Classification of Smooth Unconstrained Optimization Problems

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Abstract

We study the local convexity properties of a benchmark suite of smooth, unconstrained minimization problems drawn from the `OptimizationProblems.jl` [MOS] Julia package. For each problem, we review its origin, present the analytic form of the objective $f : \mathbb{R}^n \to \mathbb{R}$ and the standard starting point $\boldsymbol{x}_0$. We introduce a sampling-based procedure to classify the critical-point structure and verify the positive-definiteness of the Hessian in a neighborhood of a strict local minimizer. Numerical experiments confirm that while some test functions exhibit strong local convexity, others contain narrow regions of non-convexity that can slow down standard schemes. Our findings provide guidance for choosing and tuning first- and second-order methods on common benchmark problems. **TODO: Update this with the final results.** **Keywords:** Julia, Optimization, Benchmarking, Automatic Differentiation

Contents

1 Introduction

Understanding the local convexity of an objective function near strict local minimizers is fundamental to the design and convergence analysis of smooth optimization algorithms. Strong local convexity near a minimizer often guarantees rapid convergence of gradient-based and Newton-type methods, whereas narrow or nonconvex regions can result in slow progress or convergence to saddle points. Standard benchmark suites such as the Constrained and Unconstrained Testing Environment (CUTE) [**?**] offer a variety of smooth test functions with diverse convexity profiles, but a systematic comparison of their local convexity properties is lacking. In this work, we analyze the local convexity of a smooth objective functions within neighborhoods of strict local minimizers. We focus on a subset of objective functions from the *Constrained and Unconstrained Testing Environment* (CUTE) [**?**].

Our contributions are:

- We review existing techniques for classifying critical points.
- We present a sampling-based classification algorithm for determining the local convexity characteristics of the objective function f in a neighborhood of a strict local minimizer.
- **TODO:** Add other contributions

Our work is organized as follows.

- Section **??** presents a theoretical framework for classifying critical points using dynamical systems, Morse theory and spectral analysis of $\nabla^2 f(\boldsymbol{x}^*)$.
- Section **??** describes our problem selection criteria and provide analytical expressions for the objective function f and the accepted $\boldsymbol{x}_0$ for each problem. We include a brief discussion of their provenance and known properties from the literature.
- Section **??** discuss our numerical experiments for determining strict local minimizers $\boldsymbol{x}^*$ and details our sampling-based classification algorithm for determining the local convexity characteristics of f in a neighborhood of $\boldsymbol{x}^*$.
- Section **??** summarizes our findings and concludes with practical recommendations and mentions future work. Concludes with a discussion of the implications of our findings, and how they can be used to inform the design and tuning of optimization algorithms.

Our introduction proceeds as follows. We fix the notation used throughout this paper in 1.1. The general problem is stated in 1.2 and we discuss a *continuous model* 1.3 for solving the smooth minimization problem. We rigoursly define a *scheme*, discussing the properties of first and second order schemes in detail. We conclude the introduction by listing the benchmark problems under study 1.5 and describing their origins in the literature.

1.1 Preliminaries

We use the notation defined in the Appendix 3 as used by Nocedal and Wright [NW06].

Unless stated otherwise we assume $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable. Throughout we restrict our attention to a bounded path-connected open subset $\Omega \subset \mathbb{R}^n$ chosen large enough to contain all iterates and flow trajectories considered in this study. We choose our domain of interest Ω so the boundary $\partial\Omega := \overline{\Omega}\backslash\Omega$ is sufficiently smooth, meaning that f and its derivatives extend continuously to the boundary.

Add assumptions boxes used in paper as neccesasary

1.2 Unconstrained Optimization Problem

Consider the general form of a **smooth unconstrained optimization problem**

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x}), \tag{1}$$

where $\boldsymbol{x} \in \mathbb{R}^n$ is the optimization variable and $f : \mathbb{R}^n \to \mathbb{R}$ is a twice continuously differentiable objective function.

