FINDING MULTIPLE SADDLE POINTS FOR G-DIFFERENTIAL FUNCTIONALS AND DEFOCUSED NONLINEAR PROBLEMS

A Dissertation

by

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ABSTRACT

We study computational theory and numerical methods for finding multiple unstable solutions (saddle points) for two types of nonlinear variational functionals. The first type consists of Gateaux differentiable (G-differentiable) M-type (focused) problems. Motivated by quasilinear elliptic problems from physical applications, where energy functionals are at most lower semi-continuous with blow-up singularities in the whole space and G-differntiable in a subspace, and mathematical results and numerical methods for $\mathcal{C}^1$ or nonsmooth/Lipschitz saddle points existing in the literature are not applicable, we establish a new mathematical frame-work for a local minimax method and its numerical implementation for finding multiple G-saddle points with a new strong-weak topology approach. Numerical implementation in a weak form of the algorithm is presented. Numerical examples are carried out to illustrate the method. The second type consists of $\mathcal{C}^1$ W-type (defocused) problems. In many applications, finding saddles for W-type functionals is desirable, but no mathematically validated numerical method for finding multiple solutions exists in literature so far. In this dissertation, a new mathematical numerical method called a local minmaxmin method (LMMM) is proposed and numerical examples are carried out to illustrate the efficiency of this method. We also establish computational theory and present the convergence results of LMMM under much weaker conditions. Furthermore, we study this algorithm in depth for a typical W-type problem and analyze the instability performances of saddles by LMMM as well.

DEDICATION

To my mother, my father, my grandmother, and my grandfather.

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NOMENCLATURE

LMM	local minimax method
LMMM	local minmaxmin method
LMO	local min-$\perp$ method
LMO-W	local min-$\perp$ method under a weakened condition
SCP	search for critical points
MI	Morse index
DWF	defocused W-type functional
LLC	locally Lipschitz continuous
PDE	partial dierential equation
Itn	iteration number

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1. INTRODUCTION

In condensed matter physics, nonlinear optics, dynamics of biomolecules, etc, multiple solutions with different performance and instability indices exist. For example, excited states are of great interests in the study of self-guided light waves in nonlinear optics [38, 34, 37, 30, 35, 48]. All those excited states are unstable solutions. Stability is one of the main concern in control theory and system design. However, the performance and maneuverability are more desirable in many application such as system design and combat machinery. Since for most nonlinear multiple solution problems, analytic solutions are too difficult to find, development of numerical methods to compute multiple solutions becomes especially important for providing choice or balance between stability and maneuverability or performance.

Let H be a Hilbert space with its inner product $\langle \cdot, \cdot \rangle$ and norm $\| \cdot \|$. Let $J : H \to \mathbb{R}$ be a $\mathcal{C}^1$ functional. A point $u \in H$ is called a critical point of J if its Frechet derivative, $J'(u) = 0$. Critical points u that are not local extrema of J are called saddle points, or saddles, i.e., in any neighborhood of u there are v, w such that $J(v) < J(u) < J(w)$. An index-k saddle point or k-saddle is a critical point that is a local maximum of J in a k-dimensional subspace and a local minimum of J in the corresponding k-co-dimensional subspace. Critical points correspond to local equilibrium states in a physical process. Thus mathematically, a ground state as a stable local equilibrium is a local minimum point or 0-saddle, excited states, as unstable local equilibria, correspond to saddles and metastable states are among the first few saddles. Comparing to a local minimum computation, numerical search for saddles is much more challenging due to their nonlinearities, instabilites and multiplicities.

When finding critical points for variational problems, we need to investigate differentiabilities and structures of energy functionals. For the differentiability, a functional can be $\mathcal{C}^1$, locally Lipschitz continuous or others. For the structure, a functional can be M-type (focused) or W-type (defocused), see Figure 1.1 below. The methods mentioned in the survey below apply to M-type problems which are either $\mathcal{C}^1$ or locally Lipschitz continuous.

In this thesis, however, we are interested in finding multiple unstable solutions for a class of G-differential functionals with M-type structures and a class of $\mathcal{C}^1$ functionals with W-type structures. We also study computational theory and instability analysis for the relevant methods.

1.1 A Brief Survey on Methods for Solving Nonlinear PDEs

First, we give a brief review on critical point theory. Critical point theory is a classical and still very active area in mathematics. There are numerous reference books and articles on this topic. In the literature, critical points of a $\mathcal{C}^1$ functional are called smooth critical points and critical points of a locally Lipschitz continuous functional are called nonsmooth critical points. Algorithms such as the mountain pass method proposed by Choi-Mckenna [24], the linking method by Ding-Costa-Chen [28] and the local minimax method by Li-Zhou [39, 41, 45, 47, 51] were applied successfully for finding multiple smooth critical points. By using the generalized gradient of Clarke [11] for a locally Lipschitz continuous functional, nonsmooth critical points were first introduced by Chang [7] in 1981, and they were further studied by Kourogenis-Papageorgious [36, 43, 29, 42, 46] and Yao [54, 46].

Assume $J \in \mathcal{C}^2(H, \mathbb{R})$, $J''(u^*){:}H \to H$ is a self-adjoint Fredholm operator. According to the spectral theory, H has an orthogonal spectral decomposition

$$H = H^- \oplus H^0 \oplus H^+,$$

where H^-, H^0, H^+ are respectively the maximum negative definite, the null and the maximum positive definite subspace of $J''(u^*)$ in H with $dim(H^0) < \infty$, and are invariant under $J''(u^*)$. By the Morse theory, we have *Morse index* $MI(u^*) = dim(H^-)$. We call u^* a non-degenerate critical point if $H^0 = \{0\}$ and a degenerate critical point if $H^0 \neq \{0\}$. For any closed subspace W of H, let $S_W = \{u \mid u \in W, \|u\| = 1\}$ be the unit sphere in W.

Definition 1.1. *For a functional $J \in \mathcal{C}^1(H, \mathbb{R})$, we call $\{u_n\}$ a Palais-Smale (PS) sequence if $J(u_n)$ is bounded and $J'(u_n) \to 0$.*

Definition 1.2. *A functional $J \in \mathcal{C}^1(H, \mathbb{R})$ is said to satisfy the PS condition, if any PS sequence has a convergent subsequence.*

Definition 1.3. *Let L be a closed subspace of H and $L \oplus L^\perp = H$ be the orthogonal decomposition. Denote $[L, v] = \{tv + v_L \mid t \in \mathbb{R}, v_L \in L\}$ for each $v \in S_{L^\perp}$. A set-valued mapping P: $S_{L^\perp} \to 2^H$ is called the peak mapping of J $w.r.t$ $H = L \oplus L^\perp$ if $P(v)$ is the set of all local maximum points of J on $[L, v]$.*

A single-valued mapping p: $S_{L^\perp} \to H$ is called a peak selection of J $w.r.t$ L if $p(v) \in P(v)$, $\forall v \in S_{L^\perp}$. For a given $v \in S_{L^\perp}$, if such p is locally defined in $\mathcal{N}(v) \cap S_{L^\perp}$, where $\mathcal{N}(v)$ is a neighborhood of v, then p is called a local peak selection of J at v.

1.1.1 Some approaches in critical point theory

Because our objective is to find multiple critical points numerically, we select those methods which provide information about locations or local structures of critical points.

Theorem 1.1. *(Ljusternik-Schnireelmann) [17] If $J \in \mathcal{C}^1(H, \mathbb{R})$ and J is even, then $J|_{S^{m-1}}$ has at least m distinct pairs of critical points.*

Typically a minimax type critical point can be characterized by the Ljusternik-Schnirelman principle (LSP) [16]

$$\min_{A \in \mathcal{A}} \max_{u \in A} J(u),$$

where $\mathcal{A}$ is a collection of certain compact sets A, e.g., a k-D simplex. Max and Min are all in the global sense.

Theorem 1.2. *(The Mountain Pass Lemma) [1] Let $J \in \mathcal{C}^1(H, \mathbb{R})$ satisfy the PS condition. Suppose that there exists $r > 0$ and $p \in H$ with $\|p\| > r$ such that*
i) $f(0) < a$, $f(p) < a$, for some real number a,
ii) $f(x) \geq a$ for any x, $\|x\| = r$. Then

$$c = \inf_{f \in C([0,1]), f(0)=0, f(1)=p} \max_{t \in [0,1]} J(f(t))$$

is a critical value.

The Mountain Pass Lemma is a special case of LSP by using 1-D line segments as compact sets in the inner level and a global minimization is still used in the outer level.

Theorem 1.3. *(Saddle Point Theorem) [5] Let $H = L \oplus X$, where X is a subspace of H and L is a finite dimensional subspace. Assume that $J \in \mathcal{C}^1(H, \mathbb{R})$ satisfies the PS condition and*
i) there is a constant α and a bounded neighborhood $\mathcal{D}$ of 0 in L such that $J_{\partial\mathcal{D}} \leq \alpha$,
ii) there is a constant $\beta > \alpha$ such that $J|_X \geq \beta$, then

$$c = \inf_{h \in \Gamma} \max_{u \in \bar{\mathcal{D}}} J(h(u))$$

is a critical value, where $\Gamma = \{h \in C(\bar{\mathcal{D}}, H) \mid h|_{\partial\mathcal{D}} = id\}$.

Theorem 1.4. *(Linking Theorem) [5] Let $H = L \oplus X$, where X is a subspace of H and L is a finite dimensional subspace. Suppose that $J \in \mathcal{C}^1(H, \mathbb{R})$ satisfies the PS condition and*
i) there are constants ρ, $\alpha > 0$ such that $J|_{\partial B_\rho \cap X} \geq \alpha$,

ii) there is $v \in X$, $\|v\| = 1$ *and* $R > \rho$ *such that if* $Q = (\bar{B}_R \cap L) \oplus \{rv \mid 0 < r < R\}$, *then* $J|_{\partial Q} \leq 0$.

Then

$$c = \inf_{h \in \Gamma} \max_{u \in \bar{Q}} J(h(u))$$

is a critical value, where

$$\Gamma = \{h \in \mathcal{C}(\bar{Q}, H) \mid h|_{\partial Q} = id\}.$$

Theorem 1.5. *(Local Minimax Theorem) [39] Assume* $J : H \to \mathbb{R}$ *is* $\mathcal{C}^1$ *and satisfies the PS condition, and that* $L \subset H$ *is a closed subspace with* $H = L \bigoplus L^{\perp}$. *If there exists a peak selection* p *of* J *w.r.t.* L *such that*

(i) $c = \inf_{v \in O \cap S_{L^{\perp}}} J(p(v)) > -\infty$ *for some open set* $O \subset H$,

(ii) $\inf_{v \in \partial O \cap S_{L^{\perp}}} J(p(v)) = b > c$,

(iii) $p(v)$ *is continuous in* $\bar{O} \cap S_{L^{\perp}}$, *and*

(iv) $d(p(v), L) \geq \alpha$ *for some* $\alpha > 0$ *and all* $v \in O \cap S_{L^{\perp}}$,

then c *is a critical value, i.e, there exists* $v_0 \in O \cap S_{L^{\perp}}$ *such that*

$$J'(p(v_0)) = 0, J(p(v_0)) = c = \min_{v \in O \cap S_{L^{\perp}}} J(p(v)).$$

1.1.2 Some existing numerical methods to solve unstable solutions for nonlinear PDEs

All numerical methods mentioned below apply to M-type functionals which are either $\mathcal{C}^1$ or locally Lipschitz continuous.

From the algorithmic point of view, LSP is not applicable for a numerical implementation since both the maximization and minimization are in the global sense. Chio and

McKenn partly overcame this difficulty by proposing a minimax algorithm [24]. Based on the Mountain Pass Lemma and an idea from Aubin and Ekeland [14], Choi and McKenna proposed a numerical minimax algorithm called a mountain pass method to solve for a solution with $MI = 1$. Since a flow chart of the algorithm is not provided in [24], this algorithm has been modified and further rewritten in [33] as the modified mountain pass method.

Modified Mountain Pass Method [33]

Step 1. Given an initial v_0 and ε. Let $k = 0$, compute $u_k = \arg\max_{t>0} J(tu)$.

Step 2. Compute the steepest vector $d_k = -J'(u_k)$.

Step 3. If $\|d_k\| < \varepsilon$, output u_k, otherwise, continue.

Step 4. Solve for $u^k = \arg\min_{s>0} \max_{t>0} J(t(u_k + sd_k))$. Update $k = k + 1$, then go to Step 2.

The modified mountain pass method is a variational method which computes mountain pass solutions with Morse index 1 of a functional J. The merits of this algorithm are that (i) in the inner level, a maximization is taken over an affine line starting from 0 and (ii) to use the steepest descent direction to search for a local minimum in the outer level.

High Linking Method [28]

A high linking method is proposed in [28] by Ding-Costa-Chen to solve for a sign-changing solution. This method uses a constrained maximization in the first level and a local minimization in the second level and it is the first algorithm in the literature to use the idea of a "local link" to find solutions with $MI = 2$.

Step 1. Given an initial $v_0 \in H_0^1(\Omega)$ s.t. $v_0 \neq 0$ and $J(v_0) \leq 0$.

Step 2. Solve for a mountain pass solution $u_1 \in H_0^1(\Omega)$, such that for w_1, $w_2 \in H_0^1(\Omega)$ and $0 < |t| < \delta$,

$$J(u_1 + tw_1) < J(u_1), J(u_1 + tw_2) > J(u_1).$$

Step 3. Find t_1, t_2 and t_3 s.t. $J(u_1 + t_1 w_1) \leq 0$, $J(u_1 + t_2 w_1) \leq 0$, and $J(u_1 + t_3 w_2) \leq J(u_1)$. Set $g_1 = u_1 + t_1 w_1$, $g_2 = u_1 + t_2 w_1$ and $g_3 = u_1 + t_3 w_2$.

Step 4. Construct a triangle $\Delta \in H_0^1(\Omega)$ by

$$\Delta = \{\lambda_1 g_1 + \lambda_2 g_2 + (1 - \lambda_1 - \lambda_2) g_3 \mid \lambda_1 \geq 0, \lambda_2 \geq 0, \lambda_1 + \lambda_2 \leq 1\},$$

solve for $u^* \in \Delta$ such that $J(u^*) = \max_{g \in \Delta} J(g)$.

Step 5. If u^* is an interior point of the triangle Δ, go to Step 6, otherwise, set $w_2 = u^* - u_1$ and go to Step 3.

Step 6. Set $u_2 = u^*$, compute $d = J'(u_2)$. If $\|d\| < \varepsilon$, output u_2 and stop, otherwise, set $w_2 = (-d + u_2) - u_1$ and continue.

Step 7. Repeat Steps 3-5 to update the triangle and find an updated interior point w^* such that $J(u^*) = \max_{g \in \Delta} J(g)$.

Step 8. If $J(u^*) < J(u_2)$, go to Step 6, otherwise, set $d = 0.5d$, $w_2 = (-d + u_2) - u_1$ and go to Step 7.

Local Minimax Method (LMM) [39]

Step 1. Given $\varepsilon, \lambda > 0$. Let $n - 1$ critical points w_1, w_2, $\cdots$, w_{n-1} of J be previously found and w_{n-1} has the highest critical value. Set $L = [w_1, w_2, \cdots, w_{n-1}]$. Let $v_0 \in L^{\perp}$ be an ascent direction at w_{n-1}.

Step 2. Set $k = 0$, use v_0 as an initial to solve for

$$\begin{aligned} w^k &= p(v_0) = t_0 v_0 + t_1 w_1 + \cdots + t_{k-1} w_{k-1} \\ &= \arg\max\{J(s_0 v_0 + s_1 w_1 + \cdots + s_{k-1} w_{k-1}) \mid s_i \in \mathbb{R}, i = 0, 1, \cdots, n-1\}. \end{aligned}$$

Step 3. Compute $d^k = J'(w^k)$. If $\|d^k\| < \varepsilon$, output $w_n = w^k$, otherwise go to Step 4.

Step 4. Denote $v_k(s) = \dfrac{v_k + s d_k}{\|v_k + s d_k\|}$ for $s > 0$. Solve for

$$p(v_k(s)) = \arg\max\Big\{J(s_0 v_k(s) + \sum_{i=1}^{k-1} s_i w_i) \mid s_i \in \mathbb{R}, i = 0, 1, \cdots, k-1\Big\},$$

then set $w^{k+1} \equiv p(v_{k+1}) \equiv p(v_k(s^k))$, where s^k satisfies

$$s^k = \max\{s = \frac{\lambda}{2^m} \mid m \in N, J(p(v_k(s))) - J(p(v_k)) \leq -\frac{1}{4}|t_0| s \|d_k\|^2\}.$$

Step 5. Update $k = k + 1$ and go to Step 3.

LMM is a two-level optimization method to solve for multiple solutions of nonlinear PDEs in a variational order. It uses a local maximization in a subspace in the inner level which makes the numerical implementation much easier, and with the stepsize rule, the convergence of the algorithm can be established as well. The support subspace is used in the method to determine the Morse index of a solution and separate a new solution from the old ones. When the support subspace is set to be 0, LMM reduces to the modified mountain pass method. To the best of our knowledge, LMM is the first mathematically justified numerical method which can find multiple unstable critical points with high Morse index ($MI \geq 2$).

Local Min-$\perp$ Method (LMO)[45]

LMO generalizes the minimax principle which is the most popular approach in critical point theory, and it plays a crucial role for the development of our new method in Chapter 3. LMO theorem was presented in [45] and will be restated in Chapter 3. Here we just review the flow chart for it.

Given ε, $\lambda > 0$ and n previously found critical points $u_1, \cdots, u_n$ of J. u_n has the highest critical value. Let $L = [u_1, u_2, \cdots, u_n]$.

Step 1. Choose $v_k \in S_{L^\perp}$ to be an ascent direction at u_n.

Step 2. Set $k = 1$. Use v_k as an initial to solve for $u^k \equiv p(v_k) \in [L, v_k] \setminus L$ from

$$\langle J'(u^k), v_k \rangle = 0, \cdots, \langle J'(u^k), w_j \rangle = 0, j = 1, \cdots, n.$$

Step 3. Compute the steepest descent gradient $d^k = -J'(u_k)$.

Step 4. If $\|d^k\| \le \varepsilon$, then output $u_{n+1} = u^k$, stop, otherwise go to Step 5.

Step 5. Set $v_k(s) = \frac{v_k + sd^k}{\|v_k + sd^k\|}$, $s = \frac{\lambda}{2^m}$, $m \in \mathbb{N}$ and follow the same way in Step 2 to solve for $p(v_k(s))$. Let $v_{k+1} = v_k(s_{n+1})$, where s_{n+1} satisfies

$$s_{n+1} = max\{s = \frac{\lambda}{2^m} | m \in \mathbb{N}, J(p(v(s))) - J(p(v_k)) \le -\frac{1}{2} t^k s \|d^k\|^2\}.$$

Step 6. Update $k = k + 1$, and go to Step 3.

Another popular numerical method in mathematics is a Newton method. A Newton method requires a high differentiability of J and is blind to a variational structure or order. It also depends strongly on an initial guess which significantly reduces its effectiveness in finding multiple solutions. It is neither based on the min-max principle nor provides local structures of saddle points, hence we do not state its algorithm here.

1.2 Finding Multiple G-saddles

In Chapter 2, we modify LMM and study the computational theory for it in order to find multiple unstable critical points for a variational functional which is G-differential at regular points.

Consider a class of quasilinear Schrödinger equations of the form [44]

$$\mathbf{i}\frac{\partial w}{\partial t} = -\Delta_x w + V(x)w - f(|w|^2)w - \kappa\Delta_x h(|w|^2)h'(|w|^2)w, \tag{1.1}$$

where $V(x)$ is a potential density, κ is a physical constant, f and h are real functions of essentially pure power forms. Eq. (1.1) appears naturally in mathematical physics, such as in the superfluid film equation in plasma physics and fluid mechanics [8,12,4,3,2,32], in the self-channeling of a high-power ultrashort laser in matter [20,21,23,26], in the theory of Heisenberg ferromagnets and magnons [18,19,27,10, 9], in dissipative quantum mechanics [6] and in condensed matter theory [15].

For simplicity, we choose $f(|s|^2)s = |s|^{p-1}s$, a widely used form in applications and $h(s) = s$, a form used in the superfluid film equation in plasma physics [8]. However our method presented in this thesis applies to more general cases.

To study solution patterns, stability and other properties, solitary wave (solition) solutions of the form $w(x,t) = u(x)e^{-i\lambda t}$ are investigated where λ is a wave frequency and $u(x)$ is a wave amplitude function. Thus finding soliton solutions to (1.1) leads us to solve the following quasilinear elliptic equation [44]

$$-\Delta u(x) + V(x)u(x) - (\Delta(|u(x)|^2))u(x) = r(x)|u(x)|^{p-1}u(x), x \in \mathbb{R}^n. \tag{1.2}$$

Its variational functional is

$$J(u) = \int_{\mathbb{R}^n} \frac{1}{2}[(1+2u^2(x))|\nabla u(x)|^2 + V(x)u^2(x)]dx - \frac{1}{p+1}\int_{\mathbb{R}^n} r(x)|u(x)|^{p+1}dx \quad (1.3)$$

on the closed subspace

$$X = \{u \in H^1(\mathbb{R}^n) | \int_{\mathbb{R}^n} V(x)u^2(x)dx < \infty\},$$

where for simplicity we assume that the potential $V(x) \in \mathcal{C}(\mathbb{R}^n, \mathbb{R})$ satisfies $inf_{x\in\mathbb{R}^n} V(x) = 1$, and $2 < p \leq 22^*$, $2^* = \frac{n+2}{n-2}$ if $n > 2$ and $2^* = \infty$ if $n = 2$. Different $r(x)$ will be used in our numerical computation.

For many applications, $V(x)$ must be chosen to grow much fast than $|x| \to +\infty$ in order to form a potential trap and thus causes a blow-up singularity. Such a singularity can be easily handled analytically and numerically. However, the blow-up singularity due to the quasilinear term $u^2(x)|\nabla u(x)|^2$ in J will cause the main difficulty in analysis and numerical computation.

In the literature, only recently, some solution existence and other results for (1.2) are established [44]. However, so far mathematically validated numerical methods for finding multiple solutions to (1.2) are virtually none. In Chapter 2, our objective is numerically solve this problem.

1.3 Finding Multiple K-saddles for W-type Problems

In Chapter 3, we study computational theory of a new numerical method for $\mathcal{C}^1$ W-type functionals.

As a canonical model in physics, the nonlinear Schrödinger equation (NLS) is of the form

$$\mathbf{i}\frac{\partial w(x,t)}{\partial t} = -\Delta w(x,t) + v(x)w(x,t) + lf(x, |w(x,t)|)w(x,t). \quad (1.4)$$

Due to the localized property of the solutions for (1.4), finding soliton solutions of the form $w(x,t) = u(x)e^{-i\lambda t}$ under $v(x) = 0$, $l > 0$ (WLOG, $l = 1$) leads to

$$\begin{cases} -\Delta u(x) - \lambda u(x) + f(x, u(x)) = 0, & x \in \Omega, \\ u|_{\partial\Omega} = 0. \end{cases} \tag{1.5}$$

Its variational functional is

$$J(u) = \int_\Omega [\frac{1}{2}(|\nabla u(x)|^2 - \lambda u^2(x)) + F(x, u(x))]dx, \tag{1.6}$$

where $\frac{\partial}{\partial t}F(x,t) = f(x,t)$, $u \in H_0^1(\Omega)$ with norm $\|u\| = (\int_\Omega [|\nabla u|^2 + u^2]dx)^{\frac{1}{2}}$, and Ω is bounded in $\mathbb{R}^N$. $f(x,u)$ is selected to satisfy certain regularity conditions such that $J \in \mathcal{C}^1(H, \mathbb{R})$. In order to find solutions of the equation (1.5), we need to find critical points of J in (1.6).

