

# Sensitivity analysis of differential-algebraic equations and partial differential equations

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## Abstract

Sensitivity analysis generates essential information for model development, design optimization, parameter estimation, optimal control, model reduction and experimental design. In this paper we describe the forward and adjoint methods for sensitivity analysis, and outline some of our recent work on theory, algorithms and software for sensitivity analysis of differential-algebraic equation (DAE) and time-dependent partial differential equation (PDE) systems.

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## 1. Introduction

In recent years there has been a growing interest in sensitivity analysis for large-scale systems governed by both differential-algebraic equations (DAEs) and partial differential equations (PDEs). The results of sensitivity analysis have wide-ranging applications in science and engineering, including model development, optimization, parameter estimation, model simplification, data assimilation, optimal control, uncertainty analysis and experimental design.

Recent work on methods and software for sensitivity analysis of DAE and PDE systems has demonstrated that forward sensitivities can be computed reliably and efficiently. However, for problems which require the sensitivities with respect to a large number of parameters, the forward sensitivity approach is intractable and the adjoint (backward) method is advantageous. Unfortunately, the adjoint problem is quite a bit more complicated both to pose and to solve. Our goal for both DAE and PDE systems has been the development of methods and software in which generation and solution of the adjoint sensitivity system

are transparent to the user. This has been largely achieved for DAE systems. We have proposed a solution to this problem for PDE systems solved with adaptive mesh refinement (AMR).

This paper has three parts. In the first part we introduce the basic concepts of sensitivity analysis, including the forward and the adjoint method. In the second part we outline the basic problem of sensitivity analysis for DAE systems and examine the recent results on numerical methods and software for DAE sensitivity analysis based on the forward and adjoint methods. The third part of the paper deals with sensitivity analysis for time-dependent PDE systems solved by adaptive mesh refinement.

## 2. Basics of sensitivity analysis

Generally speaking, sensitivity analysis calculates the rates of change in the output variables of a system which result from small perturbations in the problem parameters. To illustrate the basic ideas of sensitivity analysis, consider a general, parameter-dependent nonlinear system

$$F(x, p) = 0, \quad (1)$$

where  $x \in \mathbb{R}^n$ ,  $p \in \mathbb{R}^m$ ,  $F : \mathbb{R}^{m+n} \rightarrow \mathbb{R}^n$  and  $\partial F/\partial x$  is nonsingular for all  $p \in \mathbb{R}^m$ . In its most basic form, sensitivity analysis calculates the sensitivities  $dx/dp$  of the solution variables with

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respect to perturbations in the parameters. In many applications, one is concerned with a function of the state variable  $x$  and parameters  $p$ , which is called a *derived function*, given by  $g(x, p) : \mathbb{R}^{m+n} \rightarrow \mathbb{R}^k$ , where  $k$  usually is much smaller than  $m$  and  $n$ . In this case, the objective of sensitivity analysis is to compute the sensitivities  $dg/dp$ . We have

$$\frac{dg}{dp} = g_x x_p + g_p, \quad (2)$$

where  $g_x = \partial g / \partial x$ ,  $x_p = \partial x / \partial p$ ,  $g_p = \partial g / \partial p$ . There are two methods for obtaining the sensitivity: the forward method and the adjoint (backward) method.

### 2.1. Forward method

Linearizing the nonlinear system (1), we obtain

$$F_x x_p + F_p = 0, \quad (3)$$

where  $x_p$  is an  $n \times m$  matrix. To compute  $dg/dp$ , we first need to solve  $m$  linear systems of (3) to obtain  $x_p$ . This is an excellent method when the dimension  $m$  of parameters is small.

### 2.2. Backward method

When the dimension  $m$  of  $p$  is large, the forward method becomes computationally expensive due to the need to compute  $x_p$ . We can avoid solving for  $x_p$  by using the backward (adjoint) method. To do this, we first multiply (3) by  $\lambda$  to obtain

$$\lambda^T F_x x_p + \lambda^T F_p = 0. \quad (4)$$

Now let  $\lambda$  solve the linear adjoint system

$$\lambda^T F_x = g_x. \quad (5)$$

Then  $g_x x_p = -\lambda^T F_p$ , thus, from (2)

$$\frac{dg}{dp} = -\lambda^T F_p + g_p. \quad (6)$$

Note that we need to solve the linear Eq. (5) just once, no matter how many parameters are involved in the system. The adjoint method is a powerful tool for sensitivity analysis. Its advantage is that when the dimension of parameters is large, we need not solve the large system for  $x_p$ , but instead only the adjoint system (5), which greatly reduces the computation time. Thus, while forward sensitivity analysis is best suited to the situation of finding the sensitivities of a potentially large number of solution variables with respect to a small number of parameters, adjoint (backward) sensitivity analysis is best suited to the complementary situation of finding the sensitivity of a scalar (or small-dimensional) function of the solution with respect to a large number of parameters.

The derivation of the adjoint sensitivity method for DAEs and PDEs follows a similar idea as above but is more complicated. In this paper we will avoid the details and focus on the introduction of the corresponding adjoint systems and software.

## 3. Sensitivity analysis for DAE systems

Recent work on methods and software for sensitivity analysis of DAE systems (Feehery, Tolsma, & Barton, 1997; Li & Petzold, 1999, 2000; Li, Petzold, & Zhu, 2000; Maly & Petzold, 1997) has demonstrated that forward sensitivities can be computed reliably and efficiently via automatic differentiation (Bischof, Carle, Corliss, Griewank, & Hovland, 1992) in combination with DAE solution techniques designed to exploit the structure of the sensitivity system. For a DAE depending on parameters,

$$\begin{cases} F(x, \dot{x}, t, p) = 0 \\ x(0) = x_0(p), \end{cases} \quad (7)$$

these problems take the form: find  $dx/dp_j$  at time  $T$ , for  $j = 1, \dots, n_p$ . Their solution requires the simultaneous solution of the original DAE system with the  $n_p$  sensitivity systems obtained by differentiating the original DAE with respect to each parameter in turn. For large systems this may look like a lot of work but it can be done efficiently, if  $n_p$  is relatively small, by exploiting the fact that the sensitivity systems are linear and all share the same Jacobian matrices with the original system.

### 3.1. The adjoint DAE

Some problems require the sensitivities with respect to a large number of parameters. For these problems, particularly if the number of state variables is also large, the forward sensitivity approach is intractable. These problems can often be handled more efficiently by the adjoint method (Errico, 1997). In this approach, we are interested in calculating the sensitivity of a derived function

$$G(x, p) = \int_0^T g(x, t, p) dt, \quad (8)$$

or alternatively the sensitivity of the integrand  $g(x, T, p)$  defined only at time  $T$ . The function  $g$  must be smooth enough that  $g_p$  and  $g_x$  exist and are bounded.

In our previous work (Cao, Li, Petzold, & Serban, 2003) we derived the adjoint sensitivity system for DAEs of index (Ascher & Petzold, 1998) up to two (Hessenberg) and investigated some of its fundamental properties. Here we summarize the main results.

The adjoint system for the DAE

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

with respect to the derived function  $G(x, p)$  (8) is given by

$$(\lambda^* F_{\dot{x}})' - \lambda^* F_x = -g_x, \quad (9)$$

where  $*$  denotes the transpose operator and prime ( $'$ ) denotes the total derivative with respect to  $t$ .

The adjoint system is solved backwards in time. For index-0 and index-1 DAE systems, the final conditions for (9) are taken to be  $\lambda^* F_{\dot{x}}|_{t=T} = 0$ , and the sensitivities of  $G(x, p)$  with respect

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