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Adjoint-based computation of the exact Hessian-vector multiplication

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We consider a scalar function depending on the numerical solution of an initial value problem, and its Hessian matrix with respect to the initial data. In many research fields such as Bayesian estimation and uncertainty quantification, the need to extract the information of the Hessian or to solve a linear system having the Hessian as a coefficient matrix often arises. These tasks often employ a Krylov subspace method such as the CG method that does not need to have all elements of the Hessian explicitly and only requires computing the multiplication of the Hessian and a given vector.

A simple approach to obtaining an approximation of such Hessian-vector multiplication is to integrate the so-called second-order adjoint (SOA) system numerically. However, the accuracy of the approximation could be limited even if the numerical integration of the SOA system is accurate enough. In this talk, we present a novel algorithm that computes the Hessian-vector multiplication *exactly* (the computed Hessian coincides with the exact one up to round-off in floating-point arithmetic). For this aim, we give a new concise derivation of the SOA system and show that the intended multiplication can be obtained by applying a particular numerical method to the SOA system. We note that the concept of canonical (partitioned) Runge–Kutta methods play an essential role in the discussion.

The discussion can be seen as an extension of the recipe presented in [2], where the computation of the gradient of a function is considered. Further details of the talk can be found in our recent preprint [1].

References

[1] S. Ito, T. Matsuda and Y. Miyatake: Adjoint-based exact Hessian computation, arXiv:1910.06524v3, 2020.

[2] J. M. Sanz-Serna: Symplectic Runge–Kutta schemes for adjoint equations, automatic differentiation, optimal control, and more, SIAM Rev., **58** (2016), 3–33.