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 then 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. **Keywords:** Julia, Optimization, Benchmarking, Automatic Differentiation

Contents

1 Introduction

Our aim is to investigate the local convexity of standard test problems from the Constrained and Unconstrained Optimization Test Environment (CUTE) [?]. We start with a brief review of continuous smooth optimization problems. We then present a set of test problems selected from the `OptimizationProblems.jl` [MOS] Julia package. Next, we provide a theoritical overview on the classification of an objective functions critical point structure. We then present a sampling procedure to classify the *critical-point* structure of the objective function $f : \mathbb{R}^n \to \mathbb{R}$ within local neighborhoods of a strict local minimizer x^*. Analytical expressions are provided for each problems objective function and the accepted initial iterate $\boldsymbol{x}_{\mathbf{0}}$.

1.1 Preliminaries

We assume the notation defined in the Appendix 3.

1.2 Continuous Unconstratined Optimization Problem

The general form of an **unconstrained optimization problem** is

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

where $\boldsymbol{x} \in \mathbb{R}^n$ is the optimization variable and $f : \mathbb{R}^n \to \mathbb{R}$ is a sufficiently smooth objective function. We requre that $f \in C^2(\overline{\Omega}; \mathbb{R})$, where the domain $\Omega \subset \mathbb{R}^n$ is a bounded open subset of $\mathbb{R}^n$; i.e., f is twice continuously differentiable at every point $\boldsymbol{x} \in \Omega$ and it's derivatives may be continuously extended to the domains boundary $\partial\Omega$. The **optimal solution** and **optimal value** of (1) is denoted by

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

where $\boldsymbol{x}^*$ satisfies the *first-order* optimality condition that $\nabla f(\boldsymbol{x}^*) = 0$.

A *critical-point* is a point satisfying the *first-order* optimality condition. Let $\boldsymbol{x}^{\boldsymbol{*}}$ denote a critical-point, and note that $\boldsymbol{x}^*$ is either a local minimizer, local maximizer, or a saddle point of f. The *second-order* optimality condition asserts that $\nabla^2 f(\boldsymbol{x}^*) \succeq 0$. A *strict local minimizer* $\boldsymbol{x}^*$ of f is a *critical-point* such that $\nabla^2 f(\boldsymbol{x}^*) \succ 0$, i.e. the Hessian of f is positive definite at $\boldsymbol{x}^*$. In general, we seek an *optimal value* $\boldsymbol{x}^*$ satisfying the *second-order* optimality condition that $\nabla^2 f(\boldsymbol{x}^*)$ is semi-positive definite.

As defined in [NW06], we say an *optimal-value* $\boldsymbol{x}^*$ is

- *global minimizer* if $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \ \forall x \in \mathbb{R}^n$
- *local minimizer* if there is a neighborhood N of $\boldsymbol{x}^*$ such that $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x} \in N$
- *strict local minimizer* if there is a neighborhood N of $\boldsymbol{x}^*$ such that $f(\boldsymbol{x}^*) < f(x)$ for all $x \in N/\{\boldsymbol{x}^*\}$
- *isolated local minimizer* if there is a neighborhood N of $\boldsymbol{x}^*$ such that $\boldsymbol{x}^*$ is the only local minimizer in N
- *stationary point* if $\nabla f(x^*) = 0$ (any local minimizer is a stationary point)

The *first-order* optimiality condition asserts $\nabla f(x^*) = 0$, which is equivalent to saying $\boldsymbol{x}^*$ is a *stationary point*. The second order optimality conditions assert that the Hessian of f at $\boldsymbol{x}^*$ is semi-positive definite, which is equivalent to saying that $\boldsymbol{x}^*$ *local minimizer*. Note, if $\nabla^2 f(x^*)$ is positive definite, we say that $\boldsymbol{x}^*$ is a *strict local minimizer*. So we arrive at the following necessary and sufficient conditions for a stationary point $\boldsymbol{x}^*$ to be a strict local minimizer

- *Necessary:* $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \succeq 0$ (positive semi-definite)
- *Sufficient:* $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \succ 0$ (positive definite).

