LEVEL SET METHODS FOR FINDING SADDLE POINTS OF GENERAL MORSE INDEX

C.H. JEFFREY PANG

Abstract. For a function $f : X \to \mathbb{R}$, a point is critical if its derivatives are zero, and a critical point is a saddle point if it is not a local extrema. In this paper, we study algorithms to find saddle points of general Morse index. Our approach is motivated by the multidimensional mountain pass theorem, and extends our earlier work on methods (based on studying the level sets of $f$) to find saddle points of mountain pass type. We prove the convergence of our algorithms in the nonsmooth case, and the local superlinear convergence of another algorithm in the smooth finite dimensional case.

Contents

1. Introduction 1
   Notation 3
2. Algorithm for critical points 3
3. Convergence properties 5
4. Optimality conditions 6
5. Another convergence property of critical points 12
6. Fast local convergence 15
7. Proof of superlinear convergence of local algorithm 20
8. Conclusion and conjectures 30
References 31

1. Introduction

For a function $f : X \to \mathbb{R}$, we say that $x$ is a critical point if $\nabla f(x) = 0$, and $y$ is a critical value if there is some critical point $x$ such that $f(x) = y$. A critical point $x$ is a saddle point if it is neither a local minimizer nor a local maximizer. In this paper, we present algorithms based on the multidimensional mountain pass theorem to find saddle points numerically.

The main purpose of critical point theory is the study of variational problems. These are problems (P) such that there exists a smooth functional $\Phi : X \to \mathbb{R}$ whose critical points are solutions of (P). Variational problems occur frequently in the study of partial differential equations.

Date: January 6, 2010.
2000 Mathematics Subject Classification. 35B38, 58E05, 58E30, 65N12.
Key words and phrases. multidimensional mountain pass, nonsmooth critical points, superlinear convergence, metric critical point theory.
At this point, we make a remark about saddle points in the study of min-max problems. Such saddle points occur in problems in game theory and in constrained optimization using the Lagrangian, and have the splitting structure

$$\min_{x \in X} \max_{y \in Y} f(x, y).$$

In min-max problems, this splitting structure is exploited in numerical procedures. See [15] for a survey of algorithms for min-max problems. In the general case, for example in finding weak solutions of partial differential equations, such a splitting structure may only be obtained after the saddle point is located, and thus is not helpful for finding the saddle point.

A critical point \(x\) is nondegenerate if its Hessian \(\nabla^2 f(x)\) is nonsingular and it is degenerate otherwise. The Morse index of a critical point is the maximal dimension of a subspace of \(X\) on which the Hessian \(\nabla^2 f(x)\) is negative definite. In the finite dimensional case, the Morse index is the number of negative eigenvalues of the Hessian.

Local maximizers and minimizers of \(f: X \to \mathbb{R}\) are easily found using optimization, while saddle points are harder to find. To find saddle points of Morse index 1, one can use algorithms motivated by the mountain pass theorem. Given points \(a, b \in X\), define a mountain pass \(p^* \in \Gamma(a, b)\) to be a minimizer of the problem

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

if it exists. Here, \(\Gamma(a, b)\) is the set of continuous paths \(p: [0, 1] \to X\) such that \(p(0) = a\) and \(p(1) = b\). Ambrosetti and Rabinowitz’s [4] mountain pass theorem states that under added conditions, there is a critical value of at least \(\max\{f(a), f(b)\}\). To find saddle points of higher Morse index, it is instructive to look at theorems establishing the existence of critical points of Morse index higher than 1. Rabinowitz [14] proved the multidimensional mountain pass theorem which in turn motivated the study of linking methods to find saddle points. We shall recall theoretical material relevant for finding saddle points of higher Morse index in this paper as needed.

While the study of numerical methods for the mountain pass problem began in the 70’s or earlier to study problems in computational chemistry, Choi and McKenna [4] were the first to propose a numerical method for the mountain pass problem to solve variational problems. Most numerical methods for finding critical points of mountain pass type rely on discretizing paths in \(\Gamma(a, b)\) and perturbing paths to lower the maximum value of \(f\) on the path. There are a few other methods of finding saddle points of mountain pass type that do not involve perturbing paths, for example [9, 2].

Saddle points of higher Morse index are obtained with modifications of the mountain pass algorithm. Ding, Costa and Chen [6] proposed a numerical method for finding critical points of Morse index 2, and Li and Zhou [13] proposed a method for finding critical points of higher Morse index.

In [12], we suggested a numerical method for finding saddle points of mountain pass type. The key observation is that the value

$$\sup \{ l \geq \max\{f(a), f(b)\} \mid a, b \text{ lie in different path components of } \{x \mid f(x) \leq l\}\}$$

is a critical value. In other words, the supremum of all levels \(l\) such that there is no path connecting \(a\) and \(b\) in the level set \(\{x \mid f(x) \leq l\}\) is a critical value. See Figure [1,1] for an illustration of the difference between the two approaches. An extensive
theoretical analysis and some numerical results of this approach were provided in [12].

In this paper, we extend three of the themes in the level set approach to find saddle points of higher Morse index, namely the convergence of the basic algorithm (Sections 2 and 3), optimality condition of sub-problem (Section 4), and a fast locally convergent method in $\mathbb{R}^n$ (Sections 6 and 7). Section 5 presents an alternative result on convergence to a critical point similar to that of Section 3.

We refer the reader to [12] for examples reflecting the limitations of the level set approach for finding saddle points of mountain pass type, which will be relevant for the design of level set methods of finding saddle points of general Morse index.

![Figure 1.1. The diagram on the left shows the classical method of perturbing paths for the mountain pass problem, while the diagram on the right shows convergence to the critical point by looking at level sets.](image)

**Notation**

$\text{lev}_{\geq b} f$: This is the level set $\{x \mid f(x) \geq b\}$, where $f : X \rightarrow \mathbb{R}$. The interpretations of $\text{lev}_{\leq b} f$ and $\text{lev}_{= b} f$ are similar.

$\mathbb{B}$: The ball of center $0$ and radius 1. $\mathbb{B}(x, r)$ stands for a ball of center $x$ and radius $r$. $\mathbb{B}^n$ denotes the $n$-dimensional sphere in $\mathbb{R}^n$.

$\mathbb{S}^n$: The $n$-dimensional sphere in $\mathbb{R}^{n+1}$.

$\partial$: Subdifferential of a real-valued function, or the relative boundary of a set.

If $h : \mathbb{B}^n \rightarrow S$ is a homeomorphism between $\mathbb{B}^n$ and $S$, then the relative boundary of $S$ is $h(S^{n-1})$.

$\text{lin}(A)$: For an affine space $A$, the lineality space $\text{lin}(A)$ is the space $\{a - a' \mid a, a' \in A\}$.

2. Algorithm for critical points

We look at the critical point existence theorems to give an insight on our algorithm for finding critical points of higher Morse index below. Here is the definition of linking sets. We take our definition from [17, Section II.8].

**Definition 2.1.** (Linking) Let $A$ be a subset of $\mathbb{R}^n$, $B$ a submanifold of $\mathbb{R}^n$ with relative boundary $\partial B$. Then we say that $A$ and $\partial B$ link if

(a) $A \cap \partial B = \emptyset$, and

(b) for any continuous $h : \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that $h \mid_{\partial B} = \text{id}$ we have $h(B) \cap A \neq \emptyset$. 
Figure 2.1 illustrates two examples of linking subsets in $\mathbb{R}^3$. In the diagram on the left, the set $A$ is the union of two points inside and outside the sphere $B$. In the diagram on the right, the sets $A$ and $B$ are the interlocking 'rings'. Note however that $A$ and $B$ link does not imply that $B$ and $A$ link, though this will be true with additional conditions. We hope this does not cause confusion.

We now recall the Palais-Smale condition.

**Definition 2.2.** (Palais-Smale condition) Let $X$ be a Banach space and $f : X \rightarrow \mathbb{R}$ be $C^1$. We say that a sequence $\{x_i\}_{i=1}^\infty \subset X$ is a Palais-Smale sequence if $\{f(x_i)\}_{i=1}^\infty$ is bounded and $\nabla f(x_i) \rightarrow 0$, and $f$ satisfies the Palais-Smale condition if any Palais-Smale sequence admits a convergent subsequence.

The classical multidimensional pass theorem originally due to Rabinowitz [14] states that under added conditions, if there are linking sets $A$ and $B$ such that $\max A f < \min B f$ and the Palais-Smale condition holds, then there is a critical value of at least $\max A f$ for the case when $f$ is smooth. (See Theorem 6.1 for a statement of the multidimensional mountain pass theorem) Generalizations in the nonsmooth case are also well-known in the literature. See for example [8].

To find saddle points of Morse index $m$, we consider finding a sequence of linking sets $\{A_i\}_{i=1}^\infty$ and $\{B_i\}_{i=1}^\infty$ such that $\text{diam}(A_i)$, the diameter of the set $A_i$, decreases to zero, and the set $A_i$ is a subset of an $m$-dimensional affine space. This motivates the following algorithm.

**Algorithm 2.3.** First algorithm for finding saddle points of Morse index $m \geq 1$.

1. Set the iteration count $i$ to 0, and let $l_i$ be a lower bound of the critical value and $u_i$ be an upper bound.
2. Find $x_i$ and $y_i$, where $(S_i, x_i, y_i)$ is an optimizing triple of

\[
\min_{S \in S_i} \max_{x, y \in S \cap \{\text{lev} \geq \frac{1}{2}(l_i + u_i)\}} |x - y|,
\]

where $U_i$ is some open set. Here, $S$ is the set of $m$-dimensional affine subspaces of $\mathbb{R}^n$ intersecting $U_i$. In the inner maximum problem above, we take the value to be 0 if $S \cap \{\text{lev} \leq \frac{1}{2}(l_i + u_i)\} \cap U_i$ is empty, making the objective function above equal to 0. For simplicity, we shall just assume that minimizers and maximizers of the above problem exist.

3. (Bisection) If the objective of (2.1) is zero, then $\frac{1}{2}(l_i + u_i)$ is a lower bound of the critical value. Set $l_{i+1} = \frac{1}{2}(l_i + u_i)$ and $u_{i+1} = u_i$. Otherwise, set $l_{i+1} = l_i$ and $u_{i+1} = \frac{1}{2}(l_i + u_i)$.
4. Increase $i$ and go back to step 2.
The critical step of Algorithm 2.3 lies in step 2. We elaborate on optimal conditions that will be a useful approximate for this step in Section 4. One may think of the set $A_i$ as the relative boundary (to the affine space $S_i$) of $S_i \cap (\text{lev} \geq l_i) \cap U_i$. A frequent assumption we will make is nondegeneracy.

**Definition 2.4.** We say that a critical point is **nondegenerate** if its Hessian is invertible.

Algorithm 2.3 requires $m > 0$, but when $m = 0$, nondegenerate critical points of Morse index zero are just strict local minimizers that can be easily found by optimization. We illustrate two special cases of Algorithm 2.3.

**Example 2.5.** (Particular cases of Algorithm 2.3) (a) For the case $m = 1$, $S$ is the set of lines. The inner maximization problem in (2.1) has its solution on the two endpoints of $S_i \cap (\text{lev} \geq \frac{1}{2}(l_i + u_i)) \cap U_i$. This means that (2.1) is equivalent to finding the local closest points between two components of $(\text{lev} \leq \frac{1}{2}(l_i + u_i)) \cap U_i$, as was analyzed in [12].

(b) For the case $m = n$, $S$ contains the whole of $\mathbb{R}^n$. Hence the outer minimization problem in (2.1) is superfluous. The level set $(\text{lev} \geq \frac{1}{2}(l_i + u_i)) \cap U_i$ gets smaller and smaller as $\frac{1}{2}(l_i + u_i)$ approaches the maximum value, till it becomes a single point if the maximizer is unique.

### 3. Convergence properties

In this section, we prove the convergence of $x_i, y_i$ in Algorithm 2.3 to a critical point when they converge to a common limit. We recall some facts about nonsmooth analysis needed for the rest of the paper. It is more economical to prove our result for nonsmooth critical points because the proofs are not that much harder, and nonsmooth critical points are also of interest in applications.

Let $X$ be a Banach space, and $f : X \to \mathbb{R}$ be a locally Lipschitz function at a given point $x$.

**Definition 3.1.** (Clarke subdifferential) [5, Section 2.1] Suppose $f : X \to \mathbb{R}$ is locally Lipschitz at $x$. The **Clarke generalized directional derivative** of $f$ at $x$ in the direction $v \in X$ is defined by

$$f^\circ(x; v) = \limsup_{t \searrow 0, y \to x} \frac{f(y + tv) - f(y)}{t},$$

where $y \in X$ and $t$ is a positive scalar. The **Clarke subdifferential** of $f$ at $x$, denoted by $\partial_C f(x)$, is the subset of the dual space $X^*$ given by

$$\{ \zeta \in X^* \mid f^\circ(x; v) \geq \langle \zeta, v \rangle \text{ for all } v \in X \}.$$

The point $x$ is a **Clarke (nonsmooth) critical point** if $0 \in \partial_C f(x)$. Here, $\langle \cdot, \cdot \rangle : X^* \times X \to \mathbb{R}$ defined by $\langle \zeta, v \rangle := \zeta(v)$ is the dual relation.

For the particular case of $C^1$ functions, $\partial_C f(x) = \{ \nabla f(x) \}$. Therefore critical points of smooth functions are also nonsmooth critical points. From the definitions above, it is clear that an equivalent definition of a nonsmooth critical point is $f^\circ(x; v) \geq 0$ for all $v \in X$. This property allows us to prove that a point is nonsmooth critical without appealing to the dual space $X^*$.

We now prove our result of convergence to nonsmooth critical points.
Proposition 3.2. (Convergence to saddle point) Let \( \tilde{z} \in X \). Suppose there is a ball \( \mathbb{B}(\tilde{z}, r) \), a sequence of triples \( \{(S_i, x_i, y_i)\}_{i=1}^\infty \) and a sequence \( l_i \) monotonically increasing to \( f(\tilde{z}) \) such that \( (x_i, y_i) \to (\tilde{z}, \tilde{z}) \) and \( (S_i, x_i, y_i) \) is an optimizing triple of (2.1) in Algorithm 2.3 for \( l_i \) with \( U_i = \mathbb{B}(\tilde{z}, r) \). Then \( \tilde{z} \) is a Clarke critical point.

Proof. Seeking a contradiction, suppose there exists some direction \( \bar{v} \) such that \( f^\circ(\tilde{z}; \bar{v}) < 0 \). This means that there is some \( \bar{\varepsilon} > 0 \) such that if \( |z - \tilde{z}| < \bar{\varepsilon} \) and \( \varepsilon < \bar{\varepsilon} \), then

\[
\frac{f(z + \varepsilon \bar{v}) - f(z)}{\varepsilon} < \frac{1}{2} f^\circ(\tilde{z}; \bar{v})
\]

\( \Rightarrow f(z + \varepsilon \bar{v}) < f(z) + \frac{1}{2} f^\circ(\tilde{z}; \bar{v}) \).

