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Increasing our understanding of the adjoint state method of model sensitivity calculation

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Abstract: The calculation of sensitivities is fundamental to model calibration, sensitivity analysis, and uncertainty quantification tasks, for which a Jacobian matrix is often required. The perturbation (i.e., finite difference) method of sensitivity calculation, in which the number of model runs required to populate a Jacobian matrix is dependent upon the number of parameters, is the most used approach. This approach is conceptually simple but can become computationally intensive when applied to numerical forward models featuring large numbers of parameters and long model run times. In this context, the adjoint state method provides an efficient alternative approach, in which the number of forward model runs required to populate a Jacobian matrix is instead dependent upon the number of constraining observations, or predictions of interest.

A literature review of over 60 published applications of adjoint sensitivities for saturated groundwater flow modelling yielded key insights for understanding the adjoint state method. Seminal applications of adjoint state sensitivities in nuclear engineering described the adjoint state variable as representing “importance”. However, this understanding was often not transferred when the method spread to other fields of science and engineering. In this way, the adjoint state variable can be understood as a means of weighting the contributions of forward model states at various locations and/or times to a specific metric (i.e., observation or prediction) of interest. In practice, forward model outputs (e.g., hydraulic heads, flow rates, or their derivatives) and adjoint model outputs (i.e., spatio-temporal distributions of the importance function) are combined through a convolution operation. For selected performance metrics, adjoint states can be viewed as impulse response functions, similar to those specified in Green’s function-based solutions, or those derived inversely from deconvolution analyses. For the calculation of cumulative-type performance metrics, the convolution of adjoint states with forward model outputs is extended over a given spatial and/or temporal interval, rather than being limited to a given location and/or time of interest.

The literature review also informed the development of three key outputs intended to increase our general understanding of the adjoint state method for calculating model sensitivities, as well as specific to groundwater flow modelling. First, a framework consisting of ten steps was developed, which provides a consistent approach when interpreting past derivations of adjoint sensitivities. Second, adjoint sensitivities of two complementary modelled states (i.e., hydraulic head and groundwater flux) to a set of commonly-used parameters were tabulated, which may be used as a reference resource. From these tabulated expressions, model parameters that do (or do not) inform a particular sensitivity of interest can also be identified. Third, simple interactive demonstration models were developed to provide clear examples of both the derivation and implementation of adjoint sensitivities, including the use of analytical solutions for benchmarking purposes, where possible.

In summary, the adjoint state method provides an efficient method of calculating the sensitivities of highly parameterised models. Applications are not restricted to simplistic forward models, as both spatially heterogeneous and non-stationary parameterisations can be accommodated. In addition, adjoint state sensitivities derived using the continuous approach can provide valuable insights into model state-parameter relationships, which can inform both data worth analyses and process understanding more generally.

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