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Abstract

Here we derive the basic forward and adjoint sensitivity approaches for fully implicit ODEs and DAEs using just basic calculus and weak formulations. The purpose of this derivation is to allow a reader to understand transient sensitivities at a first-principles level and to understand all of the assumptions and steps that go into the derivations.

Contents

1 Introduction

Here we derive forward and adjoint sensitivity methods for general ODEs and DAEs using just simple calculus and weak formulations. The goal of this derivation is to allow the reader to understand every part of the derivation and to gain understanding at a basic level.

The general fully implicit parameterized DAE (or ODE) state model that we consider is

$$
\begin{aligned}
f\left(\dot{x}(t), x(t), p, v(t), t\right) &= 0,\ t \in [t_0, t_f] && (1)\\
x(0) &= x_0(p), && (2)\\
\dot{x}(0) &= \dot{x}_0(p), && (3)
\end{aligned}
$$

where

$x : t \rightarrow x(t) \in \mathcal{X}$ for $t \in [t_0, t_f]$ are the state variables,
$\dot{x} : t \rightarrow \dot{x}(t) = d(x)/d(t) \in \mathcal{X}$ for $t \in [t_0, t_f]$ are the differential state variables,
$p \in \mathcal{P}$ are the steady-state parameters,
$v : t \rightarrow v(t) \in \mathcal{V}$ for $t \in [t_0, t_f]$ are the time-dependent parameters,
$f(\dot{x}, x, p, v, t) : \mathcal{X}^2 \times \mathcal{P} \times \mathcal{V} \times \mathbf{R} \rightarrow \mathcal{F}$ is the state DAE (ODE) residual function,
$x_0(p) \in \mathcal{P} \rightarrow \mathcal{X}$ is the initial condition function for $x(t_0)$,
$\dot{x}_0(p) \in \mathcal{P} \rightarrow \mathcal{X}$ is the initial condition function for $\dot{x}(t_0)$,
$\mathcal{X} \subseteq \mathbf{R}^{n_x}$ is the vector space for the state variables,
$\mathcal{P} \subseteq \mathbf{R}^{n_p}$ is the vector space for the steady-state parameters,
$\mathcal{V} \subseteq \mathbf{R}^{n_v}$ is the vector space for the transient parameters, and
$\mathcal{F} \subseteq \mathbf{R}^{n_x}$ is the vector space for the state DAE residual function.

Note that we assume that we have a consistent initial condition where

$$
f\left(\dot{x}_0(t_0), x_0(t_0), p, v(t_0), t_0\right) = 0. \tag{4}
$$

Remarks on notation: We use the commonly accepted convention where the unadorned identifier x for a function such as $t \rightarrow x(t)$, $t \in [t_0, t_f]$, is used to represent the function over the entire domain $t \in [t_0, t_f]$. When appropriate, the notation $x(t)$ will be used to represent a particular evaluation of the function at points t in the domain $[t_0, t_f]$. However, in some situations, the argument t of $x(t)$ will be omitted and instead a bare identifier x is used and it should be clear from the context (i.e. inside of an integral) that really a single value of the function is being represented. Cases of possible ambiguity will be addressed in the sequel.

Here we consider both distributed and terminal responses as shown by the aggregate response function:

$$
d(x, p, v) = \int_{t_0}^{t_f} g(\dot{x}(t), x(t), p, v(t), t)\,dt + h(\dot{x}(t_f), x(t_f), p), \tag{5}
$$

where:

$g(\dot{x}, x, p, v, t) : \mathcal{X}^2 \times \mathcal{P} \times \mathcal{V} \times \mathbf{R} \rightarrow \mathcal{G}$ is the distributed response function,
$h(\dot{x}, x, p) : \mathcal{X}^2 \times \mathcal{P} \rightarrow \mathcal{G}$ is the terminal response function, and
$\mathcal{G} \subseteq \mathbf{R}^{n_g}$ is the vector space for the response functions.

