More AD of Nonlinear AMPL Models: Computing Hessian Information and Exploiting Partial Separability

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Abstract

We describe computational experience with automatic differentiation of mathematical programming problems expressed in the modeling language AMPL. Nonlinear expressions are translated to loop-free code, which makes it easy to compute gradients and Jacobians by backward automatic differentiation. The nonlinear expressions may be interpreted or, to gain some evaluation speed at the cost of increased preparation time, converted to Fortran or C. We have extended the interpretive scheme to evaluate Hessian (of Lagrangian) times vector, which unfortunately takes a bit longer than approximating Hessian times vector by the finite difference of gradients (computed by AD). Detecting partially separable structure (sums of terms, each depending, perhaps after a linear transformation, on only a few variables) is of independent interest, as some solvers exploit this structure. It can be detected automatically by suitable "tree walks". Exploiting this structure permits an AD computation of the entire Hessian matrix by accumulating Hessian times vector computations for each term, and can lead to a much faster computation of the Hessian than by computing the whole Hessian times each unit vector.