If a solution of (1) exists, then we denote the **optimal value** and **optimal solution** as

$$\boldsymbol{x}^* \in \arg\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{and} \quad f^* = \min_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x}),$$

In practice we choose Ω to be the problem domain of interest. By the standing assumptions of 1.1, Ω is a bounded, path-connected, open subset of $\mathbb{R}^n$ so the closure $\overline{\Omega}$ is a bounded and closed subset of $\mathbb{R}^n$. The Heine-Borel theorem implies that the closure $\overline{\Omega}$ is compact. Consequently, the extreme value theorem asserts that a continuous real-valued function f obtains a maximum and minimum value on the compact set $\overline{\Omega}$, where continuity of f on $\overline{\Omega}$ is guaranteed by the standing C^2 assumption. So by us choosing a problem domain of interest, we can guarantee an optimal solution exists in $\overline{\Omega}$ and we can make global optimality claims about the optimal value within our chosen domain.

A point satisfying the first-order optimality condition is called a *critical point*. Such a point can be a local minimizer, local maximizer, or saddle point. We classify critical points as follows (cf. [NW06]):

- A *local minimizer* if there exists a neighborhood N of $\boldsymbol{x}^*$ such that $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x} \in N$.
- A *strict local minimizer* if there exists a neighborhood N of $\boldsymbol{x}^*$ such that $f(\boldsymbol{x}^*) < f(\boldsymbol{x})$ for all $\boldsymbol{x} \in N \setminus \{\boldsymbol{x}^*\}$.
- An *isolated local minimizer* if there exists a neighborhood N of $\boldsymbol{x}^*$ such that $\boldsymbol{x}^*$ is the unique local minimizer in N.
- A *global minimizer* if $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^n$.

Since we focus on nonlinear objective functions, global optimality generally cannot be guaranteed. However, local optimality of a critical point $\boldsymbol{x}^*$ is verified using the following conditions:

$$\begin{aligned} \text{Necessary:} \quad & \nabla f(\boldsymbol{x}^*) = 0 \;\text{ and }\; \nabla^2 f(\boldsymbol{x}^*) \succeq 0 \\ \text{Sufficient:} \quad & \nabla^2 f(\boldsymbol{x}^*) \succ 0. \end{aligned}$$

The necessary condition for $\boldsymbol{x}^*$ to be a local minimizer of f is that $\boldsymbol{x}^*$ satisfies the first-order and second-order optimality conditions. The *second-order* optimality condition states that the Hessian of f is positive semidefinite at $\boldsymbol{x}^*$. If the Hessian is strictly positive definite at $\boldsymbol{x}^*$, it is both a necessary and a sufficient condition that $\boldsymbol{x}^*$ is a strict local minimizer. It holds that strict local minimizers are isolated, corresponding precisely to points where f is strictly convex.

1.3 Continuous Model

We reinterpret the minimization problem (1) as the search for equilibria of the *gradient flow* dynamical system. Interpreting our problem as a dynamical system allows us to:

- exploit geometric structure when analyzing the critical-point landscapes;
- design time-discretisations of the gradient flow ODE (GF) and construct error bounds using the continuous model;
- leverage the stability theory of autonomous ODEs on compact manifolds.

In this section, we establish a link between the minimization of f and the trajectories of a dynamical system.

Definition 1. The *gradient-flow* dynamical system is defined by the IVP

$$\boldsymbol{\gamma}'(t) = -\nabla f\big(\boldsymbol{\gamma}(t)\big) \quad \text{subject to } \boldsymbol{\gamma}(0) = \boldsymbol{x}_0 \in \overline{\Omega} \tag{GF}$$

An integral curve $\boldsymbol{\gamma}$ satisfying the *gradient-flow* IVP is a gradient *flow-line*, or, *trajectory.*