Above, note that there may be many response functions as $n_g = |\mathcal{G}|$ may be greater than 1. The ratio $n_g/n_p = |\mathcal{G}|/|\mathcal{P}|$ has great implications when considering forward and adjoint sensitivity methods.

The implicit state solution for the DAEs in (1)–(3) at points t is signified as $x(p,v,t) \in \mathcal{X}$ and $\dot{x}(p,v,t) \in \mathcal{X}$, where v in this case is the selection of transient parameters in the range $t \in [t_0, t]$. Note that selections for v in the range $(t : t_f]$ have no influence on the implicit state solution x up to the time t. The full infinite-dimensional implicit state solution for x in $t \in [t_0, t_f]$ is signified as $x(p,v)$ where in this case v represents the entire selection for the transient parameters in $[t_0, t_f]$.

Given the implicit state function $x(p,v)$ and its time derivative $\dot{x}(p,v)$, a reduced set of auxiliary response functions are defined as

$$\hat{d}(p,v) = \int_{t_0}^{t_f} \hat{g}(p, v(t), t)dt + \hat{h}(p), \tag{6}$$

where
$\hat{g}(p, v(t), t) = g(\dot{x}(p,v,t), x(p,v,t), p, v(t), t)) : \mathcal{P} \times \mathcal{V} \times \mathbf{R} \rightarrow \mathcal{G}$ is defined on $t \in [t_0, t_f]$, and
$\hat{h}(p) = h(\dot{x}(p,v,t_f), x(p,v,t_f), p)) : \mathcal{P} \rightarrow \mathcal{G}$ is defined only at $t = t_f$.

2 Derivation of forward sensitivities

For the derivation of forward sensitivities we will ignore the transient parameters $v(t)$ for $t \in [t_0, t_f]$ since forward sensitivity methods for such problems are typically impractical[1].

The forward sensitivity problem is easily stated by differentiating (6) with respect to p to obtain

$$\frac{\partial \hat{d}}{\partial p} = \int_{t_0}^{t_f} \left(\frac{\partial g}{\partial \dot{x}} \frac{\partial \dot{x}}{\partial p} + \frac{\partial g}{\partial x} \frac{\partial x}{\partial p} + \frac{\partial g}{\partial p} \right) dt + \left. \left(\frac{\partial h}{\partial \dot{x}} \frac{\partial \dot{x}}{\partial p} + \frac{\partial h}{\partial x} \frac{\partial x}{\partial p} + \frac{\partial h}{\partial p} \right) \right|_{t=t_f}, \tag{7}$$

where

$\partial \hat{g}/\partial p \in \mathcal{G}|\mathcal{P}$ is defined on $t \in [t_0, t_f]$,
$\partial \hat{h}/\partial p \in \mathcal{G}|\mathcal{P}$ is defined only at $t = t_f$,
$\partial x/\partial p \in \mathcal{X}|\mathcal{P}$ is the forward sensitivity of the state defined on $t \in [t_0, t_f]$,
$\partial \dot{x}/\partial p \in \mathcal{X}|\mathcal{P}$ is the forward sensitivity of the state time derivative defined on $t \in [t_0, t_f]$, and
$\partial \hat{d}/\partial p \in \mathcal{G}|\mathcal{P}$ is defined independent of time.

The forward sensitivity $\partial x/\partial p$ and $\partial \dot{x}/\partial p$ in (7) is computed by solving a set of n_p independent forward sensitivity equations which are obtained by differentiating (1)–(3) with respect to p and changing the order of differentiation with respect to t and p to give

$$\begin{aligned}
\frac{\partial f}{\partial \dot{x}} \left(\frac{\partial \dot{x}}{\partial p} \right) + \frac{\partial f}{\partial x} \left(\frac{\partial x}{\partial p} \right) + \frac{\partial f}{\partial p} &= 0, \; t \in [t_0, t_f], && (8) \\
\frac{\partial x(t_0)}{\partial p} &= \frac{\partial x_0}{\partial p}, && (9) \\
\frac{\partial \dot{x}(t_0)}{\partial p} &= \frac{\partial \dot{x}_0}{\partial p}, && (10)
\end{aligned}$$

