Sensitivity Analysis of Differential-Algebraic Equations

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Background - General DAE System

$$0 = \mathbf{F}(t, \mathbf{y}, \mathbf{y}')$$

- **Mathematical structure is more complex than standard-form ODE $y' = f(t,y)$**
- **$\partial F/\partial y'$ may be singular, and in this case it is not equivalent to ODE**
- **Simple and natural formulation for modeling many physical systems**
- **Requires special consideration for formulating problem and choosing and implementing numerical methods**

Index is a measure of the degree of singularity of a DAE system

- **Standard form ODE is index-0**
- **Index is defined as the number of times the constraints must be differentiated to reach a standard form ODE system**

Background - DAE Structural Forms and Software

Semi-explicit index-1 DAE

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

Hessenberg index-2 DAE

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

Software - DASSL (Petzold (1982)), DASPK (Brown, Hindmarsh and Petzold (1994))

- **Fully-implicit DAE systems of index at most 1**
- **Backward differentiation formulas (BDF), variable-stepsize, variable order**
- **Moderate (DASSL) to large-scale (DASPK) DAE systems**

DAE Sensitivity Analysis

Given the DAE depending on parameter p,

$$F(t,x,x',p)=0, \quad x(t_0)=x_0(p)$$

sensitivity analysis finds the change in the solution with respect to perturbations in the parameters, dx/dp_i

Uses of sensitivity analysis:

- Gain physical insight into governing processes
- Parameter estimation
- Design optimization
- Optimal control
- Determine nonlinear reduced order models
- Assess uncertainty and range of validity of reduced order models

Sensitivity Analysis (Forward Mode)

General DAE problem with parameters

$$F(t,x,x',p)=0, \quad x(t_0)=x_0(p)$$

Differentiate with respect to each parameter to obtain sensitivity system

$$F(t,x,x',p)=0$$

$$\frac{\partial F}{\partial x}s_i + \frac{\partial F}{\partial x'}s'_i + \frac{\partial F}{\partial p_i} = 0$$

where $s_i \equiv \frac{dx}{dp_i}$

DASPK3.0

Solution and forward sensitivity analysis using methods of DASPK (Petzold and Li, 2000)

- **Applicable for DAE index up to two (Hessenberg)**
- **Exploit structure of sensitivity system**
- **Evaluation of sensitivity residuals by automatic differentiation**
- **Naturally parallel (MPI)**

Limitations of Forward Sensitivity Method

- Many applications require the sensitivity of a scalar derived quantity *g(x)* with respect to the initial conditions of all the solution variables