Suppose \( i \) is large enough so that \( x_i, y_i \in \mathbb{B}(\tilde{z}, \tilde{\varepsilon}) \), and that \( x_i, y_i \in A_i := S_i \cap (\text{lev}_{\geq l_i} f) \cap \mathbb{B}(\tilde{z}, r) \) are such that \( |x_i - y_i| = \text{diam}(A_i) \). Consider the set \( \hat{A} := (S_i + \varepsilon_1 \bar{v}) \cap (\text{lev}_{\geq l_i} f) \cap \mathbb{B}(\tilde{z}, r) \), where \( \varepsilon_1 > 0 \) is arbitrarily small. Let \( \hat{x}_i, \hat{y}_i \in \hat{A} \) be such that \( |\hat{x}_i - \hat{y}_i| = \text{diam}(\hat{A}) \). From the minimality of the outer minimization, we have \( |\hat{x}_i - \hat{y}_i| \geq |x_i - y_i| \). Note that \( f(\hat{x}_i) = f(\hat{y}_i) = l_i \). Then

\[
f(\hat{x}_i) < f(\hat{x}_i - \varepsilon_1 \bar{v}) + \varepsilon_1 \frac{1}{2} f^\circ(\tilde{z}; \bar{v})
\]

\( \Rightarrow f(\hat{x}_i - \varepsilon_1 \bar{v}) > f(\hat{x}_i) - \varepsilon_1 \frac{1}{2} f^\circ(\tilde{z}; \bar{v}) \)

\( > l_i \).

The continuity of \( f \) implies that we can find some \( \varepsilon_2 > 0 \) such that \( \tilde{x}_i := \hat{x}_i - \varepsilon_1 \bar{v} + \varepsilon_2(\tilde{x}_i - \tilde{y}_i) \) lies in \( A_i \). Similarly, \( \tilde{y}_i := \hat{y}_i - \varepsilon_1 \bar{v} \) lie in \( A_i \) as well. But

\[
|\tilde{x}_i - \tilde{y}_i| > |\hat{x}_i - \hat{y}_i| \geq |x_i - y_i|.
\]

This contradicts the maximality of \( |x_i - y_i| \) in \( A_i \), and thus \( \tilde{z} \) must be a critical point. \( \square \)

4. Optimality conditions

We now reduce the min-max problem (2.1) to a condition on the gradients \( \nabla f(x_i) \) and \( \nabla f(y_i) \) that is easy to verify numerically. This condition will help in the numerical solution of (2.1). We use methods in sensitivity analysis of optimization problems (as is done in [3]) to study how varying the \( m \)-dimensional affine space \( S \) in an \((m+1)\)-dimensional subspace affects the optimal value in the inner maximization problem in (2.1). We conform as much as possible to the notation in [3] throughout this section.

Consider the following parametric optimization problem \( (P_u) \) in terms of \( u \in \mathbb{R} \) as an \( m+1 \) dimensional model in \( \mathbb{R}^{m+1} \) of the inner maximization problem in (2.1):

\[
(P_u): \quad v(u) := \min \quad F(x, y, u) := -|x - y|^2 \\
\text{s.t.} \quad G(x, y, u) \in K, \\
x, y \in \mathbb{R}^{m+1},
\]

(4.1)
where \( G : (\mathbb{R}^{m+1})^2 \times \mathbb{R} \to \mathbb{R}^4 \) and \( K \subset \mathbb{R}^4 \) are defined by

\[
G(x,y,u) := \begin{pmatrix} -f(x) + b \\ -f(y) + b \\ (0,0,\ldots,0,u,1)x \\ (0,0,\ldots,0,u,1)y \end{pmatrix}, \quad K := \mathbb{R}_-^2 \times \{0\}^2.
\]

The problem \((P_u)\) reflects the inner maximization problem of \((2.1)\). Due to the standard practice of writing optimization problems as minimization problems, \((4.1)\) is a minimization problem instead. We hope this does not cause confusion.

Let \( S(u) \) be the \( m \)-dimensional subspace orthogonal to \((0, \ldots, 0, u, 1)\). The first two components of \( G(x,y,u) \) model the constraints \( f(x) \geq b \) and \( f(y) \geq b \), while the last two components enforce \( x,y \in S(u) \). Denote an optimal solution to \((P_u)\) to be \((\tilde{x}(u), \tilde{y}(u))\), and let \((\tilde{x}, \tilde{y}) := (\tilde{x}(0), \tilde{y}(0))\). We make the following assumption throughout.

**Assumption 4.1. (Uniqueness of optimizers)** \((P_0)\) has a unique solution \( \tilde{x} = 0 \) and \( \tilde{y} = (0,\ldots,0,1,0) \) at \( u = 0 \).

We shall investigate how the set of minimizers of \((P_u)\) behaves with respect to \( u \) at 0.

The derivatives of \( F \) and \( G \) with respect to \( x \) and \( y \), denoted by \( D_{x,y}F \) and \( D_{x,y}G \), are

\[
D_{x,y}F(x,y,u) = 2 \begin{pmatrix} (y-x)^T \\ (x-y)^T \end{pmatrix}, \quad (4.2)
\]

and

\[
D_{x,y}G(x,y,u) = \begin{pmatrix} -\nabla f(x)^T \\ (0,0,\ldots,0,u,1) \\ -\nabla f(y)^T \\ (0,0,\ldots,0,u,1) \end{pmatrix},
\]

where the blank terms in \( D_{x,y}G(x,y,u) \) are all zero.

The Lagrangian is the function \( L : \mathbb{R}^{m+1} \times \mathbb{R}^{m+1} \times \mathbb{R}^4 \times \mathbb{R} \to \mathbb{R} \) defined by

\[
L(x,y,\lambda, u) := F(x,y,u) + \sum_{i=1}^4 \lambda_i G_i(x,y,u).
\]

We say that \( \lambda := (\lambda_1, \lambda_2, \lambda_3, \lambda_4) \), depending on \( u \), is a Lagrange multiplier if \( D_{x,y}L(x,y,\lambda, u) = 0 \) and \( \lambda \in N_K(G(x,y,u)) \), and the set of all Lagrange multipliers is denoted by \( \Lambda(x,y,u) \). Here, \( N_K(G(x,y,u)) \) stands for the normal cone defined by

\[
N_K(G(x,y,u)) := \{ v \in \mathbb{R}^4 \mid v^T[w - G(x,y,u)] \leq 0 \text{ for all } w \in K \}.
\]

We are interested in the set \( \Lambda(\tilde{x}, \tilde{y}, 0) \). It is clear that optimal solutions must satisfy \( G(\tilde{x}, \tilde{y}, 0) = 0 \), so \( \lambda \in N_K(0) = \mathbb{R}_+^2 \times \mathbb{R}^2 \).

The condition \( D_{x,y}L(\tilde{x}, \tilde{y}, \lambda, 0) = 0 \) reduces to

\[
D_{x,y} \left( F(x,y,u) + \sum_{i=1}^4 \lambda_i G_i(x,y,u) \right) \bigg|_{x=\tilde{x}, y=\tilde{y}} = 0
\]

\[
\Rightarrow 2 \begin{pmatrix} \tilde{y} - \tilde{x} \\ \tilde{x} - \tilde{y} \end{pmatrix} + \lambda_1 \begin{pmatrix} -\nabla f(\tilde{x}) \\ 0 \end{pmatrix} + \lambda_2 \begin{pmatrix} 0 \\ -\nabla f(\tilde{y}) \end{pmatrix} + \lambda_3 \begin{pmatrix} (0,0,\ldots,0,1)^T \\ 0 \end{pmatrix} + \lambda_4 \begin{pmatrix} 0 \\ (0,0,\ldots,0,1)^T \end{pmatrix} = 0.
\]
Here, \( G_i(\bar{x}, \bar{y}, 0) \) is the \( i \)th row of \( G(\bar{x}, \bar{y}, 0) \) for \( 1 \leq i \leq 4 \). This is exactly the KKT conditions, and can be rewritten as

\[
2(\bar{y} - \bar{x}) - \lambda_1 \nabla f(\bar{x}) + \lambda_3 (0, 0, \ldots, 0, 1)^T = 0,
\]

\[
2(\bar{x} - \bar{y}) - \lambda_2 \nabla f(\bar{y}) + \lambda_4 (0, 0, \ldots, 0, 1)^T = 0.
\]

(4.3)

From (4.3), it is clear that \( \lambda_1 \) and \( \lambda_2 \) cannot be zero, and so we have

\[
\nabla f(\bar{x})^T = \left( 0, 0, \ldots, 0, \frac{\lambda_3}{\lambda_1} \right),
\]

\[
\nabla f(\bar{y})^T = \left( 0, 0, \ldots, 0, -\frac{\lambda_4}{\lambda_2} \right).
\]

Recall that \( \lambda_1, \lambda_2 \geq 0 \), so this gives more information about \( \nabla f(\bar{x}) \) and \( \nabla f(\bar{y}) \).

We next discuss the optimality of the outer minimization problem of (2.1), which can be studied by perturbations in the parameter \( u \) of (4.1), but we first recall a result on the first order sensitivity of optimal solutions.

**Definition 4.2.** (Robinson’s constraint qualification) (from [3, Definition 2.86])

We say that Robinson’s constraint qualification holds at \((\bar{x}, \bar{y}) \in \mathbb{R}^{m+1} \times \mathbb{R}^{m+1}\) if the regularity condition

\[
0 \in \text{int} \left\{ G(\bar{x}, \bar{y}, 0) + \text{Range}(D_{x,y}G(\bar{x}, \bar{y}, 0)) - K \right\}
\]

is satisfied.

**Theorem 4.3.** (Parametric optimization) (from [3, Theorem 4.26])

For problem (4.1), let \((\bar{x}(u), \bar{y}(u))\) be as defined earlier. Suppose that

(i) Robinson’s constraint qualification holds at \((\bar{x}(0), \bar{y}(0))\), and

(ii) if \( u_n \to 0 \), then \( (P_{u_n}) \) possesses an optimal solution \((\bar{x}(u_n), \bar{y}(u_n))\) that has a limit point \((\bar{x}, \bar{y})\).

Then \( v(\cdot) \) is directionally differentiable at \( u = 0 \) and

\[
v'(0) = D_u L(x, y, \lambda, 0).
\]

We proceed to prove our result.

**Proposition 4.4.** (Optimality condition on \( \nabla f(\bar{y}) \))

Consider the setup so far in this section and suppose Assumption [4.4] holds. If \( \nabla f(\bar{y}) \) is not a positive multiple of \((0, 0, \ldots, 0, 1, 0)^T\) at \( u = 0 \), then we can perturb \( u \) so that (4.1) has an increase in objective.

**Proof.** We first obtain first order sensitivity information from Theorem 4.3. Recall that by definition, Robinson’s constraint qualification holds at \((\bar{x}, \bar{y})\) if

\[
0 \in \text{int} \left\{ G(\bar{x}, \bar{y}, 0) + \text{Range}(D_{x,y}G(\bar{x}, \bar{y}, 0)) - K \right\}.
\]

From (4.3), it is clear that \( \nabla f(\bar{x}) \) and \((0, 0, \ldots, 0, 1, 0)^T\) are linearly independent, and so are \( \nabla f(\bar{y}) \) and \((0, \ldots, 0, 0, 1)^T\). From the formula of \( D_{x,y}G(\bar{x}, \bar{y}, 0) \) in (4.2), we see immediately that \( \text{Range}(D_{x,y}G(\bar{x}, \bar{y}, 0)) = \mathbb{R}^4 \), thus the Robinson’s constraint qualification indeed holds.

Suppose that \( \lim_{n \to \infty} t_n = 0 \). We prove that part (ii) of Theorem 4.3 holds by proving that \((\bar{x}(t_n), \bar{y}(t_n))\) cannot have any other limit points. Suppose that \((x', y')\) is a limit point of \( \{(\bar{x}(t_n), \bar{y}(t_n))\}_{n=1}^{\infty} \). It is clear that \( x', y' \in S(0) \).
We can find \( y_n \to \bar{y} \) such that \( y_n \in S(t_n) \) and \( f(y_n) = b \). For example, we can use the Implicit Function Theorem with the constraints
\[
\begin{align*}
  f(y) &= b, \\
g(y,u) &= 0,
\end{align*}
\]
where \( g(y,u) = (0,0,\ldots,0,u,1)^T y \). The derivatives with respect to \( y_m \) and \( y_{m+1} \) are
\[
\frac{\partial}{\partial y_m} f(\bar{y}) = -x_2, \quad \frac{\partial}{\partial y_{m+1}} f(\bar{y}) = \frac{\lambda_2}{2}, \quad \frac{\partial}{\partial y_m} g(\bar{y},0) = 0, \quad \frac{\partial}{\partial y_{m+1}} g(\bar{y},0) = 1.
\]
Therefore, for \( y_1 = y_2 = \cdots = y_{m-2} = y_{m-1} = 0 \) and any choice of \( u \) close to zero, there is some \( y_m \) and \( y_{m+1} \) such that \( y \in S(u) \) and \( f(y) = b \).

Clearly \( |\bar{x} - y_m| \leq |\bar{x}(t_n) - \bar{y}(t_n)| \). Taking limits as \( n \to \infty \), we have \( |\bar{x} - \bar{y}| \leq |x'-y'| \). Since \( (\bar{x}, \bar{y}) \) minimize \( F \), it follows that \( |\bar{x} - \bar{y}| = |x'-y'| \), and by the uniqueness of solutions to \( (P_0) \), we can assume that \( x' = \bar{x} \) and \( y' = \bar{y} \).

Theorem 4.3 implies that \( v'(0) = D_u L(x,y,\lambda,0) \). We now calculate \( D_u L(x,y,\lambda,0) \).

It is clear that \( D_u G(x,y,\lambda,0) = (0,0,0,1)^T \), and so \( D_u L(x,y,\lambda,0) = \lambda_4 \). Since \( \nabla f(\bar{y}) \) is not a multiple of \( (0,0,\ldots,0,1,0)^T \) at \( u = 0, \lambda_4 \neq 0 \), and this gives the conclusion we need.

A direct consequence of Proposition 4.4 is the following easily checkable condition.

**Theorem 4.5.** (Gradients are opposite) Let \( (S_i, x_i, y_i) \) be an optimizing triple to \( (2.1) \) for some \( l_i \), such that \( S_i \cap (\text{lev}_{\geq l_i} f) \cap U_i \) is closed, and \( (x_i, y_i) \) is the unique pair of points in \( S_i \cap (\text{lev}_{\geq l_i} f) \cap U_i \) satisfying \( |x_i - y_i| = \text{diam}(S_i \cap (\text{lev}_{\geq l_i} f) \cap U_i) \). Then \( \nabla f(x_i) \) and \( \nabla f(y_i) \) are nonzero and point in opposite directions.