where

$\partial f/\partial \dot{x} \in \mathcal{F}|\mathcal{X}$ is defined on $t \in [t_0, t_f]$,
$\partial f/\partial x \in \mathcal{F}|\mathcal{X}$ is defined on $t \in [t_0, t_f]$,
$\partial f/\partial p \in \mathcal{F}|\mathcal{P}$ is defined on $t \in [t_0, t_f]$,
$\partial x_0/\partial p \in \mathcal{X}|\mathcal{P}$ is defined only at $t = t_0$, and
$\partial \dot{x}_0/\partial p \in \mathcal{X}|\mathcal{P}$ is defined only at $t = t_0$.

Note that above, $\partial \dot{x}/\partial p = \frac{d}{dt} \partial x/\partial p = \partial/\partial p \frac{dx}{dt}$ because the order of differentiation does not matter with smooth differentiable functions, which is the assumption here.

These n_p independent sensitivity equations are solved for $\partial x/\partial p \in \mathcal{X}|\mathcal{P}$ and $\partial \dot{x}/\partial p \in \mathcal{X}|\mathcal{P}$ forward in time from t_0 to t_f. The integral in (7) can be evaluated along with the integration of (1)–(3) and (8)–(10). Note that (1)–(3) and (8)–(10) are a staggered set of DAE equations in that (1)–(3) are solved first followed by (8)–(10).

[1]Note: For some applications where n_v is not too large and where v is given a very course discretization in $t \in [t_0, t_f]$, computing forward sensitivities with respect to the discretized v can be practical.

3 Derivation of adjoint sensitivities

Here we describe a derivation for the adjoint equation and the gradient expressions that are based on simple and straightforward principles. In this derivation, we assume that the response functions $g()$ and $h()$ do not depend on $\dot{x}$.

3.1 Derivation of adjoint equation and sensitivities for steady-state parameters

In this section we begin with the basic expressions for the reduced derivative $\partial\hat{d}/\partial p$ in (7) and the forward sensitivity equations for $\partial x/\partial p$ in (8)–(10) and then perform basic manipulations in order to arrive at the adjoint equations and the adjoint sensitivities for $\partial\hat{d}/\partial p$.

We begin our derivation of the adjoint equation and sensitivities for steady-state parameters by writing the weak form of the forward sensitivity equation (8) which, in multi-vector form, is

$$\int_{t_0}^{t_f} \Lambda^T \left(\frac{\partial f}{\partial \dot{x}} \left(\frac{d}{dt} \frac{\partial x}{\partial p} \right) + \frac{\partial f}{\partial x} \left(\frac{\partial x}{\partial p} \right) + \frac{\partial f}{\partial p} \right) dt = 0, \tag{11}$$

where at this point the multi-vector function Λ, for $t \rightarrow \Lambda(t) \in \mathcal{F} | \mathcal{G}$ in $t \in [t_0, t_f]$, is any appropriate weighting function[2]. Later, Λ will be chosen to be the adjoint variables but for now Λ is nothing more than an arbitrary weighting function for the purpose of stating the weak form. The solution to the weak form of (11) is every bit as valid and is indeed more general than the strong form in (8) and we lose nothing by considering the weak form [1]. Also note that the multi-vector form of (11) really gives n_g separate weak form equations.