Let $\lambda_1 < \lambda_2 < \cdots$ be the eigenvalues of

$$\begin{cases} -\Delta u(x) = \lambda u(x), & x \in \Omega, \\ u|_{\partial\Omega} = 0, \end{cases} \tag{1.7}$$

and $\varphi_1, \varphi_2, \ldots$ be their corresponding eigenfunctions. It is clear that if $\lambda < \lambda_1$, 0 is a local minimum of J and $\lim_{t\to+\infty} J(tu) = +\infty$ in any direction u. When $\lambda_k < \lambda < \lambda_{k+1}$ for some $k = 1, 2, \cdots$, $\forall u \in [\varphi_1, \cdots, \varphi_k]$, there is $t_u > 0$ such that $t_u = \arg\min_{t>0} J(tu)$. Such a J is called a defocused W-type functional (DWF) in contrast to its counterpart, focused M-type functional (with a mountain pass structure). Solutions of DWF are called W-type solutions.

M-type functionals are numerically well-studied by LMM in documents [39, 41]. For a typical M-type functional, the functional is $\cap-$shape in $[v_1, \cdots, v_k]$, M-shape in

$[v_1, \cdots, v_k]^\perp$. But for a typical DWF, the functional is $\cup-$shape in $[v_1, \cdots, v_k]^\perp$, W-shape in $[v_1, \cdots, v_k]$. See Figure 1.1. Due to the difference in space dimensions and

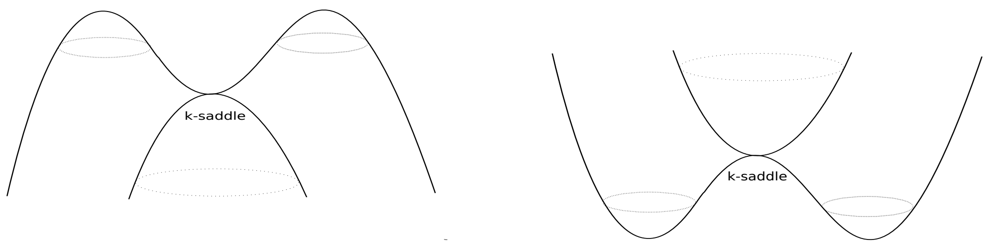

Figure 1.1: Left, M-type. $\cap-$ shape in $[v_1, \cdots, v_k]$, M-shape in $[v_1, \cdots, v_k]^\perp$. Right, W-type. $\cup-$ shape in $[v_1, \cdots, v_k]^\perp$, W-shape in $[v_1, \cdots, v_k]$.

$codim[v_1, \cdots, v_k] = +\infty$, they are not upside-down to each other, then LMM cannot be applied. A numerical method for finding multiple solutions of DWF is available for some special cases in [53]. In Chapter 3, we propose a new method called local minmaxmin method (LMMM) for general cases and numerical examples are carried out to illustrate the efficiency of this method. We also establish mathematical validation and present convergence results for LMMM under much weaker conditions. An application of LMMM to the model problem (1.6) is studied in depth and we analyze instability performance of saddles by LMMM as well.

2. FINDING SADDLES FOR G-DIFFERENTIAL M -TYPE FUNCTIONALS *

2.1 Preliminaries

By observation, J in (1.3) is at most lower semi-continuous with blow-up singularities in the whole space. In fact, under the growth condition of the nonlinearity, J is not even defined in X. Thus the following change of variables is introduced [44],

$$dv = \sqrt{1+u^2}\,du, v = h(u) = \frac{1}{2}u\sqrt{1+u^2} + \frac{1}{2}\ln(u+\sqrt{1+u^2}). \tag{2.1}$$

Hence $h'(u) = \sqrt{1+u^2} > 0$, h is strictly monotone and has an inverse $u = f(v) = h^{-1}(v)$. It follows $f'(v) = \frac{1}{h'(u)} = \frac{1}{\sqrt{1+u^2}}$. Then $J(u)$ can be rewritten as

$$I(v) = J(f(v)) = \int_{\mathbb{R}^n} \frac{1}{2}[|\nabla v(x)|^2 + V(x)f^2(v(x))]dx - \frac{1}{p+1}\int_{\mathbb{R}^n} r(x)|f(v(x))|^{p+1}dx. \tag{2.2}$$

I is defined on the space

$$H^1_G = \{v| \int_{\mathbb{R}^n} |\nabla v(x)|^2 dx < \infty, \int_{\mathbb{R}^n} V(x)f^2(v(x))dx < \infty\}, \tag{2.3}$$

with the norm

$$\|v\|_G = \|\nabla v\|_{L^2(\mathbb{R}^n)} + |v|_G, \tag{2.4}$$

where

$$|v|_G = \inf_{\xi>0} \xi\left(1 + \int_{\mathbb{R}^2} V(x)f^2(\xi^{-1}v(x))\right)dx.$$

The following results are established in [44] and provide a foundation for us to design

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a new mathematical frame-work for numerical algorithms, where and through out of the thesis, we use "$\to$" for strong convergence and "$\rightharpoonup$" for weak convergence.

Proposition 2.1. *([44]) (1) I is well defined and continuous in H^1_G.*
(2) I is Gateaux (G)-differentiable, for each $v \in H^1_G$, the G-derivative $I'(v)$ is a continuous linear functional on H^1_G, and $I'(v)$ is continuous in v in the strong-weak topology, i.e., if $v_n \to v$ in H^1_G, then $I'(v_n) \rightharpoonup I'(v)$. $\Box$

Let $J : H \to \pm\infty \cup \mathbb{R}$ be a functional. A point $u^* \in H$ is called a G-critical point of J if its G-derivative $J'(u^*) = 0$. A G-critical point u^* that is not a local minimum/maximum of J is called a G-saddle. An index-k G-saddle (k-G-saddle) is a G-critical point that is a local maximum of J in a k-dimensional subspace of H and a local minimum of J in the corresponding k-co-dimensional subspace of H. It is known that in a physical system, critical points correspond to local equilibrium states. A local minimum is a stable local equilibrium state and other saddles correspond to unstable local equilibrium states. It is clear that the solutions of (1.2) can be obtained by finding G-critical points of J and that the trivial solution $u = 0$ is the only local minimum of J among all regular points. Thus all nontrivial solutions are unstable. We are interested in numerical algorithms for finding multiple k-G-saddles in certain variational order. *The quasilinearity and lack of smoothness in J, and the multiplicity and instability of the solutions* cause the following difficulties.

• *No numerical method exists in the literature for finding multiple G-saddles.* Traditional numerical methods assume J to be $\mathcal{C}^1$, focus on finding stable solutions and emphasize solution uniqueness. One may think of a Newton method. It is well known that a Newton method requires a higher differentiability of J that we do not have, is blind to a variational structure or order, and depends strongly on an initial guess. This dependence is significantly amplified and severely reduces its effectiveness in finding multiple solutions. Thus a Newton method will not be considered in this thesis.

• The G-derivative is a directional derivative defined by $J'(u)v = \frac{d}{dt}|_{t=0}J(u+tv)$ and irrelevant to any norm on H. When in a Hilbert space H, $\langle J'(u), v\rangle = \frac{d}{dt}|_{t=0}J(u+tv)$. *This is the equation for us to evaluate the G-derivative*. Since the norm $\|\cdot\|$ cannot separate regular points from singular ones, to treat the singularity in J, the authors of [44] introduce a stronger norm $\|\cdot\|_G$ to construct a subspace H^1_G of regular points, which separates regular points from singular ones, and then study the continuity of the G-derivative J' by the norm $\|\cdot\|_G$ in Proposition 2.1. This is a very clever idea in treating singular points in analysis. Thus to avoid singular points, the problem has to be solved inside H^1_G. But it involves an implicit inverse transform f and a very complicated norm expression (2.4), which make it too difficult for us to do numerical implementation. Also the norm $\|\cdot\|_G$ does not have an associated inner product in H^1_G. Without it we cannot evaluate the G-derivative. While so far using the G-derivative as a search direction is the only hope for us to design a numerical variational algorithm, if possible, for finding multiple G-saddles. Therefore the case becomes very complicated. We must use $\langle\cdot,\cdot\rangle$, $\|\cdot\|$, $\|\cdot\|_G$ to establish a mathematical frame-work of an algorithm but use only $\langle\cdot,\cdot\rangle$, $\|\cdot\|$ in its numerical implementation.

• Since all nontrivial solutions here are unstable and they are sensitive to numerical errors, extra caution in error control must be taken in numerical computation.

Since the functional J defined in (1.3) has singularities even after an implicit inverse transform f and by Proposition 2.1, the function $I : H^1_G \to \mathbb{R}$ is only G-differentiable but not $\mathcal{C}^1$ or locally Lipschitz continuous, we conclude that mathematical results or numerical methods for smooth/nonsmooth saddles in the literatures are not applicable here.

On the other hand, recently the authors in [52] numerically solved the same problem for 1-saddles. They used the same implicit transformation $u = f(v)$ to get the variational functional $I(v)$. Then they treated $I(v)$ as $\mathcal{C}^1$ from $H^1(\mathbb{R}^n) \to \mathbb{R}$ (refer (1.7) in [52]) and applied the mountain pass lemma [1] where the min and max are actually in the global sense and the mountain pass algorithm [24], an early version of LMM of Li-Zhou with $k = 1$ or $L = \{0\}$, where the min and max are in the local sense and is designed for finding only 1-saddles of $\mathcal{C}^1$ functionals. But the functional $I(v)$ as stated in [44] is merely G-differentiable in H^1_G in the sense of Proposition 2.1 and has singularities in $H^1(\mathbb{R}^n)\backslash H^1_G$. Meanwhile the numerical results in [52] imply that the algorithm may still work for finding 1-G-saddles. Thus the mathematical validation of the numerical algorithm used in [52] becomes an interesting question to investigate. Since we want to find multiple k-G-saddles, $k = 1, 2, ...$, it becomes even more challenging.

As indicated, it was too difficult for us to use H^1_G as a constraint subspace for our numerical computation. On the other hand, the space $H^1(\mathbb{R}^n)$ has a clear and simple inner product with which we can compute G-derivatives. However, we have to deal with singularity issues in $H^1(\mathbb{R}^n) \setminus H^1_G$. We need to do more investigation on the singularity involved. It is known that when $2 < p < 2^*$, for each $u \in H^1(\mathbb{R}^n)$, the last term of J in (1.3) is well defined and under control, all other terms of J in (1.3) are nonnegative. It turns out that the only possible singularity that J may have in $H^1(\mathbb{R}^n)$ is of blow-up type or $J(u) = +\infty$ at a point $u \in H^1(\mathbb{R}^n) \setminus H^1_G$. Thus the extended functional $J : H^1(\mathbb{R}^n) \to \{+\infty\} \cup \mathbb{R}$ is well defined. It is known that such a blow-up singularity can be automatically avoided by any descent numerical algorithm starting from a regular point. On the other hand, for each regular point $u \in H^1(\mathbb{R}^n)$, we have $J(u) < +\infty$ and $v = h(u) \in H^1_G$. Then I is G-differentiable at v and

$$\langle I'(v), w\rangle = \langle J'(f(v))f'(v), w\rangle = \langle J'(u)\frac{1}{\sqrt{1+u^2}}, w\rangle, \quad \text{or} \quad J'(u) = \sqrt{1+f^2(v)}I'(v).$$

In a numerical computation, "nice" functions are used to approximate a solution and in $H^1(\mathbb{R}^n)$, the inner product is clearly and simply defined, with which the G-derivative $J'(u)$ can be evaluated at a regular point u. Also in a descent algorithm iteration, a "poor" search direct leading to a higher functional value will be automatically rejected. Thus we expect that such a “natural selection” by a descent method be able to resolve the difficulty caused by the blow-up singularity and a “poor” G-derivative.

The above observation provides us some motivation to find multiple k-G-saddles by generalizing LMM, which is so far the only method in the literature to be able to numerically find multiple smooth k-saddles. Meanwhile, we observe that the special properties of LMM

$$\min_{v\in S_{L^\perp}} \max_{u\in[L,v]} J(u)$$

imply that after a "nice" initial guess is selected, the inner level of LMM is a local maximization process above the energy level $J(0)$, which will reject any regular or singular points below the energy level $J(0)$, and the outer level of LMM has a descent property in J-value, which will select only a regular point for the next iteration. Such a combined nice property of LMM will select points only between two regular energy levels and reject any direction towards a singular point, thus can handle much more complicated singularities. However *throughout Chapter 2*, we only consider finding k-G-saddles of the following class of functionals.

Definition 2.1. *Let H be a Hilbert space with an inner product $\langle\cdot,\cdot\rangle$, its associated norm $\|\cdot\|$ and a stronger norm $\|\cdot\|_G$, and $J:H\to\{\pm\infty\}\cup\mathbb{R}$ be a functional. Assume $H_G=\{u\in H:\|u\|_G<\infty\}$ is a subspace of regular points u of J in H, i.e., $|J(u)|<+\infty$, J is continuous at u in the $\|\cdot\|_G$-norm and the G-derivative $J'(u)\in H_G$ is continuous in u in the $\|\cdot\|_G$-weak topology, or, $J'(v)\rightharpoonup J'(u)$ if $v\to u$ in the $\|\cdot\|_G$-norm.*

2.2 A Generalized Local Minimax Method (LMM)

In this section, we establish a new mathematical frame-work of LMM, by using a mixed strong-weak topology approach. First we verify a stepsize rule, then a local minimax characterization for a k-G-saddle of J in H and a descent property of LMM, which generalize the results in [39,41]

Let L be a finite-dimensional subspace of H containing regular points. For each regular point v, its local neighborhood is defined by the $\|\cdot\|_G$-norm. We can define a local selection p of J at a regular point v in the same way as in Chapter 1.

2.2.1 Computational theory

In LMM, L is spanned by previously found solutions which are regular points. The introduction of a peak selection p is important in LMM for finding multiple saddles. It separates previously found saddles spanning L from a new one to be found. We assume that LMM starts at a regular point v with a regular $p(v)$. If $p(v)$ is not a G-critical point, LMM should be able to follow certain stepsize rule to continue its iteration. It is known that for an algorithm to be successful in convergence, a descent property in J-value alone is not enough, it is important to have certain stepsize rule, such as the Armijo stepsize rule. However since LMM is a two-level algorithm, its stepsize rule is much more complicated. In proving the following stepsize rule, a linear approximation is used for $\mathcal{C}^1$ functionals in [47,51] under the assumption that p is continuous. Since such an approach cannot be used for G-saddles due to the lack of $\mathcal{C}^1$-smoothness in J, a new approach using mixed strong-weak topology involving two norms and a weak form is developed and a new bounded term w has to be introduced to LMM. It turns out that such a new approach enables us to not only establish the stepsize rule, Lemma 2.1, but also relax the continuity condition on p.

Lemma 2.1. *(Stepsize Rule) Let p be a local peak selection of J w.r.t. L at a regular point $v \in S_{L^\perp}$ s.t.*

(1) $p(v) = t_v v + u_v, u_v \in L, |t_v| > 0$*, is a regular point but not a G-critical point;*

(2) *p is weakly continuous at v in $\|.\|_G$-weak topology, or, $p(u) \rightharpoonup p(v)$ if $\|u - v\|_G \to 0$.*

Then as $s > 0$ is sufficiently small, it holds

$$J(p(v(s))) - J(p(v)) < -\frac{1}{4}s|t_v|\|d\|\|w\|, \tag{2.5}$$

where $v(s) = \frac{v+sw}{\|v+sw\|} \in S_{L^\perp}, w = -sign(t_v)\frac{d}{c}\perp[L,v], c = 1$ *if* $\|d\| \leq 1$ *and* $c = \|d\|$ *otherwise, and* $d = J'(p(v)) \in H$ *is the G-derivative with* $\|d\|_G < \infty$*. Furthermore* $p(v(s))$ *is regular.*

Proof. J is continuous at $p(v)$ in $\|.\|_G$-norm and J' is continuous at $p(v)$ in the $\|.\|_G$-weak topology. Then there is a $\|.\|_G$-neighborhood $\mathcal{N}(p(v))$ of $p(v)$ s.t. every point in $\mathcal{N}(p(v))$ is a regular point. Thus J' is continuous in $\mathcal{N}(p(v))$ in the $\|.\|_G$-weak topology. We first note that as $s \to 0$,

$$\begin{aligned}\|v(s) - v\|_G &= \|\frac{v - sw}{\|v - sw\|} - v\|_G = \|\frac{v - \|v - sw\|v}{\|v - sw\|} - \frac{sw}{\|v - sw\|}\|_G \\ &\leq \|v\|_G\frac{|1 - \|v - sw\||}{\|v - sw\|} + \frac{s\|w\|_G}{\|v - sw\|} \to 0,\end{aligned}$$

since $\|v - sw\| \to 1$ as $s \to 0$. Thus $p(v(s))$ is defined and by our assumption (2),

$$p(v(s)) = \frac{t(s)v}{\|v + sw\|} + u(s) + \frac{t(s)sw}{\|v + sw\|} \rightharpoonup p(v) = t_v v + u_v \tag{2.6}$$

for some $t(s) \to t_v, u(s) \in L, u(s) \rightharpoonup u_v$ in L as $s \to 0$. Since $t(s) \to t_v$ in $\mathbb{R}$ and $u(s) \rightharpoonup u_v$ in L, a finite-dimensional subspace, we have $u(s) \to u_v$ in $\|\cdot\|_G$-norm and consequently as $s \to 0$,

$$p(v(s)) = \frac{t(s)v}{\|v + sw\|} + u(s) + \frac{t(s)sw}{\|v + sw\|} \to p(v) = t_v v + u_v \quad \text{in} \quad \|\cdot\|_G\text{-norm} \tag{2.7}$$

as well. Next for fixed v, t close to t_v, $u \in L$ close to u_v in $\|\cdot\|_G$-norm and $s > 0$

sufficiently small such that $\frac{tv}{\|v+sw\|}+u$ and $\frac{tv}{\|v+sw\|}+u+\frac{tsw}{\|v+sw\|}$ are in $\mathcal{N}(p(v))$, since the G-derivative J' is continuous at $\frac{tv}{\|v+sw\|}+u$ in the $\|\cdot\|_G$-weak topology, we consider the variation in the direction $\frac{tsw}{\|v+sw\|}$, i.e., we define

$$g(\lambda)=J(\frac{tv}{\|v+sw\|}+u+\lambda\frac{tsw}{\|v+sw\|}).$$

Then $g(\lambda)$ is differentiable in $(0,1)$. Applying the mean-value theorem to $g(\lambda)$, there is some $\lambda_{s,t,u}\in(0,1)$ s.t.

$$\begin{aligned} & \frac{st}{\|v+sw\|}\langle d_{s,t,u},w\rangle = g'(\lambda_{s,t,u}) = g(1)-g(0) \\ = \quad & J(\frac{tv}{\|v+sw\|}+u+\frac{tsw}{\|v+sw\|})-J(\frac{tv}{\|v+sw\|}+u), \end{aligned}$$

where the G-derivative

$$d_{s,t,u}=J'(\frac{tv}{\|v+sw\|}+u+\lambda_{s,t,u}\frac{stw}{\|v+sw\|}).$$

Since p is a peak selection and $\frac{tv}{\|v+sw\|}+u\in[L,v]$, $\frac{tv}{\|v+sw\|}+u\to p(v)=t_v v+u_v$ in $\|\cdot\|_G$-norm, as $t\to t_v, u\to u_v$ in $\|\cdot\|_G$-norm and $s\to 0$, we have $J(p(v))\geq J\Big(\frac{tv}{\|v+sw\|}+u\Big)$. Hence

$$J(\frac{tv}{\|v+sw\|}+u+\frac{stw}{\|v+sw\|})-J(p(v))\leq\frac{st}{\|v+sw\|}\langle d_{s,t,u},w\rangle. \tag{2.8}$$

Once the inequality (2.8) is established, we play a continuity approach in $\|\cdot\|_G$-weak topology. It is important to note that for $t\to t_v, u\to u_v$ in $\|\cdot\|_G$-norm and $s\to 0$, we have the uniform bound for $\lambda_{s,t,u}\in(0,1)$ and the $\|\cdot\|_G$-norm convergence

$$\frac{tv}{\|v+sw\|}+u+\lambda_{s,t,u}\frac{stw}{\|v+sw\|}\to p(v)=t_v v+u_v. \tag{2.9}$$

It leads to the weak convergence $d_{s,t,u} \rightharpoonup d = J'(p(v))$ as , $t \to t_v, u \to u_v$ in $\|\cdot\|_G$-norm, $s \to 0$. Thus

$$t\langle d_{s,t,u}, w\rangle \to t_v\langle d, w\rangle = -|t_v|\|d\|\|w\| < 0$$

as $t \to t_v, u \to u_v$ in $\|\cdot\|_G$-norm, $s \to 0$. By the inequality (2.8) and the $\|\cdot\|_G$-norm convergence (2.9), for u near u_v in $\|\cdot\|_G$-norm in L, t near t_v and $s > 0$ near 0, we obtained

$$J\Big(\frac{tv}{\|v+sw\|} + u + \frac{stw}{\|v+sw\|}\Big) - J(p(v)) \leq -\frac{1}{2}\frac{s|t|}{\|v+sw\|}\|d\|\|w\|.$$

Finally by (2.7) and $\|v + sw\| \to 1$ as $s \to 0$, we conclude that

$$J(p(v(s))) - J(p(v)) < -\frac{1}{4}s|t_v|\|d\|\|w\|,$$

as $s > 0$ sufficiently small, and such a point $p(v(s))$ is regular. □

Theorem 2.1. *(Local Minimax Characterization) Let p be a local peak selection of J w.r.t. L at $v \in S_{L^\perp}$ s.t.*

(1) *p is weakly continuous at v in the $\|\cdot\|_G$-weak topology and dis$(p(v), L) > 0$,*

(2) *$J(p(v)) =$ local $\min_{u\in S_{L^\perp}} J(p(u))$ where $p(v)$ is a strict local maximum of J on $[v, L]$.*

Then $p(v)$ is a regular G-saddle of J.

Proof. By the condition (2), $p(v)$ is a regular point. If $p(v)$ is not a G-saddle point, since $p(v)$ is a strict local maximum of J on $[v, L]$, $p(v)$ cannot be a G-critical point of J either. Then by Lemma 2.1, as $s > 0$ sufficiently small,

$$J(p(v(s))) - J(p(v)) < -\frac{1}{4}s|t_v|\|d\|\|w\|,$$

where $v(s) = \frac{v+sw}{\|v+sw\|}$, $w = -\text{sign}(t_v)\frac{d}{c}$, $c = 1$ if $\|d\| \leq 1$ and $c = \|d\|$ otherwise, $p(v) = t_v v + u_v, u_v \in L, |t_v| > 0$. It leads to a contradiction to assumption (2). $\square$

Remark 2.1. (1) Since Lemma 2.1 and Theorem 2.1 assume p to be only weakly continuous, they strictly improved the corresponding results in [39,45,51];

(2) The inequality (2.5) is an important result which can be used to not only derive a local minimax characterization of k-G-saddles as in Theorem 2.1 but also design a stepsize rule for LMM, see Step 4 in the flow chart of the algorithm below. This inequality also indicates that *LMM is a strict descent method*;

(3) By the characterization in Theorem 2.1, a k-G-saddle can be obtained by solving the problem $\min_{v\in S_{L^\perp}} J(p(v))$, which leads to LMM presented previously. Note that we only assume p to be weakly continuous. The composite function $J(p(v))$ is in general not even continuous. Thus there is no way to establish a chain rule in the sense of G-derivative. Interestingly the results established in this thesis actually try to design a numerical algorithm for finding k-G-saddles of such a functional by using the G-derivative. Such an algorithm becomes possible only after we introduce the notion of a peak selection, an L-orthogonal condition $J'(p(v))\perp[v, L]$;

(4) By Lemma 2.1, the local min in Theorem 2.1 is defined in $\|\cdot\|_G$-norm. However due to the descent property of LMM, in its numerical implementation, this is not necessary.

2.2.2 Algorithm flow chart

To fit for the mixed strong-weak topology approach presented previously, we modify LMM in [39,41] by introducing a bounded term w_k^n and replacing the Frechet derivative of J by the Gateaux derivative of J.