Consequently, *strict local minimizers* are *isolated local minimizers* and such *startionary points* correspond to the optimal solution f^* being concave up.

1.3 Continous Models

Let us start by defining a *continuous model* for the general form of problem 1.

Definition 1. Let the **gradient flow** of f be a solution to the dynamical system defined as

$$\boldsymbol{\gamma}'(t) = -\nabla f(\boldsymbol{\gamma}(t)) \tag{2}$$

where the evolution of our phase space is driven by the negative gradient of f. A **gradient flow line** of f is an integral curve $\boldsymbol{\gamma} : [0, \infty) \to \Omega$ satisfying the above evolutionary ordinary-differential equation subject to $\boldsymbol{\gamma}(0) = \boldsymbol{x_0}$.

Suppose that our initial point is a stationary-point, that is, $\boldsymbol{x_0} = \boldsymbol{x^*}$. Then we aim to show the constant *gradient flow line* defined as $\boldsymbol{\gamma}(t) = \boldsymbol{x}^* \ \forall \ t \in [0, \infty)$ satisfies (2). Notice that it ought to be that $\boldsymbol{\gamma}'(t) = \boldsymbol{0}$ for all time t and since $\boldsymbol{x}^*$ is a stationary point, we have that $\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}$. Therefore, we have that

$$\boldsymbol{\gamma}'(t) = \boldsymbol{0} = -\nabla f(\boldsymbol{\gamma}(t)) = -\nabla f(\boldsymbol{x}^*) = \boldsymbol{0} \quad \text{and} \quad \boldsymbol{\gamma}(t) = \boldsymbol{x}^* \ \forall \ t \in [0, t_f]$$

So we've shown that $\boldsymbol{\gamma}(t)$ is a constant flow line of f. Consequently, by the uniqueness of solutions for ordinary differential equations, if any flow line contains a *first-order* critical point $\boldsymbol{x}^*$, it must be a constant flow line.

Lemma A. *The function $f : \omega \to \mathbb{R}$ is nonincreasing along any flow-line $\boldsymbol{\gamma}(t)$ and strictly decreasing along flow lines not containing a critical point x^*.*

Proof. Let $\boldsymbol{\gamma} : [0, t_f] \to \Omega$ be a flow line. Consider the composition $f \circ \boldsymbol{\gamma} : [0, t_f] \to \mathbb{R}$, its derivative is

$$\begin{aligned} \frac{d}{dt}\big(f(\boldsymbol{\gamma}(t))\big) &= \langle \nabla_{\boldsymbol{\gamma(t)}}(f), \frac{d\boldsymbol{\gamma}}{dt} \rangle \\ &= \langle \nabla_{\boldsymbol{\gamma(t)}}(f), -\nabla_{\gamma(t)}(f) \rangle \\ &= -\langle \nabla_{\boldsymbol{\gamma(t)}}(f), \nabla_{\gamma(t)}(f) \rangle \\ &= -|\nabla_{\boldsymbol{\gamma(t)}}(f)|^2 \\ &\leq 0 \end{aligned}$$

Therefore, $f'(\boldsymbol{\gamma(t)}) = 0$ iff $\boldsymbol{\gamma}(t)$ is on a critical point of f. In particular, if $\boldsymbol{\gamma}(t)$ does not contain in its image a critical point of f, then the above inequality implies that f is strictly decreasing along the integral curve $\boldsymbol{\gamma(t)}$. □

theorem. For all $\boldsymbol{x}$ in the closed manifold $\overline{\Omega}$, there exists uniquely $\boldsymbol{\gamma_x}(t) : \mathbb{R} \to \overline{\Omega}$ such that $\boldsymbol{\gamma_x}(0) = \boldsymbol{x}$ and the limits

$$\lim_{t\to-\infty} \boldsymbol{\gamma_x}(t) \quad \text{and} \quad \lim_{t\to\infty} \boldsymbol{\gamma_x}(t)$$

