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MASTER'S THESIS

An L-BFGS-B-NS Optimizer for Non-Smooth Functions

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Declaration of Authorship

I, Wilmer Henao, declare that this thesis titled, 'An L-BFGS-B-NS Optimizer for Non-Smooth Functions' and the work presented in it are my own. I confirm that:

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- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
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Abstract

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An L-BFGS-B-NS Optimizer for Non-Smooth Functions

by Wilmer Henao

The Thesis Abstract is written here ...

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Contents

Declaration of Authorship	i
Abstract	ii
Acknowledgements	iii
Contents	iv
List of Figures	v
1 Introduction	1
2 L-BFGS-B	3
2.1 BFGS	3
2.2 L-BFGS	4
2.3 L-BFGS-B	4
2.3.1 Gradient Projection	4
2.3.2 Subspace Minimization	5
3 Modifications to the L-BFGS-B Algorithm	7
3.1 The Armijo and Wolfe conditions	7
3.2 The Line Search Methodology	8
3.3 The Termination Condition	9
3.3.1 Termination Condition Sub-algorithm	9
3.3.2 The Solution of the Quadratic Program	10
4 Solution Tests	11
4.1 Exit Messages	11
4.2 Modified Rosenbrock Function	12
4.2.1 Performance of L-BFGS-B	14
4.2.2 Performance of L-BFGS-B-NS	15
5 Conclusions	16

List of Figures

2.1	Graphical Representation of Gradient Projection	5
3.1	Representation of the Armijo Condition in a Nutshell	7
3.2	The Idea behind the Wolfe Condition	8
4.1	Modified Rosenbrock with $p = 2$	13
4.2	Modified Rosenbrock with $p = 1$	14
4.3	Number of algorithm iterations changing p	15
4.4	Selected Runs changing dimensions using $m = 10$	15

Dedicated to my mother and Dr. Ian Malcolm

Chapter 1

Introduction

The problem addressed is to find a local minimizer of the Non-Smooth minimization problem

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ \text{s.t.} \quad & l_i \leq x_i \leq u_i, \\ & i = 1, \dots, n. \end{aligned} \tag{1.1}$$

where $f: \mathbb{R}^n \rightarrow \mathbb{R}$, is continuous but not differentiable everywhere and n is large.

The L-BFGS-B algorithm [BLNZ95] is a standard method for solving large instances of (1.1) when f is a smooth function, typically twice differentiable. The name BFGS stands for Broyden, Fletcher, Goldfarb and Shanno, the originators of the BFGS quasi-Newton algorithm for unconstrained optimization discovered and published independently by them in 1970 [Bro70, Fle70, Gol70, Sha70]. This method requires storing and updating a matrix which approximates the inverse of the Hessian $\nabla^2 f(x)$ and hence requires $\mathcal{O}(n^2)$ operations per iteration. The L-BFGS variant [Noc80], where the L stands for “Limited-Memory” and also for “Large” problems, is based on BFGS but requires only $\mathcal{O}(mn)$ operations per iteration, and less memory. Instead of storing the $n \times n$ Hessian approximations, L-BFGS stores only m vectors of dimension n , where m is a number much smaller than n . Finally, the last letter B in L-BFGS-B stands for bounds, meaning the lower and upper bounds l_i and u_i in equation (1.1). The L-BFGS-B algorithm is implemented in a FORTRAN software package [ZBNM11].

In this thesis, we first give a brief description of the L-BFGS-B algorithm at a high level and then we introduce a modified algorithm which is more suitable for functions f which may not be differentiable at their local or global optimal points. We call the new

algorithm L-BFGS-B-NS where NS stands for Non-Smooth. These changes were implemented in a modified version of the FORTRAN code [Hen14] which can be downloaded from a web repository. We report on some numerical experiments that strongly suggest that the new code should be useful for the non-smooth bound-constrained optimization problem (1.1).

We are grateful to Jorge Nocedal and his coauthors for allowing us to modify the L-BFGS-B code and post the modified version.

Chapter 2

L-BFGS-B

This section is a description of the original L-BFGS-B code [ZBNM11, ZBLN97] at a very high level. The original software is intended to find local minimizers of smooth functions. This thesis discusses how to modify the algorithm for non-smooth functions.