Suppose the initial point $\boldsymbol{x_0}$ is a critical point, then the gradient flow ODE is satisfied by the constant trajectory $\boldsymbol{\gamma}(t) = \boldsymbol{x}_0$ for any time t. Notice that constant $\boldsymbol{\gamma}(t)$ implies $\boldsymbol{\gamma}'(t) = \mathbf{0}$, substituting into the gradient-flow ODE asserts that $-\nabla f(\boldsymbol{x}_0) = \mathbf{0}$, which holds true since $\boldsymbol{x_0}$ is a critical point (i.e., $\nabla f(\boldsymbol{x}_0) = \mathbf{0}$). Consequently, the existence of a solution holds when $\boldsymbol{x}_0$ is a critical point and such points correspond to stationary equilibria in the gradient flow ODE phase space. Now we show equation (GF) is well-posed for all $\boldsymbol{x}_0 \in \overline{\Omega}$.
Let $\boldsymbol{\gamma}_{\boldsymbol{x_0}}$ be any gradient *flow-line* starting at some point $\boldsymbol{x_0}$ in $\overline{\Omega}$. Note that the trajectory $\boldsymbol{\gamma}_{\boldsymbol{x_0}}$ is driven by the steepest descent direction of the objective function f. But f is bounded below by the minimum value f^*, so the trajectory $\boldsymbol{\gamma}_{\boldsymbol{x_0}}$ cannot escape the compact set $\overline{\Omega}$ in finite time. Indeed, we will show that the trajectory $\boldsymbol{\gamma}_{\boldsymbol{x_0}}$ is guaranteed to converge to a critical point of f in $\overline{\Omega}$. But first we must establish the IVP (GF) is well-posed for all $\boldsymbol{x}_0 \in \overline{\Omega}$.

theorem (Existence)**.** For every $\boldsymbol{x_0} \in \overline{\Omega}$ the IVP (GF) admits a solution $\gamma_{\boldsymbol{x_0}} \in C^1\big([0,\infty); \overline{\Omega}\big)$ such that $\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t) \in \overline{\Omega}$ for all $t \geq 0$.

Sketch. The gradient flow ODE (GF) is a first-order, autonomous, ordinary differential equation (ODE) on the compact manifold $\overline{\Omega}$. To apply the Picard-Lindelöf theorem, it is sufficient to note $f \in C^2(\overline{\Omega})$ implies that $-\nabla f \in C^1(\overline{\Omega})$, and it follows that ∇f is Lipschitz on $\overline{\Omega}$, (i.e., f is ℓ-smooth). Consequently, the gradient flow ODE (GF) is well-posed for all interior initial conditions $\boldsymbol{x}_0 \in \Omega$ for some finite time t^*.

TODO: - Consider cleanest way to introduce the geometric approach without getting to deep into the topological / differential geometry of manifolds. - The simplest approach to "well-posedness" seems to be restricting our initial condition to the Ω, as we assume for the input of a scheme, then show that the flow lines are contained in the closure of the manifold $\overline{\Omega}$ by invoking the monotonicity of f along the flow lines and the fact that the image of $f(\overline{\Omega})$ is a compact convex (and path-connected?) set. - Define level sets, sub level sets, and the signed distance function, then introduce the alternative continuous model describing the flow of geodesics. Incorporate aspects of the Morse Theory section.

□

The following lemma characterizes the monotonicity of f along the trajectory $\boldsymbol{\gamma}_{\boldsymbol{x_0}}$.

Lemma A. *Along any trajectory $\boldsymbol{\gamma}_{x_0}(t)$ one has*

$$\frac{d}{dt} f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big) = -\|\nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big)\|^2 \;\leq\; 0, \quad t \geq 0. \tag{2}$$

Hence $f \circ \boldsymbol{\gamma}_{x_0}$ is non-increasing in t, and strictly decreasing whenever $\nabla f(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)) \neq 0$.

Proof. Differentiating the composition $f \circ \boldsymbol{\gamma}_{\boldsymbol{x_0}}$ w.r.t. t using the chain rule yields

$$\begin{aligned}
\frac{d}{dt} f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big) &= \nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big) \cdot \frac{d}{dt}\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t) \\
&= \nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big) \cdot \boldsymbol{\gamma}'_{\boldsymbol{x_0}}(t) \\
&= \nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big) \cdot \big(-\nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big)\big) \\
&= \langle \nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big), -\nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big)\rangle \\
&= -\langle \nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big), \nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big)\rangle \\
&= -\|\nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)\big)\|^2 \\
&\leq 0.
\end{aligned}$$

