NONMONOTONE LOCAL MINIMAX METHODS FOR FINDING MULTIPLE SADDLE POINTS[*]

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Abstract

In this paper, by designing a normalized nonmonotone search strategy with the Barzilai-Borwein-type step-size, a novel local minimax method (LMM), which is a globally convergent iterative method, is proposed and analyzed to find multiple (unstable) saddle points of nonconvex functionals in Hilbert spaces. Compared to traditional LMMs with monotone search strategies, this approach, which does not require strict decrease of the objective functional value at each iterative step, is observed to converge faster with less computations. Firstly, based on a normalized iterative scheme coupled with a local peak selection that pulls the iterative point back onto the solution submanifold, by generalizing the Zhang-Hager (ZH) search strategy in the optimization theory to the LMM framework, a kind of normalized ZH-type nonmonotone step-size search strategy is introduced, and then a novel nonmonotone LMM is constructed. Its feasibility and global convergence results are rigorously carried out under the relaxation of the monotonicity for the functional at the iterative sequences. Secondly, in order to speed up the convergence of the nonmonotone LMM, a globally convergent Barzilai-Borwein-type LMM (GBBLMM) is presented by explicitly constructing the Barzilai-Borwein-type step-size as a trial step-size of the normalized ZH-type nonmonotone step-size search strategy in each iteration. Finally, the GBBLMM algorithm is implemented to find multiple unstable solutions of two classes of semilinear elliptic boundary value problems with variational structures: one is the semilinear elliptic equations with the homogeneous Dirichlet boundary condition and another is the linear elliptic equations with semilinear Neumann boundary conditions. Extensive numerical results indicate that our approach is very effective and speeds up the LMMs significantly.

Mathematics subject classification: 65K10, 58E05, 49M37, 35J20.
Key words: Multiple saddle points, Local minimax method, Barzilai-Borwein gradient method, Normalized nonmonotone search strategy, Global convergence.

1. Introduction

Let X be a Hilbert space. The critical points of a continuously Fréchet-differentiable functional $E : X \to \mathbb{R}$ are defined as solutions to the associated Euler-Lagrange equation

$$E'(u) = 0, \quad u \in X,$$

where E' is the Fréchet-derivative of E. The first candidates of critical points are local minima and maxima on which traditional calculus of variations and optimization methods focus. Critical points that are not local extrema are unstable and called saddle points. When the second-order Fréchet-derivative E'' exists at some critical point u_*, the instability of u_* can be depicted by its Morse index (MI) [5]. In fact, the MI of such a critical point u_*, denoted by $\mathrm{MI}(u_*)$, is defined as the maximal dimension of subspaces of X on which the linear operator $E''(u_*)$ is negative-definite. In addition, u_* is said to be nondegenerate if $E''(u_*)$ is invertible. For a nondegenerate critical point, if its MI $= 0$, it is a strict local minimizer and then a stable critical point, while if its MI > 0, it is a saddle point and then an unstable critical point. Generally speaking, the higher the MI is, the more unstable the critical point is.

Saddle points, as unstable equilibria or transient excited states, are widely found in numerous nonlinear problems in physics, chemistry, biology and materials science [5,9,21,25,33,41,50]. They play an important role in many interesting applications, such as studying rare transitions between different stable/metastable states [10,14] and predicting morphologies of critical nucleus in the solid-state phase transformation [48,50], etc. Due to various difficulties in direct experimental observation, more and more attentions have been paid to develop effective and reliable numerical methods for catching saddle points. Compared with the computation of stable critical points, it is much more challenging to design a stable, efficient and globally convergent numerical method for finding saddle points due to the instability and multiplicity. In recent years, motivated by some early algorithms for searching for saddle points in computational physics, chemistry, biology, the dimer method [20,47], the gentlest ascent dynamics [15], the climbing string method [14,35] etc., have been proposed and successfully implemented to find saddle points. It is noted that methods mentioned above mainly consider saddle points with MI=1.

With the development of science and technology, the stable numerical computation of multiple unstable critical points with high MI has attracted more and more attentions both in theories and applications. Studies of relevant numerical methods have been carried out in the literature. Inspired by the minimax theorems in the critical point theory (see, e.g., [33]) and the work of Choi and McKenna [11], Ding *et al.* [13] and Chen *et al.* [9], a local minimax method (LMM) was developed by Li and Zhou [26,27] with its global convergence established in [27,52]. As shown in [51], for a nondegenerate critical point found by the LMM, its MI is determined a priori by the dimension of the given support space L (see the detail in Section 2.1) as MI $= \dim(L) + 1$. Therefore, the LMM is capable of selectively finding the saddle points with any given MI $= n \geq 1$ by appropriately constructing the support space L with $\dim(L) = n - 1$. Then, Xie *et al.* [41] modified the LMM with a significant relaxation for the domain of the local peak selection, which is a vital definition for the LMM (see below), and provided the global convergence analysis for this modified LMM by overcoming the lack of homeomorphism of the local peak selection. More modifications and developments of the LMM for multiple solutions of various problems, such as elliptic partial differential equations (PDEs) with nonlinear boundary conditions, quasi-linear elliptic PDEs in Banach spaces, upper semi-differentiable locally Lipschitz continuous functional and so on, have been also studied. We