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

Now it may be shown that the flow map operator $T : \overline{\Omega} \times \mathbb{R} \to \overline{\Omega}$ defined as $T(\boldsymbol{x}, t) := \boldsymbol{\gamma_x}(t)$. This implies theoretically that we may perform analysis of our phase space as constructed by a smooth union of integral curves. Consequently, by our previous lemma, if the flow map T contains a critical point $\boldsymbol{x}^*$ then it ought to be that $T(\boldsymbol{x}^*, t) \equiv \text{ const } \forall t$, otherwise, T is descending for all of time.

1.4 Optimization Schemes

A *scheme* for solving (1) is a numerical method for approximating the optimal solution $\boldsymbol{x}^*$.

Definition 2. A **scheme** for solving a general form *unconstrained optimization problem* is a one-parameter family of iteration operators:

$$T_h : \mathbb{R}^n \to \mathbb{R}^n \quad \text{where} \quad \boldsymbol{x}_{k+1} = T_h(\boldsymbol{x}_k),\ h \in (0, h_0]$$

where h_0 is a constant and h is the step size. The scheme is well-defined such that the triplet $(\boldsymbol{x}_0, h, T_h)$ satisfy

1. *Consistency*: $\forall \boldsymbol{x} \in K$
$$(T_h(\boldsymbol{x}) - \boldsymbol{x})\, h^{-1} + \nabla f(\boldsymbol{x}) \to 0 \text{ as } h \to 0.$$
implying that a single step approximates the continous gradient flow w/ local error $\mathcal{O}(h^{p+1})$ where p is the global order of the scheme.

2. *Stability*: $\exists\ c > 0, h_0 > 0\ :\ \forall h \in (0, h_0]$, and for all $\boldsymbol{x_1}, \boldsymbol{x_2}$ in a *neighborhood* $N \subset K$ around an *optimal solution* $\boldsymbol{x}^*$
$$\|T_h(\boldsymbol{x_1}) - T_h(\boldsymbol{x_2})\| \leq (1 - ch)\|\boldsymbol{x_1} - \boldsymbol{x_2}\|$$
where c is a constant that depends on the scheme and h is the step size. Or, equivalently, the scheme is *stable* if $\exists\ c > 0, h_0 > 0\ :\ \forall h \in (0, h_0]$, and for all $\boldsymbol{x}$ in a *neighborhood* about $\boldsymbol{x}^*$, each step results in a strict decrease of by atleast a factor of $1 - ch$, i.e.,
$$\|J(T_h(\boldsymbol{x}))\| \leq (1 - ch)$$
where $J(T_h(\boldsymbol{x}))$ is the Jacobian of the scheme.

3. *Convergence*: $\forall\ \boldsymbol{x_0} \in N \subset K$, s.t. N is some neighborhood around a strict minimizer x^*. and $\forall \epsilon > 0$
$$\exists\ K \in \mathbb{N}\ :\ \forall k\ > K, \boldsymbol{x}_k \in N \text{ and } d(\boldsymbol{x}_k, \boldsymbol{x}^*) \leq \epsilon.$$

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 $\|\boldsymbol{\tau}\| \leq \Delta$ 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

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.

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 $\mathrm{crit}(f)$.

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 $f(\mathrm{crit}(f))$ has Lebesque measure zero in $\mathbb{R}$.

Remark. We state a particular instance of Sard's theorem for continous 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 $\boldsymbol{x} \in \mathbb{R}^n$.
- $\mathrm{crit}(f) = \{\boldsymbol{x}^* \in \mathbb{R}^n : \nabla f(\boldsymbol{x}^*) = 0\}$ is the set of critical points of f.

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

```
# Example Code Listing
```

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.