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Level set methods for finding critical points of mountain pass type

Adrian S. Lewis [a], C.H. Jeffrey Pang [b,*]

[a] School of Operations Research and Information Engineering, Cornell University, Ithaca, NY 14853, United States

[b] Massachusetts Institute of Technology, Department of Mathematics, 2-334, 77 Massachusetts Avenue, Cambridge MA 02139-4307, United States

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ABSTRACT

Computing mountain passes is a standard way of finding critical points. We describe a numerical method for finding critical points that is convergent in the nonsmooth case and locally superlinearly convergent in the smooth finite dimensional case. We apply these techniques to describe a strategy for addressing the Wilkinson problem of calculating the distance from a matrix to a closest matrix with repeated eigenvalues. Finally, we relate critical points of mountain pass type to nonsmooth and metric critical point theory.

1. Introduction

Computing mountain passes is an important problem in computational chemistry and in the study of nonlinear partial differential equations. We begin with the following definition.

Definition 1.1. Let X be a topological space, and consider $a, b \in X$. For a function $f : X \to \mathbb{R}$, define a *mountain pass* $p^* \in \Gamma(a, b)$ to be a minimizer of the problem

$$\inf_{p\in\Gamma(a,b)} \sup_{0\le t\le 1} f \circ p(t).$$

Here, $\Gamma(a, b)$ is the set of continuous paths $p : [0, 1] \to X$ such that $p(0) = a$ and $p(1) = b$.

An important aim in computational chemistry is to find the lowest amount of energy to transition between two stable states. If a and b represent two states and f maps the states to their potential energies, then the mountain pass problem calculates this lowest energy. Early work on computing transition states includes that of Sinclair and Fletcher [1], and recent work is reviewed by Henkelman et al. [2]. We refer the reader to this paper for further references in the computational chemistry literature.

Perhaps more importantly, the mountain pass idea is also a useful tool in the analysis of nonlinear partial differential equations. For a Banach space X, variational problems are problems (P) such that there exists a smooth functional $J : X \to \mathbb{R}$ whose critical points (points where $\nabla J = 0$) are solutions of (P). Many partial differential equations are variational problems, and critical points of J are "weak" solutions. In the landmark paper by Ambrosetti and Rabinowitz [3], the mountain pass theorem gives a sufficient condition for the existence of critical points in infinite dimensional spaces. If an optimal path for solving the mountain pass problem exists and the maximum along the path is greater than $\max(f(a), f(b))$, then the maximizer on the path is a critical point distinct from a and b. The mountain pass theorem and its variants provide the

* Corresponding author.
E-mail addresses: aslewis@orie.cornell.edu (A.S. Lewis), chj2pang@mit.edu, pangchj@yahoo.com (C.H.J. Pang).

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