**Proof.** We can look at an \( m+1 \) dimensional subspace which reduces to the setting that we are considering so far in this section. By Proposition 4.4 \( \nabla f(y_i) \) is a positive multiple of \( x_i - y_i \) at optimality. Similarly, \( \nabla f(x_i) \) is a positive multiple of \( y_i - x_i \) at optimality, and the result follows.

We remark on how to start the algorithm. We look at critical points of Morse index 1 first. In this case, two local minima \( \bar{x}_1, \bar{x}_2 \) are needed before the mountain pass algorithm can guarantee the existence of a critical point \( \bar{x}_3 \). For any value above the critical value corresponding to the critical point of Morse index 1, the level set contains a path connecting \( \bar{x}_1 \) and \( \bar{x}_2 \) passing through \( \bar{x}_3 \).

To find the next critical point of Morse index 2 we remark that under mild conditions, if \( \text{lev}_{\leq a} f \) contains a closed path homeomorphic to \( S_1 \), the boundary of the disc of dimension 2, then the linking principle guarantees the existence of a critical point through the multidimensional mountain pass theorem. Theorem 6.1 which we quote later gives an idea how this is possible. We refer the reader to [10] and [3] Chapter 19 for more details on linking methods.

We now illustrate with an example that without the assumption that \( (x_i, y_i) \) is the unique pair of points satisfying \( |x_i - y_i| = \text{diam}(S_i \cap (\text{lev}_{\geq l_i} f) \cap U_i) \), the conclusion in Theorem 4.3 need not hold.

**Lemma 4.6.** (Shortest line segments) Suppose lines \( l_1 \) and \( l_2 \) intersect at the origin in \( \mathbb{R}^2 \), and let \( P \) be a point on the angle bisector as shown in the diagram on the left of Figure 4.4. The minimum distance of the line segment \( AB \), where \( A \) is a point
on \( l_1 \) and \( B \) is a point on \( l_2 \) and \( AB \) passes through \( P \), is attained when \( OAB \) is an isosceles triangle with \( AB \) as its base.

Proof. Much of this is high school trigonometry and plane geometry, but we present full details for completeness. Let \( \alpha \) be the angle \( \angle AOP \), \( \beta \) be the angle \( \angle P AO \), and \( d = |OP| \). By using the sine rule, we get

\[
|AB| = d \left( \frac{\sin \alpha}{\sin \theta} + \frac{\sin \alpha}{\sin(\pi - 2\alpha - \theta)} \right).
\]

The problem is now reduced to finding the \( \theta \) that minimizes the value above. Continuing the arithmetic gives:

\[
d \left( \frac{\sin \alpha}{\sin \theta} + \frac{\sin \alpha}{\sin(\pi - 2\alpha - \theta)} \right) = d \sin \alpha \left( \frac{1}{\sin \theta} + \frac{1}{\sin(2\alpha + \theta)} \right)
= d \sin \alpha \left( \frac{\sin \theta + \sin(2\alpha + \theta)}{\sin(\theta) \sin(2\alpha + \theta)} \right)
= d \sin \alpha \left( \frac{\sin \theta + \sin(2\alpha + \theta)}{\sin(\theta) \sin(2\alpha + \theta)} \right)
= d \sin \alpha \left( \frac{2 \sin(\alpha + \theta) \cos \alpha}{2 \sin(2\alpha) (\cos(2\alpha) - \cos(2\alpha + 2\theta))} \right)
= 2d \sin(2\alpha) \left( \frac{\sin(\alpha + \theta)}{\cos(2\alpha) - \cos(2\alpha + 2\theta)} \right)
\]

We now differentiate the \( \frac{\sin(\alpha + \theta)}{\cos(2\alpha) - \cos(2\alpha + 2\theta)} \) term above, which gives

\[
\frac{d}{d\theta} \left( \frac{\sin(\alpha + \theta)}{\cos(2\alpha) - \cos(2\alpha + 2\theta)} \right) = \frac{1}{(\cos(2\alpha) - \cos(2\alpha + 2\theta))^2} \left[ \cos(\alpha + \theta)(\cos(2\alpha) - \cos(2\alpha + 2\theta)) - 2 \sin(2\alpha + 2\theta) \sin(\alpha + \theta) \right]
\]
The numerator is simplified to be:
\[
\cos(\alpha + \theta)[\cos(2\alpha) - \cos(2\alpha + 2\theta)] - 2\sin(2\alpha + 2\theta)\sin(\alpha + \theta)
\]
\[
= \cos(\alpha + \theta)[\cos(2\alpha) - 2\cos^2(\alpha + \theta) + 1] - 4\sin^2(\alpha + \theta)\cos(\alpha + \theta)
\]
\[
= \cos(\alpha + \theta)[\cos(2\alpha) - 2\cos^2(\alpha + \theta) + 1 - 4\sin^2(\alpha + \theta)]
\]
\[
= \cos(\alpha + \theta)[\cos(2\alpha) - 2\cos^2(\alpha + \theta) + 4\cos^2(\alpha + \theta) - 3]
\]
\[
= \cos(\alpha + \theta)[\cos(2\alpha) + 2\cos^2(\alpha + \theta) - 3].
\]

With this formula, we see that the conditions for \( \frac{d}{d\theta} \left( \frac{\sin(\alpha + \theta)}{\cos(2\alpha) - \cos(2\alpha + 2\theta)} \right) = 0 \) is to have \( \cos(\alpha + \theta) = 0 \) or \( \cos(2\alpha) + 2\cos^2(\alpha + \theta) = 3 \). The first case gives us \( \theta = \frac{\pi}{2} - \alpha \), which gives us the required conclusion. The second case requires \( \alpha = 0 \) or \( \alpha = \pi \) and \( \theta = 0 \) or \( \theta = \pi \), which are degenerate cases. This gives us all optimum solutions to our problem, and concludes the proof. \( \square \)

We now create an example in \( \mathbb{R}^3 \) that illustrates that the omission of the condition of unique solutions need not give us points whose gradients point in opposite directions.

**Example 4.7.** (Gradients need not be opposite) Define the four lines \( L_1 \) to \( L_4 \) by
\[
L_1 := \{(0, 0, -1) + \lambda(1, 0, 1) \mid \lambda \in \mathbb{R}_+\}
\]
\[
L_2 := \{(0, 0, -1) + \lambda(-1, 0, 1) \mid \lambda \in \mathbb{R}_+\}
\]
\[
L_3 := \{(0, 0, 1) + \lambda(0, 1, -1) \mid \lambda \in \mathbb{R}_+\}
\]
\[
L_4 := \{(0, 0, 1) + \lambda(0, -1, -1) \mid \lambda \in \mathbb{R}_+\}
\]
The lines \( L_1 \) and \( L_2 \) lie in the \( x-z \) plane, while the lines \( L_3 \) and \( L_4 \) lie in the \( y-z \) plane. See the diagram on the right of Figure 4.1.

Consider first the problem of finding a plane \( S \) that is a minimizer of the maximum of the distances between the points defined by the intersections of \( S \) and the \( L_i \)’s. We now show that \( S \) has to be the \( x-y \) plane. The plane \( S \) intersects the \( z \) axis at some point \( (0, 0, p) \). When \( S \) is the \( x-y \) plane, the maximum distance between the points is 2. By Lemma 4.6, the distance between the points \( S \cap L_1 \) and \( S \cap L_2 \) is at least \( 2(1-p) \), while the distance between the the points \( S \cap L_3 \) and \( S \cap L_4 \) is at least \( 2(1+p) \). This tells us that the \( x-y \) plane is optimal.

With this observation, we now construct our example. Consider the function \( f : \mathbb{R}^3 \to \mathbb{R} \) defined by
\[
f(x, y, z) = -\left(\frac{x}{1+z} + \frac{y}{1-z}\right)^{4/3} - \left(\frac{x}{1+z} - \frac{y}{1-z}\right)^{4/3}.
\]
The level set \( \text{lev}_{\geq -2} f \) contains the lines \( L_1 \) to \( L_4 \). This means that \( \text{diam}(S \cap \text{lev}_{\geq -2} f) \geq 2 \). This is in fact an equation when \( S \) is the \( x-y \) plane, and the maximizers being the pairs \( \{\pm(1,0,0)\} \) and \( \{\pm(0,1,0)\} \).

The gradient \( \nabla f(x, y, z) \) is
\[
\nabla f(x, y, z) = \left(\begin{array}{c}
-\frac{4}{3} \left(\frac{x}{1+z} + \frac{y}{1-z}\right)^{1/3} - \frac{4}{3} \left(\frac{x}{1+z} - \frac{y}{1-z}\right)^{1/3} \\
-\frac{4}{3} \left(\frac{x}{1+z} + \frac{y}{1-z}\right)^{1/3} + \frac{4}{3} \left(\frac{x}{1+z} - \frac{y}{1-z}\right)^{1/3} \\
-\frac{4}{3} \left(\frac{x}{1+z} + \frac{y}{1-z}\right)^{1/3} - \frac{4}{3} \left(\frac{x}{1+z} - \frac{y}{1-z}\right)^{1/3}
\end{array}\right).
\]
With this, we can evaluate $\nabla f$ at $\pm(1,0,0)$ and $\pm(0,1,0)$ to be
\[
\nabla f(1,0,0) = \left(-\frac{8}{3},0,\frac{8}{3}\right),
\]
\[
\nabla f(-1,0,0) = \left(\frac{8}{3},0,\frac{8}{3}\right),
\]
\[
\nabla f(0,1,0) = \left(0,-\frac{8}{3},-\frac{8}{3}\right),
\]
\[
\nabla f(0,-1,0) = \left(0,\frac{8}{3},-\frac{8}{3}\right).
\]
Neither of the pairs $\{\pm(1,0,0)\}$ and $\{\pm(0,1,0)\}$ have opposite pointing gradients, which concludes our example.

5. **Another convergence property of critical points**

In this section, we look at a condition on critical points similar to Proposition 3.2 that can be helpful for numerical methods for finding critical points. Theorem 5.2 below does not seem to be easily found in the literature, and can be seen as a local version of the mountain pass theorem.

We prove Theorem 5.2 in the more general setting of metric spaces. Such a treatment includes the case of nonsmooth functions. We recall the following definitions in metric critical point theory from [7, 10, 11].

**Definition 5.1.** Let $(X,d)$ be a metric space. We call the point $x$ *Morse regular* for the function $f : X \to \mathbb{R}$ if, for some numbers $\gamma, \sigma > 0$, there is a continuous function $\phi : B(x,\gamma) \times [0,\gamma] \to X$ such that all points $u \in B(x,\gamma)$ and $t \in [0,\gamma]$ satisfy the inequality
\[
f(\phi(x,t)) \leq f(x) - \sigma t,
\]
and that $\phi(\cdot,0) : B(x,\gamma) \to B(x,\gamma)$ is the identity map. The point $x$ is *Morse critical* if it is not Morse regular.

If for some $\phi$, there is some $\kappa > 0$ such that $\phi$ also satisfies the inequality
\[
d(\phi(x,t),x) \leq \kappa t,
\]
then we call $x$ *deformationally regular*. The point $x$ is *deformationally critical* if it is not deformationally regular.

It is a fact that if $X$ is a Banach space and $f$ is locally Lipschitz, then deformationally critical points are Clarke critical. The following theorem gives a strategy for identifying deformationally critical points.

**Theorem 5.2.** (Critical points from sequences of linking sets) Let $(X,d)$ be a metric space and $f : X \to \mathbb{R}$. Suppose there is some open set $U$ of $\bar{x}$ and sequences of sets $\{\Phi_i\}_{i=1}^\infty$ and $\{\Gamma_i\}_{i=1}^\infty$ such that

1. $\Phi_i$ and $\partial \Gamma_i$ link.
2. $\Gamma_i$ are homeomorphic to $B^m$ for all $i$, and $\max_{x \in \partial \Gamma_i} f(x) < \inf_{x \in \Phi_i \cap U} f(x)$.
3. For any open set $V$ containing $\bar{x}$, there is some $I > 0$ such that $\Gamma_i \subset V$ for all $i > I$.
4. $f$ is Lipschitz in $U$. 
Then $\bar{x}$ is deformationally critical.

Proof. Suppose $\bar{x}$ is deformationally regular. Then there are $\gamma, \sigma, \kappa > 0$ and $\phi : \mathbb{B}(\bar{x}, \gamma) \times [0, \gamma] \to X$ such that the inequalities

$$f(\phi(x, t)) \leq f(x) - \sigma t \text{ and } d(\phi(x, t), x) \leq \kappa t$$

hold for all points $x \in \mathbb{B}(\bar{x}, \gamma)$ and $t \in [0, \gamma]$, and $\phi(\cdot, 0) : \mathbb{B}(\bar{x}, \gamma) \to \mathbb{B}(\bar{x}, \gamma)$ is the identity map. We may reduce $\gamma$ as necessary and assume that $U = \mathbb{B}(\bar{x}, \gamma)$.

Condition (3) implies that for any $\alpha > 0$, then there is some $I_1$ such that $\Gamma_i \subset \mathbb{B}(\bar{x}, \alpha)$ for all $i > I_1$. Consider $\Gamma_{i,t} := \phi((\Gamma_i \times \{t\}) \cup (\partial \Gamma_i \times [0, t]))$. Provided $0 < t < \frac{\alpha}{\kappa}$, we have $\Gamma_{i,t} \subset U$.

Since $f$ is Lipschitz in $U$, let $\bar{\kappa}$ be the modulus of Lipschitz continuity in $U$. We have $\max_{x \in \Gamma_i} f(x) \leq \max_{x \in \partial \Gamma_i} f(x) + \bar{\kappa} \text{diam}(\Gamma_i)$. Also,

$$\max_{x \in \Gamma_{i,t}} f(x) \leq \max_{x \in \partial \Gamma_{i,t}} f(x) + \bar{\kappa} \text{diam}(\Gamma_{i,t}) - \sigma t, \max_{x \in \partial \Gamma_{i,t}} f(x) \max_{x \in \Gamma_{i,t}} f(x) \leq \sigma t \kappa t$$

By condition (3), there is some $I_2 > 0$ such that if $i > I_2$, then diam$(\Gamma_i) < \frac{\sigma t}{\kappa}$. So for $i > \max(I_1, I_2)$, we have

$$\max_{x \in \Gamma_{i,t}} f(x) = \max_{x \in \partial \Gamma_{i,t}} f(x) < \inf_{x \in \Phi_i \cap U} f(x).$$

However, the fact that $\partial \Gamma_i$ and $\Phi_i$ link implies that $\Gamma_{i,t}$ and $\Phi_i$ must intersect, and since $\Gamma_{i,t} \subset U$, $\Gamma_{i,t}$ and $\Phi_i \cap U$ must intersect. This is a contradiction, so $\bar{x}$ is deformationally critical.