Let u_1,...,u_{k-1} be $k-1$ previously found saddles of J in H and $L = [u_1, ..., u_{k-1}]$. Given $\varepsilon, \lambda > 0$.

Step 1. Choose a regular point $\bar{u}_k^1 = v_k^1 + v_k^s \notin L$ where $v_k^1 \in S_{L^\perp}, v_k^L \in L$.

Step 2. Set $n = 1$. Use $\bar{u}_k^1$ as an initial to solve for

$$\begin{aligned} u_k^n &= p(v_k^n) = t_0^n v_k^n + t_1^n u_1 + \cdots + t_{k-1}^n u_{k-1} \\ &= \arg\max\{J(t_0 v_k^n + t_1 u_1 + \cdots + t_{k-1} u_{k-1}) | t_i \in \mathbb{R}, i = 0, 1, ..., n-1\}. \end{aligned}$$

Step 3. Find a descent direction $w_k^n = -\text{sign}(t_0^n)\frac{d_k^n}{c_k^n}$ at u_k^n, where $d_k^n = J'(u_k^n), c_k^n = 1$ if $\|d_k^n\| \le 1$ and $c_k^n = \|d_k^n\|$ otherwise.

Step 4. Denote $v_k^n(s) = \dfrac{v_k^n + s w_k^n}{\|v_k^n + s w_k^n\|}$ for $s > 0$. Use the initial point $(t_0^n, t_1^n, ..., t_{k-1}^n)$ to solve for

$$p(v_k^n(s)) = \arg\max\Big\{J(t_0 v_k^n(s) + \sum_{i=1}^{k-1} t_i u_i) | t_i \in \mathbb{R}, i = 0, 1, ..., k-1\Big\},$$

then set $u_k^{n+1} = p(v_k^{n+1}) = p(v_k^n(s_k^n)) \equiv t_0^{n+1} v_k^{n+1} + \sum_{i=1}^{k-1} t_i^{n+1} u_i$ where s_k^n satisfies

$$s_k^n = \max\{s = \frac{\lambda}{2^m} | m \in N, J(p(v_k^n(s))) - J(p(v_k^n)) \le -\frac{1}{4}|t_0^n| s \|d_k^n\| \|w_k^n\|\}.$$

Step 5. If $\|s_k^n w_k^n\| < \varepsilon$,then output u_k^{n+1} and stop, otherwise set $n = n+1$ and go to Step 3.

Remark 2.2. (1) LMM starts with $k = 1$ and $L = \{0\}$ to a find u_1, then LMM continues with $k = 2$ and $L = [u_1]$ to find u_2,..., etc. When multiple branches of solutions appear, we should follow each branch and use LMM to solve for a new solution in this branch;

(2) It is important to use the assigned initial guess in Steps 2 and 4 to continuously trace a peak selection;

(3) The G-derivative $J'(u_k^n)$ is usually obtained by solving a linear PDE. This is where a numerical solver, such as using a finite element method (FEM), a finite difference method (FDM) or a boundary element method (BEM), etc., is used;

2.2.3 Find G-derivative by a weak form

In the algorithm, we use inner product $\langle u, v\rangle = \int_\Omega [\nabla u(x)\cdot\nabla v(x) + V(x)u(x)v(x)]dx$. Denote the residual of the equation (1.2) at a point w by

$$\text{res}(w)(x) = \Delta w(x) - V(x)w(x) + (\Delta(|w(x)|^2))w(x) + r(x)|w(x)|^{p-1}w(x)$$

and denote

$$\langle u, v\rangle = \int_\Omega [\nabla u(x)\cdot\nabla v(x) + V(x)u(x)v(x)]dx.$$

The G-derivative of J or the steepest descent direction d of J at a given regular point w can be solved in weak form from a linear elliptic PDE

$$-\Delta d(x) + V(x)d(x) = \text{res}(w)(x),\ x \in \Omega, \quad d|_{\partial\Omega} = 0. \tag{2.10}$$

However many linear solvers require that the term res(w) is given as a function of x. But we failed to do so, since the term res(w) contains quasilinear terms that cannot be expressed as a function of x with piecewise linear elements. Thus to avoid using higher order finite elements or losing accuracy in numerical computation, (2.10) has to be solved in weak form

$$\langle d, \Phi\rangle = \int_\Omega \text{res}(w)(x)\Phi(x)dx, \ \ \forall\Phi \in H_0^1(\Omega). \tag{2.11}$$

Let $\varphi_i(x)$, $i = 1, ..., N$ be a nodal basis. Since G-saddles are unstable solutions and sensitive to numerical errors, according to our numerical experience, extra caution must be taken on error control in the weak form process, e.g., avoid using the numerical Laplacian operator Δ since it involves the second derivatives of a function expressed by piecewise linear finite elements. The operator Δ can be replaced by the divergence ∇ with the weak-form and the Green's identities. But the numerical divergence operation ∇ still causes unwanted errors. To avoid such a numerical differentiation, we use its expression in the divergence of the nodal basis, $\nabla\varphi_i$'s. Such a treatment leads to a significant improvement in error control. We denote

$$\begin{aligned}
\Phi(x) &= \sum_{i=1}^{N} y_i\varphi_i(x) = [\varphi_1(x), ..., \varphi_N(x)][y_1, ..., y_N]^T, \\
d(x) &= \sum_{i=1}^{N} x_i\varphi_i(x) = [\varphi_1(x), ..., \varphi_N(x)][x_1, ..., x_N]^T, \\
w(x) &= \sum_{i=1}^{N} w_i\varphi_i(x) = [\varphi_1(x), ..., \varphi_N(x)][w_1, ..., w_N]^T, \\
\nabla\Phi(x) &= \sum_{i=1}^{N} y_i\nabla\varphi_i(x) = [\nabla\varphi_1(x), ..., \nabla\varphi_N(x)][y_1, ..., y_N]^T, \\
\nabla d(x) &= \sum_{i=1}^{N} x_i\nabla\varphi_i(x) = [\nabla\varphi_1(x), ..., \nabla\varphi_N(x)][x_1, ..., x_N]^T, \\
\nabla w(x) &= \sum_{i=1}^{N} w_i\nabla\varphi_i(x) = [\nabla\varphi_1(x), ..., \nabla\varphi_N(x)][w_1, ..., w_N]^T.
\end{aligned}$$

Let $n_1, n_1, ..., n_N$ be the nodes. We denote

$$\begin{aligned}
Y &= [y_1, ..., y_N]^T = [\Phi(n_1), ..., \Phi(n_N)]^T, \\
X &= [x_1, ..., x_N]^T = [d(n_1), ..., d(n_N)]^T, \\
W &= [w_1, ..., w_N]^T = [w(n_1), ..., w(n_N)]^T, \\
F &= [r(n_1)|w(n_1)|^p, ..., r(n_n)|w(n_N)|^p]^T,
\end{aligned}$$

$$K = \begin{pmatrix} \int_\Omega \nabla\varphi_1(x)\nabla\varphi_1(x) & ... & \int_\Omega \nabla\varphi_1(x)\nabla\varphi_N(x) \\ ... & ... & ... \\ \int_\Omega \nabla\varphi_N(x)\nabla\varphi_1(x) & ... & \int_\Omega \nabla\varphi_N(x)\nabla\varphi_N(x) \end{pmatrix}, \tag{2.12}$$

$$M = \begin{pmatrix} \int_\Omega V(x)\varphi_1(x)\varphi_1(x) & ... & \int_\Omega V(x)\varphi_1(x)\varphi_N(x) \\ ... & ... & ... \\ \int_\Omega V(x)\varphi_N(x)\varphi_1(x) & ... & \int_\Omega V(x)\varphi_N(x)\varphi_N(x) \end{pmatrix}, \tag{2.13}$$

$$K_1 = \begin{pmatrix} \int_\Omega 2w^2(x)\nabla\varphi_1(x)\nabla\varphi_1(x) & ... & \int_\Omega 2w^2(x)\nabla\varphi_1(x)\nabla\varphi_N(x) \\ ... & ... & ... \\ \int_\Omega 2w^2(x)\nabla\varphi_N(x)\nabla\varphi_1(x) & ... & \int_\Omega 2w^2(x)\nabla\varphi_N(x)\nabla\varphi_N(x) \end{pmatrix}, \tag{2.14}$$

$$M_1 = \begin{pmatrix} \int_\Omega 2|\nabla w(x)|^2\varphi_1(x)\varphi_1(x) & ... & \int_\Omega 2|\nabla w(x)|^2\varphi_1(x)\varphi_N(x) \\ ... & ... & ... \\ \int_\Omega 2|\nabla w(x)|^2\varphi_N(x)\varphi_1(x) & ... & \int_\Omega 2|\nabla w(x)|^2\varphi_N(x)\varphi_N(x) \end{pmatrix}, \tag{2.15}$$

$$M_2 = \begin{pmatrix} \int_\Omega \varphi_1(x)\varphi_1(x) & ... & \int_\Omega \varphi_1(x)\varphi_N(x) \\ ... & ... & ... \\ \int_\Omega \varphi_N(x)\varphi_1(x) & ... & \int_\Omega \varphi_N(x)\varphi_N(x) \end{pmatrix}, \tag{2.16}$$

then (2.11) can be expressed as

$$Y^TKX + Y^TMX = -(Y^T(K+M)W + Y^T(K_1+M_1)W - Y^TM_2F), \forall Y \in \mathbb{R}^N.$$

Next we further denote $A = K + M$, $A_1 = K_1 + M_1, b = -(AW + A_1W - M_2F)$. Then, $d(x)$ can be obtained by solving X from the linear matrix system $Y^TAX = Y^Tb$, where A, A_1, M_2 are provided by the Matlab subroutine ASSEMPDE and other terms have to be built ourselves. As predicted in analysis, our numerical computation went smoothly without encountering any singularity difficulty.

2.3 Numerical Results

By the analysis in the previous sections, we can numerically solve (1.2) for multiple solutions simply in the space $H^1(\mathbb{R}^n)$ whose inner product can be used to evaluat the G-derivatives at a given regular point. The "natural selection" of LMM will automatically resolve the singularity issue. The term $V(x)$ in (1.2) is called a trapping potential, which is an important step toward the goal of a controlled Bose-Einstein condensate or other physical processes of excitation. In other words, for application purpose, $V(x)$ has to be properly selected so that a solution $u(x)$ has a *localized property*, i.e., $u(x) \to 0$ exponentially or at least much faster than $|x| \to +\infty$. According to the literature, we choose $V(x) = e^{|x|^2}$. Thus $\min_{x\in\mathbb{R}^n} V(x) = 1$ and $V(x) \to +\infty$ exponentially as $|x| \to +\infty$. Such a trapping potential $V(x)$ causes singularities even for $n = 2, 2^* = +\infty$. However, such $V(x)$ forms a trap for a function $u \in H^1(\mathbb{R}^n)$ to be a solution, i.e., u has to concentrate in a bounded ball centered at 0. Such a localized property enables people to solve the original problem in $\mathbb{R}^n$ numerically in a large bounded domain $\Omega \subset \mathbb{R}^n$ with a zero Dirichlet boundary condition. However, as multiple solutions are concerned, people are interested in observing the structures of different solutions, such as their symmetries, peaks and peak locations, nodal lines, etc. If the domain is selected too large, under the localized property, such structures cannot be clearly visualized from their solution profiles. So by test-solving the problem on many domains of different sizes for multiple solutions, we select the size of the domain so that both localized property and different solution profiles can be clearly visualized.

On the other hand, as it has been physically observed and mathematically verified for M-type semilinear elliptic equations (i.e., $\lim_{t\to+\infty} J(tu) = -\infty$), such as the Henon equation, the term $r(x) = |x|^m$ will cause a very different effect on a solution property. The m-value can be viewed as a bifurcation parameter. When $m < m_c$ for certain value

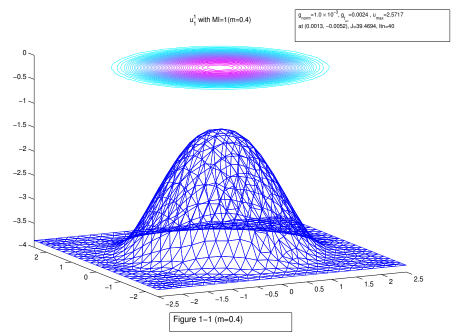
m_c, the ground state is a unique positive solution and symmetric. However when $m > m_c$, the ground state bifurcates to positive asymmetric solutions whose peak locations move away from 0. As m-value further increases, more positive solutions appear and their peaks move further away from 0 if $V(x)$ is a constant. Such a bifurcation process is called a *symmetry breaking phenomenon* which destroys the localized property. However if or not such a phenomenon will take place for the quasilinear elliptic equation (1.2) is still unknown, neither mathematically verified nor numerically observed. Actually, for (1.2), only the existence of the ground state has been mathematically established [44] and numerically computed [52]. As for the existence of other solutions, so far, it is neither mathematically verified nor numerically observed. In particular, it is interesting to numerically investigate the combined effect of the localize property and the symmetry breaking phenomenon, e.g., when $V(x) = e^{|x|^2}$ and $r(x) = |x|^m$ are both symmetric.

In the following numerical examples, we take $n = 2, p = 5, \Omega = (-2.5, 2.5)^2$. The finite elements are generated by Matlab subroutine INITMESH with piecewise linear elements.

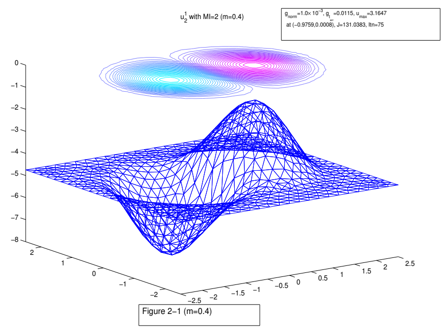
We use $g_{norm} = \|d\| = \langle d, d\rangle^{1/2} = (\int_\Omega \mathrm{res}(w)(x)d(x)dx)^{1/2} < \varepsilon = 10^{-4}$ to terminate a numerical iteration for finding 1-saddles. This ε will be increased by a factor 2^{k-1} for finding k-saddles as k increases to $2, 3, \ldots$. An initial guess $u_0 \in H_0^1(\Omega)$ is obtained flexibly from solving the equation $-\Delta u(x) + V(x)u(x) = c(x)$ by calling the Matlab subroutine ASSEMPDE, where $c(x) = -1, 1, 0$ according to the location(s) x where we want u_0 to have a positive peak, negative peak or just flat.

It is understood that due to the symmetry of the PDE (1.2), if Ω is a disk, then any solution rotated by an angle of any degree is still a solution and thus is degenerate unless it is radial symmetric; and if Ω is a square centered at 0, then any solution rotated by $\frac{\pi}{2}, \pi$ or $\frac{3\pi}{2}$ is still a solution. Thus we present only one representative solution from its equivalent class. Due to the corner effect, some solutions such as u_2 vs u_3 and u_5 vs u_6

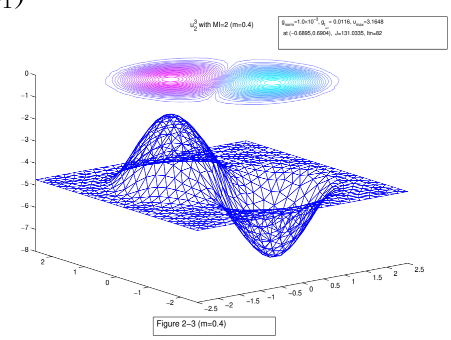
in Figure 2.1 seem to be different but actually belong to the same equivalent class when $\Omega = \mathbb{R}^2$. In order to plot the profile and contours of a solution in one figure, we have translated the profile vertically. More numerical data can be found if one zooms in at the up-right portion of each figure.



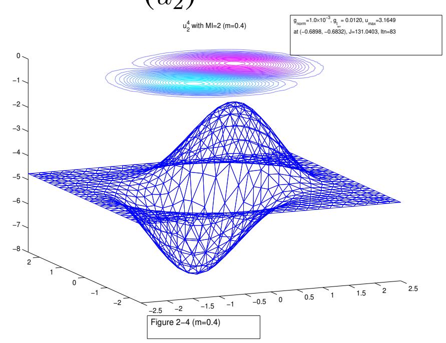
(u_1)



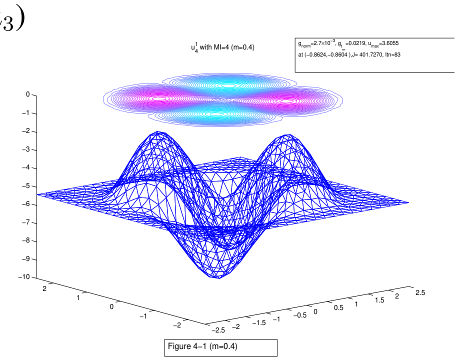
(u_2)



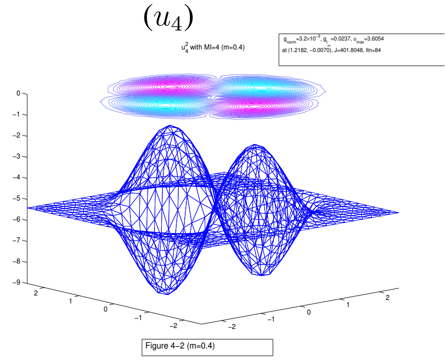
(u_3)



(u_4)

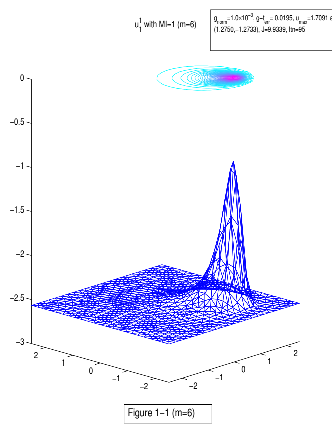


(u_5)

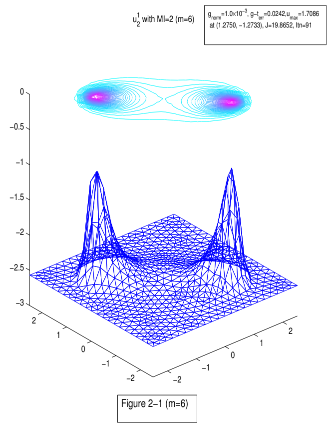


(u_6)

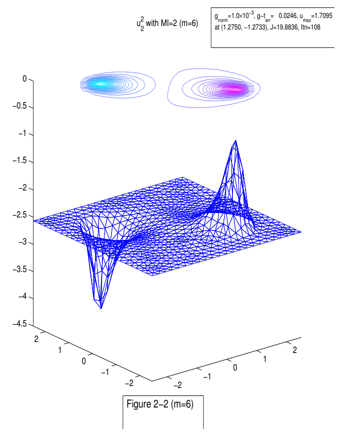
Figure 2.1: Case 1. $m = 0.4$. No bifurcation takes place. There is only one positive solution. Solutions $u_1, ..., u_6$ are found. The localized property is clearly visualized.



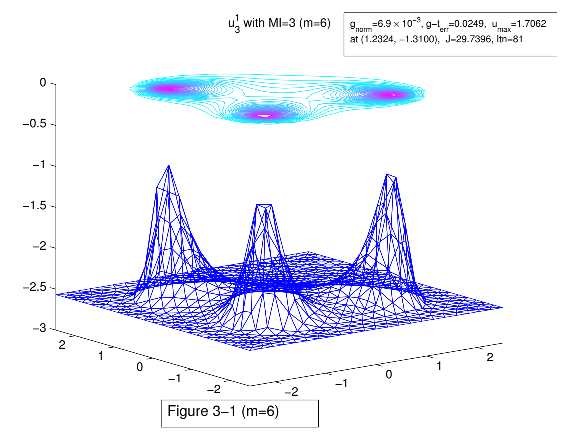
(u_1)



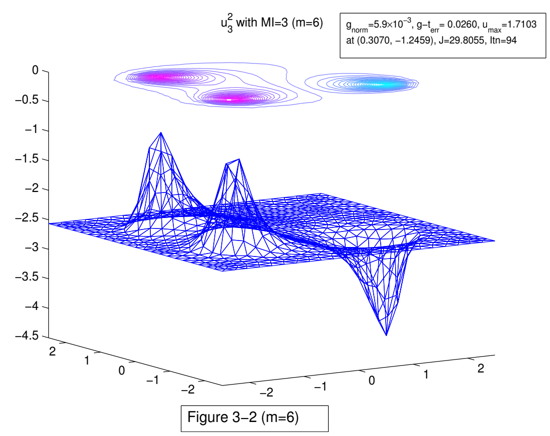
(u_2)



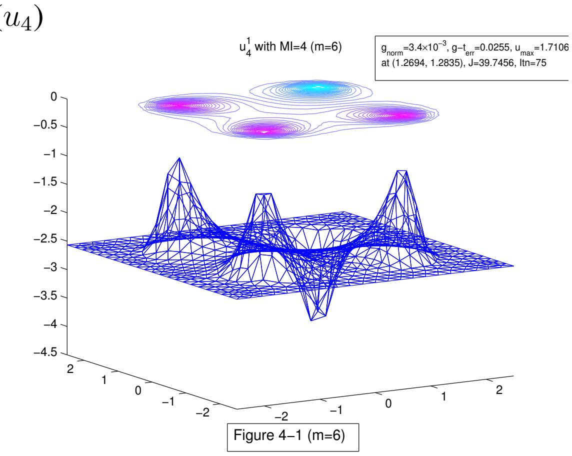
(u_3)



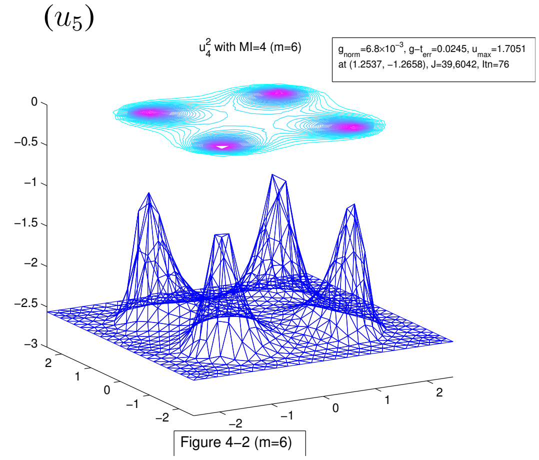
(u_4)



(u_5)

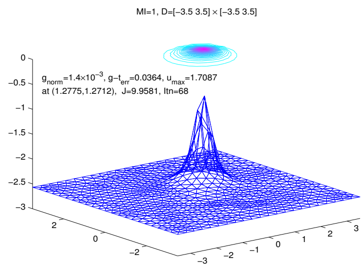


(u_6)

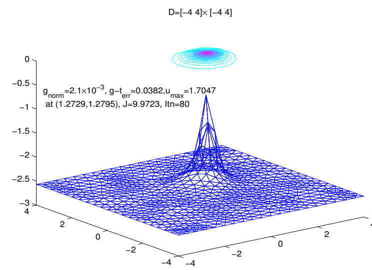


(u_7)

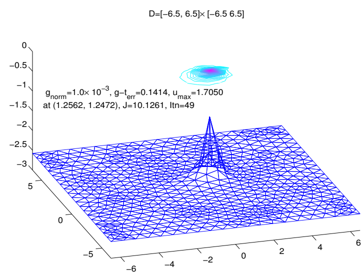
Figure 2.2: Case 2. $m = 6$. Bifurcation takes place after $m > 0.5$. We present solutions $u_1, ..., u_7$. Multiple positive solutions appeared. Thus symmetry breaking phenomenon is clearly visualized. u_5 is totally asymmetric.



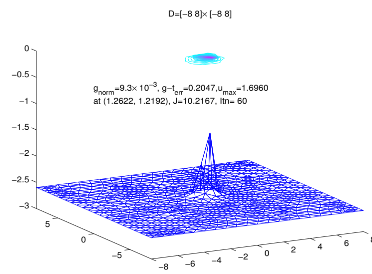
$\Omega = (-3.5, 3.5)^2$



$\Omega = (-4, 4)^2$



$\Omega = (-6.5, 6.5)^2$



$\Omega = (-8, 8)^2$.

