Searching Stationary Points of an N-dimensional Surface by a Valley Following Method A Robust Method

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A procedure is proposed [1] to follow the "minimum path" of a hypersurface. The method uses a projector technique where the projector is built by the tangent of the minimum path. The projector is applied to gradient and Hessian matrix of the given function, and it is used for predictor and corrector of a curve following. The resulting pathway is that valley floor gradient extremal which belongs to the smallest (absolute) eigenvalue of the Hessian matrix [2]. The new method avoids third derivatives. The motivation for the given procedure is that of taking into account local nonconvexity of the hypersurface.
The effectiveness of the algorithm is demonstrated by using polynomial test functions, especially the notorious Rosenbrock function, and the potentials of Lennard-Jones (LJ) clusters. Tracing the valley floor gradient extremals we locate saddle points for LJ_N with N= 3, 7, 8,15, 20, 30, and 55.

References

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