Next, we substitute the integration by parts

$$\int_{t_0}^{t_f} \left[\left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \right) \frac{d}{dt} \left(\frac{\partial x}{\partial p} \right) \right] dt = \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \frac{\partial x}{\partial p} \right) \Bigg|_{t_0}^{t_f} - \int_{t_0}^{t_f} \left[\frac{d}{dt} \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \right) \frac{\partial x}{\partial p} \right] dt \tag{12}$$

into (11) and rearrange which yields

$$\int_{t_0}^{t_f} \left(\Lambda^T \frac{\partial f}{\partial p} \right) dt + \int_{t_0}^{t_f} \left[-\frac{d}{dt} \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \right) + \Lambda^T \frac{\partial f}{\partial x} \right] \frac{\partial x}{\partial p} dt + \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \frac{\partial x}{\partial p} \right) \Bigg|_{t_0}^{t_f} = 0. \tag{13}$$

At this point in the derivation we decide to restrict the possible set of functions for Λ by forcing Λ to satisfy the differential equation

$$\frac{d}{dt} \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \right) - \Lambda^T \frac{\partial f}{\partial x} = -\frac{\partial g}{\partial x}, \; t \in [t_0, t_f]. \tag{14}$$

[2] The admissible class of weighting functions Λ are those functions that are sufficiently smooth such that the integrals of the weak form (and the modified weak form after integration by parts) are finite and well defined. Other requirements may also need to be satisfied in some cases [1].

All that we have done in (14) is to make what appears to be an arbitrary choice to help narrow the weighting function Λ from the infinite set of possible choices. It will be clear later why this choice is a convenient one. Note that the choice in (14) does not in and of itself uniquely determine Λ since boundary conditions have yet to be specified. It will be shown later that the choice of boundary condition is arbitrary but when we move toward the end of the derivation, a natural and very convenient choice for a boundary condition that uniquely specifies Λ will be obvious.

Side Note: What is critical about the choice for the adjoint equation in (14) is that the derivative $\partial g/\partial x$ appear on the RHS. What is largely arbitrary, however is the sign of the given to $\partial g/\partial x$ which of course defines the sign for the adjoint variables Λ. The Petzold papers (e.g. [2]) and the IDAS code [3] use the sign for the adjoint given in (14). However, the CVODES code [4, 3] uses the opposite sign for $\partial g/\partial x$ in the RHS and therefore gives the opposite sign for the adjoint solution Λ. With respect the the computation of the reduced response derivative, the choice for the sign of Λ is arbitrary. However, if one is going to directly interpret the adjoint solution Λ as we do in Section 4, then the sign of the adjoint becomes very important and it is critical that the user of any adjoint code know the significance of the sign of the adjoint and understand its meaning.

The derivation continues by substituting (14) into (13) and rearranging which yields

$$\int_{t_0}^{t_f} \left(\frac{\partial g}{\partial x} \frac{\partial x}{\partial p} \right) dt \quad = \quad -\int_{t_0}^{t_f} \left(\Lambda^T \frac{\partial f}{\partial p} \right) dt - \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \frac{\partial x}{\partial p} \right) \Bigg|_{t_0}^{t_f} . \tag{15}$$

Finally, substituting (15) into (7), dropping terms with $\partial g/\partial \dot{x}$ and $\partial h/\partial \dot{x}$ since we are assuming there are zero in this derivation, and rearranging gives

$$\begin{aligned} \frac{\partial \hat{d}}{\partial p} \quad &= \quad \int_{t_0}^{t_f} \left(\frac{\partial g}{\partial p} - \Lambda^T \frac{\partial f}{\partial p} \right) dt + \left(\frac{\partial h}{\partial p} \right) \Bigg|_{t=t_f} + \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \frac{\partial x}{\partial p} \right) \Bigg|_{t=t_0} \\ &\quad + \left[\left(\frac{\partial h}{\partial x} - \Lambda^T \frac{\partial f}{\partial \dot{x}} \right) \frac{\partial x}{\partial p} \right] \Bigg|_{t=t_f} . \end{aligned} \tag{16}$$

We are not finished yet since, as we stated earlier, the choice for the weighting functions Λ have not yet been uniquely specified. The first thing to consider is that, in general, the adjoint DAE in (14) is only stable if integrated backwards in time from t_f to t_0 [2]. However, as described in the following theorem, we are free to pick almost any final condition for $\Lambda(t_f)$ that is consistent with the adjoint equation at t_f and then evaluate the terms in (16) involving the resulting adjoint solution. This is established in the following theorem.