It is reasonable to choose $\Gamma_i$ to be a simplex (that is, a convex hull of $m + 1$ points) and $\Phi_i$ to be an affine space. If the sequence of sets $\{\Gamma_i\}_{i=1}^\infty$ converges to the single point $\bar{x}$ and $f$ is $C^2$ there, a quadratic approximation of $f$ using only the knowledge of the values of $f$ and $\nabla f$ on the vertices of the simplex would be good approximation of $f$ on the simplex. We outline our strategy below.

Algorithm 5.3. (Obtaining unknowns in quadratic) Let $h : \mathbb{R}^m \to \mathbb{R}$ be defined by $h(x) = \frac{1}{2}x^T Ax + b^T x + c$, and let $p_1, \ldots, p_{m+1}$ be $m + 1$ points in $\mathbb{R}^m$. Suppose that the values of $h(p_i)$ and $\nabla h(p_i)$ are known for all $i = 1, \ldots, m + 1$. We seek to obtain the values of $A$, $b$ and $c$.

1. Let $P \in \mathbb{R}^{m \times m}$ be the matrix such that the $i$th column is $p_{i+1} - p_1$, and let $D \in \mathbb{R}^{m \times m}$ be the matrix such that the $i$th column is $\nabla h(p_{i+1}) - \nabla h(p_1)$.

   Calculate $A$ with $A = DP^{-1}$.

2. Calculate $b$ with $b = \nabla h(p_1) - Ap_1$.

3. Calculate $c$ with $c = h(p_1) - \frac{1}{2}p_1^T Ap_1 - b^T p_1$.

If $h$ is $C^2$ instead of being a quadratic, then the procedure in Algorithm 5.3 can be used to approximate the values of $h$ on a simplex.

In Lemma 5.4 below, given $m + 1$ points in $\mathbb{R}^n$, we need to approximate a quadratic function on $\Delta$ as a subset of $\mathbb{R}^n$. Even though $m < n$, the procedure to obtain a quadratic estimate of $f$ in $\Delta$ is a straightforward extension of Algorithm 5.3

Lemma 5.4. (Quadratic estimate on simplex) Let $f : \mathbb{R}^n \to \mathbb{R}$ be $C^2$ and $\bar{x} \in \mathbb{R}^n$.

Let $p_1, \ldots, p_{m+1}$ be points close to $\bar{x}$. Suppose the matrix $P \in \mathbb{R}^{n \times m}$, whose $i$th column is $p_{i+1} - p_1$, has full column rank. Let $f_\Delta : \mathbb{R}^n \cap \Delta \to \mathbb{R}$ be defined as the quadratic function obtained using $f(p_1)$ and $\nabla f(p_i)$ for $i = 1, \ldots, m + 1$ with
Algorithm 5.3. For any $\epsilon > 0$, there is some $\delta > 0$ such that if $p_1, \ldots, p_{m+1} \in \mathbb{B}(\bar{x}, \delta)$, then

$$|f_\epsilon (x) - f(x)| < \frac{1}{2} \text{diam}(\Delta)^2 \epsilon (1 + \kappa \|P\|\|P^\dagger\|) \text{ for all } x \in \Delta,$$

where $\| \cdot \|$ stands for the matrix 2-norm, $P^\dagger$ is the pseudoinverse of $P$, and $\kappa$ is some constant dependent only on $n$ and $m$.

Proof. The first step of this proof is to show that step 1 of Algorithm 5.3 gives a matrix in $\mathbb{R}^{n \times n}$ which is a good approximation of how $A = \nabla^2 f(\bar{x})$ acts on the lineality space of the affine hull of $\Delta$. Since $f$ is $C^2$, for any $\epsilon > 0$, there exists $\delta > 0$ such that $|\nabla f(x) - \nabla f(x') - A(x - x')| < \epsilon |x - x'|$ for all $x, x' \in \mathbb{B}(\bar{x}, \delta)$. Thus, there is some $\kappa > 0$ depending only on $m$ and $n$ such that if $p_1, \ldots, p_{m+1} \in \mathbb{B}(\bar{x}, \delta)$, then

$$|f_\epsilon (x) - f(x)| < \frac{1}{2} \text{diam}(\Delta)^2 \epsilon (1 + \kappa \|P\|\|P^\dagger\|) \text{ for all } x \in \Delta,$$

where $\| \cdot \|$ stands for the matrix 2-norm, $P^\dagger$ is the pseudoinverse of $P$, and $\kappa$ is some constant dependent only on $n$ and $m$.

Let $P = QR$, where $Q \in \mathbb{R}^{n \times m}$ has orthonormal columns and $R \in \mathbb{R}^{m \times m}$, be a QR decomposition of $P$. For any $v \in \mathbb{R}^n$ in the range of $P$, or equivalently, $v = Qv'$ for some $v' \in \mathbb{R}^m$, we want to show that $\|Av - DR^{-1}Q^Tv\|$ is small. We note that $|v| = |v'|$, and we have the following calculation.

$$\|Av - DR^{-1}Q^Tv\| = \|AQv' - DR^{-1}Q^TQv'\| = \|AQv' - DR^{-1}v'\| \leq \|AQ - DR^{-1}\|\|v'\| \leq \|AQR - D\|\|R^{-1}\|\|v\| = \|D - AP\|\|R^{-1}\|\|v\| \leq \kappa \|P\|\|R^{-1}\|\|v\|.$$

Next, for $x, x' \in \mathbb{B}(\bar{x}, \delta)$, let $d = \text{unit}(x' - x)$. Then

$$f(x') - f(x) = \int_0^{|x' - x|} \nabla f(x + sd)^T d\mathbf{s} = \int_0^{|x' - x|} \int_0^s d^T \nabla^2 f(x + td) d t + \nabla f(x)^T d \mathbf{s}.$$

Since $f$ is $C^2$, we may reduce $\delta$ if necessary so that $\|A - \nabla^2 f(x + td)\| < \epsilon$ for all $0 \leq t \leq |x' - x|$. This tells us that

$$|d^T(DR^{-1}Q^Td - DR^{-1}Q^T \nabla^2 f(x)d)| \leq |d||DR^{-1}Q^Td - \nabla^2 f(x)d| \leq ||DR^{-1}Q^Td - Ad|| + \|Ad - \nabla^2 f(x)d\| \leq \kappa \|P\|\|R^{-1}\|\|d\| + \|A - \nabla^2 f(x)\| \leq \epsilon (1 + \kappa \|P\|\|R^{-1}\|).$$
We have
\[
\int_0^{\left| x' - x \right|} \int_0^s d^T(DR^{-1}Q^T)d \mathbf{t} + \nabla f(x)^T d \mathbf{s} \\
= \nabla f(x)^T(x' - x) + \int_0^{\left| x' - x \right|} d^T(DR^{-1}Q^T)ds \mathbf{d} \\
= \nabla f(x)^T(x' - x) + \frac{\left| x' - x \right|^2}{2}d^T(DR^{-1}Q^T)d \\
= \nabla f(x)^T(x' - x) + \frac{1}{2}(x' - x)^T(DR^{-1}Q^T)(x' - x).
\]

Continuing with the arithmetic earlier, we obtain
\[
\left| f(x') - f(x) - \left( \nabla f(x)^T(x' - x) + \frac{1}{2}(x' - x)^T(DR^{-1}Q^T)(x' - x) \right) \right| \\
\leq \int_0^{\left| x' - x \right|} \int_0^s \epsilon (1 + \kappa \|P\|\|R^{-1}\|)s \mathbf{d} \mathbf{d} \mathbf{s} \\
= \frac{1}{2}x' - x^2 \epsilon (1 + \kappa \|P\|\|R^{-1}\|).
\]
Let \( x = p_1 \) and \( x' \) be any point in \( \Delta \). Define \( f_\epsilon(x') \) by
\[
f_\epsilon(x') = f(x) + \nabla f(x)^T(x' - x) + \frac{1}{2}(x' - x)^T(DR^{-1}Q^T)(x' - x),
\]
which is the quadratic function obtained using Algorithm 5.3. We have
\[
|f_\epsilon(x') - f(x')| \leq \frac{1}{2}|x' - x|^2 \epsilon (1 + \kappa \|P\|\|R^{-1}\|) \\
\leq \frac{1}{2} \text{diam}(\Delta)^2 \epsilon (1 + \kappa \|P\|\|R^{-1}\|),
\]
which gives what we need. \( \square \)

In the statement of Lemma 5.4, we chose the domain of \( f \) to be \( \mathbb{R}^n \) so that the inequality \( 5.1 \) follows from the equivalence of finite dimensional norms. Next, the accuracy of the computed values of \( \nabla f(p_{i+1}) - \nabla f(p_i) \) might be poor, which makes the quadratic approximation strategy ineffective once we are too close to the critical point \( \bar{x} \). We remark on how we can overcome this problem by exploiting concavity.

**Remark 5.5.** (Exploiting concavity) The lineality space of the affine hull of \( \Delta \) may span the eigenspaces of the \( m \) negative eigenvalues of \( \nabla^2 f(\bar{x}) \) once we are close to the critical point \( \bar{x} \). This can be checked by calculating the Hessian as was done earlier. If this is the case, \( f \) would be concave in \( \Delta \) when \( p_1, \ldots, p_{m+1} \) are sufficiently close to \( \bar{x} \). The estimate \( f(x) \leq f(p_i) + \nabla f(p_i)^T(x - p_i) \) would hold for all \( x \in \Delta \) and \( 1 \leq i \leq m+1 \), which can give a sufficiently good estimate of \( \max_{x \in \partial \Delta} f(x) \) through linear programming.

### 6. Fast Local Convergence

In this section, we discuss how we can find good lower bounds that allow us to achieve better convergence if \( f \) is \( C^2 \) and \( X = \mathbb{R}^n \). Our method extends the local superlinearly convergent method in [12] for finding smooth critical points of mountain pass type when \( X = \mathbb{R}^n \).
Figure 6.1. Illustration of the multidimensional mountain pass theorem

Let us recall the multidimensional mountain pass theorem due to Rabinowitz [14].

**Theorem 6.1.** (Multidimensional mountain pass theorem) [14] Let \( X = Y \oplus Z \) be a Banach space with \( Z \) closed in \( X \) and \( \dim(Y) < \infty \). For \( \rho > 0 \) define

\[
M := \{ u \in Y | \| u \| \leq \rho \}, \quad M_0 := \{ u \in Y | \| u \| = \rho \}.
\]

Let \( f : X \to \mathbb{R} \) be \( C^1 \), and

\[
b := \inf_{u \in Z} f(u) > a := \max_{u \in M_0} f(u).
\]

If \( f \) satisfies the Palais Smale condition and

\[
c := \inf_{\gamma \in \Gamma} \max_{u \in M} f(\gamma(u)) \text{ where } \Gamma := \{ \gamma : M \to X \text{ is continuous} | \gamma|_{M_0} = \text{id} \},
\]

then \( c \) is a critical value of \( f \).

For the case when \( X = \mathbb{R}^3 \), we have an illustration in Figure 6.1 of the case \( f : \mathbb{R}^3 \to \mathbb{R} \) defined by \( f(x) = x_3^2 - x_1^2 - x_2^2 \). The critical point \( 0 \) has critical value \( 0 \). Choose \( Y \) to be \( \mathbb{R}^2 \times \{ 0 \} \) and \( Z \) to be \( \{ 0 \} \times \mathbb{R} \). The union of the two blue cones is the level set \( \text{lev}_{-\rho} f := f^{-1}(0) \), while the bold red ring denotes \( M_0 \) and the red disc denotes a possible image of \( M \) under \( \gamma \).

It seems intuitively clear that \( \gamma(M) \) has to intersect the vertical axis. This is indeed the case, since \( M_0 \) and \( Z \) link. (See for example [17] Example II.8.2.)

With this observation, we easily see that \( \max_{u \in M} f(\gamma(u)) \geq \inf_{z \in Z} f(z) \). Thus the critical value \( c = \inf_{\gamma \in \Gamma} \max_{u \in M} f(\gamma(u)) \) from Theorem 6.1 is bounded from below by \( \inf_{z \in Z} f(z) \). This gives a lower bound for the critical value. In the mountain pass case when \( m = 1 \), the set \( M_0 \) consists of two points, and the space \( Z \) separates the two points in \( M_0 \) so that any path connecting the two points in \( M_0 \) must intersect \( Z \).

A first try for a fast locally convergent algorithm is as follows:
Algorithm 6.2. A first try for a fast locally convergent algorithm to find saddle points of Morse index $m$ for $f : X \to \mathbb{R}$.

1. Set the iteration count $i$ to 0, and let $l_i$ be a lower bound of the critical value.
2. Find $x_i$ and $y_i$, where $(S_i, x_i, y_i)$ is an optimizing triple of
3. \[ \min_{S \in \mathcal{S}} \max_{x,y \in S \cap \{\text{lev}>l_i\}} |x-y|, \]
   where $U_i$ is an open set. Here $\mathcal{S}$ is the set of $m$-dimensional affine subspaces of $\mathbb{R}^n$ intersecting $U_i$. (The difference between this formula and (2.1) is that we take level sets of level $l_i$ instead of $\frac{1}{2}(l_i + u_i)$.)
4. For an optimal solution $(S_i, x_i, y_i)$, let $l_{i+1}$ be the lower bound of $f$ on the $(n-m)$-dimensional affine space passing through $z_i := \frac{1}{2}(x_i + y_i)$ whose linearity space is orthogonal to the linearity space of $S_i$.
5. Increase $i$ and go back to step 2.

While Algorithm 6.2 as stated works fine for the case $m = 1$ to find critical points of mountain pass type, the $l_i$’s calculated in this manner need not increase monotonically to the critical value when $m > 1$. We first present a lemma on the min-max problem (6.1) for the case of a quadratic.

Lemma 6.3. (Analysis on exact quadratic) Consider $f : \mathbb{R}^n \to \mathbb{R}$ defined by $f(x) = \sum_{j=1}^{n} a_j x_j^2$, where $a_j$ are in decreasing order, with $a_j > 0$ for $1 \leq j \leq n-m$ and $a_j < 0$ for $n-m+1 \leq j \leq n$. The function $f$ has one critical point $0$, and $f(0) = 0$. Given $l < 0$, an optimizing triple $(\bar{S}, \bar{x}, \bar{y})$ of the problem
\[ \min_{S \in \mathcal{S}} \max_{x,y \in S \cap \{\text{lev} \geq l\}} |x-y|, \]
where $\mathcal{S}$ is the set of affine spaces of dimension $m$, satisfies
\[ \bar{x} = \left( 0, 0, \ldots, 0, \pm \sqrt{\frac{l}{a_{n-m+1}}}, 0, \ldots, 0 \right), \]
where the nonzero term is in the $(n-m+1)$th position, and $\bar{y} = -\bar{x}$.

