* $Z_2^T M_\mu = 0$ *on* $\mathbb{L}_\mu$.

2. *We have* $\operatorname{rank} \hat{A}_2(z) = a$*, where* $\hat{A}_2 = Z_2^T N_\mu [I_n \, 0 \, \cdots \, 0]^T$ *such that there exists a smooth matrix function* T_2 *of size* $n \times d$*,* $d = n - a$*, and pointwise maximal rank, satisfying* $\hat{A}_2 T_2 = 0$.

3. *We have* $\operatorname{rank} F_{\dot{x}}(t,x,\dot{x}) T_2(z) = d$ *such that there exists a smooth matrix function* Z_1 *of size* $n \times d$ *and pointwise maximal rank, satisfying* $\operatorname{rank} \hat{E}_1 T_2 = d$*, where* $\hat{E}_1 = Z_1^T F_{\dot{x}}$.

Definition 2 *Given a DAE as in (1), the smallest value of* μ *such that* F *satisfies Hypothesis 1 is called the* strangeness index *of (1).*

It has been shown in [21] that if F as in (1) satisfies Hypothesis 1 with characteristic values μ, a and d, then the set $\mathbb{L}_\mu \subseteq \mathbb{R}^{(\mu+2)n+1}$ forms a (smooth) manifold of dimension $n+1$. Setting

$$\begin{aligned} \hat{F}_1(t,x,\dot{x}) &= Z_1^T F(t,x,\dot{x}), \\ \hat{F}_2(t,x) &= Z_2^T F_\mu(t,x,\hat{z}), \end{aligned}$$

where $\hat{z} = (\hat{x}^{(t)}, \ldots, \hat{x}^{(\mu+1)})$, and considering the *reduced DAE*

$$\hat{F}(t,x,\dot{x}) = \begin{bmatrix} \hat{F}_1(t,x,\dot{x}) \\ \hat{F}_2(t,x) \end{bmatrix} = 0, \tag{5}$$

one has the following (local) relation between the solutions of (1) and (5).

Theorem 3 *[19, 21] Let* F *as in (1) satisfy Hypothesis 1 with values* μ*,* a*, and* d*. Then every sufficiently smooth solution of (1) also solves (5).*

It also has been shown in [21] that if $x^* \in C^1(\mathbb{I}, \mathbb{R}^n)$ is a sufficiently smooth solution of (1) then there exist an operator $\hat{\mathcal{F}} \colon \mathbb{D} \to \mathbb{Y}$, $\mathbb{D} \subseteq \mathbb{X}$ open, given by

$$\hat{\mathcal{F}}(x)(t) = \begin{bmatrix} \dot{x}_1(t) - \mathcal{L}(t, x_1(t)) \\ x_2(t) - \mathcal{R}(t, x_1(t)) \end{bmatrix}, \tag{6}$$

with $\mathbb{X} = \{x \in C(\mathbb{I}, \mathbb{R}^n) \mid x_1 \in C^1(\mathbb{I}, \mathbb{R}^d),\ x_1(\underline{t}) = 0\}$ and $\mathbb{Y} = C(\mathbb{I}, \mathbb{R}^n)$. Then x^* is a *regular solution* of (6), i. e., there exist neighborhoods $\mathbb{U} \subseteq \mathbb{X}$ of x^*, and $\mathbb{V} \subseteq \mathbb{Y}$ of the origin such that for every $b \in \mathbb{V}$ the equation $\hat{\mathcal{F}}(x) = b$ has a unique solution $x \in \mathbb{U}$ that depends continuously on f.

The requirements of Hypothesis 1 and that of a well-defined differentiation index are equivalent up to some (technical) smoothness requirements, see [18, 21]. For uniquely solvable systems, however, the differentiation index aims at a reformulation of the given problem as an ODE, whereas Hypothesis 1 aims at a reformulation as a DAE with two parts, one part which states all constraints and another part which describes the dynamical behavior. If the appropriate smoothness conditions hold then $\nu = 0$ if $\mu = a = 0$ and $\nu = \mu + 1$ otherwise.

2.3 The perturbation index

Motivated by the desire to classify the difficulties arising in the numerical solution of DAEs, the *perturbation index* [16] was introduced which studies the effect of a perturbation η in

$$F(t, \hat{x}, \dot{\hat{x}}) = \eta, \tag{7}$$

with sufficiently smooth η and initial condition $\hat{x}(\underline{t}) = \underline{\hat{x}}$.

