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Adjoint-based constant-mass partial derivatives

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ABSTRACT

In transport theory, adjoint-based partial derivatives with respect to mass density are constant-volume derivatives. Likewise, adjoint-based partial derivatives with respect to surface locations (i.e., internal interface locations and the outer system boundary) are constant-density derivatives. This paper derives the constant-mass partial derivative of a response with respect to an internal interface location or the outer system boundary and the constant-mass partial derivative of a response with respect to the mass density of a region. Numerical results are given for a multiregion two-dimensional (r-z) cylinder for three very different responses: the uncollided gamma-ray flux at an external detector point, k_{eff} of the system, and the total neutron leakage. Results from the derived formulas compare extremely well with direct perturbation calculations.

1. Introduction

It is well known that the adjoint equation in transport theory provides an economical means of computing derivatives of a system response to system parameters. It is also well known, though not often remarked on, that adjoint-based partial derivatives with respect to mass density (Greenspan, 1982; Favorite et al., 2017; Bledsoe et al., 2011) are *constant-volume* derivatives. Likewise, adjoint-based partial derivatives with respect to surface locations (Bledsoe et al., 2011; Favorite and Bledsoe, 2010; Favorite and Gonzalez, 2017) (i.e., internal interface locations and the outer system boundary) are *constant-density* derivatives.

In this paper, we derive a formula for the *constant-mass* partial derivative of a response with respect to an internal interface location or the outer system boundary. We also derive two formulas for the *constant-mass* partial derivative of a response with respect to the mass density of a region. These formulas use the constant-density partial derivatives with respect to surface locations and the constant-volume partial derivatives with respect to densities, which may be computed using adjoint methods or numerical differences. The only surface perturbations that we consider are those in which surfaces are translated along coordinate axes.

When relationships among thermodynamic properties are derived, people are careful to denote the quantity that is held constant in the partial differentiation (Black and Hartley, 1985; Bejan, 2016). This paper will adopt that specificity, and we recommend it for all work with sensitivities in nuclear engineering.

This paper includes numerical comparisons for a two-dimensional (r-z) cylinder that also demonstrate the correctness of the regular adjoint-based derivatives for surface locations. Three very different responses are considered: the uncollided gamma-ray flux at an external detector point, k_{eff} of the system, and the total neutron leakage. Adjoint-based partial derivatives for the neutron problems were computed using the new SENSMG code (Favorite, 2017) at Los Alamos National Laboratory.

Section 2 presents the derivations of the constant-mass partial derivatives. Section 3 presents results for numerical test problems. Section 4 is a summary.

2. Derivations

Consider a radiation transport problem with some response of interest R. We will be examining how R changes as the mass m, volume V, and/or mass density ρ of any of the materials in the system change. This treatment will ignore gasses and all temperature dependencies. The equation of state for the materials is simply

$$\rho = m/V. \tag{1}$$

The three equations for the total differential of R with respect to mass, volume, and mass density are

$$dR = \left(\frac{\partial R}{\partial m}\right)_V dm + \left(\frac{\partial R}{\partial V}\right)_m dV, \tag{2}$$

$$dR = \left(\frac{\partial R}{\partial \rho}\right)_V d\rho + \left(\frac{\partial R}{\partial V}\right)_\rho dV, \tag{3}$$

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and

$$dR = \left(\frac{\partial R}{\partial m}\right)_{\rho} dm + \left(\frac{\partial R}{\partial \rho}\right)_{m} d\rho, \tag{4}$$

where the subscripts on the partial derivatives indicate the quantities to be held constant. Holding a volume constant implies holding all of its bounding surfaces constant.

The derivations in this paper apply regardless of whether the transport problem is homogenous or inhomogeneous (i.e., an eigenvalue problem or a fixed-source problem). The derivations also apply to diffusion theory or any physical system in which a response depends on mass, volume, and density.