Figure 2.3: Case 3. $m = 6$. A ground state u_1 with the same potential $V(x)$ but different Ω. Refer Figure 2.2 (u_1) for $\Omega = (-2.5, 2.5)^2$. By comparison, it is clear that in the appearance of both the potential $V(x)$ and the symmetry breaking term $r(x)$, the effect of the trapping potential $V(x)$ is decisive and the localized property is preserved.

2.4 Conclusion

In this chapter, to find G-saddles of a class of functionals $J : H \to \{\pm\infty\} \cup \mathbb{R}$ that are just G-differential at regular points, a mixed strong-weak topology approach is proposed to establish a new mathematical frame-work and LMM is modified accordingly. The weak format is used when solving the gradient involved in the algorithm due to the singularity caused by the quasilinear term. The modified LMM is implemented successfully with various numerical examples of multiple k-G-saddles presented. This project is finished and the related paper is published [56]. No future work was planned.

3. FINDING SADDLES FOR $\mathcal{C}^1$ W-TYPE NONLINEAR PDES

We investigate the boundary value problem (1.5) , which is also our model problem in this chapter. We restate it here

$$\begin{cases} -\Delta u(x) - \lambda u(x) + f(x, u(x)) = 0, \quad x \in \Omega, \\ u|_{\partial\Omega} = 0. \end{cases} \tag{3.1}$$

Its variational functional is

$$J(u) = \int_\Omega [\frac{1}{2}(|\nabla u(x)|^2 - \lambda u^2(x)) + F(x, u(x))]dx, \tag{3.2}$$

where $\frac{\partial}{\partial t}F(x,t) = f(x,t)$, $u \in H = H_0^1(\Omega)$ with norm $\|u\| = (\int_\Omega [|\nabla u|^2 + u^2]dx)^{\frac{1}{2}}$, and Ω is bounded in $\mathbb{R}^N$. $f(x, u)$ is selected such that $J \in \mathcal{C}^1(H, \mathbb{R})$. In order to find solutions of the equation (3.1), we need to find critical points of J in (3.2).

As we stated previously in Chapter 1, we could not apply the numerical methods that are designed only for solving M-type problems here since (3.2) has a W-type structure. We propose a new numerical method, a local minmaxmin method (LMMM), and establish its computational theory in this chapter.

3.1 Local Min-$\perp$ Method under Weakened Conditions (LMO-W)

We generalize the previous definition of the unit sphere S_W to develop computational theory for the new method LMMM. In this chapter, we denote $S_W = \{w \in W \mid \|w\| \approx 1\}$ for any subspace $W \subset H$, we use $\|w\| \approx 1$ instead of $\|w\| = 1$. Then we generalize the definition of a L-$\perp$ selection accordingly and it is stated below.

Definition 3.1. *Let L be a closed subspace of H and $L \oplus L^\perp = H$ be the orthogonal decomposition. Let $S_{L^\perp} = \{v \in L^\perp \mid \|v\| \approx 1\}$ and $[L, v] = \{tv + v_L \mid t \in \mathbb{R}, v_L \in L\}$*

for each $v \in S_{L^\perp}$. A set-valued mapping P: $S_{L^\perp} \to 2^H$ is called an L-$\perp$ mapping of J $w.r.t$ $H = L \oplus L^\perp$ if

$$P(v) = \{u \in [L, v] \mid J'(u) \perp [L, v]\}, \forall v \in S_{L^\perp}. \tag{3.3}$$

A single-valued mapping p: $S_{L^\perp} \to H$ is called an L-$\perp$ selection of J if $p(v) \in P(v)$, $\forall v \in S_{L^\perp}$. For a given $v \in S_{L^\perp}$, if such p is locally defined in $\mathcal{N}(v) \cap S_{L^\perp}$, where $\mathcal{N}(v)$ is a neighborhood of v, then p is called a local L-$\perp$ selection of J at v.

It is not hard to prove that if $p(v)$ is a local maximum of J in $[L, v]$, then such a $p(v)$ is also an L-$\perp$ point of J in $[L, v]$. Thus Definition 3.1 generalizes the notion of a peak mapping in [39, 41].

Let us recall the local min-$\perp$ method (LMO) in [45].

Theorem 3.1. *(LMO Characterization of Saddle Points [45]) For any closed subspace $L \subset H$, let $v^* \in S_{L^\perp} = \{v \in L^\perp \mid \|v\| = 1\}$, p is a local L-$\perp$ selection of J w.r.t. L at v^*, i.e., $p(v) \in [L, v]$, $J'(p(v)) \perp [L, v]$ for any $v \in \mathcal{N}(v^*)$. Assume (i) $p(v^*)$ is continuous at v^*, (ii) $d(p(v^*), L) > \alpha$ for some $\alpha > 0$. If*

$$v^* = \arg \min_{v \in \mathcal{N}(v^*) \cap S_{L^\perp}} J(p(v)),$$

then $u^* = p(v^*)$ is a critical point of J, i.e., $J'(u^*) = 0$.

LMO principle is now well-known in the literature. It has some very useful applications, such as the generalized Nehari manifold method, etc. Note that $\|v\| = 1$ was used in the notation $S_{L^\perp}$ for the above LMO characterization and the condition (i) posed on p is continuity, but $p(v)$ is implicitly defined, it is very difficult to determine its continuity. We hope we can weaken the condition (i) such that LMO can be applied to the case when p is not continuous. By replacing $\|v\| = 1$ by $\|v\| \approx 1$, we restudy LMO under a weakened condition of continuity and rename it by LMO-W, namely, a local min-$\perp$ method under a weakened condition.

First we define a locally directional Lipschitz continuity.

Definition 3.2. *For a map $F : M \to N$, at a given $m_0 \in M$, if for some $m \in M$, there is a constant l_0 depending on m_0 and m, such for all $s > 0$ small, it holds*

$$\|F(m_0 + sm) - F(m_0)\| \le l_0 s\|m\|, \tag{3.4}$$

F is said to be locally directional Lipschitz continuous at the given m_0 in the direction m. If for any $m \in M$, there is a constant l_0 depending on m_0 and m, such for all $s > 0$ small, (3.4) holds, we say F is locally directional Lipschitz continuous at the given m_0.

Let p be a local L-$\perp$ selection. Note that if $v \in S_{L^\perp}$ is given, when $s > 0$ is small, we have $\|v + sw\| \approx 1$. For $v(s) = \frac{v+sw}{\|v+sw\|}$, we have $[L, v(s)] = [L, v + sw]$ and then

$$p(v(s)) = t_s \frac{v(s) + u(s)}{\|v(s) + u(s)\|} = p(v + sw) = t(s)(v + sw + u'(s)),$$

where $u(s) \in [L, v(s)]$, $t(s) = \frac{t_s}{\|v+sw\|\|v(s)+u(s)\|}$, $u'(s) = \frac{t_s}{t(s)} \frac{t_s u(s)}{\|v(s)+u(s)\|}$.

By Definition 3.2, if a local L-$\perp$ selection p is locally directional Lipschitz continuous at a given $v \in S_{L^\perp}$, then for each $w \in L^\perp$, there is a constant l_0 depending on v and w, such that for all $s > 0$ small, it holds

$$\|p(v + sw) - p(v)\| \le l_0 s\|w\|,$$

where the term $\|w\|$ can be removed since l_0 depends on w. It implies

$$\|p(v(s)) - p(v)\| \le l_0|s|\|w\| = O(s).$$

It is clear that a locally directional Lipschitz continuity at v implies a locally directional continuity at v but not a necessary continuity at v. If the constant l_0 does not depend on w, p becomes locally Lipschitz continuous at v. If furthermore such a constant l_0 is independent of w and v, then p becomes locally lipschitz continuous.

Assume the G-derivative of p exists at v in a direction w and

$$\lim_{s\to 0}\frac{1}{s}(p(v+sw)-p(v)) = \delta p(v;w) \neq 0,$$

where $\delta p(v;\alpha w) = \alpha\delta p(v;w)$ for any scalar α, but not necessarily linear in w. Denote $l = \frac{2}{\|w\|}|\delta p(v;w)| > 0$, then there is $s_0 > 0$ such that when $s_0 > |s| > 0$, it holds

$$\|p(v+sw)-p(v)\| < l|s|\|w\|,$$

i.e., p is locally directional Lipschitz continuous at v in the direction w. In other words, a nonzero G-derivative of p at v in w implies a locally directional continuity but not continuity. It is clear that a locally directional continuity does not indicate a weak-continuity since the later implies a continuity in any finite-dimensional space.

With the above weakened condition on p, we are able to improve the computational theory for LMO.

Lemma 3.1. *(Stepsize Rule of LMO-W) For a given $v \in S_{L^\perp}$, assume that p is a local L-$\perp$ selection at v s.t.*

(i) *p is locally directional Lipschitz continuous at v,*

(ii) *$dis(p(v), L) > 0$,*

(iii) *$d = -J'(p(v)) \neq 0$.*

Then there is $s_0 > 0$ such that when $s_0 > s > 0$, we have

$$J(p(v(s))) - J(p(v)) < -\frac{1}{4C} t_v s \|J'(p(v))\|^2, \tag{3.5}$$

where $v(s) = \frac{v+sw}{\|v+sw\|}$, $w = \frac{d}{C}$, $C = \max\{1, \|d\|\}$, $p(v) = t_v v + u_v$, for $t_v > 0$ and $u_v \in L$.

Proof. If p is a local L-$\perp$ selection of J at $v \in S_{L^\perp}$, then $J'(p(v)) \perp [L, v]$ by the definition. Denote $p(v(s)) = t_s v(s) + u(s)$, $p(v) = t_v v + u_v$ for $t_v, t_s > 0$, $u_v, u(s) \in L$, it is clear that $t_s \to t_v$ as $s \to 0$ and

$$p(v(s)) = p(v + sw).$$

Since p is locally directional Lipschitz continuous at v in w, there exists $l > 0$ depending on v and w, s.t. $\|p(v + sw) - p(v)\| < l|s|$. So we have

$$\begin{aligned}
J(p(v(s))) - J(p(v)) &= \langle J'(p(v)), p(v(s)) - p(v)\rangle + o(\|p(v(s)) - p(v)\|) \\
&= \langle J'(p(v)), p(v(s))\rangle + o(\|p(v + sw) - p(v)\|) \\
&= \langle J'(p(v)), t_s \frac{v + sw}{\|v + sw\|} + u(s)\rangle + o(\|p(v + sw) - p(v)\|) \\
&= \frac{t_s}{\|v + sw\|}\langle J'(p(v)), v + sw\rangle + o(\|p(v + sw) - p(v)\|) \\
&= \frac{t_s s}{\|v + sw\|}\langle J'(p(v)), w\rangle + o(\|p(v + sw) - p(v)\|) \\
&= -\frac{t_s s}{\|v + sw\|}\frac{\|J'(p(v))\|^2}{C} + o(s) \\
&< -\frac{1}{4C} t_v s \|J'(p(v))\|^2.
\end{aligned}$$

Then (3.5) holds. □

Theorem 3.2. *(LMO-W Characterization) For any closed subspace $L \subset H$ and a given $v^* \in S_{L^\perp}$, let p be a local L-$\perp$ selection at v^*. Assume* *(i)* p *is locally directional Lipschitz continuous at* v^**,*

(ii) $p(v^*) \notin L$*,*

(iii) $v^* = \arg\min_{v\in\mathcal{N}(v^*)\cap S_{L^\perp}} J(p(v))$*, where* $\mathcal{N}(v^*)$ *is a neighborhood of* v^**.*

Then $u^* \equiv p(v^*)$ *is a critical point of* J*, i.e.,* $J'(u^*) = 0$*.*

Proof. Denote $p(v^*) = t_{v^*}v^* + u_{v^*}$ with $t_{v^*} > 0$, $u^* \in L$. If $d = -J'(p(v^*)) \neq 0$, set $w = \frac{d}{C}$ where $C = max\{1, \|d\|\}$ and $v(s) = \frac{v^*+sw}{\|v^*+sw\|}$, then by the Stepsize Rule of LMO-W, for $s > 0$ sufficiently small, we have

$$J(p(v(s))) - J(p(v^*)) < -\frac{1}{4C}t_{v^*}s\|d\|^2,$$

which contradicts assumption (iii). Therefore $p(v^*)$ is a critical point of J. $\square$

The analysis of LMO-W above provides us a mathematical support for the numerical method LMMM we will discuss below.

3.2 Local Minmaxmin Method (LMMM)

As stated before, $\lambda_1 < \lambda_2 < \cdots$ are the eigenvalues of $-\Delta u(x) = \lambda u(x)$ with the same zero boundary condition and $\varphi_1, \varphi_2, \ldots$ are the corresponding eigenfunctions. Notice that J in (3.2) is bounded from below, and if $\lambda < \lambda_1$, 0 is a local minimum of J and $\lim_{t\to+\infty} J(tu) = +\infty$ in any direction u. When $\lambda_k < \lambda < \lambda_{k+1}$, there is $t_u > 0$ such that $t_u = \arg\min_{t>0} J(tu)$ for $\forall u \in [\varphi_1, \cdots, \varphi_k]$. Motivated by LMO-W, we propose LMMM for W-type problems,

$$\min_{v\in L^\perp} \max_{u\in[L,v],\|u\|\approx 1} J(t_u u), \tag{3.6}$$

where $t_u = \arg\min_{t>0} J(tu)$, and (3.6) can be rewritten as

$$\min_{v \in S_{L^\perp}} \max_{u \in [L,v], \|u\| \approx 1} \min_{t>0} J(tu). \tag{3.7}$$

Define

$$p(v) = \arg \max_{u \in [L,v], \|u\| \approx 1} \min_{t>0} J(tu), \tag{3.8}$$

$$T(u) = t_u u, \tag{3.9}$$

then $p(v) = t_u u = T(u) \in [L, v]$ for some $u \in [L, v]$ with $\|u\| \approx 1$, and it holds

$$J(p(v)) = \max_{u \in [L,v], \|u\| \approx 1} \min_{t>0} J(tu). \tag{3.10}$$

Consequently we can state LMMM as

$$\min_{v \in S_{L^\perp}} J(p(v)) \equiv \min_{v \in S_{L^\perp}} \max_{u \in [L,v], \|u\| \approx 1} J(T(u)) \equiv \min_{v \in S_{L^\perp}} \max_{u \in [L,v], \|u\| \approx 1} \min_{t>0} J(tu). \tag{3.11}$$

Now we are able to verify the following property for p locally defined in (3.8) under the weakened condition, i.e. locally directional Lipschitz continuity on T.

Lemma 3.2. *(L-$\perp$ Property) T is defined as in (3.9), $p(v)$ is locally defined as in (3.8) with $p(v) = t_u u$ for some $u \in [L, v]$, $\|u\| \approx 1$. Assume T is locally directional Lipschitz continuous at such u, then $J'(p(v)) \perp [L, v]$.*

Proof. Since $p(v) = t_u u$ for some $u \in [L, v]$, $\|u\| \approx 1$, it follows that $J'(p(v)) \perp u$. Suppose $J'(p(v)) \perp [L, v]$ does not hold, we define

$$u(s) = \frac{u + sw}{\|u + sw\|} \in S_{[L,v]}, s > 0, \tag{3.12}$$

where $w = J'(p(v))_{[L,v]} \neq 0$ is the projection of $J'(p(v))$ onto the closed subspace $[L, v]$. Denote $T(u(s)) = t_s u(s)$, it is clear that when $s > 0$ is small, we have

$$t_s u(s) = T(u(s)) = T(u + sw) = t'_s(u + sw),$$

where $t'_s = \frac{t_s}{\|u+sw\|}$. Since $J'(p(v)) \perp u$,$u \in [L, v]$, and $J'(p(v)) - J'(p(v))_{[L,v]} \in [L, v]^{\perp}$, we get $\langle J'(p(v))_{[L,v]}, u\rangle = \langle J'(p(v)), u\rangle - \langle J'(p(v)) - J'(p(v))_{[L,v]}, u\rangle = 0$, namely, $J'(p(v))_{[L,v]} \perp u$. By the assumption, T is locally directional Lipschitz continuous at u in w, then there is $l_1 > 0$ depending on u and w such that when $|s|$ is small, it holds

$$\|T(u + sw) - T(u)\| < l_1|s|.$$

It is clear that $T(u(s)) \to T(u)$ as $s \to 0$. Then when $s_0 > s > 0$, we get

$$\begin{aligned}
J(T(u(s))) - J(T(u)) &= \langle J'(T(u)), T(u(s)) - T(u)\rangle + o(\|T(u(s)) - T(u)\|) \\
&= \langle J'(p(v)), T(u(s))\rangle - \langle J'(p(v)), T(u)\rangle + o(\|T(u + sw) - T(u)\|) \\
&= \langle J'(p(v)), T(u(s))\rangle + o(\|T(u + sw) - T(u)\|) \\
&= \frac{t_s}{\|u + sw\|}(\langle J'(p(v)), u\rangle + s\langle J'(p(v)), w\rangle) + o(\|T(u + sw) - T(u)\|) \\
&= \frac{t_s s}{\|u + sw\|}\langle w + J'(t_u u)_{[L,v]^{\perp}}, w\rangle + o(\|t_s u(s) - t_u u\|) \\
&= \frac{t_s s}{\|u + sw\|}\|w\|^2 + o(|s|) \\
&> \frac{t_u s}{2}\|w\|^2 > 0.
\end{aligned}$$

That is to say, if $\|J'(p(v))_{[L,v]}\| \neq 0$, we always can find $s > 0$, $T(u(s)) \in S_{[L,v]}$, such that $J(T(u(s))) > J(p(v)) + \frac{t_u s}{2}\|w\|^2$, which contradicts (3.10). Consequently $J'(p(v)) \perp [L, v]$. $\square$

LMMM seems to be a three-level algorithm, but in many problems, t_u can be expressed as a real functional of u and $J(t_u u)$ has an explicit expression. Then it becomes a two-level algorithm. Furthermore if we denote $R(t,u) = \langle J'(tu), u\rangle$, by the implicit function theorem, when

$$R'_t = \langle J''(t_u u), u\rangle \neq 0,$$

$t'(u) = T'(u)$ is locally continuous at u and thus $T(\cdot)$ is locally directional Lipschitz continuous at u. Therefore the assumption on T in Lemma 3.2 makes sense.

Note that proof process of Lemma 3.2 suggest a stepsize rule for approximating $p(v)$ defined in (3.8).

3.2.1 Computational theory for LMMM

According to Lemma 3.2, clearly, if $p(v)$ is locally defined as in (3.8), then p is a local L-$\perp$ selection. Therefore, LMMM is within LMO-W frame-work, but with a clearer structure $p(v) = \arg\max_{u\in[L,v],\|u\|\approx 1} \min_{t>0} J(tu)$. Hence we can establish the computational theory for LMMM in a similar way. All the proofs can be obtained in the same ways.

Lemma 3.3. *(LMMM Stepsize Rule) For $v \in S_{L^\perp}$, assume p is locally defined as in (3.8) and*

(i) *p is locally directional Lipschitz continuous at v,*

(ii) *$dis(p(v), L) > 0$,*

(iii) *$d = -J'(p(v)) \neq 0$.*

Then there is $s_0 > 0$ such that when $s_0 > s > 0$, we have

$$J(p(v(s))) - J(p(v)) < -\frac{1}{4C} t_v s \|J'(p(v))\|^2, \tag{3.13}$$

where $v(s) = \frac{v+sw}{\|v+sw\|}$, $w = \frac{d}{C}$, $C = \max\{1, \|d\|\}$, $p(v) = t_v v + u_v$, *for* $t_v > 0$ *and* $u_v \in L$.

Lemma 3.3 can be used to not only derive a local characterization of a saddle point as stated in Theorem 3.1 but also that the inequality (3.13) designs a stepsize rule for the main algorithm of LMMM.

Theorem 3.3. *(LMMM Characterization) For any closed subspace* $L \subset H$*, let* $v^* \in S_{L^\perp}$ *and* p *be locally defined at* v^* *as in (3.8). Assume*

1. p *is locally directional Lipschitz continuous at* v^**,*

2. $p(v^*) \notin L$*,*

3. $v^* = \arg\min_{v \in \mathcal{N}(v^*) \cap S_{L^\perp}} J(p(v))$*, where* $\mathcal{N}(v^*)$ *is a neighborhood of* v^**.*

Then $u^* = p(v^*)$ *is a critical point of* J*, i.e.,* $J'(u^*) = 0$*.*

3.2.2 Algorithm flow chart

Now we are able to design the algorithm for LMMM in the following way.

Given $\varepsilon, \lambda > 0$ and n previously found critical points $u_1, \cdots, u_n$ of J, of which u_n has the highest critical value. Let $L = [u_1, u_2, \cdots, u_n]$.

Step One. Choose $v^k \in S_{L^\perp}$ to be an ascent direction at u_n.

Step Two. Set $k = 1$. Use v^k as an initial to solve for $u^k_{n+1} \equiv p(v^k) \in [L, v^k] \setminus L$ and $p(v^k) \equiv t^k_{n+1}\tilde{u}^k_{n+1}$, where $\tilde{u}^k_{n+1} \in [L, v^k]$.

The following algorithm is for this step only.

Given $\varepsilon_0 > 0$, $\lambda_0 > 0$, $w^{k_0} = v^k$.

Step 1. Take $w^{k_0} \in [L, v^k]$ as an initial, set $k_0 = 1$, compute $t^{k_0}_u = \arg(local)_{t>0} J(tw^{k_0})$ to get $p^{k_0}(v^k) = t^{k_0}_u w^{k_0}$.

Step 2. Compute the steepest descent direction d^{k_0}= $J'(t_u^{k_0}w^{k_0})$ of J at $p^{k_0}(v^k) = t_u^{k_0}w^{k_0}$, and compute

$$pd^{k_0} \equiv (d^{k_0})_{[L,v^k]},$$

which is the projection of d^{k_0} onto $[L, v^k]$.

Step 3. If $\|pd^{k_0}\| < \varepsilon_0$, output $p(v^k) \equiv p^{k_0}(v^k) = t_u^{k_0}w^{k_0}$, and $t_{n+1}^k \equiv t_u^{k_0}$, $\tilde{u}_{n+1}^k = w^{k_0}$. Otherwise, continue.

Step 4. Set $w^{k_0}(s) = \frac{w^{k_0}+s(pd^{k_0})}{\|w^{k_0}+s(pd^{k_0})\|} \in [L, v^k]$, $s = \frac{1}{2^n}$, $n \in \mathbb{N}$, and solve for $t_u^{k_0}(s) = \arg_{t>0} J(tw^{k_0}(s))$. Set $w^{k_0+1} = w^{k_0}(s^{k_0})$, $t_u^{k_0+1} = t_u^{k_0}(s^{k_0})$, where s^{k_0} satisfies

$$s^{k_0} = max\{s = \frac{\lambda}{2^n}|n \in \mathbb{N}, J(t_u^{k_0}(s)w^{k_0}(s)) - J(t_u^{k_0}w^{k_0}) \geq \frac{1}{2}t_u^{k_0}s\|pd^{k_0}\|^2\}.$$

Let $p^{k_0+1}(v^k) = t_u^{k_0+1}w^{k_0+1}$.

Step 5. Update $k_0 = k_0 + 1$ and go to step 2.

Step Three. Compute the steepest descent vector $d_{n+1}^k = -J'(u_{n+1}^k) = -J'(t_{n+1}^k\tilde{u}_{n+1}^k)$.

Step Four. If $\|d^k\| \leq \varepsilon$, then output $u_{n+1} = u_{n+1}^k$, stop, otherwise go to Step Five.