A direct consequence of the positive-definiteness property of a norm is that the final inequality is strict for all points $\boldsymbol{\gamma}_{\boldsymbol{x_0}}(t)$ that aren't critical. □

theorem. For all $\boldsymbol{x}_0 \in \overline{\Omega}$, the flow operator maps to a unique integral curve $\boldsymbol{\gamma}_{\boldsymbol{x}_0}(t)$ of the gradient flow ODE (GF) such that

$$\boldsymbol{\gamma}_{\boldsymbol{x}_0}(t) = T(\boldsymbol{x}_0; t) := \boldsymbol{x}_0 - \int_0^t \nabla f\big(\boldsymbol{\gamma}_{\boldsymbol{x}_0}(s)\big) ds \tag{3}$$

and $\boldsymbol{\gamma}_{\boldsymbol{x}_0}(t)$ is a continuous map from $\mathbb{R}$ to the closure of the manifold $\overline{\Omega}$, i.e., $\boldsymbol{\gamma}_{\boldsymbol{x}_0}(t) : \mathbb{R} \to \overline{\Omega}$. $\boldsymbol{\gamma}_{\boldsymbol{x}}(t) : \mathbb{R} \to \overline{\Omega}$ such that $\boldsymbol{\gamma}_{\boldsymbol{x}}(0) = \boldsymbol{x}$ and the limits

$$\lim_{t \to -\infty} \boldsymbol{\gamma}_{\boldsymbol{x}}(t) \quad \text{and} \quad \lim_{t \to \infty} \boldsymbol{\gamma}_{\boldsymbol{x}}(t)$$

exist and converge to *critical-points* of f.

TODO: - Complete the compact-domain formulation of the gradient flow dynamical system and demonstrate that trajectories provably descend the objective and terminate at critical points inside $\overline{\Omega}$. -For completeness, connect connect "critical points" to the "stationary points" of the gradient flow ODE and explain the relationship between the two and their synonymous use in the literature.

1.4 Optimization Schemes

We introduce a *scheme* for solving a *unconstrained optimization problem* based on the *gradient flow* dynamical system 1.

Definition 2. An **optimization scheme** is a one-parameter family of iteration operators $T_h : \overline{\Omega} \to \overline{\Omega}$, indexed by a step size $h \in (0, h_0]$ where h_0 is constant, that generates an iterative sequence using the rule

$$\boldsymbol{x}_{k+1} = T_h(\boldsymbol{x}_k) \text{ for } k = 0, 1, 2, \dots \tag{4}$$

starting from an initial point $\boldsymbol{x}_0 \in \overline{\Omega}$. The scheme is well-defined such that the triplet $(\boldsymbol{x}_0, h, T_h)$ satisfy:

1. Consistency: the iteration operator T_h is *consistent* with the (GF) ODE if the following limit holds:

   $$\frac{(T_h(\boldsymbol{x}) - \boldsymbol{x})}{h} + \nabla f(\boldsymbol{x}) \to 0 \text{ as } h \to 0 \text{ for all } \boldsymbol{x} \in \overline{\Omega},$$

   A consistent scheme approximates the continuous gradient flow w/ a local error of $\mathcal{O}(h^{p+1})$ committed at each step k; where p is the global order. Consistent schemes reproduce the exact optimality condition in the limit as $h \to 0$.

2. Stability: let $\boldsymbol{x}^*$ be a strict local minimizer of f. The operator T_h is *stable*, or *locally contractive*, at $\boldsymbol{x}^*$ if there exist constants $c > 0$ and $h_0 \le \frac{2}{L}$, and an open neighborhood $N \subset \overline{\Omega}$ with $x^* \in N$, such that

   $$\|T_h(x) - T_h(y)\| \le \big(1 - ch\big) \|x - y\| \quad \forall\ x, y \in N,\ \forall\ h \in (0, h_0].$$

   Equivalently, by the mean-value theorem, the Jacobian of T_h must satisfy the following uniform spectral-radius bound

   $$\rho\big(D\ T_h(\boldsymbol{x}^*)\big) \ \le\ 1 - ch \quad \forall\ h \in (0, h_0]$$

   where $\rho(\cdot)$ denotes the spectral radius. In either form, the contraction factor $1 - ch$ lies strictly inside $(0, 1)$, so that the iterates produced by the scheme remain in N and satisfy

   $$\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\| \le (1 - ch)\|\boldsymbol{x}_k - \boldsymbol{x}^*\|,$$

   implying convergence whenever $h \in (0, h_0]$ is fixed.