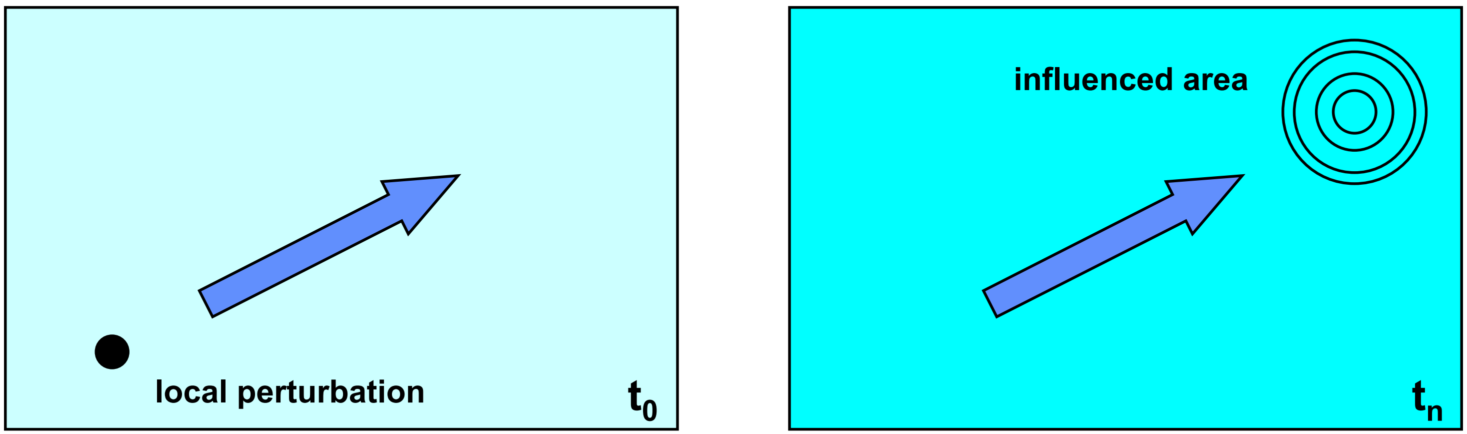
- Forward sensitivity analysis computes

$$\frac{dg(x)}{dx_0} = \left(\frac{dg(x)}{dx_n}\right)\left(\frac{dx_n}{dx_0}\right)$$

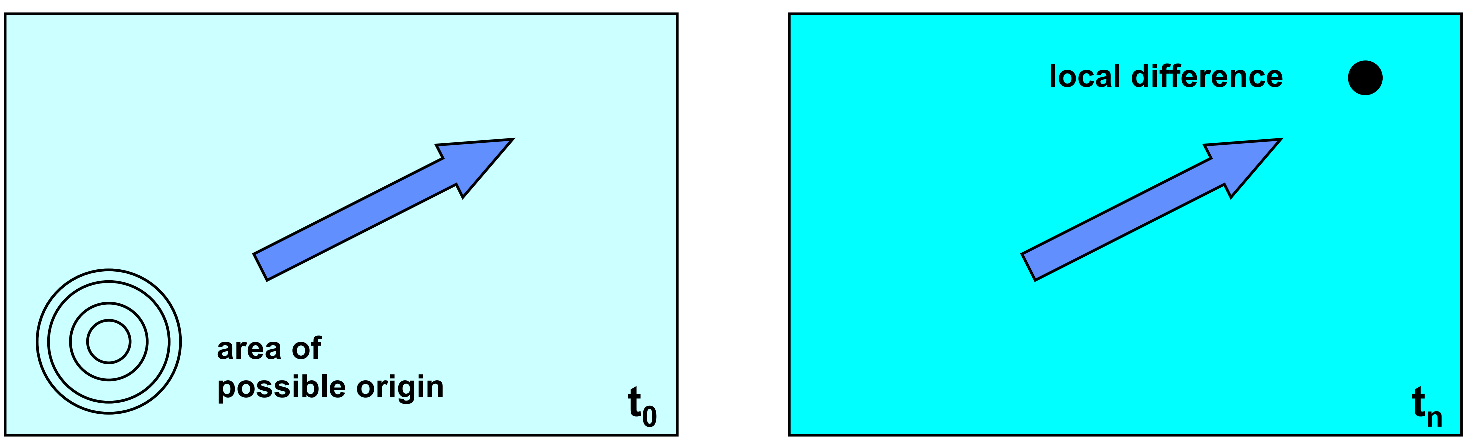
- If the dimension of *x* is large, this can be very expensive

Forward vs. Adjoint Sensitivity Analysis

Forward Model



Adjoint Model



Basic Idea and Derivation of the Adjoint Method

Given the nonlinear system $F(x, p) = 0$

with derived function $g(x, p)$

We wish to compute $\frac{dg}{dp}$

We have $\frac{dg}{dp} = g_x x_p + g_p$

Linearizing the original nonlinear system, $F_x x_p + F_p = 0$

The forward sensitivity method computes x_p **for each p. But this is too costly if p is large.**

To derive the adjoint method, first multiply by λ^T **to obtain**

$$\lambda^T F_x x_p + \lambda^T F_p = 0$$

Now let λ **solve** $\lambda^T F_x = g_x$

Then $\frac{dg}{dp} = -\lambda^T F_p + g_p$

DAE Sensitivity Analysis (Adjoint Method)

Given the DAE depending on parameters p,

$$F(t,x,x',p)=0, \qquad x(t_0)=x_0(p)$$

and a function

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

or a function at the end point (t=T): g(x,p,T)

Sensitivity analysis finds the change dG/dp or dg/dp of these functions with respect to perturbations in the parameters p. The function we choose depends on the application problem. Usually the dimension of G or g is much smaller than that of x or p.