2.1 BFGS

BFGS is a standard tool for optimization of smooth functions [NW99]. It is a line search method. The search direction is of type $d = -B_k \nabla f(x_k)$ where B_k is the k^{th} approximation to the inverse Hessian of f .¹ This k^{th} step approximation is calculated via the BFGS formula

$$B_{k+1} = \left(I - \frac{s_k y_k^T}{y_k^T s_k} \right) B_k \left(I - \frac{y_k s_k^T}{y_k^T s_k} \right) + \frac{s_k s_k^T}{y_k^T s_k} \quad (2.1)$$

where $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$ and $s_k = x_{k+1} - x_k$. BFGS exhibits super-linear convergence on generic problems but it requires $\mathcal{O}(n^2)$ operations per iteration [NW99].

In the case of non-smooth functions, BFGS typically succeeds in finding a local minimizer [LO13]. However, this requires some attention to the line search conditions. These conditions are known as the Armijo and weak Wolfe line search conditions and they are a set of inequalities used for the computation of an appropriate step length that reduces the objective function “sufficiently”. These inequalities will be explained later in section 3.1.

¹When it is exactly the inverse Hessian the method is known as Newton’s method. Newton’s method has quadratic convergence but requires the explicit calculation of the Hessian at every step.

2.2 L-BFGS

L-BFGS stands for Limited-memory BFGS. This algorithm approximates BFGS using only a limited amount of computer memory to update an approximation to the inverse of the Hessian of f . Instead of storing a dense $n \times n$ matrix, L-BFGS keeps a record of the last m iterations where m is a small number that is chosen in advance². For this reason the first m iterations of BFGS and L-BFGS produce exactly the same search directions if the initial approximation B_0 is set to the identity matrix.

Because of this construction, the L-BFGS algorithm is less computationally intensive and requires only $\mathcal{O}(mn)$ operations per iteration. So it is much better suited for problems where the number of dimensions n is large.

2.3 L-BFGS-B

Finally L-BFGS-B is an extension of L-BFGS. The B stands for the inclusion of Boundaries. L-BFGS-B requires two extra steps on top of L-BFGS. First, there is a step called *gradient projection* that reduces the dimensionality of the problem. Depending on the problem, the gradient projection could potentially save a lot of iterations by eliminating those variables that are on their bounds at the optimum reducing the initial dimensionality of the problem and the number of iterations and running time. After this *gradient projection* comes the second step of *subspace minimization*. During the *subspace minimization* phase, an approximate quadratic model of (1.1) is solved iteratively in a similar way that the original L-BFGS algorithm is solved. The only difference is that the step length is restricted as much as necessary in order to remain within the *lu*-box defined by equation (1.1).

2.3.1 Gradient Projection

The L-BFGS-B algorithm was designed for the case when n is large and f is smooth. Its first step is the gradient projection similar to the one outlined in [CGT88, MT89] which is used to determine an active set corresponding to those variables that are on either their lower or upper bounds. The active set defined at point x^* is:

$$\mathcal{A}(x^*) = \{i \in \{1 \dots n\} | x_i^* = l_i \vee x_i^* = u_i\} \quad (2.2)$$

²In this thesis $m < 20$, and in practice numbers between 5 and 10 are regularly used. There is no way of knowing *a priori* what choice of m will provide the best results as will be illustrated later in this thesis

Working with this active set is more efficient in large scale problems. A pure line search algorithm would have to choose a step length short enough to remain within the box defined by u_i and l_i . So if at the optimum, a large number \mathcal{B} of variables are either on the lower or the upper bound, as many as \mathcal{B} of iterations might be needed. Gradient projection tries to reduce this number of iterations. In the best case, only 1 iteration is needed instead of \mathcal{B} .

Gradient projection works on the linear part of the approximation model:

$$m_k(x) = f(x_k) + \nabla f(x_k)^T(x - x_k) + \frac{(x - x_k)^T H_k(x - x_k)}{2} \quad (2.3)$$

where H_k is a L-BFGS-B approximation to the Hessian $\nabla^2 f$ stored in the implicit way defined by L-BFGS.