Theorem 1 *If Λ_1 and Λ_2 are any two particular bounded solutions to the adjoint equation (14) (each associated with a different bounded consistent final condition on $\Lambda(t_f)$) then*

$$\left. \frac{\partial \hat{d}}{\partial p} \right|_{\Lambda=\Lambda_1} = \left. \frac{\partial \hat{d}}{\partial p} \right|_{\Lambda=\Lambda_2} \tag{17}$$

where $\left(\partial \hat{d}/\partial p\right)\big|_{\Lambda=\Lambda_1}$ and $\left(\partial \hat{d}/\partial p\right)\big|_{\Lambda=\Lambda_1}$ represent the reduced derivative in (16) evaluated using the adjoint solutions Λ_1 and Λ_2 respectively.

Proof

Here we prove (17) by proving that

$$\begin{aligned} D_2 - D_1 &= \left.\frac{\partial \hat{d}}{\partial p}\right|_{\Lambda=\Lambda_2} - \left.\frac{\partial \hat{d}}{\partial p}\right|_{\Lambda=\Lambda_1} \\ &= \int_{t_0}^{t_f} (\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial p} dt + \left.\left[(\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial \dot{x}} \frac{\partial x}{\partial p}\right]\right|_{t_0}^{t_f} = 0 \end{aligned} \tag{18}$$

for any two particular solutions Λ_1 and Λ_2 to the adjoint equation (14). Above, the expression in (18) comes from substituting Λ_1 and Λ_2 into (16), subtracting the two expressions, dropping out zero terms, and rearranging.

We start the proof by substituting (8) into (18) which yields

$$D_2 - D_1 = \int_{t_0}^{t_f} (\Lambda_2 - \Lambda_1)^T \left[-\frac{\partial f}{\partial \dot{x}} \left(\frac{d}{dt} \frac{\partial x}{\partial p} \right) - \frac{\partial f}{\partial x} \left(\frac{\partial x}{\partial p} \right) \right] dt + \left.\left[(\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial \dot{x}} \frac{\partial x}{\partial p}\right]\right|_{t_0}^{t_f}. \tag{19}$$

Substituting the integration by parts

$$-\int_{t_0}^{t_f} \left[\left((\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial \dot{x}} \right) \frac{d}{dt} \left(\frac{\partial x}{\partial p} \right) \right] dt = \int_{t_0}^{t_f} \left[\frac{d}{dt} \left((\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial \dot{x}} \right) \frac{\partial x}{\partial p} \right] dt - \left.\left[(\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial \dot{x}} \frac{\partial x}{\partial p}\right]\right|_{t_0}^{t_f}$$

into (19), canceling terms, and rearranging yields

$$D_2 - D_1 = \int_{t_0}^{t_f} \left[\frac{d}{dt} \left((\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial \dot{x}} \right) - (\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial x} \right] \left(\frac{\partial x}{\partial p} \right) dt. \tag{20}$$

Next, substituting the solutions Λ_1 and Λ_2 into (14) and subtracting these two adjoint equations yields

$$-\frac{d}{dt} \left((\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial \dot{x}} \right) + (\Lambda_2 - \Lambda_1)^T \frac{\partial f}{\partial x} = 0, \; t \in [t_0, t_f]. \tag{21}$$

Finally, substituting (21) into (20) yields

$$D_2 - D_1 = 0 \tag{22}$$

which completes the proof. □

The above theorem establishes that there are an infinite number of choices for the final condition for the adjoint solution that all yield the same reduced derivative $\partial \hat{d} / \partial p$. While a wide variety of final conditions for $\Lambda(t_f)$ can be chosen to close the adjoint equation, rather than picking just any final condition, selecting the final condition

$$\left(\frac{\partial h}{\partial x} - \Lambda^T \frac{\partial f}{\partial \dot{x}} \right) \bigg|_{t=t_f} = 0, \tag{23}$$

is rather convenient since it zeros out the last term in (16) and allows us to avoid the computation of $\partial x/\partial p$ at $t = t_f$ which we do not readily have with an adjoint method. This specification of the final condition closes the adjoint equation and uniquely defines the adjoint Λ in all of the cases of state DAEs what we will consider here[3].

