Enclosures of Higher Order Derivative Tensors on the Basis of Univariate Taylor Expansions

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This contribution considers the problem of evaluating all pure and mixed partial derivatives of some vector function

$$\boldsymbol{y} \;=\; \boldsymbol{f}(\boldsymbol{x}) \quad \text{with } \boldsymbol{f} : \mathcal{D} \subset \mathbb{R}^{\bar{n}} \mapsto \mathbb{R}^m,$$

defined by a computer program. In order to provide the required derivative information Automatic Differentiation (AD) can be applied.

Even though the reverse mode of AD may be more efficient when the number of dependent variables is small compared to the number of independents, only the forward mode will be considered here. The mechanics of this direct application of the chain rule are completely independent of the number m of dependent variables so that it is possible to restrict the analysis to a scalar-valued function

$$y \;=\; f(\boldsymbol{x}) \quad \text{with} \quad f : \mathcal{D} \subset \mathbb{R}^{\bar{n}} \mapsto \mathbb{R}.$$

This greatly simplifies the notation, and the full tensors can then easily be obtained by an outer loop over the component index.

The natural approach to evaluate derivative tensors seems to be their recursive calculation using the usual forward mode of AD. This technique has been implemented by Berz [1], Neidinger [3], and others. The only complication using this multi-variant approach is the need to utilize the symmetry in the higher derivative tensors, which leads to fairly complex addressing schemes.

Much simpler data access patterns and similar or lower computational counts can be achieved through propagating a family of univariate Taylor series of an arbitrary degree. At the end, their values are used to compute the desired tensor coefficients [2].

Using exact arithmetic, both approaches yield the same derivative information. Obviously, the situation changes if the computations are performed in floating point or interval arithmetic. We analyze the effects of using interval arithmetic for both methods to evaluate derivatives. Furthermore the quality of the enclosures achieved are compared and discussed.

References

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