If a scheme is order-p consistent and stable in a neighborhood of a strict local minimizer, then consistent of order p and stable within a neighborhood of a strict local minimizer, then $\boldsymbol{x_k} \to \boldsymbol{x}^*$ as $k \to \infty$ and the scheme is said to be *convergent*.

The following iteration operators are examples of schemes for solving (1).

- **Gradient Descent (GD)**: $T_h(\boldsymbol{x}) = \boldsymbol{x} - h\nabla f(\boldsymbol{x})$ is first-order ($p = 1$) and contractive when $\nabla^2 f \succeq \mu I \succeq 0$.
- **Newton's Method (NM)**: $T_h(\boldsymbol{x}) = \boldsymbol{x} - h\nabla^2 f(\boldsymbol{x})^{-1}\nabla f(\boldsymbol{x})$ is second-order ($p = 2$) and contractive when $\nabla^2 f \succeq \mu I \succeq 0$.
- **Trust Region (TR)**: $T_h(\boldsymbol{x}) = \boldsymbol{x} + \arg\min_{\boldsymbol{\tau}} m_{\boldsymbol{x}}(\boldsymbol{\tau})$ where $m_{\boldsymbol{x}}(\boldsymbol{\tau}) = f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{\tau}\rangle + \frac{1}{2}\langle \boldsymbol{\tau}, \nabla^2 f(\boldsymbol{x})\boldsymbol{\tau}\rangle$ is the quadratic approximation of f at $\boldsymbol{x}$ and $\|\boldsymbol{\tau}\| \le \Delta$ is the trust region constraint.

- **Quasi-Newton (QN)**: $T_h(\boldsymbol{x}) = \boldsymbol{x} - hB\nabla f(\boldsymbol{x})$ where $B \approx \nabla^2 f^{-1}(\boldsymbol{x})$ is a positive-definite approximation of the Hessian. the quasi-newton method is a first-order ($p = 1$) scheme and contractive when $\nabla^2 f \succeq \mu I \succeq 0$.

- **TODO** Make this a table

TODO: numerics disscusion, introduce the ϵ order stationary points.

Analysis of Gradient Descent (GD)

TODO: use the following notes and provide an example of the analysis of GD. Relate the step choices below to the Wolfe conditions, cite Nocedal and Wright.

theorem. Assume f is ℓ-smooth and α-strongly convex and that $\epsilon > 0$. If we iterate the gradient descent *scheme* with $h = h_0 = \frac{1}{\ell}$ held fixed, i.e.,

$$T_h(\boldsymbol{x}_k) = \boldsymbol{x}_k - \frac{1}{\ell}\nabla f(\boldsymbol{x}_k),$$

then $d(x_k, x^*) \leq \epsilon$ for all $k > K$ where K is chosen to satisfy

$$\frac{2\ell}{\alpha} \cdot \log\left(\frac{d(x_0, x^*)}{\epsilon}\right) \leq K.$$

Remark. Under *ℓ-smoothness* and *α-strong convexity* assumptions in a neighborhood Ω about $\boldsymbol{x}^*$, it may be shown directly from the above theorem above that the *GD scheme* converges linearly to the optimal solution $\boldsymbol{x}^*$ at a rate of

$$\frac{d(\boldsymbol{x}_k, \boldsymbol{x}^*)}{d(\boldsymbol{x}_{k-1}, \boldsymbol{x}^*)} \leq 1 - \frac{\alpha}{\ell}$$

where $d(\boldsymbol{x}_k, \boldsymbol{x}^*)$ is the distance between the current iterate $\boldsymbol{x}_k$ and the optimal solution $\boldsymbol{x}^*$. The convergence rate is linear in the sense that the distance between the current iterate and the optimal solution decreases by a factor of $1 - \frac{\alpha}{\ell}$ at each iteration. (Ref: TODO)

Remark. Convergence to a first-order stationary point trivally implies convergence to a ϵ-first-order stationary point. Similarly, convergence to a second-order stationary point trivially implies convergence to a ϵ-second-order stationary point.