2.1. Constant-mass partial derivative with respect to interface location

In Eq. (2), we use

$$dm = \left(\frac{\partial m}{\partial \rho}\right)_{V} d\rho + \left(\frac{\partial m}{\partial V}\right)_{\rho} dV = V d\rho + \rho dV \tag{5}$$

and

$$\left(\frac{\partial R}{\partial m}\right)_{V} = \left(\frac{\partial R}{\partial \rho}\right)_{V}\left(\frac{\partial \rho}{\partial m}\right)_{V} = \frac{1}{V}\left(\frac{\partial R}{\partial \rho}\right)_{V}, \tag{6}$$

yielding

$$\begin{aligned} dR =& \frac{1}{V}\left(\frac{\partial R}{\partial \rho}\right)_{V}(V d\rho + \rho dV) + \left(\frac{\partial R}{\partial V}\right)_{m} dV \\ =& \left(\frac{\partial R}{\partial \rho}\right)_{V} d\rho + \frac{\rho}{V}\left(\frac{\partial R}{\partial \rho}\right)_{V} dV + \left(\frac{\partial R}{\partial V}\right)_{m} dV. \end{aligned} \tag{7}$$

Subtracting Eq. (7) from Eq. (3) yields

$$0 = \left(\frac{\partial R}{\partial V}\right)_{\rho} dV - \frac{\rho}{V}\left(\frac{\partial R}{\partial \rho}\right)_{V} dV - \left(\frac{\partial R}{\partial V}\right)_{m} dV. \tag{8}$$

Factoring out the dV, setting the sum of the rest to zero, and rearranging yields

$$\left(\frac{\partial R}{\partial V}\right)_{m} = -\frac{\rho}{V}\left(\frac{\partial R}{\partial \rho}\right)_{V} + \left(\frac{\partial R}{\partial V}\right)_{\rho}. \tag{9}$$

Because the volume V is fully specified as a function of the linear dimensions, each linear dimension r can be written uniquely as a function of V and the other dimensions. Therefore, use the chain rule for each of the derivatives with respect to volume to yield

$$\left(\frac{\partial R}{\partial r}\right)_{m}\left(\frac{\partial r}{\partial V}\right) = -\frac{\rho}{V}\left(\frac{\partial R}{\partial \rho}\right)_{V} + \left(\frac{\partial R}{\partial r}\right)_{\rho}\left(\frac{\partial r}{\partial V}\right), \tag{10}$$

and divide through by $(\partial r/\partial V)$ to yield

$$\left(\frac{\partial R}{\partial r}\right)_{m} = -\frac{\rho}{V}\left(\frac{\partial V}{\partial r}\right)\left(\frac{\partial R}{\partial \rho}\right)_{V} + \left(\frac{\partial R}{\partial r}\right)_{\rho}. \tag{11}$$

Now consider a particular internal interface, designated r_i, as shown in Fig. 1. On the negative side of interface r_i (left or below or "inside") is region 1 with volume, mass, and mass density V_1, m_1, and ρ_1, respectively. On the positive side of interface r_i (right or above or "outside") is region 2 with volume, mass, and mass density V_2, m_2, and ρ_2, respectively. The first term on the right side of Eq. (11) becomes the sum of terms for regions 1 and 2.

Generalizing this concept to all regions $j = 1,\ldots J$ that border surface i yields

$$\left(\frac{\partial R}{\partial r_i}\right)_{m} = -\sum_{j=1}^{J}\frac{\rho_j}{V_j}\left(\frac{\partial V_j}{\partial r_i}\right)_{r_k, k\neq i}\left(\frac{\partial R}{\partial \rho_j}\right)_{V} + \left(\frac{\partial R}{\partial r_i}\right)_{\rho}, \tag{12}$$

where subscripts V, m, and ρ without indices imply all volumes, masses, and densities. Also, subscript "r_k, $k \neq i$" means that all surfaces are held constant except r_i. All the derivatives with respect to r_i in Eq. (12) correspond to moving r_i in the positive coordinate direction. Let $\hat{\mathbf{n}}_j$ be the outward unit normal vector for surface i relative to volume j and $\hat{\mathbf{e}}_i$ be the positive coordinate direction in which $(\partial R/\partial r_i)_m$ and $(\partial V_j/\partial r_i)_{r_k,k\neq i}$ are calculated. If moving surface r_i in direction $\hat{\mathbf{e}}_i$ causes volume j to increase, then $\hat{\mathbf{e}}_i$ must be pointing outward. In this case $\hat{\mathbf{e}}_i \cdot \hat{\mathbf{n}}_j = 1$, and therefore