Finally, substituting (23) and $\partial x_0/\partial p$ for $\partial x/\partial p$ at $t = t_0$ in (16) we arrive the final expression for reduced derivative

$$\frac{\partial \hat{d}}{\partial p} = \int_{t_0}^{t_f} \left(\frac{\partial g}{\partial p} - \Lambda^T \frac{\partial f}{\partial p} \right) dt + \left(\frac{\partial h}{\partial p} \right) \bigg|_{t=t_f} + \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \right) \bigg|_{t=t_0} \frac{\partial x_0}{\partial p}. \tag{24}$$

In conclusion, (14) and (23) define the set of adjoint DAE equations that specify a unique adjoint solution Λ which are integrated backwards in time and (24) gives the expression for the computation of $\partial \hat{d}/\partial p$ in terms of the computed adjoint Λ. Note that the integral in (24) can be evaluated at the same time that the adjoint is being solved backward in time. Therefore, no storage of the adjoint is needed beyond what is needed for the time stepping algorithm.

3.2 Derivation of adjoint sensitivities for transient parameters

Here we consider the derivation of the reduced sensitivity with respect to transient parameters

$$\frac{\partial \hat{d}}{\partial v(t)} \in \mathcal{G}|\mathcal{V}, \text{ for } t \in [t_0, t_f]. \tag{25}$$

Our derivation for these sensitivities for the transient parameters v will be a little different than for the steady-state parameters p. The primary reason for using a different derivation is that the infinite-dimensional transient parameters v are fundamentally different than finite-dimensional steady-state parameters p. Because of the infinite-dimensional nature of v, we use a different tool of functional analysis. The tool we use is the application of the infinite-dimensional operator $\partial \hat{d}/\partial v$ to the infinite-dimensional perturbation δv where we will then use to identify $\partial \hat{d}/\partial v(t)$ in the integrand of

$$\frac{\partial \hat{d}}{\partial v} \delta v = \int_{t_0}^{t_f} \frac{\partial \hat{d}}{\partial v(t)} \delta v(t) dt. \tag{26}$$

The integral in (26) is the definition the infinite-dimensional operator application $(\partial \hat{d}/\partial v)\delta v$.

[3]A uniquely defined adjoint Λ requires that certain regularity conditions are satisfied by the state DAE (see [2]) but for the purposes of this derivation we assume that such a condition is always satisfied.

We begin the derivation with the variational derivative of $\hat{d}(v)$ with respect to v along the variation δv which is simply

$$\frac{\partial \hat{d}}{\partial v}\delta v = \int_{t_0}^{t_f} \left(\frac{\partial g}{\partial x}\frac{\partial x}{\partial v}\delta v + \frac{\partial g}{\partial v}\delta v \right) dt + \left(\frac{\partial h}{\partial x}\frac{\partial x}{\partial v}\delta_v \right)\bigg|_{t=t_f}. \tag{27}$$

Next, we write the weak form of the linearization of the state equation (about a solution for $f(\dot{x},x,p,v,t)=0$) with respect to v along the variation δv which is

$$\int_{t_0}^{t_f} \Lambda^T \left[\frac{\partial f}{\partial \dot{x}} \left(\frac{d}{dt}\frac{\partial x}{\partial v} \right) \delta v + \frac{\partial f}{\partial x}\frac{\partial x}{\partial v}\delta v + \frac{\partial f}{\partial v}\delta_v \right] dt = 0 \tag{28}$$

and has initial condition $(\partial x/\partial v)\delta v|_{t=t_0} = 0$. The sensitivity equation that is used in the weak form in (28) can be derived using a simple Taylor expansion of the state equation about a solution $f(\dot{x},x,p,v,t)=0$ in the variation δv and then dropping off the $O(||\delta v||^2)$ and higher terms.