theorem. Assume f is ℓ-smooth, then for any $\epsilon > 0$, if we iterate the GD scheme with $h = h_0 = \frac{1}{\ell}$ held fixed starting from $\boldsymbol{x}_0 \in \Omega$ where Ω is a neighborhood of x^*, then the number of iterations K required to achieve the stopping condition $\|\nabla f(\boldsymbol{x}_k)\| \leq \epsilon$ is at most

$$\left\lceil \frac{\ell}{\epsilon^2}\left(f(\boldsymbol{x}_0) - f(\boldsymbol{x}^*)\right) \right\rceil$$

Remark. **TODO and Questions**

- State how we use theorems in when performing analysis from the results of our experimewts.

- What is the relationship between ℓ and α?

- In practice do we know how to compute ℓ and α?

- What is the relationship between ℓ and ρ?
- In practice do we know how to compute ℓ and ρ?

1.5 Benchmark Problems

We select a subset of the `OptimizationProblems.jl` [MOS] Julia package that support automatic differentiation (AD) natively through operator overloading. (TODO: Cite ForwardDiff.jl, Flux.jl, etc.) Each problem is implemented as `ADNLPModel` instance, which is a wrapper around the `NLPModel` interface whose backend AD engine is configurable to support forward-mode or reverse-mode.

2 Theory

Note that Ω is a bounded subset of $\mathbb{R}^n$, so its closure $\overline{\Omega} = \Omega \cup \partial\Omega$ is a compact subset of $\mathbb{R}^n$, by the Heine-Borel Theorem. Also, the boundary $\partial\Omega$ is sufficiently smooth, so we can apply the theory of smooth manifolds. The closure $\overline{\Omega}$ is a compact subset of $\mathbb{R}^n$ and is a smooth manifold with boundary $\partial\Omega$. The interior Ω is an open subset of $\mathbb{R}^n$ and is a smooth manifold.

Move the above bit to 1.3

Definition 3. A point $\boldsymbol{x}^* \in \Omega$ is a **critical point** of f if the differentiable map $df_p : T_p\Omega \to \mathbb{R}$ is zero. (Here $T_p\Omega$ is a tangent space of the Manifold M at p.) The set of critical points of f is denoted by $\text{crit}(f)$.

Definition 4. A point $\boldsymbol{x}^* \in \Omega$ is a **non-degenerate critical point** of f if the Hessian $H_p f$ is non-singular.

Definition 5. The **index** of a *non-degenerate critical point* $\boldsymbol{x}^*$ is defined to be the dimension of the negative eigenspace of the Hessian $H_p f$.

- local minima at $\boldsymbol{x}^*$ have index 0.
- local maxima at $\boldsymbol{x}^*$ have index n.
- saddle points at $\boldsymbol{x}^*$ have index k where $0 < k < n$.

We reserve the integers $c_0, c_1, \ldots, c_i, \ldots, c_n$ to denote the number of critical points of index i.

Definition 6. A **Morse function** is a smooth function $f : \Omega \to \mathbb{R}$ such that all critical points of f are non-degenerate.

2.1 Morse Theory in a Metric Space

theorem. Let f be a Morse function on Ω, then the Euler characteristic of Ω is given by

$$\chi(\Omega) = \sum_{i=0}^{n} (-1)^i c_i$$

where c_i is the number of critical points of index i.

Remark. The Euler characteristic $\chi(\Omega)$ is a topological invariant of the manifold Ω and is independent of the choice of Morse function f. The Euler characteristic is a measure of the "shape" of the manifold and can be used to distinguish between different topological spaces. The Euler characteristic may be defined by the alternating sum of the Betti numbers b_i of the manifold Ω

$$\chi(\Omega) = \sum_{i=0}^{n} (-1)^i b_i$$

where b_i is the i-th Betti number of the manifold Ω.

theorem. (Sard's theorem) Let f be a Morse function on Ω, then the image $f(\text{crit}(f))$ has Lebesque measure zero in $\mathbb{R}$.