Step Five. Set $v^k(s) = \frac{v^k+sd^k}{\|v^k+sd^k\|}$, $s = \frac{\lambda}{2^m}$, $m \in \mathbb{N}$ and solve for $p(v^k(s))$ using the method in Step Two. Then let $v^{k+1} = v^k(s_{n+1})$, where s_{n+1} satisfies

$$s_{n+1} = max\{s = \frac{\lambda}{2^m}|m \in \mathbb{N}, J(p(v^k(s))) - J(p(v^k)) \leq -\frac{1}{2}t_{n+1}^k s\|d^k\|^2\}.$$

Denote $u_{n+1}^{k+1} = p(v^{k+1}) = t_{n+1}^{k+1}\tilde{u}_{n+1}^{k+1}$.

Step Six. Update $k = k + 1$, and go to Step Three.

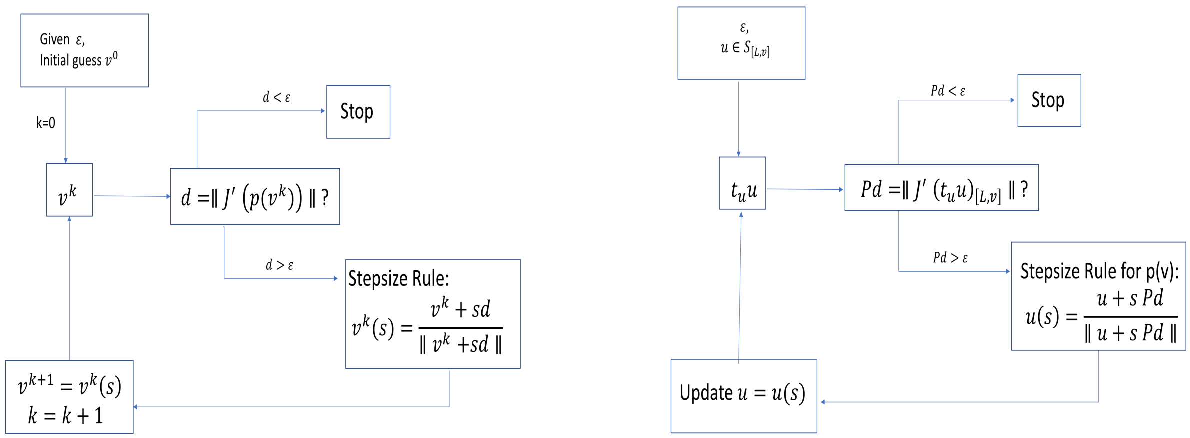


Figure 3.1: Left, main algorithm of LMMM. Right, an algorithm for finding $p(v)$.

3.3 Numerical Results

3.3.1 Tests on finite-dimensional benchmark problems

Example 3.1. *Consider finding 1-saddles of a W-type problem*

$$J(x, y) = (1 - x^2 - y^2)^2 + y^2/(x^2 + y^2). \tag{3.14}$$

It is known that it has two local minima $u_l = (-1, 0)$ and $u_r = (1, 0)$, two $1-saddles$ $(0, 1)$ and $(0, -1)$, and a local maximum $(0, 0)$. The graph and the contour of J are shown in Figure 3.2. Both the local minima and maxima can be obtained by the $Matlab$ subroutine $FMINCON$ or some other numerical methods such as the steepest descent method. When using the newly introduced LMMM above in order to find 1-saddles, we choose a point in the upper half plane as an initial to find $(0, 1)$, and choose a point in the lower half plane as an initial to find $(0, -1)$. The numerical results are displayed as in Table 3.1.

Example 3.2. *Find 1-saddle points of a W-type function with a triple-well potential func-*

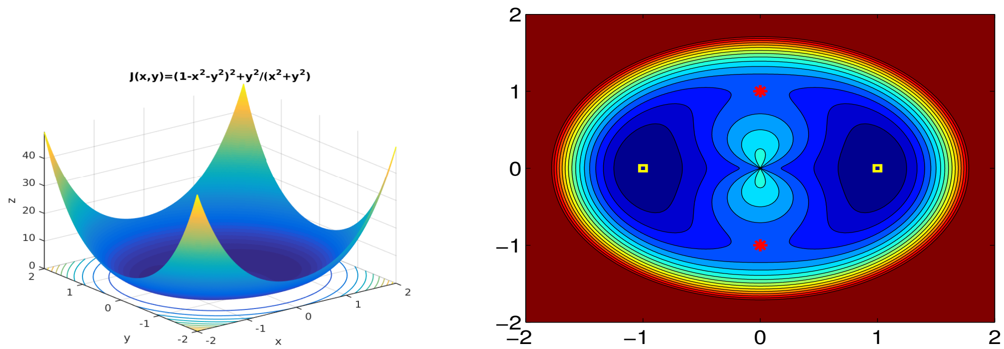


Figure 3.2: Example 3.1. Two local minima ($\square$) at $(1, 0)$, $(-1, 0)$, two 1-saddles ($*$) at $(0, 1)$, $(0, -1)$ and one local maximum at $(0, 0)$.

Saddles	Energy	$\|J'(.)\|$	Itn
(0.000000006639, 1.000006922069)	1.000000000192	0.00006	3
(-0.000000104723, -1.000006922069)	1.000000000192	0.00006	3

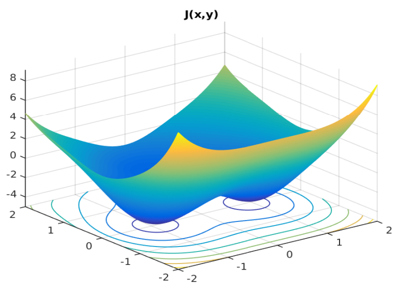
Table 3.1: Numerical results for Example 3.1 by LMMM.

tion

$$J(x,y) = 3e^{-x^2-(y-\frac{1}{3})^2} - 3e^{-x^2-(y-\frac{5}{3})^2} - 5e^{-(x-1)^2-y^2} - 5e^{-(x+1)^2-y^2} + 0.2x^4 + 0.2(y-\frac{1}{3})^4.$$

J has a local maximum at $(x_0, y_0) = (4.94e - 07, 0.5191867342)$. Note that for the innermost level of LMMM, we need $\min_{t>0} J(tu)$ for a fixed $u \in [L, v]$. However, for this function, since $(0, 0)$ is not a local maximum, we could not guarantee that a local minimum along the direction u can be achieved. Therefore, we make a shift $J(x, y) \to \tilde{J}(x, y) = J(x + x_0, y + y_0)$ such that $(0, 0)$ is a local maximum for the new function $\tilde{J}$. Apply LMMM to $\tilde{J}$ to find its critical point (x, y), then $(x + x0, y + y0)$ is the corresponding critical point for $J(x, y)$.

In Table 3.2, the critical points of J are displayed.



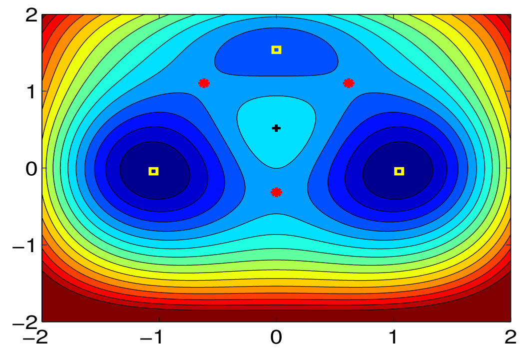


Figure 3.3: Example 3.2. Three local minima ($\square$), one local maximum ($+$) and three 1-saddles ($*$).

	Critical Points	$\|J'(.)\|$	Itn
Local Min	(-4.94e-07, 0.5191867339)	0.00009	12
Local Min	(1.048054981, -0.0420936579)	0.00001	4
Local Min	(-1.0480549862, -0.0420936639)	0.00001	4
1-Saddle	(0.000000016, -0.31585285080)	0.00009	4
1-Saddle	(0.617273599, 1.1027353229)	0.00007	10
1-Saddle	(-0.6172852270, 1.1027945720)	0.00007	4

Table 3.2: Numerical results for Example 3.2 by LMMM.

Example 3.3. *We compute 1-saddles of the Muller function. Muller function is not a W-type function, but it has local W-type structures near its saddle points.*

$$J(x,y) = \sum_{i=1}^{4} K_i e^{[a_i(x-x_i^0)^2 + b_i(x-x_i^0)(y-y_i^0) + c_i(y-y_i^0)^2]},$$

where the vectors $K = (-200, -100, -170, 15)$, $a = (-1, -1, -6.5, 0.7)$, $b = (0, 0, 11, 0.6)$, $c = (-10, -10, -6.5, 0.7)$, $x^0 = (1, 0, -0.5, -1)$, *and* $y^0 = (0, 0.5, 1.5, 1)$.

By viewing the graph and the contour of J in Figure 3.3, we have an intuition that it is

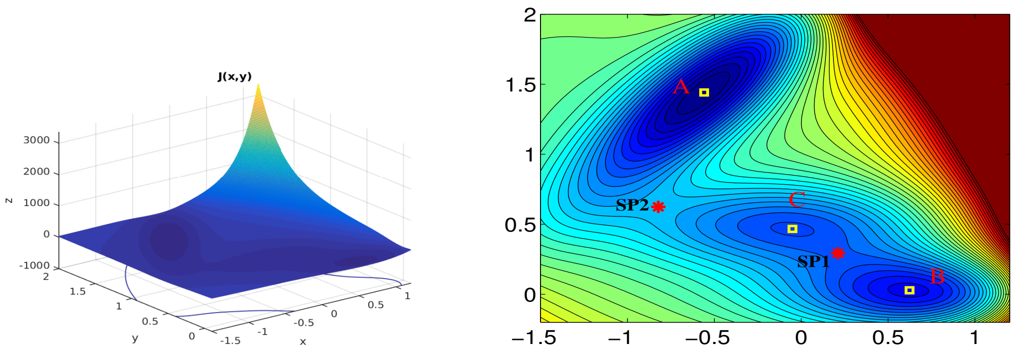


Figure 3.4: Example 3.3. Three local minima A,B,C and two 1-saddles SP1, SP2.

harder to find 1-saddles compared with the previous two benchmark problems since there is no symmetrical property. By LMMM, we get three local minima A,B,C and the first 1-saddle SP1 which are displayed in Table 3.3. For the second 1-saddle SP2, similar with Example 3.2, we shift J to $\tilde{J}$ such that we can get a local minimum along the positive direction of $u \in [L, v]$. Here we select $(x_0, y_0) = (-0.4, 0.95)$, make a shift $J(x, y) \to \tilde{J}(x, y) \equiv J(x+x_0, y+y_0)$, then apply LMMM to $\tilde{J}$. By using an initial point $(-0.4, -0.5)$ in LMMM for $\tilde{J}$, we get one 1-saddle of $\tilde{J}$ and shift it back to get the corresponding 1-saddle SP2=$(-0.821999939540670, 0.624313366549593)$ of J.

	Critical points	Initial	Energy	$\|J'(.)\|$	Itn
Local Min	(-0.5582, 1.4417)	(-0.5,1.5)	-146.70	0.00008	15
Local Min	(0.6235, 0.0280)	(0.5,0.05)	-108.17	0.00005	15
Local Min	(-0.0500, 0.4700)	(-0.1, 0.5)	-80.77	0.00005	14
1-Saddle SP1	(0.2125, 0.2930)	(0.1, 0.15)	-72.25	0.00179	8
1-Saddle SP2	(-0.8220, 0.6243)	(-0.4,-0.5)	-40.66	0.00097	6

Table 3.3: Numerical results for Example 3.3 by LMMM.

Remark 3.1. *For the above three benchmark problems, they are in a finite dimensional space (actually 2 dimensions). According to our algorithm experience, when finding 1-saddles for functionals with W-type structures (finite dimension or infinite dimension), we let $L = [u_0]$, where u_0 is a local minimum with $MI = 0$. Therefore, LMMM becomes two-level optimization when being applied to the above benchmark problems,*

$$J(u^*) = \max_{u \in [L,v], \|u\| \approx 1} \min_{t>0} J(tu),$$

where u^* is the critical points of J and $J(p(v)) = J(u^*)$. Meanwhile, in the main algorithm of LMMM, we use $J'(p(v)) \perp [L, v]$ to terminate Step Two in the flow-chart to solve for $p(v)$, then we just need to judge whether $J'(p(v)) = 0$ or not since the dimension is two, and the algorithm becomes much simpler.

3.3.2 Apply LMMM to infinite-dimensional W-type problems

As stated previously in Chapter 1, for a typical M-type functional, the functional is $\cap$-shape in $[v_1, \cdots, v_k]$, M-shape in $[v_1, \cdots, v_k]^\perp$, and saddle points appear in the M-shape . But for a typical W-type functional, it is $\cup$-shape in $[v_1, \cdots, v_k]^\perp$, W-shape in $[v_1, \cdots, v_k]$, and we need to find saddle points from the W-shape . Due to the finite dimension of the W-shape space , the algorithm is very sensitive when searching for critical points since it may go out the scope of W-shape and enter the $\cup$-shape. On the other hand, even though the innermost level of LMMM is a local minimization, it is very easy that the local maximization in the middle level will pull local minima back to "0", then we will get the trivial solution "0" and the algorithm stops. So how to keep the searching for saddle points strictly inside W-shape and away from "0" becomes important and we will discuss how to overcome such difficulties in Section 3.5. In this section, we only present the numerical results.

When $\Omega = [-1, 1] \times [-1, 1]$, compute the eignevalues $\lambda_1 < \lambda_2 < \cdots$ and their corresponding eigenfunctions $\varphi_1, \varphi_2, \cdots$ of (1.7) to get

(a) $\lambda_1 = 4.9348$, $\varphi_1 = cos(\frac{\pi x}{2})cos(\frac{\pi y}{2})$. (b) $\lambda_2 = 12.3370$, $\varphi_2 = sin(\pi x)cos(\frac{\pi y}{2})$.

(c) $\lambda_3 = 12.3370$, $\varphi_3 = cos(\frac{\pi x}{2})sin(\pi y)$. (d) $\lambda_4 = 19.7392$, $\varphi_4 = sin(\pi x)sin(\pi y)$.

(e) $\lambda_5 = 24.6740$, $\varphi_5 = cos(\frac{3\pi x}{2})cos(\frac{\pi y}{2})$. (f) $\lambda_6 = 24.6740$, $\varphi_6 = cos(\frac{\pi x}{2})cos(\frac{3\pi y}{2})$.

For all the following numerical examples, we use the above eigenfunctions or combinations of them as initial guesses when finding multiple W-type critical points.

3.3.2.1 Apply LMMM to the model (typical W-type) problem, case 1

Now return to our model problem (3.1) in this chapter. We typically select $f(x, u(x)) = |u(x)|^{p-1}u(x)$ and get the following BVP

$$\begin{cases} -\Delta u(x) - \lambda u(x) + |u(x)|^{p-1}u(x) = 0, \quad x \in \Omega, \\ u|_{\partial\Omega} = 0. \end{cases} \tag{3.15}$$

The corresponding energy function is a W-type functional,

$$J(u) = \int_\Omega (\frac{1}{2}|\nabla u(x)|^2 - \lambda u^2(x))dx + \frac{1}{p+1}\int_\Omega |u(x)|^{p+1}dx.$$

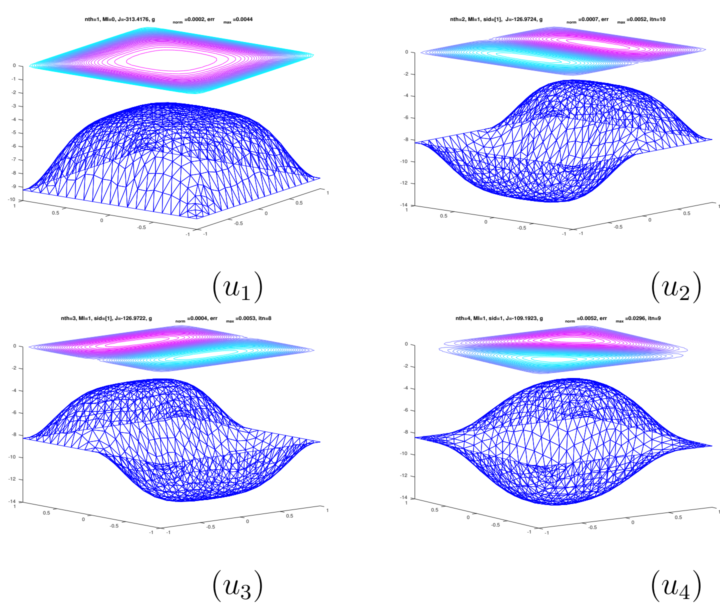
We select $p = 3$ and $\Omega = [-1, 1] \times [-1, 1]$ when solving for numerical solutions for it. As computed previously, the eigenvalues for the Laplacian operator based on the same domain are: 4.9348, 12.3370, 12.3370, 19.7392, 24.6740, 24.6740, 32.0762, 32.0762, $\cdots$. In literature [17, 31], it has been proved that when $\lambda_n < \lambda < \lambda_{n+1}$, there are at least n different solutions for (3.15).

Theoretically there are at least six different solutions when $\lambda = 28$ and there are at least four different solutions when $\lambda = 20$. By LMMM, we find the following numerical solutions from (u_1) to (u_{10}) when $\lambda = 28$, which are displayed in Table 3.4 and Figure 3.5

& 3.6, and multiple critical points from $(\bar{u}_1)$ to $(\bar{u}_6)$ when $\lambda = 20$, which are displayed in Table 3.5 and Figure 3.7.

nth	Figure	MI	Support	Energy	$\|J'(.)\|$	err_{max}	Itn
1	(u_1)	0	NA	-313.4176	0.0002	0.0044	8
2	(u_2)	1	1	-126.9724	0.0007	0.0052	10
3	(u_3)	1	1	-126.9722	0.0004	0.0053	8
4	(u_4)	1	1	-109.1923	0.0052	0.0296	9
5	(u_5)	1	1	-109.1914	0.006	0.0719	6
6	(u_6)	2	[1,2]	-31.7034	0.001	0.0075	7
7	(u_7)	3	[1,2,6]	-5.1074	0.0029	0.0457	5
8	(u_8)	3	[1,2,6]	-5.1073	0.0014	0.0304	6
9	(u_9)	3	[1,2,4]	-4.2985	0.001	0.0215	4
10	(u_{10})	3	[1,2,4]	-4.2607	0.0011	0.0709	5

Table 3.4: Numerical values of W-type solutions of (3.15) when $\lambda = 28$.



(u_1) (u_2) (u_3) (u_4)

Figure 3.5: W-type solutions of (3.15) when $\lambda = 28$. $(u_1) - (u_4)$

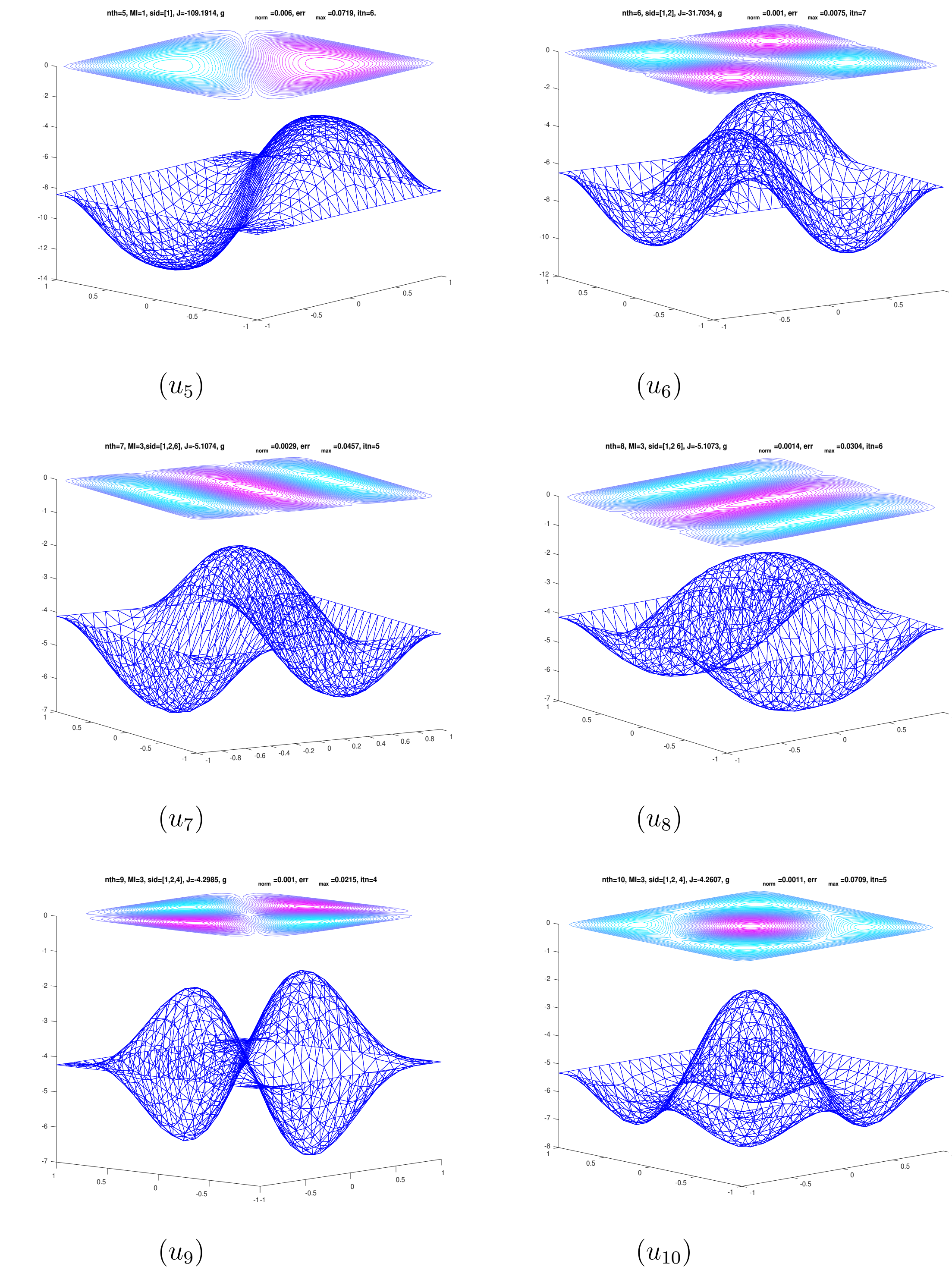


Figure 3.6: W-type solutions of (3.15) when $\lambda = 28$. $(u_5) - (u_{10})$

nth	Figure	MI	Support	Energy	$\|J'(.)\|$	err_{max}	Itn
1	$(\bar{u}_1)$	0	NA	-125.7075	0.0009	0.0114	8
2	$(\bar{u}_2)$	1	1	-28.5324	0.0008	0.0075	5
3	$(\bar{u}_3)$	1	1	-28.5321	0.0007	0.0068	5
4	$(\bar{u}_4)$	1	1	-24.3427	0.0025	0.0263	5
5	$(\bar{u}_5)$	1	1	-24.3426	0.0019	0.0177	6
6	$(\bar{u}_6)$	2	[1,2]	-0.0303	0.0005	0.0099	2

Table 3.5: Numerical values of W-type solutions of (3.15) when $\lambda = 20$.