In this first stage of the algorithm a piece-wise linear path starts at the current point x_k in the direction $-\nabla f(x_k)$. Whenever this direction encounters one of the constraints, the path turns corners in order to remain feasible. The path is nothing but the feasible piece-wise projection of the negative gradient direction on the constraint box determined by the values \vec{l} and \vec{u} . At the end of this stage, the value of x that minimizes $m_k(x)$ restricted to this piece-wise gradient projection path is known as the “Cauchy point” x^c . See Figure 2.1.

2.3.2 Subspace Minimization

The problem with gradient projection is that its search direction does not take advantage of information provided implicitly by the Hessian H_k , and therefore the speed of convergence is at best linear. It is for this reason that a stage two is necessary. Stage 2 (subspace minimization) uses an L-BFGS implicit approximation of the inverse Hessian matrix restricted to the free variables that are not in the active set $\mathcal{A}(x^c)$.

The starting position for stage two will be the previously found Cauchy point and the goal is to find a new $\bar{x} = x^c + \alpha^* \hat{d}$. The idea at a higher level is to minimize (2.3) over the free variables subject to their lower and upper bounds. First, the L-BFGS algorithm provides a new search direction \hat{d}^u of the *unconstrained* problem that takes implicit advantage of approximations of the Hessian matrix restricted to the free variables. After an unconstrained search direction has been found, the constraints are taken into account and the search direction is restricted to the l, u bounding box via a step length factor α^* . The step length is chosen so that the new point \bar{x} satisfies the Armijo and Wolfe³

³The Armijo and weak Wolfe conditions will be explained on section 3.1

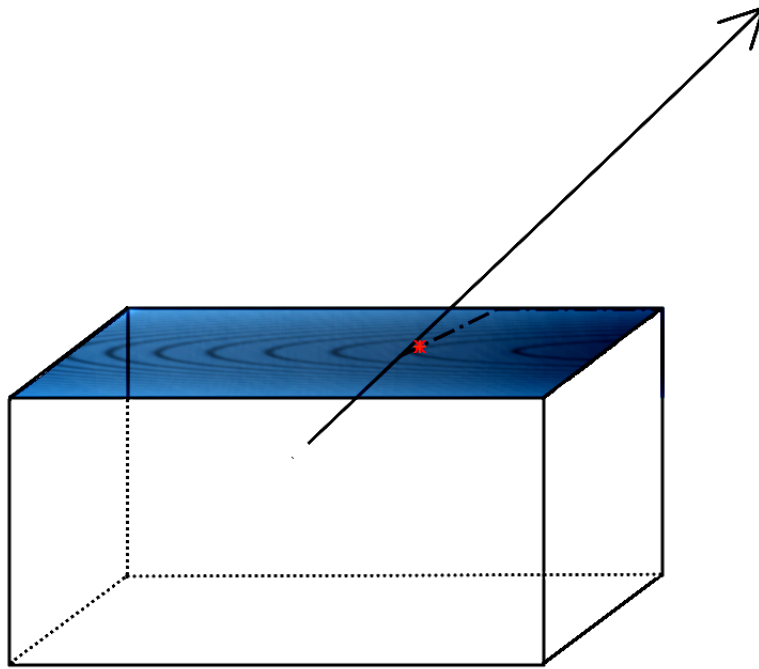


FIGURE 2.1: The arrow represents the direction of the negative gradient. The dotted path represents the projected gradient path. The contours represent the level sets of the model. The optimal point (the '*' in red) is the Cauchy point x^c

conditions. A restriction on the step length is added so that the next iteration stays feasible. Sometimes it is not possible to satisfy the Wolfe condition due to the bounded nature of the problem, so in these cases, only the Armijo condition needs to be satisfied. Once this step length is found, the next step is to check the termination condition. If the termination condition fails, a new gradient projection and subspace minimization will be needed and the method repeats. If the termination condition is successful, the program exits with an appropriate exit message.

Chapter 3

Modifications to the L-BFGS-B Algorithm

We made three main changes to the original L-BFGS-B algorithm. They concern the line search Wolfe conditions, the line search methodology, and the termination condition.

3.1 The Armijo and Wolfe conditions

It is accepted that the Armijo and Wolfe conditions work very well whenever the function f is smooth [LF01]. The Armijo condition, also known as the sufficient decrease requirement in the direction d_k , is defined as

$$f(x_k + \alpha_k d_k) \leq f(x_k) + c_1 \alpha_k d_k^T \nabla f(x_k) \quad (3.1)$$

where $0 < c_1 < 1$ is a constant, often $c_1 = 10^{-4}$ [NW99]. This condition guarantees “sufficient decrease” of the function. It is possible to continue decreasing without ever reaching the optimum if the Armijo condition is not required as is shown in Figure 3.1.

