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Level set methods for finding critical points of mountain pass type

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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

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

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

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primary ways to establish the existence of critical points and to find critical points numerically. For more on the mountain pass theorem and some of its generalizations, we refer the reader to [4].

In [5], Choi and McKenna proposed a numerical algorithm for the mountain pass problem by using an idea from [6] to solve a semilinear partial differential equation. This is extended to finding solutions of *Morse index* 2 (that is, the maximum dimension of the subspace of X on which J'' is negative definite) in [7], and then to finding ones of higher Morse index by Li and Zhou [8].

Li and Zhou [9], and Yao and Zhou [10] proved convergence results showing that their minimax method is sound for obtaining weak solutions to nonlinear partial differential equations. Moré and Munson [11] proposed an "elastic string method", and proved that the sequence of paths created by the elastic string method contains a limit point that is a critical point.

The prevailing methods for numerically solving the mountain pass problem are motivated by finding a sequence of paths (by discretization or otherwise) such that the maxima along these paths decrease to the optimal value. Indeed, many methods in [2] approximate a mountain pass in this manner. As far as we are aware, only [12,13] deviate from this strategy. We make use of a different approach by looking at the path connected components of the lower level sets of f instead.

One easily sees that l is a lower bound of the mountain pass problem if and only if a and b lie in two different path connected components of $\text{lev}_{\leq l} f$. A strategy for finding an optimal mountain pass is to start with a lower bound l and keep increasing l until the path connected components of $\text{lev}_{\leq l} f$ containing a and b respectively coalesce at some point. However, this strategy requires one to determine whether the points a and b lie in the same path connected component, which is not easy. We turn to finding saddle points of mountain pass type, as defined below.

Definition 1.2. For a function $f : X \to \mathbb{R}$, a *saddle point of mountain pass type* $\bar{x} \in X$ is a point such that there exists an open set U such that $\bar{x}$ lies in the closure of two path components of $(\text{lev}_{<f(\bar{x})} f) \cap U$.

We shall refer to saddle points of mountain pass type simply as saddle points. As an example, for the function $f : \mathbb{R}^2 \to \mathbb{R}$ defined by $f(x) = x_1^2 - x_2^2$, the point $\mathbf{0}$ is a saddle point of mountain pass type: we can choose $U = \mathbb{R}^2, a = (0, 1), b = (0, -1)$. When f is $\mathcal{C}^1$, it is clear that saddle points are critical points. As we shall see later (in Propositions 6.1 and 6.2), saddle points of mountain pass type can, under reasonable conditions, be characterized as maximal points on mountain passes, acting as "bottlenecks" between two components. In fact, if f is $\mathcal{C}^2$, the Hessians are nonsingular and several mild assumptions hold, these bottlenecks are exactly critical points of Morse index 1. We refer the reader to the lecture notes of Ambrosetti [14]. Some of the methods in [2] actually find saddle points instead of solving the mountain pass problem.

We propose numerical methods for finding saddle points using the strategy suggested in Definition 1.2. We start with a lower bound l and keep increasing l until the components of the level set $\text{lev}_{\leq l} f \cap U$ containing a and b coalesce, reaching the objective of the mountain pass problem. The first method that we propose in Algorithm 2.1 is purely metric in nature. One appealing property of this method is that calculations are now localized near the critical point and we keep track of only two points instead of an entire path. Our algorithm enjoys a monotonicity property: the distance between two components decreases monotonically as the algorithm progresses, giving an indication of how close we are to the saddle point. In a practical implementation, local optimality properties in terms of the gradients (or generalized gradients) can be helpful for finding saddle points. Such optimality conditions are covered in Section 9.

It follows from the definitions that our algorithm, if it converges, converges to a saddle point. We then prove that any saddle point is deformationally critical in the sense of metric critical point theory [15–17], and is Morse critical under additional conditions. This implies in particular that any saddle point is Clarke critical in the sense of nonsmooth critical point theory [18,19] based on nonsmooth analysis in the spirit of [20–23]. It seems that there are few existing numerical methods for finding either critical points in a metric space or nonsmooth critical points. Currently, we are only aware of [24].

One of the main contributions of this paper is to give a second method (in Section 3) which converges locally superlinearly to a nondegenerate smooth critical point, i.e., critical points where the Hessian is nonsingular, in $\mathbb{R}^n$. A potentially difficult step in this second method is that where we have to find the closest point between two components of the level sets. While the effort needed to perform this step accurately may be great, the purpose of this step is to make sure that the problem is well aligned after this step. Moreover, this step need not be performed to optimality. In our numerical example in Section 8, we were able to obtain favorable results without performing this step.

Our initial interest in the mountain pass problem came from computing the 2-norm distance of a matrix A to the closest matrix with repeated eigenvalues. This is also known as the Wilkinson problem, and this value is the smallest 2-norm perturbation that will make the eigenvalues of matrix A behave in a non-Lipschitz manner. Alam and Bora [25] showed how the Wilkinson problem can be reduced to a global mountain pass problem. We do not solve the global mountain pass problem associated with the Wilkinson problem, but we demonstrate that locally our algorithm converges quickly to a smooth critical point of mountain pass type.

Outline: Section 2 illustrates a local algorithm for finding saddle points of mountain pass type, while Sections 3–5 are devoted to the statement, proof of convergence, and additional observations of a fast local algorithm for finding nondegenerate critical points of Morse index 1 in $\mathbb{R}^n$.

Section 6 discusses the relationship between mountain passes, saddle points, and critical points in the sense of metric critical point theory and nonsmooth analysis, and does not depend on material in Sections 3–5.