Definition 4 *If $x \in C^1(\mathbb{I}, \mathbb{C}^n)$ is a solution, then (3) is said to have* perturbation index $\kappa \in \mathbb{N}$ *along x, if κ is the smallest number such that for all sufficiently smooth $\hat{x}$ satisfying (7) the estimate (with appropriate norms in the relevant spaces)*

$$\|\hat{x} - x\| \leq C(\|\underline{\hat{x}} - \underline{x}\|_\infty + \|\eta\| + \|\dot{\eta}\| + \cdots + \|\eta^{(\kappa-1)}\|), \tag{8}$$

holds with a constant C independent of $\hat{x}$. It is said to have perturbation index $\kappa = 0$ *if the estimate*

$$\|\hat{x} - x\| \leq C(\|\underline{\hat{x}} - \underline{x}\|_\infty + \max_{t \in \mathbb{I}} \| \textstyle\int_{\underline{t}}^{t} \eta(s)\, ds\|_\infty) \tag{9}$$

holds.

For the linear variable coefficient case, the following relation holds.

Theorem 5 *[21] Let the strangeness index μ of (3) be well-defined and let x be a solution of (3). Then the perturbation index κ of (3) along x is well-defined with $\kappa = 0$ if $\mu = a = 0$ and $\kappa = \mu + 1$ otherwise.*

The reason for the two cases in the definition of the perturbation index is that in this way the perturbation index equals the differentiation index if defined. Counting in the way of the strangeness index according to the estimate (8), there would be no need in the extension (9).

It has been shown in [21] that the concept of the perturbation index can also be extended to the non-square case.

3 The tractability index

A different index concept [14, 23, 24] is formulated in its current form for DAEs *with properly stated leading term*,

$$F \frac{\mathrm{d}}{\mathrm{d}t}(Dx) = f(x, t), \ t \in \mathbb{I} \tag{10}$$

with $F \in C(\mathbb{I}, \mathbb{C}^{n,l})$, $D \in C(\mathbb{I}, \mathbb{C}^{l,n})$, $f \in C(\mathbb{I}, \mathbb{C}^n)$ sufficiently smooth such that $\operatorname{kernel} F(t) \oplus \operatorname{range} D(t) = \mathbb{C}^l$ for all $t \in \mathbb{I}$ and such there exists a projector $R \in C^1(\mathbb{I}, \mathbb{C}^{l,l})$ with $\operatorname{range} R(t) = \operatorname{range} D(t)$, and $\operatorname{kernel} R(t) = \operatorname{kernel} F(t)$ for all $t \in \mathbb{I}$. One introduces the chain of matrix functions

$$\mathcal{G}_0 = FD, \ \mathcal{G}_1 = \mathcal{G}_0 + \mathcal{B}_0 \mathcal{Q}_0, \ \mathcal{G}_{i+1} = \mathcal{G}_i + \mathcal{B}_i \mathcal{Q}_i, \ i = 1, 2, \ldots, \tag{11}$$

where $\mathcal{Q}_i$ is a projector onto $\mathcal{N}_i = \text{kernel}\,\mathcal{G}_i$, with $\mathcal{Q}_i\mathcal{Q}_j = 0$ for $j = 0, \ldots, i-1$, $\mathcal{P}_i = I - \mathcal{Q}_i$, $\mathcal{B}_0 = f_x$, and $\mathcal{B}_i = \mathcal{B}_{i-1}\mathcal{P}_{i-1} - \mathcal{G}_i D^- \frac{\mathrm{d}}{\mathrm{d}t}(D\mathcal{P}_1 \ldots \mathcal{P}_i D^-)D\mathcal{P}_{i-1}$, where D^- is the reflexive generalized inverse of D satisfying $(DD^-) = R$ and $(D^-D) = \mathcal{P}_0$.