Remark. We state a particular instance of Sard's theorem for continuous scalar-valued functions f, which was first proved by Anothony P. Morse in 1939. The theorem asserts that the image of the critical points of a Morse function is a set of measure zero in $\mathbb{R}$. This means that the critical points of a Morse function are "rare" in the sense that they do not form a dense subset of the manifold Ω. Consequently, selecting $\boldsymbol{x} \in \Omega$ at random will almost never yeild a critical point of f.

Remark. The property that $\boldsymbol{x}^* \in \Omega$ being a *critical point* of a Morse function f is not dependent of the metric of $\Omega \subset \mathbb{R}^n$ (and consequently, the norm induced by the metric)

3 Apendix

Notation

We assume the following notation throughout

- $\|\cdot\|$ denotes the usual ℓ_2 norm for vectors $\boldsymbol{x}$ in $\mathbb{R}^n$ and $p = 2$ norm for matrices in $\mathbb{R}^{n\times m}$. i.e.,

$$\|x\| := \left(\sum_i x_i^2\right)^{1/2}$$
$$\|A\| := (\lambda_{\max}(A^\top A))^{1/2} = \max(\sigma(A))$$

- $\sigma(A) := \{\text{singular values of } A\}$.
- $A \in \mathbb{R}^{n\times n} \implies \sigma(A) = \{\text{eigenvalues of } A \text{ (i.e. spectrum)}\}$
- $\sigma_{\max}(A) := \max(\sigma(A))$ and $\sigma_{\min}(A) := \min(\sigma(A))$.
- $A \in \mathbb{R}^{n\times n} \implies \lambda_{\max}(A) := \sigma_{\max}(A)$ and $\lambda_{\min}(A) = \sigma_{\min}(A)$
- $\langle\cdot,\cdot\rangle$ denotes the usual inner product on $\mathbb{R}^n$, i.e.,

$$\langle \boldsymbol{x}, \boldsymbol{y}\rangle := \boldsymbol{x}^\top \boldsymbol{y} = \sum_{i=1}^n \boldsymbol{x}_i \boldsymbol{y}_i = \|\boldsymbol{x}\|\|\boldsymbol{y}\|\cos(\theta)$$

  where θ is the angle between $\boldsymbol{x}$ and $\boldsymbol{y}$.

- $\mathcal{B}_r(\boldsymbol{x}) := \{\boldsymbol{y} \in \mathbb{R}^n : \|\boldsymbol{y} - \boldsymbol{x}\| < r\}$ is the open ball of radius r centered at $\boldsymbol{x} \in \mathbb{R}^n$.
- $\text{crit}(f) = \{\boldsymbol{x}^* \in \mathbb{R}^n : \nabla f(\boldsymbol{x}^*) = 0\}$ is the set of critical points of f.

Definitions

Definition 7. f is **L-Lipschitz** if $\forall\ \boldsymbol{x_1}, \boldsymbol{x_2}$

$$\exists\ L \geq 0\ :\ \|f(\boldsymbol{x_1}) - f(\boldsymbol{x_2})\| \leq L\|\boldsymbol{x_1} - \boldsymbol{x_2}\|$$

Definition 8. f has **ℓ-Lipschitz gradient**, or, f is **ℓ-smooth** if $\forall\ \boldsymbol{x_1}, \boldsymbol{x_2}$

$$\exists\ \ell \geq 0\ :\ \|\nabla f(\boldsymbol{x_1}) - \nabla f(\boldsymbol{x_2})\| \leq \ell\|\boldsymbol{x_1} - \boldsymbol{x_2}\|$$

Definition 9. f has **ρ-Lipschitz Hessian** if $\forall\ \boldsymbol{x_1}, \boldsymbol{x_2}$

$$\exists\ \rho \geq 0\ :\ \|\nabla^2 f(\boldsymbol{x_1}) - \nabla^2 f(\boldsymbol{x_2})\| \leq \rho\|\boldsymbol{x_1} - \boldsymbol{x_2}\|$$

Definition 10. f is **convex** if $\forall\ \boldsymbol{x_1}, \boldsymbol{x_2}$

$$\begin{aligned} f(\boldsymbol{x_2}) &\geq f(\boldsymbol{x_1}) + \langle \boldsymbol{x_2} - \boldsymbol{x_1}, \nabla f(\boldsymbol{x_1})\rangle \\ &= f(\boldsymbol{x_1}) + \nabla f(\boldsymbol{x_1})^T(\boldsymbol{x_2} - \boldsymbol{x_1}) \end{aligned}$$