The other condition, which is the one that was actually changed, is the curvature condition, of which the most popular version is the “strong Wolfe” curvature condition:

$$|d_k^T \nabla f(x_k + \alpha_k d_k)| \leq c_2 |d_k^T \nabla f(x_k)| \quad (3.2)$$

Here d_k represents the search direction and c_2 is a constant such that $0 < c_1 < c_2 < 1$; often $c_2 = 0.9$ [NW99]. The strong Wolfe condition is a natural choice for optimization

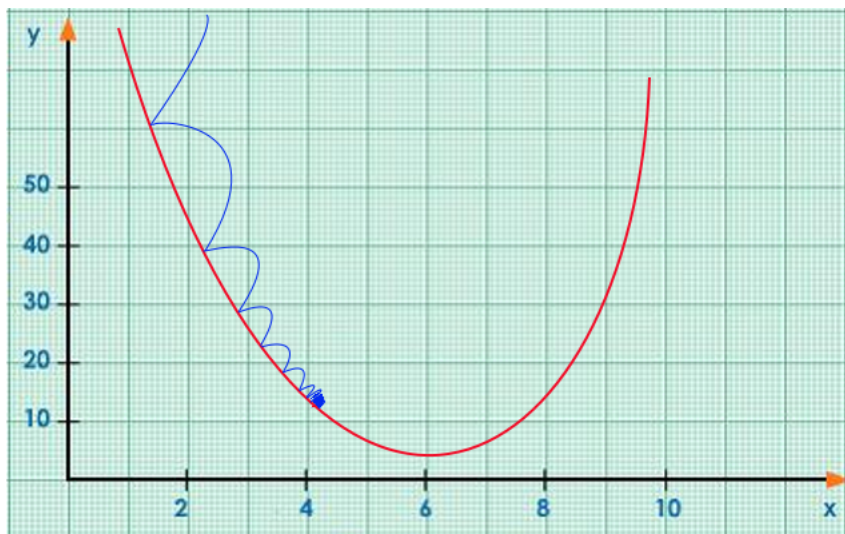


FIGURE 3.1: In this figure, the iterations always reduce the value of the function a little bit, but never enough to go below 12

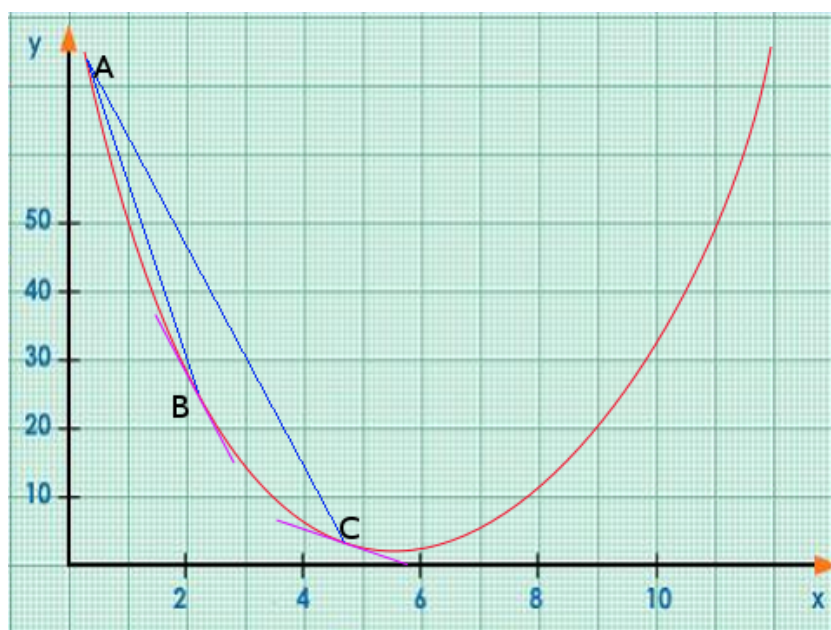


FIGURE 3.2: The logic of the Wolfe conditions is this. Starting at point A, Point B is a step in the right direction, however, point C offers a “flatter” tangent and should be closer to the optimum which has a tangent of zero (Smooth case).

of smooth functions. Its goal is to find a step length long enough that the slope has been reduced “sufficiently” as illustrated in figure (3.2), but the problem is that the condition, as it is, does not work well for the non-smooth case. This is because near the minimal points there may be abrupt changes in the gradient. A good example of this problem is the function $f(x) = |x|$, where the slope never becomes flat near the optimal point.