Proof. Let $S_{\bar{x},V} := \{ \bar{z} + Vw \mid w \in \mathbb{R}^m \}$, where $V \in \mathbb{R}^{n \times m}$ is a matrix with orthonormal columns. Let the matrix $A \in \mathbb{R}^{n \times n}$ be the diagonal matrix with entries $a_j$ in the $(j,j)$th position. The ellipse $S_{\bar{x},V} \cap \{\text{lev} \geq l\}$ can be written as a union of elements of the form $\bar{z} + Vw$, where $w$ satisfies
\[ \begin{align*}
(\bar{z} + Vw)^T A (\bar{z} + Vw) &\geq l \\
\iff w^T V^T A V w + 2\bar{z}^T A V w + \bar{z}^T A \bar{z} &\geq l.
\end{align*} \]

If the matrix $V^T A V$ has a nonnegative eigenvalue, then $S_{\bar{x},V} \cap \{\text{lev} \geq l\}$ is unbounded. Otherwise, the set
\[ \{ \bar{z} + Vw \mid w^T V^T A V w + 2\bar{z}^T A V w + \bar{z}^T A \bar{z} \geq l \} \]
is bounded. Therefore the inner maximization problem of (6.2) corresponding to $S = S_{\bar{x},V}$ has a (not necessarily unique) pair of minimizers. We continue completing the square with respect to $w$ and let the symmetric matrix $C$ be the square root $C = [-V^T A]^{\frac{1}{2}}$.
\[ -w^T C^2 w + 2\bar{z}^T A V w + \bar{z}^T A \bar{z} \geq l \]
\[ \iff -(C w - C^{-1} V^T A \bar{z})^T (C w - C^{-1} V^T A \bar{z}) + \bar{z}^T A \bar{z} + \bar{z}^T A C^{-2} V^T A^T \bar{z} \geq l. \]
The maximum length between two points of an ellipse is twice the distance between the center and the furthest point on the ellipse. (This fact is easily proved by reducing to, and examining, the two dimensional case.) The distance between the center and the furthest point on the ellipse $S_{z,v} \cap \text{lev}_{\geq 1} f$ can be calculated to be
\[
\sqrt{\frac{1}{\alpha} (\bar{z}^T A \bar{z} + \bar{z}^T A V C^{-2} V^T A^T \bar{z} - l)},
\]
where $\alpha$ is the square of the smallest eigenvalue in $C$, or equivalently the negative of the largest eigenvalue of $V^T AV$. The term $(\bar{z}^T A \bar{z} + \bar{z}^T A V C^{-2} V^T A^T \bar{z})$ is $\max \{f(x) \mid x \in S_{z,v}\}$, which we refer to as $\max_{S_{z,v}} f$. We now proceed to minimize $\max_{S_{z,v}} f$ and maximize $\alpha$ separately.

**Claim 1:** $\max_{S_{z,v}} f \geq 0$.

We first prove that the subspace
\[
Z := \{z \mid z_n = z_{n-1} = \cdots = z_{n-m+1} = 0\}
\]
must intersect $S_{z,v}$. Recall that $V^T AV$ is negative definite. Therefore for any $w \neq 0$, $w^T V^T AV w < 0$. Since the first $n - m$ eigenvalues of $A$ are positive, $V w$ cannot be all zeros in its last $m$ components. This shows that the $m \times m$ matrix $V((n - m + 1) , n, 1 : m)$ is invertible. We can find some $\bar{w}$ such that the last $m$ components of $\bar{z} + V \bar{w}$ are zeros. This shows that $S_{z,v} \cap Z \neq \emptyset$, so $\max_{S_{z,v}} f \geq \min \{f(x) \mid x \in Z\} = 0$.

**Claim 2:** $\alpha \leq -a_{n-m+1}$.

To find the maximum value of $\alpha$, we recall that it is the negative of the largest eigenvalue of $V^T AV$. Since $V \in \mathbb{R}^{n \times m}$, the Courant-Fischer Theorem, gives $\alpha \leq -a_{n-m+1}$.

Choose the affine space $\bar{S} := \{0\} \times \mathbb{R}^m$. This minimizes $\max_S f$ and maximizes $\alpha$ as well, giving the optimal solution in the statement of the lemma.

It should be noted however that the minimizing subspace need not be unique, even if the values of $a_j$ are distinct. The example below highlights how Algorithm 6.2 can fail.

**Example 6.4.** (Failure of Algorithm 6.2) Suppose $f(x) = x_1^2 - x_2^2 - 3x_3^2$. The subspace $S = \{x \mid x_1 = x_3\}$ intersects the level set $\text{lev}_{\leq -1} f$ in the disc
\[
\left\{ \lambda \left( \frac{1}{\sqrt{2}} \sin \theta, \cos \theta, \frac{1}{\sqrt{2}} \sin \theta \right) \mid 0 \leq \theta \leq 2\pi, 0 \leq \lambda \leq 1 \right\}.
\]
The largest distance between two points on the disc is 2, and the subspace $S$ can be verified to give the optimal value to the min-max problem \([6.1]\) by Lemma 6.3.

On the ray $S^\perp = \{\lambda(1,0,-1) \mid \lambda \in \mathbb{R}\}$, the function $f$ is concave, hence there is no minimum. This example illustrates that Algorithm 6.2 can fail in general. See Figure 6.2.

Example 6.4 shows that even if there are only 2 negative eigenvalues, it might be possible to find a two-dimensional subspace $\bar{S}$ on which the Hessian is negative definite on both $S$ and $S^\perp$. Therefore, we amend Algorithm 6.2 by determining the eigenspace corresponding to the $m$ smallest eigenvalues.

**Algorithm 6.5.** Fast local method to find saddle points of Morse index $m$.

1. Set the iteration count $i$ to 0, and let $l_i$ be a lower bound of the critical value.
Figure 6.2. An example where Algorithm 6.2 fails.

(2) Find $x_i$ and $y_i$, where $(S'_i, x_i, y_i)$ is an optimizing triple of
\begin{equation}
\min_{S \in \mathcal{S}} \max_{x, y \in S \cap (\text{lev} \leq l_i) \cap U_i} |x - y|,
\end{equation}
where $U_i$ is an open set. Here $\mathcal{S}$ is the set of $m$-dimensional affine subspaces of $\mathbb{R}^n$ intersecting $U_i$. We emphasize that the space where minimality is attained in the outer minimization problem is $S'_i$. After solving the above problem, find the subspace $S_i$ that approximates the eigenspace corresponding to the $m$ smallest eigenvalues using Algorithm 6.6 below.

(3) For an optimizing triple $(S_i, x_i, y_i)$ found in step 2, let $l_{i+1}$ be the lower bound of $f$ on the $(n - m)$-dimensional affine space passing through $z_i := \frac{1}{2}(x_i + y_i)$ whose lineality space is orthogonal to the lineality space of $S_i$.

(4) Increase $i$ and go back to step 2 till convergence.

A local algorithm is needed in Algorithm 6.5 to find the subspace $S_i$ in step 2.

**Algorithm 6.6. Finding the subspace $S_i$ in step 2 of Algorithm 6.5**

1. Let $X_1 = \text{span}\{x_i - y_i\}$, where $x_i, y_i$ are found in step 2 of Algorithm 6.5 and let $j$ be 1.
2. Find the closest point from $z_i := \frac{1}{2}(x_i + y_i)$ to $\text{lev} \leq l_i \cap (z_i + X_j^\perp)$, which we call $\bar{p}_{j+1}$.
3. Let $X_{j+1} = \text{span}\{X_j, \bar{p}_{j+1} - z_i\}$ and increase $j$ by 1. If $j = m$, let $S_i$ be $z_i + X_m$ and the algorithm ends. Otherwise, go back to step 2.

Step 2 of Algorithm 6.6 finds the negative eigenvalues and eigenvectors, starting from the eigenvalues furthest from zero. Once all the eigenvectors are found, then $S_i$ is the span of these eigenvectors.

In some situations, the lineality space of $S_i$ are known in advance, or do not differ too much from the previous iteration. In this case, we can get around using Algorithm 6.6 and use the estimate instead.

We are now ready to prove the convergence of Algorithm 6.5.
7. **Proof of Superlinear Convergence of Local Algorithm**

We prove our result on the convergence of Algorithm 6.5 in steps. The first step is to look closely at a model problem.

**Assumption 7.1.** Given $\delta > 0$, suppose $h : \mathbb{R}^n \rightarrow \mathbb{R}$ is $C^2$, 
\[
|\nabla h(x) - Ax| \leq \delta |x|, \\
|h(x) - \frac{1}{2} x^T Ax| \leq \frac{1}{2} \delta |x|^2 
\]
for all $x \in \mathbb{B}$, where $A \in \mathbb{R}^{n \times n}$ is an invertible diagonal matrix with diagonal entries ordered decreasingly, of which $a_i = A_{ii}$ and 
\[
a_1 > a_2 > \cdots > a_{n-m} > 0 > a_{n-m+1} > \cdots > a_n.
\]

Define $h_{\min} : \mathbb{R}^n \rightarrow \mathbb{R}$ and $h_{\max} : \mathbb{R}^n \rightarrow \mathbb{R}$ by:
\[
h_{\min}(x) = \frac{1}{2} x^T (A - \delta I)x \quad \text{and} \quad h_{\max}(x) = \frac{1}{2} x^T (A + \delta I)x.
\]

It is clear that $\nabla h(0) = 0$, $h(0) = 0$, $\nabla^2 h(0) = A$, and the Morse index is $m$. Here is a simple observation that bounds the level sets of $h$:

**Proposition 7.2.** (Level set property) The level sets of $h$ satisfy 
\[
\mathbb{B} \cap \text{lev}_{\geq 1} h_{\min} \subset \mathbb{B} \cap \text{lev}_{\geq 1} h \subset \mathbb{B} \cap \text{lev}_{\geq 1} h_{\max},
\]
and 
\[
\mathbb{B} \cap \text{lev}_{\leq 1} h_{\max} \subset \mathbb{B} \cap \text{lev}_{\leq 1} h \subset \mathbb{B} \cap \text{lev}_{\leq 1} h_{\min}.
\]

**Proof.** This follows easily from $|h(x) - \frac{1}{2} x^T Ax| \leq \frac{1}{2} \delta |x|^2$ for all $x \in \mathbb{B}$. \hfill \square

For convenience, we highlight the standard problem below:

**Problem 7.3.** Suppose $g : \mathbb{R}^n \rightarrow \mathbb{R}$ is $C^2$, with critical point $0$ of Morse index $m$, $g(0) = 0$ and the Hessian $\nabla^2 g(0)$ has distinct eigenvalues that are all nonzero. Consider the problem
\[
\min_{S \in \mathcal{S}} \max_{x,y \in S \cap \text{lev}_{\geq 1} g} |x - y|,
\]
where $S$ is the set of $m$ dimensional affine subspaces.

Note that in Problem 7.3, we have limited the region where $x$ and $y$ lie in by $\mathbb{B}$. Here is a result on the optimizing pair $(\bar{x}, \bar{y})$ of the inner maximization problem in Problem 7.3

**Lemma 7.4.** (Convergence to eigenvector and saddle point) For all $\delta > 0$ sufficiently small, suppose that $h : \mathbb{R}^n \rightarrow \mathbb{R}$ is such that Assumption 7.1 holds. Assume that for the optimizing triple $(\bar{S}, \bar{x}, \bar{y})$ of Problem 7.3 for $g = h$, $(\bar{x}, \bar{y})$ is the unique pair of points in $\bar{S} \cap (\text{lev}_{\geq 1} h) \cap \mathbb{B}$ such that $|\bar{x} - \bar{y}| = \text{diam}(\bar{S} \cap (\text{lev}_{\geq 1} h) \cap \mathbb{B})$. Then there exists $\epsilon > 0$ such that if $0 < \epsilon < 1$ and $(\bar{x}, \bar{y})$ are such that $|\bar{y} - \bar{x}| \leq \epsilon |\bar{y} - \bar{x}|$ converges to the $(n-m+1)$th eigenvector as $\delta \rightarrow 0$, and $|\frac{1}{2} (\bar{x} + \bar{y})|^2/|l| \rightarrow 0$ as $\delta \rightarrow 0$.

**Proof.** Since $\text{lev}_{\leq 1} h_{\max} \cap \mathbb{B} \subset \text{lev}_{\leq 1} h \cap \mathbb{B}$, we look at the the optimal solution of the min-max problem for $h_{\max}$ first. The objective of Problem 7.3 for $g = h_{\max}$ is $2 \sqrt{\frac{l}{a_{n-m+1} + \delta}}$ by Lemma 6.3. This gives an upper bound for the min-max problem for $h$. Similarly, by considering $h_{\min}$ instead, we deduce that Problem 7.3 has optimal solution bounded from below by $2 \sqrt{\frac{l}{a_{n-m+1} - \delta}}$. 


Recall the optimality condition in Proposition 4.5. We now proceed to find the first pair of points with opposite pointing gradients. Let $\bar{x}$ and $\bar{y}$ be optimal points at level $l_i$. Now,

$$\bar{y} - \bar{x} = \lambda_1 \nabla h(\bar{x}),$$

and

$$\bar{x} - \bar{y} = \lambda_2 \nabla h(\bar{y}),$$

for some $\lambda_1, \lambda_2 > 0$. Then

$$\lambda_1 \nabla h(\bar{x}) + \lambda_2 \nabla h(\bar{y}) = 0$$

and

$$|\lambda_1 A\bar{x} + \lambda_2 A\bar{y}| \leq |\lambda_1 A\bar{x} - \nabla h(\bar{x})| + \lambda_2 |A\bar{y} - \nabla h(\bar{y})|$$

$$\leq \delta|\lambda_1 |\bar{x}| + \lambda_2 |\bar{y}|\rangle$$

$$|A(\lambda_1 \bar{x} + \lambda_2 \bar{y})| \leq \delta|\lambda_1 |\bar{x}| + \lambda_2 |\bar{y}|\rangle$$

$$\Rightarrow |\lambda_1 \bar{x} + \lambda_2 \bar{y}| \leq |A^{-1}||A(\lambda_1 \bar{x} + \lambda_2 \bar{y})|$$

$$\leq |A^{-1}|\delta|\lambda_1 |\bar{x}| + \lambda_2 |\bar{y}|\rangle.$$

This means that there are points $x'$ and $y'$ such that $\lambda_1 x' + \lambda_2 y' = 0$, $|\bar{x} - x'| \leq |A^{-1}|\delta|\bar{x}|$ and $|\bar{y} - y'| \leq |A^{-1}|\delta|\bar{y}|$. With this, we now concentrate on pairs of points that are negative multiples of each other.