From here the derivation proceeds almost identically to the case for the steady-state parameters p described in the previous section.

Substituting the integration by parts

$$\int_{t_0}^{t_f} \left[\left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \right) \frac{d}{dt} \left(\frac{\partial x}{\partial v}\delta v \right) \right] dt = \left(\Lambda^T \frac{\partial f}{\partial \dot{x}}\frac{\partial x}{\partial v}\delta v \right)\bigg|_{t_0}^{t_f} - \int_{t_0}^{t_f} \left[\frac{d}{dt} \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \right) \frac{\partial x}{\partial v}\delta v \right] dt \tag{29}$$

into (28) and rearranging yields

$$\int_{t_0}^{t_f} \left(\Lambda^T \frac{\partial f}{\partial v}\delta v \right) dt + \int_{t_0}^{t_f} \left[-\frac{d}{dt} \left(\Lambda^T \frac{\partial f}{\partial \dot{x}} \right) + \Lambda^T \frac{\partial f}{\partial x} \right] \frac{\partial x}{\partial v}\delta v dt + \left(\Lambda^T \frac{\partial f}{\partial \dot{x}}\frac{\partial x}{\partial v}\delta v \right)\bigg|_{t_0}^{t_f} = 0. \tag{30}$$

Substituting the choice for the adjoint equation (14) into (30) and rearranging yields

$$\int_{t_0}^{t_f} \left(\frac{\partial g}{\partial x}\frac{\partial x}{\partial v}\delta v \right) dt \quad = \quad -\int_{t_0}^{t_f} \left(\Lambda^T \frac{\partial f}{\partial v}\delta v \right) dt - \left(\Lambda^T \frac{\partial f}{\partial \dot{x}}\frac{\partial x}{\partial v}\delta v \right)\bigg|_{t_0}^{t_f}. \tag{31}$$

Substituting (31) into (27) and rearranging yields

$$\begin{aligned} \frac{\partial \hat{d}}{\partial v}\delta v \quad = \quad & \int_{t_0}^{t_f} \left(\frac{\partial g}{\partial v} - \Lambda^T \frac{\partial f}{\partial v} \right) \delta v dt + \left(\Lambda^T \frac{\partial f}{\partial \dot{x}}\frac{\partial x}{\partial v}\delta v \right)\bigg|_{t=t_0} \\ & + \left[\left(\frac{\partial h}{\partial x} - \Lambda^T \frac{\partial f}{\partial \dot{x}} \right) \frac{\partial x}{\partial v}\delta v \right]\bigg|_{t=t_f}. \end{aligned} \tag{32}$$

Using the choice for the final condition in (23) and noting that $(\partial x/\partial v)\delta v|_{t=t_0} = 0$ (since v can not affect x at $t=t_0$ because v only appears in the DAE RHS, not the initial condition), then (32) reduces to

$$\frac{\partial \hat{d}}{\partial v}\delta v = \int_{t_0}^{t_f} \left(\frac{\partial g}{\partial v} - \Lambda^T \frac{\partial f}{\partial v} \right) \delta v dt. \tag{33}$$

Finally, by comparing (33) with (26) it is clear that

$$\frac{\partial \hat{d}}{\partial v(t)} = \frac{\partial g}{\partial v(t)} - \Lambda(t)^T \frac{\partial f}{\partial v(t)},\ t \in [t_0, t_f] \tag{34}$$

is the reduced derivative object that we are seeking.

4 Significance and interpretation of the adjoint

In this section we consider another reason for choosing (23) as the final condition to close the adjoint equation (14). This choice of the final condition makes the adjoint variables Λ become the first-order sensitivity of the auxiliary response function $d(x)$ with respect the perturbations in the constraints through the state solution. This is easy to see by simply considering the case where $g(x,v,t) = g(x)$, $h(x) = h(x)$, and $f(\dot{x},x,v,t) = f(\dot{x},x,t) - v$ which, when substituted into (34), gives

$$\frac{\partial \hat{d}}{\partial v(t)} = \Lambda(t)^T,\ t \in [t_0, t_f], \tag{35}$$

where $v(t) \in \mathcal{F}$ are the perturbations in the state constraints $f(\dot{x},x,t)$.