Definition 11. f is **strictly convex** if

$$\begin{aligned}\exists\ \mu > 0\ :\ \nabla^2 f \succeq \mu I\\ \iff \lambda_{\min}(\nabla^2 f) \geq \mu > 0\end{aligned}$$

Definition 12. f is α-**strongly convex** if $\forall\ \boldsymbol{x_1}, \boldsymbol{x_2} \exists\ \alpha > 0$ s.t.

$$\begin{aligned}f(\boldsymbol{x_2}) &\geq f(\boldsymbol{x_1}) + \langle \nabla f(\boldsymbol{x_1}), \boldsymbol{x_2} - \boldsymbol{x_1} \rangle + \frac{\alpha}{2} \|\boldsymbol{x_2} - \boldsymbol{x_1}\|^2\\ \iff \lambda_{\min}(\nabla^2 f(\boldsymbol{x})) &\geq -\alpha.\end{aligned}$$

Definition 13. $\boldsymbol{x^*}$ is a **first-order stationary point** if $\|\nabla f(x^*)\| = 0$.

Definition 14. $\boldsymbol{x^*}$ is an ϵ-**first-order stationary point** if $\|\nabla f(x^*)\| \leq \epsilon$.

Definition 15. $\boldsymbol{x}^* \in \mathbb{R}^n$ is a **second-order stationary point** if $\|\nabla f(x^*)\| = 0$ and $\nabla^2 f(x^*) \succeq 0$.

Definition 16. if f has ρ-Lipschitz Hessian, $\boldsymbol{x}^* \in \mathbb{R}^n$ is a ϵ-**second-order stationary point** if

$$\|\nabla f(x^*)\| \leq \epsilon \text{ and } \nabla^2 f(x^*) \succeq -\sqrt{\rho\epsilon}$$

Remark. Note that the Hessian is not required to be positive definite, but it is required to have a small eigenvalue.

Definition 17. A point $\boldsymbol{x^*} \in \Omega$ is a **critical point** of f if the differentiable map $df_p : T_p\Omega \to \mathbb{R}$ is zero. (Here $T_p\Omega$ is a tangent space of the Manifold M at p.) The set of critical points of f is denoted by crit(f).

Definition 18. A point $\boldsymbol{x^*} \in \Omega$ is a **non-degenerate critical point** of f if the Hessian $H_p f$ is non-singular.

Definition 19. The **index** of a *non-degenerate critical point* $\boldsymbol{x^*}$ is defined to be the dimension of the negative eigenspace of the Hessian $H_p f$.

- local minima at $\boldsymbol{x^*}$ have index 0.
- local maxima at $\boldsymbol{x^*}$ have index n.
- saddle points at $\boldsymbol{x^*}$ have index k where $0 < k < n$.

We reserve the integers $c_0, c_1, \ldots, c_i, \ldots, c_n$ to denote the number of critical points of index i.

Remark. For each objective function f we are interested in determining the critical points of f

Remark. The **Morse function** is a smooth function $f : \Omega \to \mathbb{R}$ such that all critical points of f are non-degenerate.

3.1 Test Problems

Generalized Rosenbrock function:

$$f(x) = \sum_{i=1}^{n-1} \left(c(x_{i+1} - x_i^2)^2 + (1 - x_i)^2 \right),$$

$$x_0 = [-1.2, 1, -1.2, 1, \ldots, -1.2, 1], \quad c = 100.$$

3.2 Code Listings

Below are the code listings for the experiments conducted in this report.

Code 1: Algorithm 16.5

```
# TODO: Add Code Listings
```

References

[MOS] Tangi Migot, Dominique Orban, and Abel Soares Siqueira. Optimizationproblems.jl: A collection of optimization problems in julia. If you use this software, please cite it using the metadata from this file.

[NW06] Jorge Nocedal and Stephen J. Wright. *Numerical Optimization*. Springer, New York, NY, USA, second edition, 2006.