Now,

$$\lambda_1 \nabla h(\bar{x}) = \bar{y} - \bar{x}$$

$$\Rightarrow \nabla h(\bar{x}) = \frac{1}{\lambda_1}(\bar{y} - \bar{x})$$

$$\Rightarrow |A\bar{x} - \frac{1}{\lambda_1}(\bar{y} - \bar{x})| \leq \delta|\bar{x}|.$$

Similarly, this gives us

$$|A(-\bar{y}) - \frac{1}{\lambda_2}(\bar{y} - \bar{x})| \leq \delta|\bar{y}|.$$

Therefore,

$$|A(\bar{y} - \bar{x}) + \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)(\bar{y} - \bar{x})| \leq \delta(|\bar{x}| + |\bar{y}|).$$

This gives:

$$|A(y' - x') + \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)(y' - x')|$$

$$\leq |A(y' - x') - A(\bar{y} - \bar{x})| + \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)|((y' - x') - (\bar{y} - \bar{x})|$$

$$+ |A(\bar{y} - \bar{x}) + \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)(\bar{y} - \bar{x})|$$

$$\leq |A||A^{-1}|\delta(|\bar{x}| + |\bar{y}|) + \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)|A^{-1}|\delta(|\bar{x}| + |\bar{y}|) + \delta(|\bar{x}| + |\bar{y}|)$$

$$= \delta(|\bar{x}| + |\bar{y}|) \left(|A||A^{-1}| + \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)|A^{-1}| + 1\right).$$

(7.1)
Next, we relate $|\vec{y} - \vec{x}|$ and $|\vec{x}| + |\vec{y}|$. We have

\[
|\vec{x}| \leq |\vec{x}'| + |A^{-1}| \delta |\vec{x}|
\]

\[
\Rightarrow (1 - |A^{-1}| \delta) |\vec{x}| \leq |\vec{x}'|
\]

and similarly, $(1 - |A^{-1}| \delta) |\vec{y}| \leq |\vec{y}'|$. It is clear that $|\vec{y}' - \vec{x}'| = |\vec{x}'| + |\vec{y}'|$, and we get

\[
|\vec{x}| + |\vec{y}| \leq \frac{1}{1 - |A^{-1}| \delta} (|\vec{x}'| + |\vec{y}'|)
\]

\[
= \frac{1}{1 - |A^{-1}| \delta} |\vec{y}' - \vec{x}'|
\]

\[
\leq \frac{1}{1 - |A^{-1}| \delta} (|\vec{y} - \vec{x}| + |A^{-1}| \delta (|\vec{x}| + |\vec{y}|))
\]

\[
\Rightarrow (1 - 2|A^{-1}| \delta) (|\vec{x}| + |\vec{y}|) \leq |\vec{y} - \vec{x}|
\]

To show that (1) in (7.1) converges to 0 as $\delta \searrow 0$, we need to show that $(\frac{1}{\lambda_1} + \frac{1}{\lambda_2})$ remains bounded as $\delta \searrow 0$. Note that

\[
\nabla h(\vec{x}) - \nabla h(\vec{y}) = \left( \frac{1}{\lambda_1} + \frac{1}{\lambda_2} \right) (\vec{y} - \vec{x})
\]

\[
\Rightarrow |\frac{1}{\lambda_1} + \frac{1}{\lambda_2}| = \frac{|\nabla h(\vec{x}) - \nabla h(\vec{y})|}{|\vec{y} - \vec{x}|}
\]

\[
\leq \frac{1}{|\vec{y} - \vec{x}|} |\vec{A}(\vec{x} - \vec{y})| + \delta (|\vec{x}| + |\vec{y}|)
\]

\[
\leq \frac{1}{|\vec{y} - \vec{x}|} (|\vec{A}| \delta - \vec{y} - \vec{x}) + \frac{1}{1 - 2|A^{-1}| \delta} |\vec{y} - \vec{x}|
\]

\[
= |\vec{A}| + \frac{\delta}{1 - 2|A^{-1}| \delta}.
\]

Since the eigenvectors depend continuously on the entries of a matrix when the eigenvalues remain distinct, we see that $\frac{1}{|\vec{y} - \vec{x}|} (\vec{y}' - \vec{x}')$ converges to an eigenvector of $\vec{A}$ as $\delta \to 0$ from formula (7.1).

Next, we show that $\frac{1}{|\vec{y} - \vec{x}|} (\vec{y}' - \vec{x})$ converges to an eigenvector corresponding to the eigenvalue $a_{n-m+1}$. Recall that $2 \sqrt{\frac{l}{a_{n-m+1}-\delta}} \leq |\vec{x} - \vec{y}|$ and $|\vec{x} - \vec{y}) - (\vec{x}' - \vec{y}')| \leq 2|A^{-1}| \delta$. So $\frac{1}{|y - x|} (y' - x)$ has the same limit as $\frac{1}{|y - x|} (y' - x')$. If $\vec{x}'$ and $\vec{y}'$ are such that $\frac{1}{|y - x|} (y' - x')$ converges to a eigenvector corresponding to $a_k$, then Lemma 7.5 below gives us the following chain of inequalities:

\[
|\vec{x} - \vec{y}| \leq |\vec{x}| + |\vec{y}|
\]

\[
\leq 2 \sqrt{(1+\theta)^2 + (n-1)\theta^2} \frac{l}{(a_k + \delta)(1-\theta)^2 + (n-1)(a_1 + \delta)\theta^2},
\]

where $\theta \to 0$ as $\delta \searrow 0$. We note that $k \geq n - m + 1$ because $a_k$ cannot be nonnegative. As $\delta \searrow 0$, the limit of the RHS of the above is $2 \sqrt{\frac{l}{a_k}}$. This gives a contradiction if $k > n - m + 1$, so $k = n - m + 1$. 


To show $\frac{1}{2}(\bar{x} + \bar{y}) \to 0$ as $\delta \searrow 0$: We now work out an upper bound for $\left|\frac{1}{2}(\bar{x} + \bar{y})\right|$ using Lemma 7.5. We get

$$\left|\frac{1}{2}(\bar{x} + \bar{y})\right| \leq \frac{1}{2}(x' + y') + \frac{1}{2}|A^{-1}\delta(\bar{x} + |\bar{y}|)$$

$$= \frac{1}{2}|x' - |y'|| + \frac{1}{2}|A^{-1}|\delta(|\bar{x}| + |\bar{y}|)$$

$$\leq \frac{1}{2}|\bar{x} - |y'|| + |A^{-1}|\delta(|\bar{x}| + |\bar{y}|)$$

$$\leq \frac{1}{2} \sqrt{\left|\frac{(1 + \theta)^2 + (n - 1)\theta^2}{(a_{n-m+1} + \delta)(1 - \theta)^2 + (n - 1)(a_1 + \delta)\theta^2} \right|} \left|\frac{l}{(a_{n-m+1} - \delta)(1 + \theta)^2 + (n - 1)(a_n - \delta)\theta^2} + |A^{-1}|\delta(|\bar{x}| + |\bar{y}|)\right|.$$  

Here, $\theta > 0$ is such that $\theta \to 0$ as $\delta \to 0$. At this point, we note that the final formula above can be written as $\frac{1}{2}\left(\sqrt{\frac{T}{c_1} - \sqrt{\frac{T}{c_2}}} + |A^{-1}|\delta(|\bar{x}| + |\bar{y}|)\right)$, where $c_1, c_2 < 0$, with $|c_1| < |c_2|$, and $c_1, c_2 \to a_{n-m+1}$ as $\delta \to 0$. Therefore

$$\left|\frac{1}{2}(\bar{x} + \bar{y})\right| \leq \frac{1}{2}\left(\sqrt{\frac{T}{c_1} - \sqrt{\frac{T}{c_2}}} + |A^{-1}|\delta(|\bar{x}| + |\bar{y}|)\right)$$

$$= \frac{1}{2} \frac{\sqrt{T} - \sqrt{T}}{\sqrt{c_1} + \sqrt{c_2}} + |A^{-1}|\delta(|\bar{x}| + |\bar{y}|)$$

$$\leq \frac{1}{2c_1c_2} \frac{l(c_2 - c_1)}{2\sqrt{\frac{T}{c_2}}} + |A^{-1}|\delta(|\bar{x}| + |\bar{y}|)$$

$$\leq \frac{c_2 - c_1}{4c_1} \frac{l}{\sqrt{\frac{T}{c_2}}} + |A^{-1}|\delta(|\bar{x}| + |\bar{y}|).$$

It is clear that as $\delta \to 0$, the above formula goes to zero, so $\left|\frac{1}{2}(\bar{x} + \bar{y})\right|^2/l \to 0$ as $\delta \to 0$ as needed. \qed

In Lemma 7.5 below, we say that $e_i$ is the $i$th elementary vector if it is the $i$th column of the identity matrix. It is also the eigenvector corresponding to the eigenvalue $a_k$ of $A$.

**Lemma 7.5. (Length estimates of vectors)** Let $h : \mathbb{R}^n \to \mathbb{R}$ and $A \in \mathbb{R}^{n \times n}$ satisfy Assumption 7.1 for some $\delta > 0$. Suppose $h(\bar{x}) = h(\bar{y}) = l < 0$. Suppose $\theta > 0$ is such that $|d_{\bar{x}} - e_k|_\infty < \theta$ for some $d_{\bar{x}}$ pointing in the same direction as $\bar{x}$, and that the same relation holds for $\bar{y}$.

Then $|\bar{x}|$ and $|\bar{y}|$ are bounded from below and above by

$$(1 - \theta)\sqrt{\frac{1}{(a_k - \delta)(1 + \theta)^2 + (n - 1)(a_n - \delta)\theta^2}} \leq |\bar{x}|, |\bar{y}|,$$

$$|\bar{x}|, |\bar{y}| \leq \sqrt{\frac{1}{(1 + \theta)^2 + (n - 1)\theta^2}} \frac{l}{(a_k + \delta)(1 + \theta)^2 + (n - 1)(a_1 + \delta)\theta^2}. $$
Proof. Necessarily we must have $k \geq n - m + 1$ because if $k < n - m + 1$, then the eigenvalue $a_k$ is positive, making the direction $e_k$ and its nearby directions directions of ascent. Let $d := d_x$. From $|d - e_k|_{\infty} < \theta$, we obtain $1 - \theta \leq d_k \leq 1 + \theta$ and $|d_j| < \theta$ for $j \neq k$.

For the direction $d$, we find the largest and smallest value for the norm of $\bar{x}$ if $\text{unit}(\bar{x}) = \text{unit}(d)$. This is also the largest and smallest possible value of $t$ such that $h(t \text{ unit}(d)) = l$. Here, $\text{unit}(\cdot)$ maps a nonzero vector to the unit vector of the same direction. Now

$$h(t \text{ unit}(d)) \leq \sum_{i=1}^{n} (a_i - \delta)(t \text{ unit}(d)_i)^2$$

$$= t^2 \sum_{i=1}^{n} (a_i - \delta) \frac{d_i^2}{\sum_{j=1}^{n} d_j^2}$$

$$\leq \frac{t^2}{\sum_{j=1}^{n} d_j^2} \left( (a_k - \delta)d_k^2 + (a_n - \delta) \sum_{j \neq k} d_j^2 \right)$$

$$\leq \frac{t^2}{(1 - \theta)^2} [(a_k - \delta)(1 + \theta)^2 + (n - 1)(a_n - \delta)\theta^2].$$

Since $h(t \text{ unit}(d)) = l$, we have

$$t \leq (1 - \theta) \sqrt{\frac{l}{(a_k - \delta)(1 + \theta)^2 + (n - 1)(a_n - \delta)\theta^2}}.$$

Next,

$$h(t \text{ unit}(d)) \geq \sum_{i=1}^{n} (a_i + \delta)(t \text{ unit}(d)_i)^2$$

$$= \frac{t^2}{\sum_{j=1}^{n} d_j^2} \sum_{i=1}^{n} (a_i + \delta)d_i^2$$

$$\geq \frac{t^2}{(1 + \theta)^2 + (n - 1)\theta^2} [(a_k + \delta)(1 - \theta)^2 + (n - 1)(a_1 + \delta)\theta^2].$$

Again, since $h(t \text{ unit}(d)) = l$, we have

$$t \geq \sqrt{[(1 + \theta)^2 + (n - 1)\theta^2] \frac{l}{(a_k + \delta)(1 - \theta)^2 + (n - 1)(a_1 + \delta)\theta^2}}.$$

□

Here are some lemmas on the completion of orthogonal matrices. In Lemmas 7.6 and 7.7 let $|\cdot|$ denote a norm for matrices (which need not be a matrix norm).

**Lemma 7.6.** (Completion to orthogonal matrix) Let $E_k \in \mathbb{R}^{n \times k}$ be the first $k$ columns of the $n \times n$ identity matrix. Then for all $\epsilon > 0$, there exists $\delta > 0$ such that if $V_k \in \mathbb{R}^{n \times k}$ has orthonormal columns and $|V_k - E_k| < \delta$, then $V_k$ can be completed to an orthogonal matrix $V_n \in \mathbb{R}^{n \times n}$ such that $|I - V_n| < \epsilon$.

The above lemma is an easy consequence of the following result.
Lemma 7.7. (Finding orthogonal vector) For all $\epsilon > 0$, there exists a $\delta > 0$ such that if $V_k \in \mathbb{R}^{n \times k}$ has orthonormal columns and $|V_k - E_k| < \delta$, then there is a vector $v_{k+1} \in \mathbb{R}^n$ such that $|v_{k+1}| = 1$ and is orthogonal to all columns of $V_k$, and the concatenation $V_{k+1} := [V_k, v_{k+1}]$ satisfies $|V_{k+1} - E_{k+1}| < \epsilon$.

Proof. Since all finite dimensional norms are equivalent, we can assume that the norm $|\cdot|$ on $\mathbb{R}^{n \times k}, \mathbb{R}^{n \times (k+1)}$ is the $\infty$-norm for vectors, that is $|M| = \max_{i,j} |M(i,j)|$. Suppose $|V_k - E_k| < \delta$. Then $|V_k(i,j)| < \delta$ if $i \neq j$ and $|V_k(i,i) - 1| < \delta$. We now construct the vector $v_{k+1}$ using the Gram-Schmidt process.

