A New Automatic Differentiation Mode for Sparse Hessian Matrices

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ABSTRACT

In the context of nonlinear programming, many algorithms boil down to the application of Newton’s method to the system constituted by the first order Lagrangian conditions, [1, 5]. The calculation of Hessian matrices is necessary in this class of solvers. Our focus is on the exact calculation, within machine precision, of Hessian matrices through automatic differentiation.

We present and demonstrate a closed formula for the Hessian matrix of a function expressed as generic composition of maps. We show how this formula can be useful in designing automatic differentiation algorithms for the computation of Hessian matrices. In order to illustrate, we deduce an existing algorithm and elaborate a new one. Implementation details are provided on how to take advantage of sparsity and symmetry.

As a by-product, we obtain a promising algorithm for automatically obtaining the sparsity pattern of Hessian matrices, a necessary step in a class of methods used for computing Hessian matrices via graph coloring, [2, 3].

Complexity analysis and computational tests are presented, comparing the new methods to existing software, [6, 4].

Key Words: automatic differentiation, sparse Hessians, sparsity pattern of symmetric matrices.

References


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