Definition 6 *[23] A DAE of the form (10) with properly stated leading term is said to be* regular with tractability index τ on the interval $\mathbb{I}$, *if there exist a sequence of continuous matrix functions (11) such that*

1. *$\mathcal{G}_i$ is singular and has constant rank $\bar{r}_i$ on $\mathbb{I}$ for $i = 0, \ldots, \tau - 1$,*
2. *$\mathcal{Q}_i$ is continuous and $D\mathcal{P}_1 \ldots \mathcal{P}_i D^-$ is continuously differentiable on $\mathbb{I}$ for $i = 0, \ldots, \tau - 1$,*
3. *$\mathcal{Q}_i\mathcal{Q}_j = 0$ holds on $\mathbb{I}$ for all $i = 1, \ldots, \tau - 1$ and $j = 1, \ldots, i - 1$,*
4. *$\mathcal{G}_\mu$ is nonsingular on $\mathbb{I}$.*

The chain of projectors and spaces allows to filter out an ODE for the differential part of the solution $u = D\mathcal{P}_1 \ldots \mathcal{P}_{\tau-1}D^-Dx$ of the linear version of (10) with $f(x,t) = A(t)x(t) + q(t)$, see [23], which is given by

$$\dot{u} - \frac{d}{dt}(D\mathcal{P}_1 \ldots \mathcal{P}_{\tau-1}D^-)u - D\mathcal{P}_1 \ldots \mathcal{P}_{\tau-1}\mathcal{G}_\mu^{-1}AD^-u = D\mathcal{P}_1 \ldots \mathcal{P}_{\tau-1}\mathcal{G}_\mu^{-1}q.$$

Instead of using derivative arrays here derivatives of projectors are used. The advantage is that the smoothness requirements for the inhomogeneity can be explicitly specified and in this form the tractability index can be extended to the infinite dimensional systems. However, if the projectors have to be computed numerically, then difficulties in obtaining the derivatives can be anticipated.

It is still a partially open problem to characterize the exact relationship between the tractability index and the other indices. Partial results have been obtained in [5, 6, 24, 22], showing that (except again for different smoothness requirements) the tractability index is equal to the differentiation index and thus by setting $\tau = 0$ if $\mu = a = 0$ one has $\tau = \mu + 1$ if $\tau > 0$.

3.1 The geometric index

The geometric theory to study DAEs as differential equations on manifolds was developed first in [30, 32, 33]. One constructs a sequence of sub-manifolds and their parameterizations via local charts (corresponding to the different constraints on different levels of differentiation). The largest number of differentiations needed to identify the DAE as a differential equation on a manifold is then called the *geometric index* of the DAE. It has been shown in [21] that any solvable regular DAE with strangeness index $\mu = 0$ can be locally (near a given solution) rewritten as a differential equation on a manifold and vice versa. If one considers the reduced system (5), then starting with a solution $x^* \in C^1(\mathbb{I}, \mathbb{R}^n)$ of (1), the set $\mathbb{M} = \hat{F}_2^{-1}(\{0\})$ is nonempty and forms the desired sub-manifold of dimension d of $\mathbb{R}^n$, where the differential equation evolves and that contains the consistent initial values. The ODE case trivially is a differential equation on the manifold $\mathbb{R}^n$. Except for differences in the smoothness requirements, the geometric index is equal to the differentiation index [5]. This then also defines the relationship to the other indices.

3.2 The structural index

A combinatorially oriented index was first defined for the linear constant coefficient case. Let $(E(p), A(p))$ be the parameter dependent pencil that is obtained from (E, A) by substituting the nonzero elements of E and A by independent parameters p_j. Then the unique integer that equals the Kronecker index of $(E(p), A(p))$ for all p from some open and dense subset of the parameter set is called the *structural index*, see [25] and in a more general way [26]. For the nonlinear case a local linearization is employed.

Although it has been shown in [31] that the differentiation index and the structural index can be arbitrarily different, the algorithm of [25] to determine the structural index is used heavily in applications, see e. g., [38] by employing combinatorial information to analyze which equations should be differentiated and to introduce extra variables for index reduction [36]. A sound analysis when this approach is fully justified has, however, only been given in special cases [10, 20, 36].

4 Conclusions

Different index concepts for systems of differential-algebraic equations have been discussed. Except for different technical smoothness assumptions (and in the case of the strangeness-index, different counting) for regular and uniquely solvable systems, these concepts are essentially equivalent to the differentiation index. However, all have advantages and disadvantages when it comes to generalizations, numerical methods or control techniques. The strangeness index and the perturbation index also extend to non-square systems, while the tractability index allows a direct generalization to infinite dimensional systems.

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