The knowledge that this selection for the adjoint Λ is the sensitivity of a functional of interest $d(x)$ with respect to the changes in the constraints makes the adjoint a useful quantity in and of itself. This is why the adjoint is useful in more contexts other than just computing reduced derivatives. Examples of other areas where adjoints are useful are sensitivity analysis and error estimation [5]

Note that the sign given the adjoint in the choice for the adjoint equation (14) determines the interpretation for the adjoint in this analysis. If the opposite sign for the adjoint would have been chosen, then we must interpret the perturbation to the state equation as $f(\dot{x},x,v,t) = f(\dot{x},x,t) + v$. The only issue here is whether adding a constant to a state equation will increase or decrease the reduced response function $\hat{d}(p)$. However, since most people just look at the magnitude of this sensitivity inherent in the adjoint, the sign of the adjoint again becomes unimportant.

5 The adjoint, the reduced gradient and the augmented adjoint

We now restate the adjoint in (14) and (23), and the reduced sensitivities in (24) and (34) in standard column-wise multi-vector form for Λ which yields the adjoint DAE equations

$$\frac{d}{dt}\left(\frac{\partial f}{\partial \dot{x}}^T \Lambda\right) - \frac{\partial f}{\partial x}^T \Lambda + \frac{\partial g}{\partial x}^T = 0,\ t \in [t_0, t_f], \tag{36}$$

$$\left.\left(\frac{\partial f}{\partial \dot{x}}^T \Lambda\right)\right|_{t=t_f} = \left.\frac{\partial h}{\partial x}^T\right|_{x=x(t_f)}, \tag{37}$$

and the reduced gradient expressions

$$\frac{\partial \hat{d}}{\partial p}^T = \int_{t_0}^{t_f} \left(\frac{\partial g}{\partial p}^T - \frac{\partial f}{\partial p}^T \Lambda\right) dt + \left.\frac{\partial h}{\partial p}^T\right|_{t=t_f} + \frac{\partial x_0}{\partial p}^T \left.\left(\frac{\partial f}{\partial \dot{x}}^T \Lambda\right)\right|_{t=t_0}. \tag{38}$$

and

$$\frac{\partial \hat{d}}{\partial v(t)}^T = \frac{\partial g}{\partial v(t)}^T - \frac{\partial f}{\partial v(t)}^T \Lambda(t),\ t \in [t_0, t_f] \tag{39}$$

As described in [2], for some classes of DAEs (including some implicit ODEs), the form of the adjoint in (36)–(37) may be unstable while the following *augmented adjoint DAE system* (created by defining the augmented adjoint varaibles $\hat{\Lambda} = \partial f / \partial \dot{x} \Lambda$)

$$\frac{d}{dt}(\hat{\Lambda}) - \frac{\partial f}{\partial x}^T \Lambda + \frac{\partial g}{\partial x}^T = 0,\ t \in [t_0, t_f], \tag{40}$$

$$\hat{\Lambda} - \frac{\partial f}{\partial \dot{x}}^T \Lambda = 0,\ t \in [t_0, t_f], \tag{41}$$

$$\hat{\Lambda}\Big|_{t=t_f} = \left.\frac{\partial h}{\partial x}^T\right|_{x=x(t_f)}, \tag{42}$$

generally is stable when the forward DAE (up to index 2) is stable. In addition, when considering time-stepping algorithms for state and adjoint equations, only the augmented adjoint DAE is guaranteed to be stable for the same time-step used by the forward DAE [2]. Therefore, the augmented adjoint DAE system is to be preferred in a software implementation and only imparts a small additional space/time cost.

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