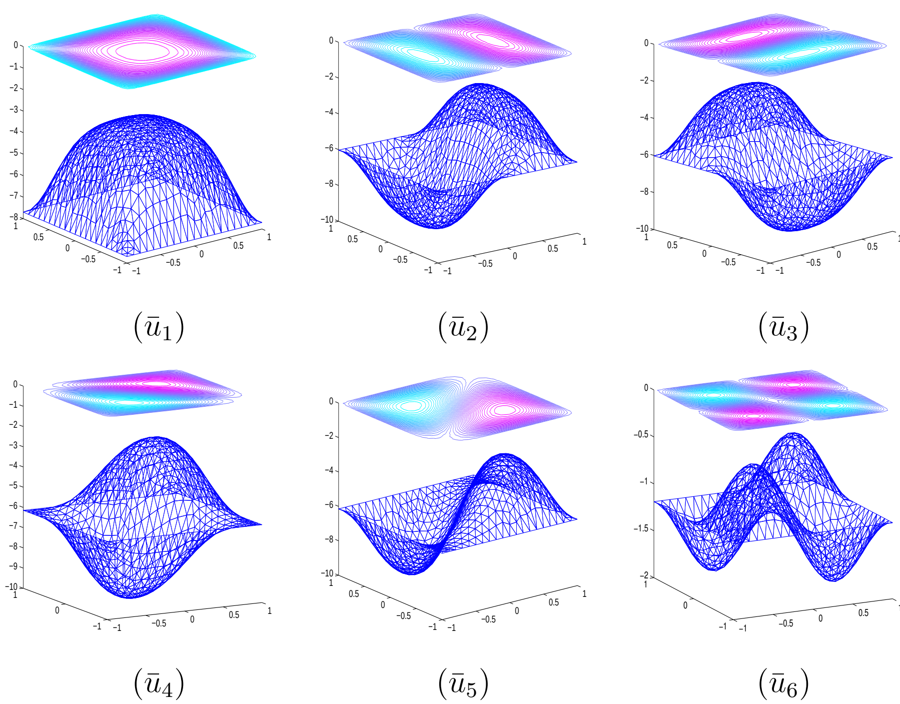


Figure 3.7: W-type solutions of (3.15) when $\lambda = 20$.

Notice that for the numerical solutions above, in the case when $\lambda = 28$, we can treat u_2, u_3 as the same solution since one can be obtained by rotating the other one. In this sense, u_4, u_5 are the same solution, and so are u_7, u_8. Then we found seven different numerical solutions by LMMM. Similarly, in the case when $\lambda = 20$, we found four different numerical solutions which is consistent with $\lambda_4 < 20 < \lambda_5$.

3.3.2.2 Apply LMMM to the model problem, case 2

For the model problem (3.1), if we select $f(x, u(x)) = k|x|^r|u(x)|^{p-1}u(x)$, then we get the following BVP

$$\begin{cases} -\Delta u(x) - \lambda u(x) + k|x|^r|u(x)|^{p-1}u(x) = 0, \quad x \in \Omega, \\ u|_{\partial\Omega} = 0. \end{cases} \tag{3.16}$$

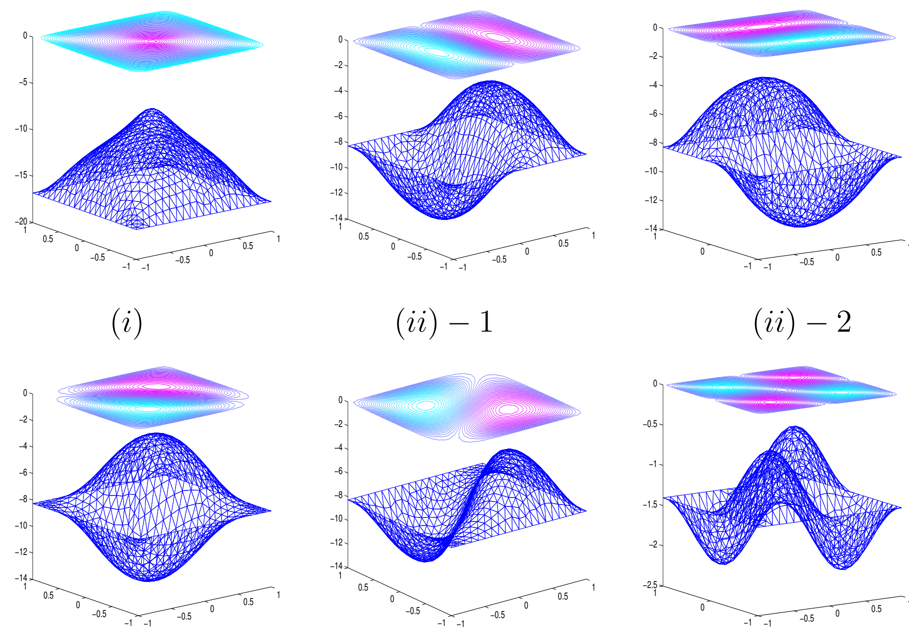
The corresponding energy function is

$$J(u) = \int_{\Omega} [\frac{1}{2}(|\nabla u(x)|^2 - \lambda u^2(x)) + \frac{k}{p+1}|x|^r|u(x)|^{p+1}]dx.$$

This is a more general case of W-type problem. When taking $r = 0$ and $k = 1$, it becomes the typical W-type problem case 1. We select $p = 3$, $k = 1$, $\lambda = 20$, $\Omega = [-1, 1] \times [-1, 1]$ and $r = 1$ when applying LMMM to compute the multiple saddle points. The results are shown below.

nth	Figure	MI	Support	Energy	$\|J'(.)\|$	err_{max}	Itn
1	(i)	0	NA	-295.4434	0.0008	0.0158	15
2	(ii)-1	1	1	-48.7262	0.0015	0.0255	6
3	(ii)-2	1	1	-48.7260	0.0012	0.0251	5
4	(iii)-1	1	1	-41.9065	0.0027	0.0266	5
5	(iii)-2	1	1	-41.9064	0.0019	0.0277	6
6	(iv)	2	[1,2]	-0.0420	0.0010	0.0205	3

Table 3.6: Numerical values of W-type solutions of (3.16).



(i) $(ii)-1$ $(ii)-2$

$(iii)-1$ $(iii)-2$ (iv)

Figure 3.8: W-type solutions of (3.16).

3.3.2.3 Apply LMMM to a M-type problem with a locally W-type structure (W-M type)

In this section, we apply LMMM to the following concave-convex elliptic problem,

$$\begin{cases} -\Delta u(x) = a(x)|u(x)|^{q-1}u(x) + |u(x)|^{p-1}u(x), \quad x \in \Omega, \\ u|_{\partial\Omega} = 0, \end{cases} \tag{3.17}$$

where $u \in H = H_0^1(\Omega)$, $\Omega \subset \mathbb{R}^N$ is open bounded, $0 < q < 1 < p < 2^*$, $2^* = \frac{N+2}{N-2}$ if $N \geq 3$, $2^* = \infty$ if $N = 1, 2$. $a(x)$ is a nonnegative function in Ω. Its corresponding energy function is

$$J(u) = \int_\Omega [\frac{1}{2}|\nabla u(x)|^2 - \frac{a(x)}{q+1}|u(x)|^{q+1} - \frac{1}{p+1}|u(x)|^{p+1}]dx. \tag{3.18}$$

This problem has a combined effect of concave and convex nonlinearities [25]. It has various applications in mathematical physics and population dynamics [49]. The sublinear and superlinear terms together make (3.18) be a combination of focused and defocused system. It has a structure in the Figure 3.9. It is clear that it is a M-type problem but with a locally W-type structure.

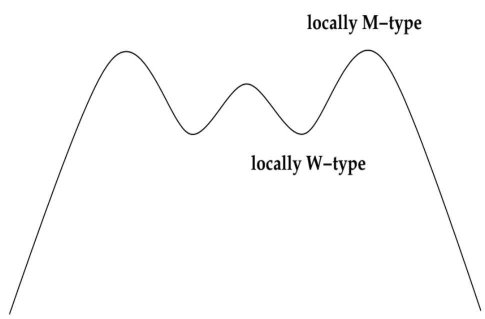


Figure 3.9: M-type with a locally W-type structure.

For the above problem, we can apply LMM to find critical points with positive energies (M-type critical points), hence they are not our interest in this thesis. We are interested in finding critical points with negative energies (W-type critical points). We select $p = 4$, $q = 0.05$, $a(x) = 1.4$ and $\Omega = [-1, 1] \times [-1, 1]$ when applying LMMM to (3.18) and get the numerical solutions displayed in Table 3.7 and Figure 3.10 & 3.11.

nth	Figure	MI	Support	Energy	$\|J'(.)\|$	u_{max}	u_{max} at	Itn
1	(a)	0	NA	-0.4314	0.0002	0.3898	(-0.0005, -0.0032)	6
2	(b1)	1	1	-0.1589	0.0006	0.1426	(0.5003, 0.0031)	7
3	(b2)	1	1	-0.1589	0.0009	0.1428	(-0.0035, 0.4980)	7
4	(c1)	1	1	-0.1445	0.0008	0.1481	(0.3944, 0.3906)	8
5	(c2)	1	1	-0.1445	0.0006	0.1480	(-0.3909, 0.3912)	8
6	(d)	2	[1,2]	-0.0930	0.0008	0.0902	(-0.5012, 0.4955)	9
7	(e1)	3	[1,2,6]	-0.0756	0.0008	0.0660	(-0.0057, -0.0003)	11
8	(e2)	3	[1,2,6]	-0.0756	0.0008	0.0659	(-0.6659, 0.0042)	11
9	(f)	3	[1,4,5]	-0.0671	0.0017	0.0716	(0.0024, 0.6072)	10
10	(g)	3	[1,4,5]	-0.0732	0.0013	0.1026	(-0.0005, -0.0032)	11

Table 3.7: Numerical values of W-type solutions of (3.17).

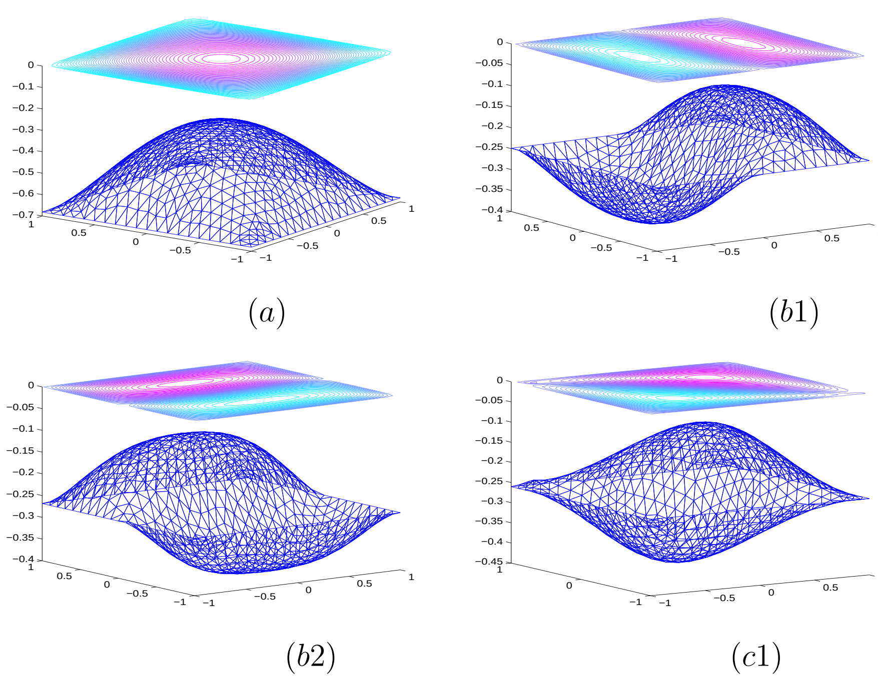


Figure 3.10: W-type solutions of (3.17). $(a) - (c1)$

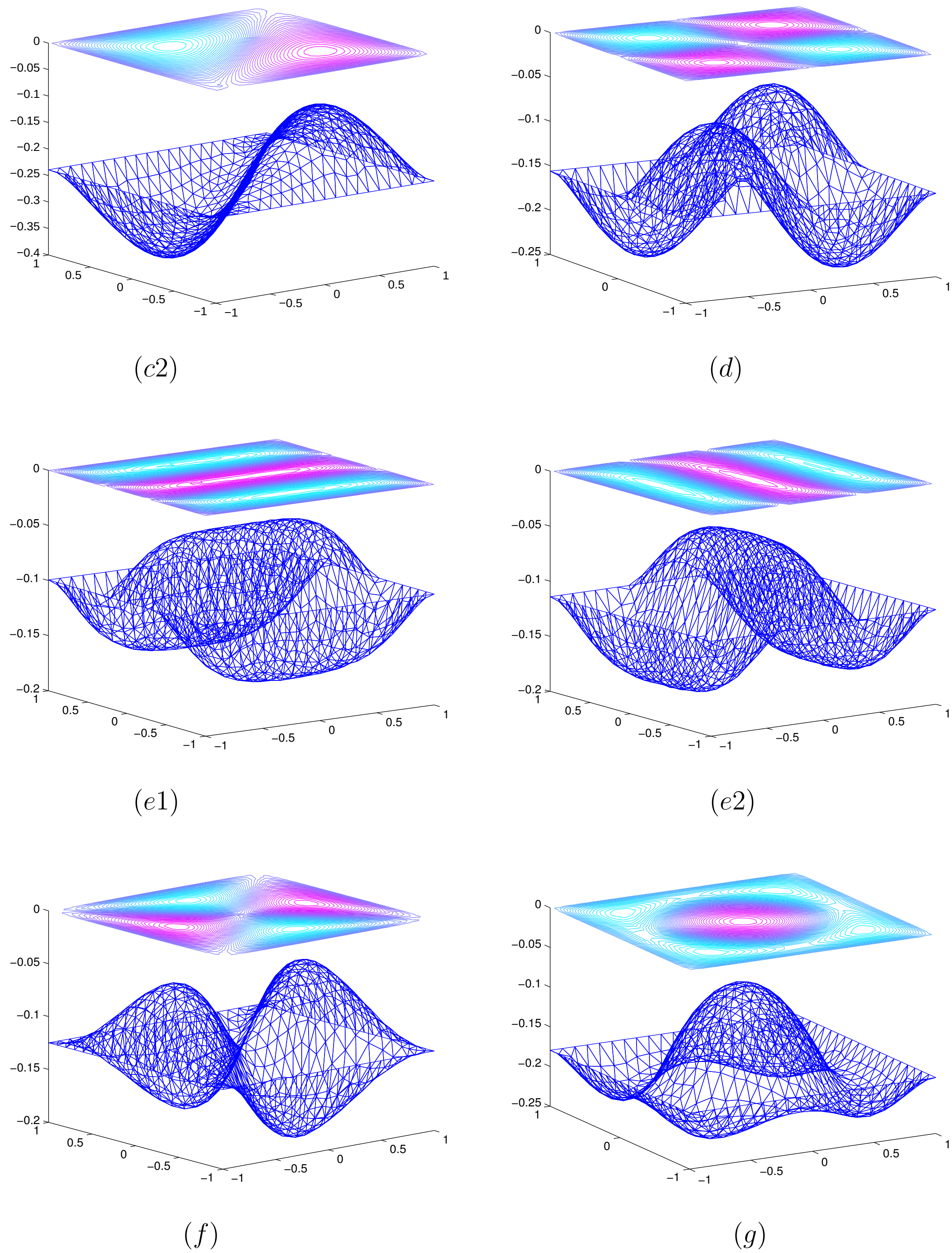


Figure 3.11: W-type solutions of (3.17). $(c2) - (f)$

3.4 Convergence Analysis for LMMM

In order to establish a convergence result for LMMM, we need PS condition as well as an uniform stepsize rule. PS condition is define as in (1.2) in Chapter 1, and the uniform stepsize rule is presented below.

Lemma 3.4. *(Uniform Stepsize Rule) Let p be locally defined as in (3.8) at $v_0 \in S_{L^\perp}$ with $d_0 = -J'(p(v_0)) \neq 0$. Assume (1) p is locally directional Lipschitz continuous at v_0, (2) p is continuous near v_0, (3) $p(v_0) = t_0 v_0 + v_0^L \notin L$. Then there are $\delta > 0$, $s_0 > 0$, s.t. when $\|v - v_0\| < \delta$, $0 < s < s_0$, we have*

$$J(p(v(s))) - J(p(v)) < -\frac{1}{4C} t_0 s \|J'(p(v))\|^2,$$

where $v(s) = \frac{v+sw}{\|v+sw\|} \in S_{L^\perp}$, $w = \frac{-J'(p(v))}{C}$, $C = \max\{1, \|J'(p(v))\|\}$.

Now we present a convergence result for LMMM.

Theorem 3.4. *(Convergence) Let $p(v)$ be defined as in (3.8), $\{v^k\}$ and $\{u_{n+1}^k\}$ be sequences generated by LMMM. Assume J satisfies PS condition. If (a) p is locally directional continuous and continuous, (b) $dist(L, u_{n+1}^k) > \alpha > 0$ for $\forall k = 0, 1, 2, \cdots$, (c) $\inf_{v \in S_{L^\perp}} J(p(v)) > -\infty$. Then*

(a) there is $\{v^{k_i}\} \subset \{v^k\}$ s.t. $v^{k_i} \to v^*$, $u^* = p(v^*)$, $J'(u^*) = 0$,

(b) if u^* is isolated then $v^k \to v^*$.

The proofs for Lemma 3.4 and Theorem 3.4 are similar with the proofs in [57].

3.5 Algorithm Analysis in Applications

In this section, we analyze the algorithm LMMM when it is applied to the model problem (3.1), which we restate here

$$\begin{cases} -\Delta u(x) - \lambda u(x) + f(x, u(x)) = 0, & x \in \Omega, \\ u|_{\partial\Omega} = 0. \end{cases} \tag{3.19}$$

Its variational functional is

$$J(u) = \int_\Omega [\frac{1}{2}(|\nabla u(x)|^2 - \lambda u^2(x)) + F(x, u(x))]dx, \tag{3.20}$$

where Ω is bounded in $\mathbb{R}^N$, $u \in H_0^1(\Omega)$ with norm $\|u\| = (\int_\Omega [|\nabla u|^2 + u^2]dx)^{\frac{1}{2}}$ and $\frac{\partial}{\partial t}F(x,t) = f(x,t)$. Solutions of (3.19) correspond to critical points of J in (3.20).

In this section, we always suppose $f(x, \xi)$ satisfies the following hypothesis.

(f1) $f(x, \xi)$ is locally Lipschitz on $\bar{\Omega} \times \mathbb{R}$.

(f2) There are positive constants a_1 and a_2 s.t

$$|f(x, \xi)| \leq a_1 + a_2|\xi|^s, \tag{3.21}$$

where $0 \leq s < \frac{N+2}{N-2}$ for $n > 2$. If $n = 2$,

$$|f(x, \xi)| \leq a_1 exp(\phi(\xi)), \tag{3.22}$$

where $\phi(\xi)\xi^{-2} \to \infty$.

(f3) $f(x, \xi) = o(|\xi|)$ as $\xi \to 0$, and $f(x, \xi)\xi > 0$ when $x\xi \neq 0$. Note that (f3) implies that for some δ small, there exist $c > 0$ and $m > 1$, s.t. for all $x \in \bar{\Omega}$ and $|\xi| < \delta$,

$$|f(x, \xi)| < c|\xi|^m, \tag{3.23}$$

and there exists $d > 0$, s.t. for all $x \in \bar{\Omega}$ and $|\xi| < \delta$,

$$|F(x,\xi)| < d|\xi|^{m+1}. \tag{3.24}$$

(f4) There are constants $\mu > 2$ and $r \geq 0$ s.t. for $\xi \geq r$,

$$0 < \mu F(x,\xi) \leq \xi f(x,\xi), \tag{3.25}$$

where $F(x,\xi) = \int_0^\xi f(x,t)dt$. Notice that (f4) implies that there exist positive numbers a_3 and a_4 s.t. for all $x \in \bar{\Omega}$, $\xi \in \mathbb{R}$,

$$F(x,\xi) \geq a_3|\xi|^\mu - a_4, \tag{3.26}$$

and there exists positive numbers a_5 and a_6 s.t. for all $x \in \bar{\Omega}$ and $\xi \in \mathbb{R}$,

$$|f(x,\xi)| \geq a_5|\xi|^{\mu-1} - a_6. \tag{3.27}$$

(f5) $\frac{f(x,\xi)}{|\xi|}$ is strictly increasing w. r. t. ξ.

When we establish the convergence result for LMMM, we assume that J satisfies PS condition. The following lemma indicates that J in (3.20) indeed satisfies PS condition.

Lemma 3.5. *J in (3.20) satisfies PS condition.*

In order to prove it, we need to use Proposition 3.1 [17] and Rellich Embedding Theorem [50].

Proposition 3.1. *let $\Omega \subset \mathbb{R}^N$ be a bounded domain and let g satisfies*

(g1) $g \in \mathcal{C}(\bar{\Omega} \times \mathbb{R}, \mathbb{R})$,

(g2) There are constants $r, t \geq 1$ and $a_1 \geq 0$, $a_2 \geq 0$ such that

$$|g(x,\xi)| \leq a_1 + a_2|\xi|^{\frac{r}{t}},$$

for all $x \in \bar{\Omega}$, $\xi \in \mathbb{R}$.

Then the map $\varphi(x) \to g(x, \varphi(x))$ belongs to $\mathcal{C}(L^r(\Omega), L^t(\Omega))$.

Rellich Embedding Theorem. If $|\Omega| < \infty$, the following embedding are compact

$$H_0^1(\Omega) \hookrightarrow L^p(\Omega), 1 \leq p < 2^*,$$

where $2^* = \infty$ when $N = 1, 2$, $2^* = \frac{2N}{N-2}$ when $N \geq 3$.

Now we are able to prove Lemma 3.5.

Proof. We use an equivalent norm $\|u\| = \int_\Omega u(x)^2 dx$ here. Let $\{u_n\}$ be a PS sequence, i.e. $J(u_n)$ is bounded and $J'(u_n) \to 0$, by (f4) we get $F(x, u_n(x)) \geq a|u_n(x)|^\mu - b$, for some $\mu > 2$, $a > 0$, $b > 0$. Denote $\Omega_1 = \{x \in \Omega \mid |u_n(x)|^{\mu-2} \geq \frac{1}{2a}\lambda\}$, then when $x \in \Omega_1$, $a|u_n(x)|^\mu - b \geq \frac{1}{2}\lambda u_n(x)^2 - b$. Denote $G(u) = \frac{1}{2}\lambda\int_\Omega u^2 dx - \int_\Omega F(x, u(x))dx$, then $J(u) = \frac{1}{2}\|u\|^2 - G(u)$ and we have

$$\begin{aligned}
&G(u_n) = \frac{1}{2}\lambda\int_\Omega u_n^2 dx - \int_\Omega F(x, u_n(x))dx \\
&= \int_{\Omega_1} (\frac{1}{2}\lambda u_n^2 - F(x, u_n(x))dx + \int_{\Omega/\Omega_1} (\frac{1}{2}\lambda u_n^2 - F(x, u_n(x))dx \\
&\leq \int_{\Omega_1} (\frac{1}{2}\lambda u_n^2 - (a|u_n(x)|^\mu - b)) + C_0 \\
&\leq \int_{\Omega_1} (\frac{1}{2}\lambda u_n^2 - (\frac{1}{2}\lambda u_n^2 - b)) + C_0 \\
&\leq C.
\end{aligned}$$

Since there exists a constant M such that $J(u_n) < M$, it follows that $\frac{1}{2}\|u_n\|^2 = J(u_n) + G(u_n) \leq M + C$. That means $\{u_n\}$ is bounded in $H = H_0^1(\Omega)$. Consequently there must exist one subsequence of $\{u_n\}$, denoted by $\{u_n\}$ again, such that $u_n \rightharpoonup u \in H$. By the Rellich Embedding Theorem, $u_n \to u$ in $L^p(\Omega)$. Meanwhile we have

$$
\begin{aligned}
&\langle J'(u_n) - J'(u), u_n - u\rangle = \langle J'(u_n), u_n - u\rangle - \langle J'(u), u_n - u\rangle \\
&= \int_\Omega (-\Delta u_n)(u_n - u)dx - \int_\Omega (-\Delta u)(u_n - u)dx - \lambda \int_\Omega u_n(u_n - u)dx + \lambda \int_\Omega u(u_n - u)dx \\
&+ \int_\Omega f(x, u_n)(u_n - u)dx - \int_\Omega f(x, u)(u_n - u)dx \\
&= \int_\Omega -\Delta(u_n - u)(u_n - u)dx - \lambda \int_\Omega (u_n - u)^2 dx + \int_\Omega (f(x, u_n) - f(x, u)(u_n - u))dx \\
&= \|u_n - u\|^2 - \lambda \int_\Omega (u_n - u)^2 dx + \int_\Omega (f(x, u_n) - f(x, u)(u_n - u))dx.
\end{aligned}
$$

Isolate $\|u_n - u\|^2$ to the left side to get

$$
\|u_n - u\|^2 = \langle J'(u_n) - J'(u), u_n - u\rangle + \lambda \int_\Omega (u_n - u)^2 dx + \int_\Omega (f(x, u_n) - f(x, u)(u_n - u))dx.
$$

Now we discuss each term from the right side of the above equation separately.