The direction of $v_{k+1}$ obtained by the Gram-Schmidt process is:

$$
(I - V_k V_k^T) e_{k+1} = e_{k+1} - V_k V_k^T e_{k+1} = e_{k+1} - \sum_{i=1}^k V_k(i, k+1) V_k(:, i).
$$

Since $|V_k(i,j)| < \delta$ for all $i \neq j$, the sum $\alpha_{k+1} \in \mathbb{R}^n$ defined by $\alpha_{k+1} = \sum_{i=1}^k V_k(i, k+1) V_k(:, i)$ has components obeying the bounds

$$
|\alpha_{k+1}(j)| \leq \begin{cases} 
  k\delta^2 & \text{if } j \geq k + 1, \\
  (k-1)\delta^2 + \delta & \text{if } j < k + 1.
\end{cases}
$$

Then $v_{k+1} = \text{unit}(e_{k+1} + \alpha_{k+1})$. We first analyze the maximum error in $v_{k+1}(j)$ for $j \neq k + 1$. The 2-norm of $e_{k+1} + \alpha_{k+1}$ is at least

$$
|e_{k+1} + \alpha_{k+1}|_2 \geq |e_{k+1}|_2 - |\alpha_{k+1}|_2
\geq 1 - \sqrt{\sum_{i=1}^n |\alpha_{k+1}(i)|^2}
\geq 1 - \sqrt{(n-k)k\delta^2 + k((k-1)\delta^2 + \delta)}
\geq 1 - \sqrt{n k \delta^2 + k \delta}.
$$

If $\delta < \min\{1, \frac{1}{4(n+1)k}\}$, then $\sqrt{n k \delta^2 + k \delta} \leq \frac{1}{2}$, and so $|e_{k+1} + \alpha_{k+1}|_2 \geq \frac{1}{2}$. In this case, the maximum error in $v_{k+1}(j)$ is $2((k-1)\delta^2 + \delta)$ for $j \neq k$. For $j = k + 1$, we note that $|v_{k+1}(k+1)| = 1$, which tells us that

$$
|v_{k+1}(k+1)|^2 = 1 - \sum_{1 \leq i \leq n, i \neq k} |v_{k+1}(i)|^2
\geq 1 - 4(n-1)[(k-1)\delta^2 + \delta]^2
\Rightarrow v_{k+1}(k+1) \geq \sqrt{1-4(n-1)[(k-1)\delta^2 + \delta]^2}
= \sqrt{1-4(n-1)\delta^2[(k-1)\delta + 1]^2}.
$$

If $\delta < \min\{1, \frac{1}{2k\sqrt{n-1}}\}$, then $4(n-1)\delta^2[(k-1)\delta + 1]^2 < 1$, which gives

$$
v_{k+1}(k+1) \geq \sqrt{1-4(n-1)\delta^2[(k-1)\delta + 1]^2}
\geq 1 - 4(n-1)\delta^2[(k-1)\delta + 1]^2
\Rightarrow |v_{k+1}(k+1)| - 1 \leq 4(n-1)\delta^2[(k-1)\delta + 1]^2.
$$

If $\delta < \min\{\frac{\epsilon}{2k}, \frac{\epsilon}{2k\sqrt{n-1}}\}$, then

$$
|\langle V_k, v_{k+1} \rangle - E_{k+1}| \leq \max\{2((k-1)\delta^2 + \delta), 4(n-1)\delta^2[(k-1)\delta + 1]^2\}
\leq \epsilon.
$$
and we are done.

The next result shows that we get a closer estimate to the critical value after each iteration of step 2 in Algorithm 6.5.

**Lemma 7.8. (Lower bound on critical value)** Let \( \delta > 0 \) be sufficiently small, and suppose \( h : \mathbb{R}^n \to \mathbb{R} \) satisfies Assumption 7.7. Let \( S_{\bar{z},V} := \{ \bar{z} + Vw \mid w \in \mathbb{R}^{n-m} \} \), and \( V \in \mathbb{R}^{n \times (n-m)} \) be such that \( V \) has orthonormal columns, with \( |\bar{z} - 0| < \delta \) and \( |V - E_{n-m}| < \delta \), where \( E_{n-m} \in \mathbb{R}^{n \times (n-m)} \) is the first \( n-m \) columns of the identity matrix. Then

\[
-\frac{1}{2} |A - \delta I| (1 + ||V^T (A - \delta I) V||^{-1} ||V^T A - \delta I||^2) |\bar{z}|^2 \leq \min_{s \in S_{\bar{z},V} \cap B} h(s).
\]

**Proof.** We find a lower bound for the smallest value of \( h \) on \( S_{\bar{z},V} \). The function \( h_{\bar{z},V} : \mathbb{R}^{n-m} \to \mathbb{R} \) defined by \( h_{\bar{z},V}(w) := h(\bar{z} + Vw) \) satisfies

\[
h_{\bar{z},V}(w) = h(\bar{z} + Vw) \geq \frac{1}{2} (\bar{z} + Vw)^T (A - \delta I) (\bar{z} + Vw).
\]

Let us denote \( h_{\bar{z},V,\min} : \mathbb{R}^{n-m} \to \mathbb{R} \) by \( h_{\bar{z},V,\min}(w) = \frac{1}{2} (\bar{z} + Vw)^T (A - \delta I) (\bar{z} + Vw) \). The Hessian of \( h_{\bar{z},V,\min} \) is \( V^T (A - \delta I) V \), which tells us that \( h_{\bar{z},V,\min} \) is strictly convex. Therefore, we seek to find the minimizer of \( h_{\bar{z},V,\min} \).

The minimizing value of \( w \), which we denote as \( \bar{w}_{\min} \), satisfies \( \nabla h_{\bar{z},V,\min}(\bar{w}_{\min}) = 0 \). This gives us

\[
V^T (A - \delta I) \bar{z} + V^T (A - \delta I) V \bar{w}_{\min} = 0 \\
\Rightarrow \bar{w}_{\min} = -[V^T (A - \delta I) V]^{-1} V^T (A - \delta I) \bar{z}.
\]

An easy bound on \( |\bar{w}_{\min}| \) is \( |\bar{w}_{\min}| \leq ||V^T (A - \delta I) V||^{-1} ||V^T A - \delta I|| |\bar{z}| \). So \( h_{\bar{z},V,\min} \) is bounded from below by

\[
\min_w h_{\bar{z},V,\min}(w) = \min_w \frac{1}{2} (\bar{z} + Vw)^T (A - \delta I) (\bar{z} + Vw) \\
= \frac{1}{2} (\bar{z} + V\bar{w}_{\min})^T (A - \delta I) (\bar{z} + V\bar{w}_{\min}) \\
\geq -\frac{1}{2} |\bar{z} + V\bar{w}_{\min}| (A - \delta I) |\bar{z} + V\bar{w}_{\min}| \\
= -\frac{1}{2} |A - \delta I||\bar{z} + V\bar{w}_{\min}|^2 \\
\geq -\frac{1}{2} |A - \delta I||\bar{z}| + |V\bar{w}_{\min}|^2 \\
= -\frac{1}{2} |A - \delta I||\bar{z}| + |\bar{w}_{\min}|^2 \\
\geq -\frac{1}{2} |A - \delta I|(||\bar{z}| + ||V\bar{w}_{\min}||)^2 \\
= -\frac{1}{2} |A - \delta I| (1 + ||V^T (A - \delta I) V||^{-1} ||V^T A - \delta I||^2) |\bar{z}|^2.
\]

We shall prove Lemma 7.9 about the approximation of the eigenvectors corresponding to the smallest eigenvalues. This lemma analyzes Algorithm 6.6. We clarify our notation. In the case of an exact quadratic, Algorithm 6.6 first finds
It is clear that as $e_n$, followed by $e_{n-1}$, $e_{n-2}$ and so on, all the way to $e_{n-m+2}$.

We define $I_k$ and $I_k^\perp$ as subsets of $\{1, \ldots, n\}$ by

$$I_k := \{n - m + 1\} \cup \{n - k + 2, n - k + 3, \ldots, n\}$$

$$I_k^\perp := \{1, \ldots, n\} \setminus I_k.$$

Next, we define $E_k^\perp$ and $E_k^\perp$. The matrix $E_k^\perp \in \mathbb{R}^{n \times k}$ has the $k$ columns $e_{n-m+1}, e_n, e_{n-1}, \ldots, e_{n-k+2}$, while the matrix $E_k^\perp \in \mathbb{R}^{n \times (n-k)}$ contains all the other columns in the $n \times n$ identity matrix. The columns of $E_k^\perp$ and $E_k^\perp$ are chosen from the $n \times n$ identity matrix from the index sets $I_k$ and $I_k^\perp$ respectively.

We will need to analyze the eigenvalues of $(V_k^\perp)^T(A \pm \delta I)V_k^\perp$ in the proof of Lemma 7.9 where $|V_k^\perp - E_k^\perp|$ is small. Note that the matrix $(E_k^\perp)^T(A \pm \delta I)E_k^\perp$ is principle minor of $A \pm \delta I$, and its eigenvalues are the eigenvalues of $A \pm \delta I$ chosen according to the index set $I_k^\perp$. Furthermore,

$$|(V_k^\perp)^T(A \pm \delta I)V_k^\perp - (E_k^\perp)^T(A \pm \delta I)E_k^\perp| \leq |(V_k^\perp)^T(A \pm \delta I)V_k^\perp - (V_k^\perp)^T(A \pm \delta I)E_k^\perp| + |(V_k^\perp)^T(A \pm \delta I)E_k^\perp - (E_k^\perp)^T(A \pm \delta I)E_k^\perp| \leq |(V_k^\perp)^T(A \pm \delta I)||V_k^\perp - E_k^\perp| + |(V_k^\perp)^T - (E_k^\perp)^T||(A \pm \delta I)E_k^\perp|$$

It is clear that as $|V_k^\perp - E_k^\perp| \to 0$, $|(V_k^\perp)^T(A \pm \delta I)V_k^\perp - (E_k^\perp)^T(A \pm \delta I)E_k^\perp| \to 0$. The eigenvalues of a matrix varies continuously with respect to the entries when the eigenvalues are distinct, so we shall let $\tilde{a}_i$ denote the eigenvalue of $(V_k^\perp)^T(A + \delta I)V_k^\perp$ that is closest to $a_i$, and $\tilde{a}_i$ denote the eigenvalue of $(V_k^\perp)^T(A - \delta I)V_k^\perp$ that is closest to $a_i$.

**Lemma 7.9.** (Estimates of eigenvectors to negative eigenvalues) Let $h : \mathbb{R}^n \to \mathbb{R}$. Given a fixed $l < 0$ sufficiently close to 0, let $p$ be the closest point to $\bar{z}$ in the set $\text{lev}_{\mathbb{R}^n} h \cap S_{\bar{z}, V_k^\perp}$, where $S_{\bar{z}, V_k^\perp} := \{\bar{z} + V_k^\perp w \mid w \in \mathbb{R}^{n-k}\}$ and $V_k^\perp \in \mathbb{R}^{n \times (n-k)}$. Then for all $\epsilon > 0$, there exists $\delta > 0$ such that if

1. $h : \mathbb{R}^n \to \mathbb{R}$ satisfies Assumption 7.7.
2. $|\bar{z}| < \delta$ and
3. $|V_k^\perp - E_k^\perp| < \delta$, where $V_k^\perp$ has orthogonal columns.

then $|h(p) - h_{\bar{z}, V_k^\perp, \max}(p) - e_{n-k+1}| < \epsilon$. As a consequence, $|V_m^\perp - E_m^\perp| \to 0$ as $\delta \to 0$.

**Proof.** The first step is to find an upper bound on the distance between $\bar{z}$ and $p$. The upper bound is obtained from looking at the closest distance between $\bar{z}$ and $\text{lev}_{\mathbb{R}^n} h \cap S_{\bar{z}, V_k^\perp}$.

We look at the function $h_{\bar{z}, V_k^\perp, \max} : \mathbb{R}^{n-k} \to \mathbb{R}$ defined by $h_{\bar{z}, V_k^\perp, \max}(w) := h_{\bar{z}, V_k^\perp, \max}(\bar{z} + V_k^\perp w)$. We have

$$h_{\bar{z}, V_k^\perp, \max}(w) = h_{\bar{z}, V_k^\perp, \max}(\bar{z} + V_k^\perp w)$$

$$= \frac{1}{2}(\bar{z} + V_k^\perp w)^T(A + \delta I)(\bar{z} + V_k^\perp w)$$

$$\Rightarrow \nabla h_{\bar{z}, V_k^\perp, \max}(w) = (V_k^\perp)^T(A + \delta I)\bar{z} + (V_k^\perp)^T(A + \delta I)V_k^\perp w.$$
for this critical value is \( \frac{1}{2} |\bar{z} + V_k^\perp \bar{w}| |A + \delta I||\bar{z} + V_k^\perp \bar{w}| \), which is in turn bounded by:

\[
\frac{1}{2} |\bar{z} + V_k^\perp \bar{w}| |A + \delta I||\bar{z} + V_k^\perp \bar{w}|
\]

\[
= \frac{1}{2} |A + \delta I| |\bar{z} + V_k^\perp \bar{w}|^2
\]

\[
\leq \frac{1}{2} |A + \delta I| (1 + \left| \left( (V_k^\perp)^T (A + \delta I)V_k^\perp \right)^{-1} \left( (V_k^\perp)^T |A + \delta I| \right)^2 \right| \bar{z}|^2.
\]

(following calculations similar to that of (7.2)).

Then an upper bound of the distance \( d(\bar{z}, \text{lev}_{\leq l} h_{\text{max}} \cap S_{\bar{z}, V_k^\perp}) \) can be calculated by:

\[
d(\bar{z}, S_{\bar{z}, V_k^\perp} \cap \text{lev}_{\leq l} h_{\text{max}})
\]

\[
\leq |\bar{z} - (\bar{z} + V_k^\perp \bar{w}_{\text{max}})| + d(\bar{z} + V_k^\perp \bar{w}_{\text{max}}, S_{\bar{z}, V_k^\perp} \cap \text{lev}_{\leq l} h_{\text{max}})
\]

\[
\leq |\bar{w}_{\text{max}}| + \sqrt{\frac{l - \frac{1}{2} |A + \delta I| (1 + \left| \left( (V_k^\perp)^T (A + \delta I)V_k^\perp \right)^{-1} \left( (V_k^\perp)^T |A + \delta I| \right)^2 \right| \bar{z}|^2}{\beta}}.
\]

The extra term \(-\frac{1}{2} |A + \delta I| \cdots \bar{z}|^2\) compensates for the fact that the critical value of \( h_{\bar{z}, V_k^\perp, \text{max}} \) is not necessarily zero. To simplify notation, let \( \beta \) be the right hand side of the above formula as marked.

We now figure the possible intersection between \( B(\bar{z}, \beta) \) and \( S_{\bar{z}, V_k^\perp} \cap \text{lev}_{\leq l} h \).