The weak Wolfe condition defined as

$$d_k^T \nabla f(x_k + \alpha_k d_k) \geq c_2 d_k^T \nabla f(x_k) \quad (3.3)$$

can be used in the non-smooth case. It is all that is needed to guarantee that the BFGS updated inverse Hessian approximation is positive definite [NW99]. This weak version is suited for the problems in this thesis and it was implemented as part of the line search algorithm explained in the next section.

3.2 The Line Search Methodology

The original FORTRAN software [ZBNM11] contains a line search subroutine. It was partially changed for the purpose of this thesis. The old version of the code was commented out.

The old version has a problem with the function *dcstep* in the non-smooth case. The function *dcstep* was designed to work only with smooth functions in mind. The algorithm in *dcstep* takes advantage of quadratic and cubic approximations to the function in order to calculate step lengths that satisfy Armijo and Wolfe conditions. Unfortunately, these second and third order approximations do not work in the non-smooth case, and the optimizer breaks down using the line search as it is. Function *dcstep* is available at the repository [Hen14]

The solution to this particular issue is to use a line search similar to the one suggested in [LO13] and in [OS12]. This approach is to double the step length while the Armijo condition is violated, and once the interval has been bracketed, do bisection until both the Armijo and Wolfe conditions are satisfied. The only difference with the approach in this thesis is that the line search in HANSO can double its step length up to 30 times, whereas in this thesis, the step length can double only as long as it is less than the maximum value that guarantees feasibility of the solution (the maximum established in the first step of the original line search).

3.3 The Termination Condition

In the case of smooth functions, L-BFGS-B checks whether the algorithm has converged by means of the *projected gradient* which is nothing but the projection of the negative gradient onto the bounding box defined by l and u . If this projected gradient has a small norm the algorithm terminates. In the case of non-smooth functions however, the function at the minimum may have a “wedge”. In this wedge the projected gradient

may not vanish (it is not defined at the “bottom” of the wedge, such as is the case for $f(x) = |x|$ at $x = 0$). Furthermore, if there is a sequence of points that approaches the optimum x in a direction \vec{p} , the projected gradients corresponding to this sequence of points might be completely different from the projected gradients associated with a sequence of points that approach the optimum x from a different direction.

3.3.1 Termination Condition Sub-algorithm

Lewis and Overton formulate an algorithm that gives a practical solution to this problem in section 6.3 of [LO13] in the case of unconstrained non-smooth optimization. They suggest computing the norm of the smallest vector that is part of the convex hull of gradients evaluated at points near the optimum candidate x and terminate if this is sufficiently small. The neighborhood is defined as those points at which the gradient has already been evaluated with a distance to x smaller than a small tolerance $\tau_x > 0$ and no more than $J \in \mathbb{N}$ iterations back in history. This list of gradients is referred to as the set \mathcal{G} [LO13].

With this list \mathcal{G} of gradients at hand, the next step is to find the vector with the minimal norm contained in the convex hull of these gradients. If the minimum such norm is smaller than another tolerance τ_d , the algorithm terminates.

In order to find this vector, there is the need to solve a quadratic problem. Every vector in the convex hull can be expressed as a convex combination Gz of those vectors in \mathcal{G} , where G is the matrix with columns made up of gradients in \mathcal{G} and z is such that $\sum z_i = 1$ and $z_i \geq 0$.

The objective is to find the right combination of z that minimizes the norm $\|Gz\|_2$. This is equivalent to solving the following optimization problem

$$\begin{aligned} \min \quad & q(z) = \|Gz\|_2^2 = z^T G^T G z \\ \text{s.t.} \quad & \sum z_i = 1 \\ & z_i \geq 0. \end{aligned} \tag{3.4}$$

The solution to this problem z^* defines the associated vector Gz^* , so if $\|Gz^*\|_2 < \tau_d$ the algorithm terminates.