(i) Since $u_n \rightharpoonup u$,$\langle J'(u), u_n - u\rangle \to 0$. Besides, $|\langle J'(u_n), u_n - u\rangle| \leq \|J'(u_n)\|_{L^2}\|u_n - u\| \to 0$. So $\langle J'(u_n) - J'(u), u_n - u\rangle \to 0$ as $n \to \infty$.

(ii) $\int_\Omega (u_n - u)^2 dx \to 0$ by Rellich Embedding Theorem.

(iii) We have $s + 1 < \frac{2N}{N-2}$ by (f2) and $u_n \to u$ in $L^{s+1}(\Omega)$ by Rellich Embedding Theorem. Let $r = s + 1$, $t = \frac{s+1}{s}$ in Proposition 3.1, then $f(x, u_n) \to f(x, u)$ in L^t. On the other hand, by the Hölder inequality,

$$
|\int_\Omega (f(x, u_n) - f(x, u)(u_n - u))dx| \leq \|f(x, u_n) - f(x, u)\|_{L^t}\|u_n - u\|_{L^{s+1}} \to 0.
$$

In view of (i), (ii),(iii), we get $\|u_n - u\| \to 0$, which means that any PS sequence has one convergent subsequence, so J in (3.20) satisfies PS condition. $\square$

In the previous sections, we denoted the eigenvalues of (1.7) by $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k \leq \cdots$ and the corresponding eigenfuncitons by $\{\varphi_i\}$. In this section, we use the same notations but assume $\{\varphi_i\}$ are orthonormal and we always take λ in (3.19) such that $\lambda_k < \lambda < \lambda_{k+1}$. Now we can prove the following lemma.

Lemma 3.6. *For each $w \in X \subset [\varphi_1, \varphi_2, \cdots, \varphi_k]$ with $\|w\| = 1$, there exists $t_w > 0$ such that $t_w = \arg\min_{t>0} J(tw)$. Furthermore, if we denote $\gamma_0^v = \{t_w w | w \in X, \|w\| = 1\}$, then there exists $\delta > 0$, such that $\gamma_0^v \cap B(0, \delta) = \emptyset$.*

Proof. For $\forall\, w \in X$ with $\|w\| = 1$, w can be written as $w = \sum_{i=1}^k a_i\varphi_i$, where $\sum_{i=1}^k a_i^2 = 1$, then it follows that

$$
\begin{aligned}
&\int_\Omega (|\nabla w|^2 - \lambda w^2)dx \\
&= \int_\Omega (-\Delta w - \lambda w)w dx \\
&= \int_\Omega [(-\sum_{i=1}^k a_i \Delta\varphi_i + \sum_{i=1}^k a_i\varphi_i) - (\lambda+1)\sum_{i=1}^k a_i\varphi_i](\sum_{i=1}^k a_i\varphi_i)dx \\
&= \sum_{i=1}^k a_i^2 - (\lambda+1)\int_\Omega (\sum_{i=1}^k a_i\varphi_i)(\sum_{i=1}^k a_i\varphi_i) \\
&= \sum_{i=1}^k a_i^2 - (\lambda+1)\int_\Omega [\sum_{i=1}^k a_i(\frac{\lambda_i}{\lambda_i+1}\varphi_i + \frac{1}{\lambda_i+1}\varphi_i)](\sum_{i=1}^k a_i\varphi_i) \\
&= \sum_{i=1}^k a_i^2 - (\lambda+1)\int_\Omega [\sum_{i=1}^k a_i(\frac{-\Delta\varphi_i}{\lambda_i+1} + \frac{1}{\lambda_i+1}\varphi_i)](\sum_{i=1}^k a_i\varphi_i) \\
&= \sum_{i=1}^k a_i^2 - (\lambda+1)\sum_{i=1}^k \frac{a_i^2}{\lambda_i+1} \\
&= \sum_{i=1}^k (1 - \frac{\lambda+1}{\lambda_i+1})a_i^2 < 0.
\end{aligned}
$$

It is very clear that for $\forall\, w \in X$ with $\|w\| = 1$, $t > 0$, we have

$$J(tw) = \int_\Omega [\frac{t^2}{2}(|\nabla w(x)|^2 - \lambda w^2(x)) + F(x, tw(x))]dx.$$

On one hand, $F(x, tw) \geq a_3|tw|^\mu - a_4$ by (3.26), then for any fixed w, $J(tw) \to +\infty$ as $t \to \infty$. On the other hand, $|F(x, tw)| < d|tw|^{m+1}$ by (3.24), then $J(tw) < 0$ for sufficiently small $t > 0$. As a result, there must exist at least one local minimum $t_w > 0$ such that $t_w = \arg\min_{t>0} J(tw)$.

If J obtains its local minimum at t_w for any $w \in X$, we have $\frac{dJ(tw)}{dt}|_{t=t_w} = 0$, i.e.

$$\begin{aligned}
&\frac{dJ(tw)}{dt} = t\int_\Omega (|\nabla w|^2 - \lambda w^2)dx + \int_\Omega f(x, tw)wdx \\
&= t[\int_\Omega (|\nabla w|^2 - \lambda w^2)dx + \int_\Omega \frac{f(x, tw)}{t} wdx] \\
&= 0.
\end{aligned}$$

Since $t_w > 0$, we get $\int_\Omega (|\nabla w|^2 - \lambda w^2)dx + \int_\Omega \frac{f(x,t_w w)}{t_w} wdx = 0$. If $\gamma_0^v \cap B(0, \delta) = \emptyset$ does not hold for any $\delta > 0$, then there exist $\{t_{w_n} w_n\} \subset \gamma_0^v$ such that $t_{w_n} w_n \to 0$, so $t_{w_n} \to 0$ as $n \to \infty$. For each w_n, we have $t_{w_n} > 0$, it it clear that

$$\int_\Omega (|\nabla w_n|^2 - \lambda w_n^2)dx + \int_\Omega \frac{f(x, t_{w_n} w_n)}{t_{w_n}} w_n dx = 0. \tag{3.28}$$

By (3.23), when n is large enough, $|f(x, t_{w_n} w_n)| < c|t_{w_n}|^m |w_n(x)|^m$ for all $x \in \bar{\Omega}$. Then

$$\frac{f(x, t_{w_n} w_n)}{t_{w_n}} w_n = \frac{|f(x, t_{w_n} w_n)|}{t_{w_n}} |w_n| \leq c|t_{w_n}|^{m-1} |w_n(x)|^{m+1}. \tag{3.29}$$

Since $m+1>2$,

$$\int_\Omega |w_n(x)|^{m+1}dx \le C\int_\Omega |w_n(x)|^2 dx \le C. \tag{3.30}$$

In view of (3.29), (3.30), we can get

$$\int_\Omega \frac{f(x,t_{w_n}w_n)}{t_{w_n}} w_n dx \le C_1|t_{w_n}|^{m-1} \to 0, n\to\infty.$$

Since (3.28) holds, then

$$\int_\Omega (|\nabla w_n|^2 - \lambda w_n^2)dx \to 0, n\to\infty. \tag{3.31}$$

However, if we denote $w_n = \sum_{i=1}^k a_i^{(n)}\varphi_i$, where $\sum_{i=1}^k (a_i^{(n)})^2 = 1$, we can compute

$$\int_\Omega (|\nabla w_n|^2 - \lambda w_n^2)dx = \sum_{i=1}^k (1-\frac{\lambda+1}{\lambda_i+1})(a_i^{(n)})^2.$$

In view of (3.31), since $1-\frac{\lambda+1}{\lambda_i+1}<0$ for all $i=1,\cdots,k$, we get

$$(a_i^{(n)})^2 \to 0, n\to\infty,$$

which is in contradiction with $\sum_{i=1}^k (a_i^{(n)})^2 = 1$. So there must exist $\delta>0$, such that $\gamma_0^v \cap B(0,\delta)=\emptyset$. $\square$

Lemma 3.6 is helpful in several ways. First, at the beginning of this chapter, we pointed out that the model problem (3.1) has a W-type structure since it is W-shape in a finite dimensional subspace $V=[v_1,\cdots,v_k]$, but we don't know which space V is. This lemma indicates that such a subspace exists and we can find it, namely, it is the eigenfunction space $E=[\varphi_1,\varphi_2,\cdots,\varphi_k]$ of (1.7). The dimension of E depends on the value of λ in

(3.20). Second, when we compute numerical solutions for W-type problems in infinitely dimensional space, we need to keep the search for critical points (SCP) inside the W-shape and away from "0". This lemma indicates that we can keep SCP inside the W-shape and away from "0" if we search critical points inside E. Unfortunately, our problems are not so easy. J is W-shape in E does not mean that multiple saddle points are in E. For some $w \in H \setminus E$, $J(tw)$ can also obtain its local minimum and it is W-shape in the direction w. The innermost minimization of LMMM searches all local minima for all directions $u \in [L, v]$, and those u's are often not in E. However, Lemma 3.6 provides us hints to select appropriate initial guesses which should be from E, and our numerical examples showed an efficiency of such selections.

Lemma 3.7. *For a fixed* $u \in H$ *with* $\|u\| = 1$*, regard the function* $J(tu)$ *in (3.20) as a function of* $t \geq 0$*, then* $J(tu)$ *satisfies either (i)* $J(tu)$ *is increasing on* $[0, \infty)$ *with* $J(tu) = 0$ *if and only if* $t = 0$*, or (ii)* $J(tu)$ *has an unique local minimum at* $t_u > 0$ *such that* $J(t_u u) < 0$*, where* $t_u = \arg\min_{t>0} J(tu)$.

Proof. Given $u \in S_H$, $J(tu) = \int_\Omega [\frac{t^2}{2}(|\nabla u(x)|^2 - \lambda u^2(x)) + F(x, tu(x))]dx$,

$$\frac{dJ(tu)}{dt} = t \int_\Omega (|\nabla u|^2 - \lambda u^2)dx + \int_\Omega f(x, tu)udx. \tag{3.32}$$

We can separate our discussion into two cases.

(i) Case 1, $\int_\Omega (|\nabla u|^2 - \lambda u^2)dx \geq 0$. In this case, $\int_\Omega f(x, tu)udx \geq 0$ by (f3), hence $\frac{dJ(tu)}{dt} \geq 0$ for all $t > 0$, i.e. $J(tu)$ is increasing on $[0, \infty)$.

Suppose there is another $t_1 > 0$ such that $J(t_1 u) = 0$. By the increasing property of $J(tu)$, we have $J(tu) = 0$ for all $t \in (0, t_1)$ and $\frac{dJ(tu)}{dt} = 0$ as well. Look at (3.32), we must have $\int_\Omega (|\nabla u|^2 - \lambda u^2)dx = 0$ and $\int_\Omega f(x, tu)udx = 0$. By (f3), $f(x, tu)u = 0$ almost everywhere in Ω, then $u(x) = 0$ almost everywhere and hence $\int_\Omega |\nabla u|^2 dx = 0$. But it is impossible since $\|u\| = 1$. As a result, $J(tu) = 0$ if and only if $t = 0$.

(ii) Case 2, $\int_\Omega(|\nabla u|^2 - \lambda u^2)dx < 0$. In this case, it is clear that $J(tu) < 0$ for sufficiently small t and $J(tu) \to \infty$ when $t \to \infty$. Then $J(tu)$ has at lease one local minimum, denoted by $t_u > 0$, then $\frac{dJ(tu)}{dt}|_{t=t_u} = 0$, i.e

$$t_u \int_\Omega (|\nabla u|^2 - \lambda u^2)dx + \int_\Omega f(x, t_u u)udx = 0.$$

Divide both sides of the above equation by t_u, we get

$$\int_\Omega (|\nabla u|^2 - \lambda u^2)dx = -\int_\Omega \frac{f(x, t_u u)}{t_u} udx. \tag{3.33}$$

Let $\Omega_0 = \{x \in \Omega | u(x) = 0\}$, $\Omega_- = \{x \in \Omega | u(x) < 0\}$ and $\Omega_+ = \{x \in \Omega | u(x) > 0\}$, we can write

$$\int_\Omega \frac{f(x, t_u u)}{t_u} udx = \int_{\Omega_0} \frac{f(x, t_u u)}{t_u} udx + \int_{\Omega_-} \frac{f(x, t_u u)}{t_u u} u^2 dx + \int_{\Omega_+} \frac{f(x, t_u u)}{t_u u} u^2 dx.$$

Suppose there is another t'_u s.t $\frac{dJ(tu)}{dt}|_{t=t'_u} = 0$, then (3.33) holds as well. W.L.O.G., assume $t'_u > t_u$. By (f3), $f(x, 0) = 0$, then $\int_{\Omega_0} \frac{f(x,t_u u)}{t_u} udx = 0$. By (f5),

$$\frac{f(x, t_u u)}{t_u u} < \frac{f(x, t'_u u)}{t'_u u}, \forall x \in \Omega_+.$$

When $x \in \Omega_-$, $t'_u u < t_u u$. By (f5) again, we get

$$\frac{f(x, t'_u u)}{t'_u u} = -\frac{f(x, t'_u u)}{|t'_u u|} > -\frac{f(x, t_u u)}{|t_u u|} = \frac{f(x, t_u u)}{t_u u}.$$

As a result, $\int_\Omega \frac{f(x,t_u u)}{t_u} udx < \int_\Omega \frac{f(x,t'_u u)}{t'_u} udx$. However, the left side of (3.33) is fixed, which leads to a contradiction, so t_u is unique. $\square$

Let's recall LMMM as $\min_{v\in S_{L^\perp}} \max_{u\in[L,v],\|u\|\approx 1} \min_{t>0} J(tu)$, and we used (1) $\|v\| \approx 1$ in the notation $S_{L^\perp}$ rather than $\|v\| = 1$, (2) $\|u\| \approx 1$ rather than $\|u\| = 1$ in the middle-level optimization when developing the computational theory under the weakened conditions. So the middle level of LMMM is a local maximization over $\{u \in [L, v] \mid \|u\| \approx 1\}$ and the outermost level is a local minimization over $\{v \in L^\perp \mid \|v\| \approx 1\}$. In fact, for any fixed $v \in H$,

$$\max_{u\in[L,v],\|u\|\approx 1} \min_{t>0} J(tu) = \max_{u\in[L,v],\|u\|=1} \min_{t>0} J(tu),$$

since $\arg\min_{t>0} J(tu)$ is the same no matter whether $\|u\| \approx 1$ or $\|u\| = 1$. Then we have

$$\min_{v\in L^\perp,\|v\|\approx 1} \max_{u\in[L,v],\|u\|\approx 1} \min_{t>0} J(tu) = \min_{v\in L^\perp,\|v\|\approx 1} \max_{u\in[L,v],\|u\|=1} \min_{t>0} J(tu).$$

Meanwhile $[L, v] = [L, cv]$ for any constant c, so it follows that

$$\min_{v\in L^\perp,\|v\|\approx 1} \max_{u\in[L,v],\|u\|=1} \min_{t>0} J(tu) = \min_{v\in L^\perp,\|v\|=1} \max_{u\in[L,v],\|u\|=1} \min_{t>0} J(tu).$$

To sum up, LMMM is equivalent to

$$\min_{v\in L^\perp,\|v\|=1} \max_{u\in[L,v],\|u\|=1} \min_{t>0} J(tu).$$

From this point to the end of this chapter, we treat LMMM as

$$\min_{v\in S_{L^\perp}} \max_{u\in[L,v],\|u\|=1} \min_{t>0} J(tu),$$

and S_W is defined as the unit sphere $S_W = \{w \in W \mid \|w\| = 1\}$ for any subspace $W \subset H$.

For a fixed $u \in S_{[L,v]}$, consider the performance of $J(tu)$ in t on the interval $[0, \infty)$. by Lemma 3.7, we have either (i)$\int_\Omega (|\nabla u|^2 - \lambda u^2)dx \geq 0$, $J(tu) \geq 0$ for all $t > 0$ and the equality holds if and only if $t = 0$, J is $\cup-$ shape in this case, or (ii) $\int_\Omega(|\nabla u|^2 - \lambda u^2)dx < 0$, $J(tu)$ can achieve the unique minimum at $t_u > 0$ and $J(t_u u) < 0$, J is W-shape in this case. We are interested at those u's such that $\int_\Omega(|\nabla u|^2 - \lambda u^2)dx < 0$ since our objective is to search for multiple solutions of J in W-shape, not in $\cup-$ shape. Now we can define

Definition 3.3. $L_v = \{u \mid u \in S_{[L,v]}, \int_\Omega(|\nabla u|^2 - \lambda u^2)dx < 0\}$.

Definition 3.4. $\gamma^v = \{t_u u \mid u \in L_v, t_u = \arg\min_{t>0} J(tu)\}$.

The following corollary follows immediately by Lemma 3.7.

Corollary 3.1. *For a given $w \in [L, v]$, if $J(w) \leq 0$ and $w \neq 0$, then $\frac{w}{\|w\|} \in L_v$.*

Remark 3.2. *Suppose $L_v \neq \emptyset$. For any $u \in L_v$, by Definition 3.3, $\int_\Omega(|\nabla u|^2 - \lambda u^2)dx < 0$. Let $G(u) = \int_\Omega(|\nabla u|^2 - \lambda u^2)dx$, since $J(u) \in \mathcal{C}^1$, then $G(u) \in \mathcal{C}^1$ hence it is continuous. So there exists $r_0 > 0$, such that $\int_\Omega(|\nabla u'|^2 - \lambda u'^2)dx < 0$ when $u' \in B(u, r_0) \cap S_{[L,v]}$. Therefore $u' \in L_u$. That is to say, if $L_v \neq \emptyset$, L_v is either open in $S_{[L,v]}$ or $L_u = S_{[L,v]}$.*

Let T be defined as in (3.9), i.e. $T(u) = t_u u$ with $t_u = \arg\min_{t>0} J(tu)$, and let $T|_{L_v}$ be the same map T but restricted on L_v. If $L_v = \emptyset$, J is $\cup$-shape in $[L, v]$. If $L_v \neq \emptyset$, the range of $T|_{L_v}$ is γ^v defined in Definition 3.4, and it is obvious that $0 \notin \gamma^v$.

Lemma 3.8. *The map $T|_{L_v} : L_v \to \gamma^v$ is one-to-one and continuous.*

Proof. It is obvious that $T|_{L_v}$ is one-to-one. $J \in \mathcal{C}^2$ under the hypothesis. Denote $R(t, u) = \langle J'(tu), u\rangle$, by the implicit function theorem, when

$$R'_t = \langle J''(t_u u), u\rangle \neq 0,$$

$t'(u) = T'(u)$ is locally continuous at u hence $T|_{L_v}$ is continuous. $\square$

Due to Lemma 3.8 and the three possibilities of L_v as in Remark 3.2, γ^v has three possibilities as well. (i) γ^v is empty, corresponding to the $\cup$-shape of J in $[L, v]$. (ii) γ^v is compact. In this case, it is defined for all $u \in S_{[L,v]}$, corresponding to the W-shape of J in $[L, v]$. (iii) γ^v is not compact, and we will show γ^v approaches 0 later for this case.

Lemma 3.9. *Assume $L_v \neq 0$, then $L_v = S_{[L,v]}$ if and only if $B(0, \delta) \cap \gamma^v = \emptyset$ for some $\delta > 0$.*

Proof. (i) Suppose $L_v = S_{[L,v]}$, if $B(0, \delta) \cap \gamma^v = \emptyset$ does not hold for any $\delta > 0$, then there exist $\{t_{u_n} u_n\} \subset \gamma^v$ such that $t_{u_n} u_n \to 0$ as $n \to 0$. Since L_u is compact, $T|_{L_v}$ is continuous and one-to-one, γ^v must be compact as well. That means $0 \in \gamma^v$, which is impossible since $0 \notin \gamma^v$. So there exists $\delta > 0$ such that $B(0, \delta) \cap \gamma^v = \{\varnothing\}$.

(ii) Suppose $B(0, \delta) \cap \gamma^v = \emptyset$ for some $\delta > 0$. $J \in \mathcal{C}^2$ under the hypothesis, then there exist $d > 0$ such that $J(t_u u) < -d$ for all $t_u u \in \gamma^v$. If $L_v = S_{[L,v]}$ does not hold, then γ^v is not compact by the analysis stated previously.

Let $w \notin \gamma^v$ be any point satisfying $t_{u_n} u_n \to w$ with $t_{u_n} u_n \in \gamma^v$, then $J(t_{u_n} u_n) \to J(w)$. Since $J(t_{u_n} u_n) \leq -d$, then $J(w) \leq -d$. By Corollary 3.1, $\frac{w}{\|w\|} \in L_v$. Denote $w_0 = \frac{w}{\|w\|}$, if we can prove that $w = t_{w_0} w_0$, where $t_{w_0} = \arg\min_{t>0} J(t w_0)$, then we can get $w \in \gamma^v$, so it is a contradiction.

Now we prove $w = t_{w_0} w_0$. Consider the Map H:$v \to \frac{v}{\|v\|} \to t_v v$, by Lemma 3.8, H is continuous at w.

If $t_{w_0} w_0 \neq w$, denote $\varepsilon = \|w - t_{w_0} w_0\| > 0$. Since $t_{u_n} u_n \to w$, then $\exists N$, when $n > N$

$$\|t_{u_n} u_n - w\| < \frac{\varepsilon}{3}. \tag{3.34}$$

For such $n > N$, notice that $H(t_{u_n}u_n) = t_{u_n}u_n$ and $H(w) = t_{w_0}w_0$ and we have

$$\|H(t_{u_n}u_n) - H(w)\| = \|t_{u_n}u_n - t_{w_0}w_0\| \tag{3.35}$$

$$= \|w - t_{w_0}w_0 + t_{u_n}u_n - w\| \tag{3.36}$$

$$\geq \|w - t_{w_0}w_0\| - \|t_{u_n}u_n - w\| \tag{3.37}$$

$$> \frac{2}{3}\varepsilon. \tag{3.38}$$

Since H is continuous, there exists $\delta > 0$, for all w' satisfying $\|w' - w\| < \delta$, $\|H(w') - H(w)\| < \frac{1}{3}\varepsilon$. For such a δ, since $t_{u_n}u_n \to w$, then $\exists\ N_0$ big enough, such that when $n > N_0$, $\|t_{u_n}u_n - w\| < \delta$, and it holds that

$$\|t_{u_n}u_n - t_{w_0}w_0\| < \frac{1}{3}\varepsilon. \tag{3.39}$$

Take $N_1 = \max\{N, N_0\}$, both (3.38) and (3.39) hold, which is impossible. So $t_{w_0}w_0 = w$.

$\square$

Lemma 3.9 indicates that if $\gamma^v \neq \emptyset$ and is not defined for all $u \in S_{[L,v]}$, then for any $\delta > 0$, $B(0,\delta) \cap \gamma^v \neq \emptyset$, hence γ^v approaches 0. So far, we have very clear structure for γ^v. When applying LMMM to W-type problems, we need to avoid $\gamma^v = \emptyset$ since J is $\cup$-shape. We also need to avoid case (iii) since we will find a trivial solution "0". We hope we can keep SCP strictly inside W-shape and away from "0". Then a question arises, can we find v such that $L_v = S_{[L,v]}$?

Due to the multiplicities and instabilities of the saddles points, it is very hard for us to discuss those saddles with high instability index. We research on saddle points with $MI = 1$ by LMMM.