Again, since \( S_{\bar{z}, V_k^\perp} \cap \text{lev}_{\leq l} h \subset S_{\bar{z}, V_k^\perp} \cap \text{lev}_{\leq l} h_{\text{min}} \), we look at the intersection of \( B(\bar{z}, \beta) \) and \( S_{\bar{z}, V_k^\perp} \cap \text{lev}_{\leq l} h_{\text{min}} \). We find the critical point of \( h_{\bar{z}, V_k^\perp, \text{min}} : \mathbb{R}^{n-k} \rightarrow \mathbb{R} \) defined by \( h_{\bar{z}, V_k^\perp, \text{min}}(w) := \frac{1}{2} (\bar{z} + V_k^\perp w)^T (A - \delta I)(\bar{z} + V_k^\perp w) \). The gradient of \( h_{\bar{z}, V_k^\perp, \text{min}} \) can be found to be

\[
\nabla h_{\bar{z}, V_k^\perp, \text{min}}(w) = (V_k^\perp)^T (A - \delta I)\bar{z} + (V_k^\perp)^T (A - \delta I)V_k^\perp w.
\]

Once again, the critical point is \( \bar{w}_{\text{min}} = ((V_k^\perp)^T (A - \delta I)V_k^\perp)^{-1} (V_k^\perp)^T (A - \delta I)\bar{z} \). So \( B(\bar{z}, \beta) \subset B(\bar{z} + V_k^\perp \bar{w}_{\text{min}}, \beta + |\bar{w}_{\text{min}}|) \).

Consider \( p \in B(\bar{z} + V_k^\perp \bar{w}_{\text{min}}, \beta + |\bar{w}_{\text{min}}|) \cap (S_{\bar{z}, V_k^\perp} \cap \text{lev}_{\leq l} h_{\text{min}}) \). Let us introduce a change of coordinates such that \( p = \sum_{i \in I_k^c} \tilde{p}_i \tilde{v}_i + \bar{w}_{\text{min}} \), where \( \tilde{v}_i \in \mathbb{R}^{n-k} \) correspond to the eigenvectors of \( (V_k^\perp)^T (A - \delta I)V_k^\perp \) (in turn corresponding to the eigenvalues \( \tilde{a}_i \) and \( \tilde{\mu}_i \)). Then the condition \( \bar{z} + V_k^\perp p \in B(\bar{z} + V_k^\perp \bar{w}_{\text{min}}, \beta + |\bar{w}_{\text{min}}|) \) and \( \bar{z} + V_k^\perp p \in S_{\bar{z}, V_k^\perp} \cap \text{lev}_{\leq l} h_{\text{min}} \) can be represented as the following constraints respectively:

\[
\sum_{i \in I_k^c} \tilde{p}_i^2 \leq (\beta + |\bar{w}_{\text{min}}|)^2,
\]

\[
\sum_{i \in I_k^c} \tilde{a}_i \tilde{p}_i^2 \leq 1 + \frac{1}{2} ((\bar{z} + V_k^\perp \bar{w}_{\text{min}})^T (A - \delta I)(\bar{z} + V_k^\perp \bar{w}_{\text{min}})).
\]

As \( \delta \rightarrow 0 \), the only admissible solution is \( \tilde{p}_{n-k+1} = \sqrt{\frac{1}{\tilde{a}_{n-k+1}}} \) and the rest of the \( \tilde{p}_i \)’s are zero. The above constraints are linear in \( \tilde{p}_i^2 \). We consider the minimum
possible value of \( \bar{\rho}_{n-k+1} \) is defined by \( \bar{\rho}_{n-k+1} = \sqrt{\frac{\bar{p}_{n-k+1}}{\sum p_i^2}} \), which is the dot product between the unit vectors in the direction of \( \bar{v}_{n-k+1} \) and \( p - (\bar{z} + V_k^+ \bar{w}_{\min}) \). This is equivalent to the linear fractional program in \( p_i^2 \) of minimizing \( \frac{\bar{p}_{n-k+1}}{\sum p_i^2} \) subject to the constraints in \( (7.3) \).

This linear fractional program can be transformed into a linear program by \( q = \frac{1}{\sum p_i^2} \) and \( q_i = \frac{\tilde{p}_i^2}{\sum p_i^2} \), which gives:

\[
\min \quad q_{n-k+1} \quad \text{s.t.} \quad q \geq \frac{1}{(\beta + |\bar{w}_{\min}|)^2},
\]

\[
\sum_{i \in I_k^+} \tilde{a}_i q_i \leq \left[ l + \frac{1}{2}(\bar{z} + V_k^+ \bar{w}_{\min})^T (A - \delta I)(\bar{z} + V_k^+ \bar{w}_{\min}) \right] q + \tilde{a}_{n-1},
\]

\[
\sum_{i \in I_k^+} q_i = 1, \quad q_i \geq 0 \text{ for all } i \in I_k^+.
\]

The constraints of the linear program above gives

\[
\sum_{i \in I_k^+} (-\tilde{a}_i + \tilde{a}_{n-k}) q_i \geq - \left[ l + \frac{1}{2}(\bar{z} + V_k^+ \bar{w}_{\min})^T (A - \delta I)(\bar{z} + V_k^+ \bar{w}_{\min}) \right] q + \tilde{a}_{n-1}
\]

\[
\Rightarrow \quad \sum_{i \in I_k^+} (-\tilde{a}_i + \tilde{a}_{n-k}) q_i \geq - \frac{l + \frac{1}{2}(\bar{z} + V_k^+ \bar{w}_{\min})^T (A - \delta I)(\bar{z} + V_k^+ \bar{w}_{\min})}{(\beta + |\bar{w}_{\min}|)^2} + \tilde{a}_{n-1}.
\]

Since only \( -\tilde{a}_{n-k+1} + \tilde{a}_{n-k} \) is positive and the other \( -\tilde{a}_i + \tilde{a}_{n-k} \) are nonpositive, we have

\[
\frac{(-\tilde{a}_{n-k+1} + \tilde{a}_{n-k}) q_{n-k+1}}{(-\tilde{a}_{n-k+1} + \tilde{a}_{n-k}) \sum_{i \in I_k^+} (\tilde{a}_i + \tilde{a}_{n-k}) q_i} \geq - \frac{l + \frac{1}{2}(\bar{z} + V_k^+ \bar{w}_{\min})^T (A - \delta I)(\bar{z} + V_k^+ \bar{w}_{\min})}{(\beta + |\bar{w}_{\min}|)^2} + \tilde{a}_{n-k}
\]

\[
\Rightarrow q_{n-k+1} \geq \frac{1}{-\tilde{a}_{n-k+1} + \tilde{a}_{n-k}} \left( - \frac{l + \frac{1}{2}(\bar{z} + V_k^+ \bar{w}_{\min})^T (A - \delta I)(\bar{z} + V_k^+ \bar{w}_{\min})}{(\beta + |\bar{w}_{\min}|)^2} + \tilde{a}_{n-k} \right).
\]

The limit of the right hand side goes to 1 as \( \delta \to 0 \), so this means that \( \bar{z} - p \) is close to the direction of the eigenvector corresponding to the eigenvalue \( \tilde{a}_{n-k+1} \) in \( (V_k^+)^T AV_k^+ \), which in turn converges to \( e_{n-k+1} \). The proof of this lemma is complete.

The conclusion that \( |V_m^+ - E_m^+| \to 0 \) as \( \delta \to 0 \) follows from the first part of this lemma and Lemma 7.6.

With these lemmas set up, we are now ready to prove the fast local convergence of Algorithm 6.5 to the critical point and critical value. We recall that Q-linear convergence of a sequence of positive numbers \( \{\alpha_i\}_{i=1}^\infty \) converging to zero is defined by \( \lim \sup_{i \to \infty} \frac{\alpha_{i+1}}{\alpha_i} < 1 \), while Q-superlinear convergence is defined by \( \lim_{i \to \infty} \frac{\alpha_{i+1}}{\alpha_i} = 0 \). Next, R-linear convergence and R-superlinear convergence of a
Theorem 7.10. (Fast convergence of Algorithm 6.5) Suppose that

Theorem 7.10. Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is $C^2$ and $0$ is a nondegenerate critical point of $f$ of Morse index $m$, and $h(0) = 0$.

There is some $R > 0$ such that if $0 < r < R$, then for $U_i = B(0, r)$ and $l_0 < 0$ (depending on $r$) sufficiently close to 0, Algorithm 6.5 converges $R$-superlinearly to the critical point $0$ and $Q$-superlinearly to the critical value $0$ provided that at each iteration, there exists an optimizing triple $(S_i, x_i, y_i)$ for which $(x_i, y_i)$ is the unique pair of points $S_i \cap (\text{lev}_{\geq l_i}) \cap B(0, r)$ such that $|x_i - y_i| = \text{diam}(S_i \cap (\text{lev}_{\geq l_i}) \cap B(0, r))$.

If a sufficiently good approximate for the lineality space of each $S_i$ is available in step 2 of Algorithm 6.5 instead, then Algorithm 6.5 converges $R$-linearly to the critical point and $Q$-linearly to the critical value.

Proof. As a reminder, $Q$-linear convergence of the critical value is defined to be $\limsup_{i \to \infty} \frac{|l_{i+1}|}{|l_i|} < \infty$, and $Q$-superlinear convergence of the critical value is defined to be $\lim_{i \to \infty} \frac{|l_{i+1}|}{|l_i|} = 0$. From the $Q$-linear ($Q$-superlinear) convergence of $l_i$, we obtain the $R$-linear ($R$-superlinear) convergence of the critical point by observing that $\limsup_{i \to \infty} \frac{|l_i|}{\sqrt{|l_i|}} < \infty$, and that $\sqrt{|l_i|}$ converges $Q$-linearly ($Q$-superlinearly).

Since $f$ is $C^2$, for all $\delta > 0$, we can find $R > 0$, such that

$$|f(x) - x^T Ax| < \delta |x|^2$$

for all $x \in B(0, R)$.

The function $f_R : \mathbb{R}^n \to \mathbb{R}$ defined by $f_R(x) := \frac{1}{R^2} f(Rx)$ satisfies Assumption 7.1 with $A := \nabla^2 f_R(x) = \nabla^2 f(x)$.

We want to show that if $\delta > 0$ is sufficiently small, then for all $l < 0$ sufficiently small, a step in Algorithm 6.5 gives good convergence to the critical value. Given an iterate $l_i$, the next iterate $l_{i+1}$ is

$$\min_{x \in S_{l_i}, V_{l_i} \cap B(0, R)} f(x) = \min_{x \in S_{l_i}, \sqrt{\delta} \cap B} R^2 f_R(x),$$

where $V_{l_i}$, which approximates the first $n-m$ eigenvectors, is defined before Lemma 7.9.

We seek to find $\frac{|l_{i+1}|}{|l_i|}$. The value of $l_{i+1}$ depends on how well the last $m$ eigenvectors are approximated, and how well the critical point is estimated, which in turn depends on $\delta$. The ratio $\frac{|l_{i+1}|}{|l_i|}$ is bounded from above by

$$\frac{1}{2} |A - \delta I| (1 + \frac{1}{2} (V_{l_i}^T (A - \delta I) V_{l_i}^{-1} + (V_{l_i}^{-1})^T A - \delta I)^2 |z_i|^2 / l_i,$$

which converges to 0 as $\delta \to 0$ by Lemmas 7.4, 7.6, 7.8 and 7.9.

The conclusion in the second part of the theorem follows a similar analysis. \[QED\]

8. Conclusion and conjectures

In this paper, we present a strategy to find saddle points of general Morse index, extending the algorithms for finding critical points of mountain pass type as was done in [12]. Algorithms 6.5 and 6.6 may not be easily implementable, especially when $m$ is large. However, Algorithm 6.6 can be performed only as needed in a practical implementation. It is hoped that this strategy can augment current
methods for finding saddle points, and can serve as a foundation for further research on effective methods of finding saddle points.

Here are some conjectures:

- How do the algorithms presented fare in real problems? Are there difficulties in the infinite dimensional case when implementing Algorithm 6.5?
- Are there ways to integrate Algorithms 6.5 and 6.6 to give a better algorithm?
- Are there better algorithms than Algorithm 6.6 to approximate $S_i$?
- Can the uniqueness assumption in Theorem 7.10 be lifted? If not, how does it affect the design of algorithms?

Acknowledgement. I thank the Fields Institute in Toronto, where much of this paper was written. They have provided a wonderful environment for working on this paper.

References

[1] A. Ambrosetti and P.H. Rabinowitz, *Dual variational methods in critical point theory and applications*, J. Funct. Anal., 14 (1973), 349-381
[2] V. Barutello and S. Terracini, *A bisection algorithm for the numerical mountain pass*, Nonlinear differ. equ. appl. 14 (2007) 527-539.
[3] J.F. Bonnans and A. Shapiro, *Perturbation Analysis of Optimization Problems*, Springer, NY, 2000.
[4] Y.S. Choi and P. J. McKenna, *A mountain pass method for the numerical solution of semilinear elliptic problems*, Nonlinear Anal., 20 (1993), pp. 417-437.
[5] F.H. Clarke, *Optimization and Nonsmooth Analysis*. Wiley, New York, 1983. Republished as Vol. 5, Classics in Applied Mathematics, SIAM, 1990.
[6] Zhonghai Ding, David Costa and Goong Chen, *A high-linking algorithm for sign-changing solutions of semilinear elliptic equations*, Nonlinear Analysis 38 (1999) 151-172.
[7] M. Degiovanni and M. Marzocchi, *A critical point theory for nonsmooth functionals*, Ann. Math. Pura. Appl. 167 (1994), pp. 73-100
[8] Y. Jabri, *The Mountain Pass Theorem: Variants, Generalizations and Some Applications*, Cambridge, UK, 2003.
[9] J. Horák, *Constrained mountain pass algorithm for the numerical solution of semilinear elliptic problems*, Numerische Mathematik 98 (2004) 251-276.
[10] A.D. Ioffe and E. Schwartzman, *Metric critical point theory 1: Morse regularity and homotopic stability of a minimum*, J. Math Pures Appl. 75 (1996), pp. 125-153.
[11] G. Katriel, *Mountain pass theorem and a global homeomorphism theorem*, Ann. Institut Henri Poincaré, Analyse Non Linéaire, 11 (1994), pp. 189-209.
[12] A.S. Lewis and C.H.J. Pang, *Level set methods for finding critical points of mountain pass type*, submitted, 2009. Available at http://arxiv.org/abs/0906.4466
[13] Yongxin Li and Jianxin Zhou, *A minmax method for finding multiple critical points and its applications to semilinear PDES*, SIAM J. Sci. Comput., Vol 23, No. 3, pp 840-865, 2001.
[14] P.H. Rabinowitz, *Some critical point theorems and applications to semilinear elliptic partial differential equations*, Ann. Scuola Norm. Sup. Pisa, 5, 412-424 (1977)
[15] B. Rustem and M. Howe, *Algorithms for Worst-Case Design and Applications to Risk Management*, Princeton, NJ, 2003
[16] M. Schechter, *Linking Methods in Critical Point Theory*, Birkhauser, Boston, 1999.
[17] M. Struwe, *Variational Methods*, 3rd edition, Springer, 2000.

Current address: Department of Combinatorics and Optimization, Mathematics, University of Waterloo.

E-mail address: chj2pang@math.uwaterloo.ca