DAE Adjoint Equations

For G, we solve

$$F_{\dot{x}}^T \dot{\lambda} - (F_x^T - \frac{dF_{\dot{x}}^T}{dt})\lambda = -g_x^T$$

$$(F_{\dot{x}}^T \lambda)\Big|_{t=T} = 0$$

The corresponding sensitivities are

$$\frac{dG}{dp} = \int_0^T g_p dt - \int_0^T \lambda^T F_p dt + (\lambda^T F_{\dot{x}})\Big|_{t=0} \frac{dx_0}{dp}$$

For g, we solve

$$F_{\dot{x}}^T \dot{\xi} - (F_x^T - \frac{dF_{\dot{x}}^T}{dt})\xi = 0$$

$$(F_{\dot{x}}^T \xi)\Big|_{t=T} = (\frac{dF_{\dot{x}}^T}{dt}\lambda - F_{\dot{x}}^T \dot{\lambda})\Big|_{t=T}$$

Here we need to get the boundary condition from the end point of $\dot{\lambda}(T)$ but we need not solve for $\lambda(t)$. The corresponding sensitivities are

$$\frac{dg}{dp} = g_p - (\xi^T F_p)\Big|_{t=T} - \int_0^T \xi^T F_p dt + (\xi^T F_{\dot{x}})\Big|_{t=0} \frac{dx_0}{dp}$$

Properties of the DAE Adjoint System - Stability

If the original system is stable, will the adjoint system also be stable? Consider

$$e^t \dot{x} + \frac{1}{2} e^t x = 0$$

This system is equivalent to the stable system

$$\dot{x} + \frac{1}{2} x = 0$$

The adjoint system is

$$e^t \dot{\lambda} - \frac{1}{2} e^t \lambda + e^t \lambda = 0$$

Which is equivalent to the unstable (backwards) system

$$\dot{\lambda} + \frac{1}{2} \lambda = 0$$

Properties of the DAE Adjoint System - Stability

Original DAE system

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

Augmented adjoint system

$$\dot{\bar{\lambda}} - F_x^* \lambda = -g_x^*$$

$$\bar{\lambda} - F_{\dot{x}}^* \lambda = 0$$

If the original DAE system is stable then

- **The adjoint DAE system is stable (ODE, index-1 DAE, index-2 Hessenberg DAE and combinations)**
- **The adjoint DAE system may not be stable, however the augmented adjoint system is stable (fully-implicit index 0 and index 1 DAE)**

Numerical Stability

If a numerical method with a given stepsize is stable for the original DAE system, will it also be stable for the adjoint system?

If the original DAE system is numerically stable then

- **The adjoint DAE system is numerically stable (ODE, semi-explicit index-1 DAE, index-2 Hessenberg DAE and combinations)**
- **The adjoint DAE system may not be numerically stable, however the augmented adjoint DAE system is numerically stable (fully-implicit ODE and DAE)**

DAE Adjoint Sensitivity Software

DASPKADJOINT (Li and Petzold, 2001)

Adjoints, adjoints everywhere

- Time-dependent PDE systems with adaptive mesh refinement (ADDA method), to appear soon on website
- Conditioning and error estimation, subspace error estimate for linear systems, www.engineering.ucsb.edu/~cse
- Conditioning and error estimation for matrix equations – Sylvester, Lyapunov, Algebraic Riccati (in progress)
- Error estimates for reduced/simplified models (in progress)