In our algorithm, L is usually spanned by the previously found critical points. This is very important since the separation condition $d(L, p(v)) > \alpha$ guarantees we can find a new one. Note that when $L = 0$, LMMM finds a stable nontrivial critical point with $J < 0$. How to find this critical point has been done before by many other methods, so is not a main concern in our study. In the following paragraphs, we denote it by u_0. λ_i, φ_i are the same as the previous ones in this section.

Lemma 3.10. *Let* $L = [u_0]$, $k \in \mathbf{N}$, $k > 2$, *then we can find* $v \in S_{L^\perp}$ *such that* $L_v = [L, v]$.

Proof. Select $\bar{v} = \sum_{i=1}^{k} a_i \varphi_i$, consider the following linear system

$$\begin{cases} \langle u_0, \sum_{i=1}^{k} a_i \varphi_i \rangle = 0, \\ \int_\Omega (-\Delta u_0 - \lambda u_0)(\sum_{i=1}^{k} a_i \varphi_i) dx = 0. \end{cases} \tag{3.40}$$

It is equivalent to

$$\begin{cases} \langle u_0, \varphi_1 \rangle a_1 + \cdots + \langle u_0, \varphi_k \rangle a_k = 0, \\ \int_\Omega (-\Delta u_0 - \lambda u_0)\varphi_1) dx a_1 + \cdots + \int_\Omega (-\Delta u_0 - \lambda u_0)\varphi_k) dx a_k = 0. \end{cases}$$

Since $k > 2$, the above linear system is homogeneously undetermined, then there must be infinitely many nontrivial solutions.

Denote the solution space by Γ, and $V_0 = \{\sum_{i=1}^{k} a_i \varphi_i | \sum_{i=1}^{k} a_i^2 = 1, (a_1, \cdots, a_k) \in \Gamma\}$. Now we prove that for any $v \in V_0$, $L_v = S_{[L,v]}$.

If $v \in V_0$, then $\|v\| = 1$ and $v \in S_{L^\perp}$ by the first equation of (3.40).

Since u_0 is a global minimum of J with $J(u_0) < 0$, we get $\frac{u_0}{\|u_0\|} \in L_v$ by Corollary 3.1 and $\int_\Omega (-\Delta u_0 - \lambda u_0) u_0 dx < 0$ by Definition 3.3. We also have $\int_\Omega (-\Delta v - \lambda v) v dx < 0$ by Lemma 3.6. Then $\forall w \in S_{[L,v]}$, $w = a u_0 + b v$, and by the second equation of the system, we get

$$\begin{aligned}
&\int_\Omega (-\Delta w - \lambda w) w dx \\
&= \int_\Omega [(-\Delta a u_0 - \lambda a u_0) + (-\Delta b v - \lambda b v)](a u_0 + b v) dx \\
&= a^2 \int_\Omega [(-\Delta u_0 - \lambda u_0) u_0 dx + b^2 \int_\Omega [(-\Delta v - \lambda v) v dx < 0.
\end{aligned}$$

then we get $w \in L_v$, so $L_v = S_{[L,v]}$. $\square$

Remark 3.3. *We know that when $k = 1$, J has only one nontrivial solution, which is a global minimum and stable, so we will always assume $k \geq 2$. Notice that if Ω is a rectangle in $\mathbb{R}^2$, λ_2 has multiplicity 2, so the above lemma holds as well.*

Now we can establish the following theorem.

Theorem 3.5. *Assume $L = [u_0]$, V_0 is noted as in the proof of Lemma 3.10. For $\forall v \in V_0$, let L_v, γ^v be defined as in Definition 3.3, 3.4. then*

$$A = \max_{u \in [L,v], \|u\|=1} \min_{t>0} J(tu)$$

can be achieved and $A < 0$.

Proof. Lemma 3.10 shows that $L_v = S_{[L,v]}$ for $\forall v \in V_0$. By Lemma 3.9, there exist $\delta > 0$ such that $B(0,\delta) \cap \gamma^v = \emptyset$. Since $J \in \mathcal{C}^2$, then $J(\gamma^v) < -d$ for some constant $d > 0$. It also holds that γ^v is compact since L_v is compact and $T|_{L_v}$ is a continuous, one-to-one map. Then J must achieve the maximum in γ^v. Namely, $A = \max_{u \in [L,v], \|u\|=1} \min_{t>0} J(tu)$ can be achieved and $A < 0$. $\square$

By the above theorem, we can intentionally select an initial $v \in V_0 \subset S_{L^\perp}$ s.t. $J(p(v)) < -d$ for some constant $d > 0$. Simultaneously, the stepsize rule indicates the algorithm is decreasing, which means that SCP can be kept strictly inside W-shape and away from "0", and the algorithm has to stop at somewhere since J is bounded below.

3.6 Instability Analysis of Saddles by LMMM

When multiple solutions exist in a nonlinear system, some of them are stable and others are unstable. For those unstable solutions, their instability behaviors can be very different. Stability/instability is one of main concern in system design and control theory. The performance or maneuverability of saddles for W-type problems is desirable in many applications .

Assume $J''(u^*)$:$H \to H$ is a self-adjoint Fredholm operator with an orthogonal spectral decomposition: $H = H^- \oplus H^0 \oplus H^+$. By the Morse theory [22], we have *Morse index* $MI(u^*) = dim(H^-)$. If u^* is a non-degenerate critical point, i.e, $H^0 = \{0\}$, $MI(u^*) = 0$ implies that J is increasing in any direction at u^*, hence u^* is a local minimum and a stable solution of J. If $MI(u^*) > 0$, then in any neighborhood $\mathcal{N}(u^*)$ of u^*, $\exists v, w \in \mathcal{N}(u^*)$, such that $J(v) < J(u^*) < J(w))$, so it is unstable and a saddle point.

For a non-degenerate critical point u^*, the value $MI(u^*)$ can be used to measure its local instability [13]. That is to say, $MI(u^*)$ can be used as a local instability index. However, in order to get the local instability index, one usually need to go through two steps, first to numerically compute the unstable solution u^* and then to numerically solve for the number of negative eigenvalues (counting multiplicity) of the linear operator $J''(u^*)$. Such a process to get $MI(u^*)$ is always very expensive, which makes it not to be applicable.

Recently, for M-type problems, based on a local minimax characterization of saddle points, several estimates of the Morse index were established in [40, 47] and a local minimax index (MMI) which is closely related to the Morse index was proposed therein to measure the local instability of saddle points not necessarily non-degenerate. Later on, analogous instability analysis of unstable solutions based on LMO has been carried out. Unlike those early results, these new estimates can provide some guidance in finding saddle points numerically with a prescribed Morse index [55]. However, to the best of our knowledge, instable performance of saddles for DWF is not analyzed yet. In this section, We mathematically analyze the Morse index of saddles for DWF to get $dim(L) \leq MI(u^*) + dim(H^0 \cap [L, v^*]) \leq dim(L) + 1$. Narrowing the estimates is an interesting topic for the future researchers.

Local instability index: For a critical point $u^* \in H$ of J in H, a vector $v \in H$ is said to be a decreasing (increasing) direction of J at u^* if there exists $t_0 > 0$, such that

$$J(u^* + tv) < (>) J(u^*), \forall t_0 > t > 0.$$

In general, the set of all decreasing (or increasing) vectors of J at a critical point does not form a linear vector space. The maximum dimension of a subspace of decreasing directions of J at a critical point u^* is called the *local instability index.*

For a functional with mountain pass structure, LMM works very well and the following estimate of Morse index has been established.

Theorem 3.6. *(Instability Analysis of Saddles by LMM [47]) Let $v^* \in S_{L^\perp}$. If J has a local peak selection p at v^* w.r.t. L such that p is continuous at v^*, $v^* = \arg\min_{v \in S_{L^\perp}} J(p(v))$, and $u^* = p(v^*) \notin L$. Furthermore, assume p is differentialble at v^*, then u^* is a critical point with*

$$dim(L) + 1 = MI(u^*) + dim(H^0 \cap [L, v^*]), \tag{3.41}$$

where H^0 is the null space of the linear operator $J''(u^*)$ in H.

The following Lemma 3.11, Lemma 3.12, and Lemma 3.13 have very important roles in our study of instabilities for DWF.

Lemma 3.11. *[55] Let $v^* \in S_{L^\perp}$, assume that there exists a neighborhood $\mathcal{N}(v^*)$ of v^* and a locally defined mapping $p : \mathcal{N}(v^*) \cap S_{L^\perp} \to H$, s.t. $p(v) \in [L, v]$ for every $v \in \mathcal{N}(v^*) \cap S_{L^\perp}$, and in particular, $p(v^*) = t_0 v^* + v_L^*$ for some $v_L^* \in L$. If p is differentiable at v^* and $t_0 \neq 0$, then*

$$p'(v^*)([L, v^*]^\perp) \oplus [L, v^*] = H. \tag{3.42}$$

Lemma 3.12. *Let $v^* = \arg\min_{v \in S_{L^\perp}} J(p(v))$, where p is a local L-$\perp$ selection of J and differentiable at v^*. If $u^* = p(v^*) \notin L$, then u^* is a critical point of J with*

$$p'(v^*)([L, v^*]^\perp) \cap (H^- \oplus (H^0 \cap [L, v^*])) = 0. \tag{3.43}$$

Proof. u^* is a critical point follows immediately from Theorem 3.1. If (3.43) does not hold, there exists $w \in [L, v^*]^\perp$, such that $0 \neq p'(v^*)(w) \in H^- \oplus (H^0 \cap [L, v^*])$. Let $p'(v^*)(w) = h^- + h^0$, where $h^- \in H^-$ and $h^0 \in H^0 \cap [L, v^*]$. By Lemma 3.11, $p'(v^*)([L, v^*]^\perp) \oplus [L, v^*] = H$, so $p'(v^*)([L, v^*]^\perp) \bigcap [L, v^*] = \{0\}$. As a result, $h^- \neq 0$.

The second Taylor expansion for J near $u^* = p(v^*)$ is

$$J(u) = J(u^*) + \frac{1}{2}\langle J''(u^*)(u - u^*), u - u^* \rangle + o(\|u - u^*\|^2). \tag{3.44}$$

Denote $v^*(t) = \frac{v^* + tw}{\|v^* + tw\|}$, it is obvious that $v^*(t) \in N(v^*) \cap S_{L^\perp}$ for $|t|$ small, and $\frac{dv^*(t)}{ds}|_{t=0} = w$. We also have $v^*(t) \to v^*$, and $p(v^*(t)) \to p(v^*)$ as $t \to 0$. By the first Taylor expansion for p as a function of t near $t = 0$, it then follows that

$$u(t) \equiv p(v^*(t)) = p(v^*) + tp'(v^*)(w) + o(|t|). \tag{3.45}$$

Since $p'(v^*)(w) \in H^- \oplus (H^0 \cap [L, v^*])$ with $h^- \neq 0$, we have

$$\langle J''(u^*)(p'(v^*)(w)), p'(v^*)(w)\rangle < 0.$$

In view of (3.44) and (3.45), for $|t|$ sufficiently small, we get

$$\begin{aligned} J(p(v^*(t))) &= J(u^*) + \frac{1}{2}\langle J''(u^*)(tp'(v^*)(w) + o(|t|)), tp'(v^*)(w) \\ &\quad + o(|t|)\rangle + o(\|tp'(v^*)(w) + o(|t|)\|^2) \\ &= J(u^*) + \frac{t^2}{2}\langle J''(u^*)(p'(v^*)(w)), p'(v^*)(w)\rangle + o(|t|^2) \\ &< J(u^*), \end{aligned}$$

which contradicts that v^* is a local minimum of $J(p(v))$ for $v \in S_{L^\perp}$, thus (3.43) holds. $\square$

Lemma 3.13. *[55] Let $L = [u_1, u_2, \cdots, u_n]$, where $\{u_i\} \subset H$ are linearly independent. Assume p is a local L-$\perp$ selection of J at $v^* \in S_{L^\perp}$, s.t. (a) p is continuous at v^*, (b) $u^* = p(v^*) \notin L$, (c) $v^* = \arg\min_{v \in S_{L^\perp}} J(p(v))$. Let*

$$Q = \begin{pmatrix} \langle J''(u^*)v^*, v^*\rangle & \langle J''(u^*)u_1, v^*\rangle & \cdots & \langle J''(u^*)u_n, v^*\rangle \\ \langle J''(u^*)v^*, u_1\rangle & \langle J''(u^*)u_1, u_1\rangle & \cdots & \langle J''(u^*)u_n, u_1\rangle \\ \cdots & \cdots & \cdots & \cdots \\ \langle J''(u^*)v^*, u_n\rangle & \langle J''(u^*)u_1, u_n\rangle & \cdots & \langle J''(u^*)u_n, u_n\rangle \end{pmatrix},$$

(Note, $Q \in \mathbb{R}^{(n+1)\times(n+1)}$ is a symmetric matrix. We denote by Q^+, Q^-, $ker(Q)$ the positive definite, negative definite and null subspaces of Q in $\mathbb{R}^{n+1}$. Obviously, $\mathbb{R}^{n+1} = Q^- \oplus Q^+ \oplus$

$ker(Q)$.) and define

$$G^{+} = \{t_0 v^* + t_1 u_1 + \cdots + t_n u_n \mid (t_0, t_1, \cdots, t_n)^T \in Q^{+}\} \subseteq [L, v^*],$$

$$G^{-} = \{t_0 v^* + t_1 u_1 + \cdots + t_n u_n \mid (t_0, t_1, \cdots, t_n)^T \in Q^{-}\} \subseteq [L, v^*],$$

$$G^{0} = \{t_0 v^* + t_1 u_1 + \cdots + t_n u_n \mid (t_0, t_1, \cdots, t_n)^T \in ker(Q)\} \subseteq [L, v^*].$$

Then the following statements hold,

(i) u^* is a critical point of J,

(ii) $[L, v^*] = G^{-} \oplus G^{0} \oplus G^{+}$,

(iii) $dim(H^0 \cap [L, v^*]) \leq dim(G^0) = dim(ker(Q))$,

(iv) $dim(L) + 1 - dim(Q^{+}) \leq MI(u^*) + dim(H^0 \cap [L, v^*])$,

(v) $dim(L) + 1 - dim(Q^{+}) \leq MI(u^*) + dim(ker(Q))$.

So far, we can establish a bound estimate of Morse index by LMO.

Theorem 3.7. *(Instability Analysis of Saddles by LMO) Let $L = [u_1, u_2, \cdots, u_n]$, where $\{u_i\} \subset H$ are linearly independent. Let $v^* = \arg\min_{v \in S_{L^\perp}} J(p(v))$, where p is a local L-$\perp$ selection of J at $v^* \in S_{L^\perp}$, and differentiable at v^*. Assume $u^* = p(v^*) \notin L$ and define Q, G^+, G^0, G^- as in Lemma 3.13, then u^* is a critical point of J and the following bound estimates hold*

$$dim(L) + 1 - dim(Q^{+}) \leq MI(u^*) + dim(H^0 \cap [L, v^*]) \leq dim(L) + 1. \quad (3.46)$$

Proof. According to Lemma 3.13, it is known that u^* is a critical point of J with

$$dim(L) + 1 - dim(Q^{+}) \leq MI(u^*) + dim(H^0 \cap [L, v^*]),$$

so we just need to prove

$$MI(u^*) + dim(H^0 \cap [L, v^*]) \leq dim(L) + 1. \tag{3.47}$$

By Lemma 3.11, we have the decomposition

$$H = p'(v^*)([L, v^*]^\perp) \oplus [L, v^*],$$

then we can write H as

$$H = H^- \oplus (H^0 \cap [L, v^*]) \oplus (H^0 \cap [L, v^*]^\perp_{H^0}) \oplus H^+.$$

Suppose (3.47) does not hold, namely, $MI(u^*) + dim(H^0 \cap [L, v^*]) > dim(L) + 1$, then

$$(H^- \oplus (H^0 \cap [L, v^*])) \cap p'(v^*)([L, v^*]^\perp) \neq \{0\},$$

which contradicts to (3.43). That means the inequality (3.47) holds and (3.46) holds consequently. □

Remark 3.4. *1, The result in Theorem 3.6 provides a way to evaluate the Morse index for a saddle point of a M-type functional without actually computing $dim(H^-)$, which is very expensive. Additionally, for a degenerate saddle point u^*, it implies that $dim(L) + 1$ is better than Morse index to measure its instability.*

2, Theorem 3.7 provides a bound estimate for $MI(u^*)+dim(H^0\cap[L, v^*])$ when saddle points can be found by LMO. Note that when $p(v)$ is a peak selection of J, LMO becomes LMM and in Theorem 3.7, $Q^+ = \{0\}$ for LMM, then we have the same result as previously [55].

3, For LMMM in this thesis, we proved that it fits into LMO frame-work, so we also *have the same bound estimate in Theorem 3.7. On the other side, LMMM has a much clearer structure than LMO, so we should have a better instability analysis for such a saddle point found by it.*

So far, we can establish the following bound estimate of the Morse index by LMMM.

Theorem 3.8. *Let $L = [u_1, u_2, \cdots, u_n]$, $\{u_i\} \subset H$ and they are linearly independent. $p(v)$ is defined as in (3.8), i.e., $p(v) = \arg\max_{w\in[L,v],\|w\|=1} \min_{t>0} J(tw)$ for $v \in S_{L^\perp}$ and $p(v) = t_w w$ for some $w \in S_{[L,v]}$, where $t_w = \arg\min_{t>0} J(tw)$. T is defined as in (3.9). Assume that*

(i) T is locally Lipschitz continuous at w,

(ii) $v^* = \arg\min_{v\in S_{L^\perp}} J(p(v))$,

(iii) $u^* = p(v^*) \notin L$,

(iv) J is non-degenerate in the direction u^*,

(v) p is differentiable at v^*.

Q, G^+, G^-, G^0 are defined as in Lemma 3.13. Then the following statements hold

(a) $u^* = p(v^*)$ is a critical point of J,

(b) $dim(Q^+) = 1$,

(c) $dim(L) \leq MI(u^*) + dim(H^0 \cap [L, v^*]) \leq dim(L) + 1$.

Proof. (a) follows directly from Lemma 3.13.

Now we prove (b).

Denote $u^* = p(v^*) = t_u u$ for some $u \in [L, v^*]$ with $\|u\| = 1$, $t_u = \arg\min_{t>0} J(tu)$, by Lemma 3.13, $[L, v^*] = G^+ \oplus G^0 \oplus G^-$, then we have the following decomposition of u

$$u = u^+ + u^0 + u^-, \tag{3.48}$$

where $u^+ \in G^+$, $u^0 \in G^0$ and $u^- \in G^-$.

First we claim that $u^+ \neq 0$. If $u^+ = 0$, since J is non-degenerate in the direction u^*, i.e.$\langle J''(u^*)u^*, u^*\rangle \neq 0$, then $\langle J''(u^*)u, u\rangle < 0$. However, $J(tu)$ achieves its local minimum at t_u, so

$$\langle J''(u^*)u, u\rangle > 0, \tag{3.49}$$

which is a contradiction. Since $u^+ \neq 0$, $u^+ \in G^+$, then $dim(Q^+) = dim(G^+) \geq 1$. If we can prove $dim(Q^+) \leq 1$, statement (b) holds immediately.

Now we prove $dim(Q^+) \leq 1$. If it does not hold, then $dim(Q^+) \geq 2$. Since $dim(Q^+) = dim(G^+)$, there are at least one vector $u^1 \in G^+$ with $\|u^1\| = 1$ such that

$$\langle J''(u^*)u^+, u^1\rangle = 0. \tag{3.50}$$

Denote $u(r) = \frac{u+ru^1}{\|u+ru^1\|} \in [L, v^*], r > 0$, then $\|u(r)\| = 1$. Let $t_r = \arg\min_{t>0} J(tu(r))$, we have

$$\|u - u(r)\| \leq \frac{2r\|u^1\|}{\|u + ru^1\|} = \frac{2r}{\|u + ru^1\|}. \tag{3.51}$$

Since T is locally Lipschitz continuous at u, there exist $d_0 > 0$, $l_0 > 0$ such that for all $u' \in [L, v^*]$ with $\|u'\| = 1$, when $\|u - u'\| < d_0$, it holds

$$\|t_u u - t'u'\| \leq l_0\|u - u'\|, \tag{3.52}$$

where $t' = \arg\min_{t>0} J(tu')$, and that $u(r) \in [L, v^*]$, $u(r) \to u$, $t' \to t_u$ as $r \to 0$. In view of (3.51) and (3.52), there are $l_1 > 0$ and $r_0 > 0$, s.t

$$\|t_u u - t_r u(r)\| \leq l_1|r|, \forall r_0 > r > 0. \tag{3.53}$$

Look at the definition for $u(r)$, we know $u(r) \in [u, u^1]$, then $(t_u u - t_r u(r)) \in [u, u^1]$. Denote $t_u u - t_r u(r) = su + s^1 u^1$, by (3.53), both s, s^1 can be very small when r is very small. In view of (3.48), (3.50), (3.49), (3.53), when r is sufficiently small

$$
\begin{aligned}
&J(t_r u(r)) = J(u^* + t_r u(r) - t_u u) \\
&= J(u^*) + \frac{1}{2}\langle J''(u^*)(t_r u(r) - t_u u), t_r u(r) - t_u u\rangle + o(\|t_r u(r) - t_u u\|^2) \\
&= J(u^*) + \frac{1}{2}\langle J''(u^*)(su + s^1 u^1), su + s^1 u^1\rangle + o(\|su + s^1 u^1\|^2) \\
&= J(u^*) + \frac{1}{2}(\langle J''(u^*)su, su\rangle + \langle J''(u^*)s^1 u^1, s^1 u^1\rangle) + o(\|su + s^1 u^1\|^2) \\
&> J(u^*),
\end{aligned}
$$

which contradicts to $u^* = p(v^*) = \arg\max_{w \in S_{[L,v^*]}} \min_{t>0} J(tw)$. So $dim(Q^+) \leq 1$.
To sum up, we must have $dim(Q^+) = 1$.
(c) If $p(v)$ is defined as in (3.8), by Lemma 3.2, p is a local L-$\perp$ selection of J. Then (c) follows immediately from (b). $\square$

3.7 Conclusion

In this chapter, a local minmaxmin method (LMMM) is proposed to solve multiple saddles for defocused W-type problems. First, with the new weakened conditions, we verify that LMMM fits into min-$\perp$ frame-work and justify the stepsize rule, then LMMM characterization follows immediately. Second, the algorithm for LMMM is carried out with numerical results displayed successfully. Third, by the difficulties we encountered due to our numerical experience, we analyze its feasibility when applied to the model problem. Finally, the instability analysis is studied to get a bound estimate of Morse index for Saddles by LMMM.

4. SUMMARY

Search and study of multiple unstable states for new applications are of great interests in modern science and advanced engineering. Extensive numerical methods were carried out in literature to compute multiple unstable solutions for variational problems. However, neither G-saddles for M-type problems nor multiple saddles for W-type problems can be obtained by the existing methods.

In this thesis, we studied two types of nonlinear variational functionals. we established computational theory and designed numerical methods for finding multiple unstable saddle points of them. The first type consists of Gateaux differentiable M-type problems. Such type of functionals are at most lower semi-continuous. They have blow-up singularities in the whole space caused by quasilinear terms and they are just G-differentiable in a subspace. With a new strong-weak topology approach, we established a new mathematical frame-work for a local minimax method and presented its numerical implementation for finding multiple G-saddles. Numerical examples are carried out to illustrate the method. Some interesting phenomenons were observed. The second type consists of $\mathcal{C}^1$ W-type problems. Finding saddles for W-type functionals in a variational order is desirable in many applications. Motivated by local min-$\perp$ method, we proposed a new mathematical numerical method called a local minmaxmin method (LMMM). By verifying that LMMM fits into min-$\perp$ frame work, we established its mathematical validation such as stepsize rule and LMMM characterization. Numerical examples are carried out to illustrate the efficiency of this method. Due to the difficulties caused by the structures of such type of functionals, we investigated the algorithm in depth when applied to typical W-type problems. We aslo presented the convergence results of LMMM under much weaker conditions. Lastly, we analyzed the instability performances of saddles by LMMM.

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