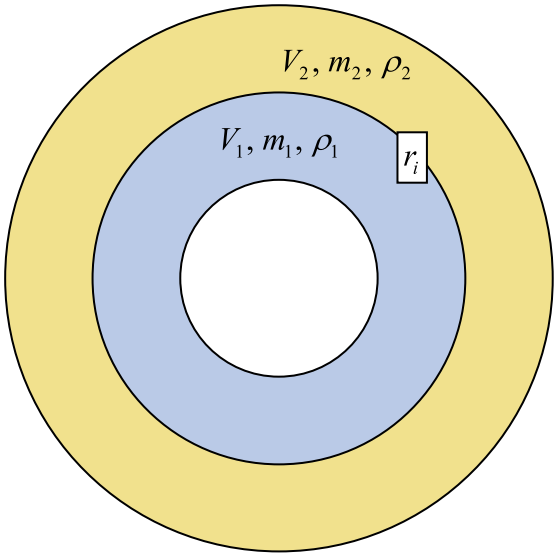

Fig. 1. Interface r_i and the regions on either side of it.

$$\left(\frac{\partial V_j}{\partial r_i}\right)_{r_k,k\neq i} = (A_j)\hat{\mathbf{e}}_i \cdot \hat{\mathbf{n}}_j, \tag{13}$$

where A_j is the area of surface r_i in contact with volume j. Likewise, if moving surface r_i in direction $\hat{\mathbf{e}}_i$ causes volume j to decrease, then $\hat{\mathbf{e}}_i$ must be pointing inward, $\hat{\mathbf{e}}_i \cdot \hat{\mathbf{n}}_j = -1$, and Eq. (13) is still satisfied. Using Eq. (13) in Eq. (12) yields

$$\left(\frac{\partial R}{\partial r_i}\right)_{m} = -\sum_{j=1}^{J}\frac{\rho_j A_j}{V_j}\left(\frac{\partial R}{\partial \rho_j}\right)_{V}\hat{\mathbf{e}}_i \cdot \hat{\mathbf{n}}_j + \left(\frac{\partial R}{\partial r_i}\right)_{\rho}. \tag{14}$$

Define the relative sensitivity of R to the mass density of region j as (Greenspan, 1982; Favorite et al., 2017)

$$S_{R,\rho_j} \equiv \frac{\rho_j}{R}\left(\frac{\partial R}{\partial \rho_j}\right)_{V}. \tag{15}$$

(Typically, the relative sensitivity is defined with a partial derivative that is merely assumed to be the constant-volume partial derivative. Here, we are explicit.) Using Eq. (15) in Eq. (14) yields

$$\left(\frac{\partial R}{\partial r_i}\right)_{m} = -R\sum_{j=1}^{J}\frac{A_j}{V_j}S_{R,\rho_j}\hat{\mathbf{e}}_i \cdot \hat{\mathbf{n}}_j + \left(\frac{\partial R}{\partial r_i}\right)_{\rho}. \tag{16}$$

The sensitivities to densities and the constant-density partial derivative with respect to the surface location [on the right side of Eq. (16)] can all be computed with adjoint-based methods.

If r_i is the outer boundary, then there is no term in Eq. (16) for a region outside of r_i.

Eq. (16) represents the change in R as r_i moves in the positive coordinate direction with respect to the coordinate system. Eq. (16) preserves the masses of all regions adjacent to r_i (and therefore all masses in the system).