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Finding saddle points of mountain pass type with quadratic models on affine spaces

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The problem of computing saddle points is important in certain problems in numerical partial differential equations and computational chemistry, and is often solved numerically by a minimization problem over a set of mountain passes. We propose an algorithm to find saddle points of mountain pass type to find the bottlenecks of optimal mountain passes. The key step is to minimize the distance between level sets by using quadratic models on affine spaces similar to the strategy in the conjugate gradient algorithm. We discuss parameter choices, convergence results, and how to augment the algorithm to a path based method. Finally, we perform numerical experiments to test the convergence of our algorithm.

Comments: This paper has been withdrawn because the important ideas have been poorly developed here. A new submission has since subsumed the material in this paper. 20 pages, 4 figures

Subjects: Numerical Analysis (math.NA)

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