In this case, it is important to notice that instead of the gradient we have to work with the projected gradient and this is because the gradient may not vanish in all directions. In the unconstrained case, if a component of the gradient is not zero this yields a direction of descent. But in the bounded case, this may be impossible to continue working on those

directions because the boundary may have been reached. For this reason the gradients have to be projected onto the bounding box, and it is these projected gradients that we incorporate in the termination condition of L-BFGS-B-NS.

3.3.2 The Solution of the Quadratic Program

The solution of the quadratic program (3.4) is obtained using a practical primal-dual method. This is the same method implemented by Skajaa [Ska10] in his thesis. His code `qpspecial` was implemented in FORTRAN for this thesis. The method is the well known Mehrotra's Predictor-Corrector algorithm applied to quadratic programming, as explained in chapter 16 of [NW99].

Chapter 4

Solution Tests

The L-BFGS-B implementation was tested on the high performance cluster machines at NYU. In order to run these tests it was necessary to create a series of PBS files¹ using a PBS generator script. This script generator created PBS files which in turn run bash shell scripts². Several of these shell scripts are available the the repository [Hen14]. The main reason to run scripts this way is because it achieves parallelism, and because the system sends confirmation e-mails and statistics about the different stages of the processes giving a lot of control to the practitioner.

4.1 Exit Messages

The original L-BFGS-B optimizer displays different messages depending on the condition that triggered the exit. The following is a list of some of the most common exit messages in the original L-BFGS-B optimizer.

- “ABNORMAL_TERMINATION_IN_LNSRCH” This message means that there was a problem and the program’s exit was premature. It is typically found for non-smooth functions where the line search breaks down. But the message could also be symptomatic of other problems.
- “CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_LT_PGTOL”: Means that convergence was achieved because the norm of the projected gradient is small

¹PBS stands for Portable Batch System. This is software that performs job scheduling. It is used by High Performance Computing at NYU (and many other High Performance Computing Centers) to allocate computational tasks. In order to run jobs at the high performance clusters, a series of PBS batch files need to be created

²Bash is a command processor. Each Bash script that was created includes a series of computer commands, namely execution of the original L-BFGS-B software and the new code L-BFGS-B-NS

enough. Notice that this convergence message does not apply to L-BFGS-B-NS because of particular requirements for non-smooth functions involving the convex hull of projected gradients instead as explained in section 3.3. Instead it is replaced by

- “CONVERGENCE: ZERO_GRAD_IN_CONV_HULL” This means that the termination condition discussed on section 3.3 was satisfied³.
- “CONVERGENCE: REL_REDUCTION_OF_F_LT_FACTR*EPSMCH”: This convergence condition is achieved whenever the relative reduction of the value of function f is smaller than a predefined factor times machine ϵ . This exit message does not apply to L-BFGS-B-NS either. It was disabled by setting the factor “FACTR” to zero.

The limit on the number of iterations was set to 10,000.

4.2 Modified Rosenbrock Function

Consider a modified version of the Rosenbrock function problem [Ros61]:

$$f(x) = (x_1 - 1)^2 + \sum_{i=2}^n |x_i - x_{i-1}^2|^p \quad (4.1)$$

We can study the properties of function f based on the properties of the function $\phi(t_i)$. Where $\phi(t_i) = |t_i|^p$ and $t_i = x_i - x_{i-1}^2$. The properties of the function depend on the value of the p parameter⁴. This function can be proven to be locally Lipschitz continuous whenever $p \geq 1$. However, its second derivative blows up at zero whenever $p < 2$.

The properties can be separated into different cases. Whenever $p > 1$ the derivative can be represented as:

$$\frac{d}{dt}\phi(t) = \pm p|t|^{p-1} \quad (4.2)$$

and therefore, the limit of the derivative exists and is equal to zero near $t = 0$

$$\lim_{t \rightarrow 0} \frac{d}{dt}\phi(t) = 0$$

From here we conclude that f has a smooth first derivative.

³This does not mean that the resulting vector is exactly equal to zero 0, but it is small enough to satisfy the termination condition.

⁴The original Rosenbrock function had a value of $p = 2$ and the second term is multiplied by 100.

However, if $p = 1$, $\phi(t) = |t|$, and absolute value is not differentiable at $t = 0$. However, $\phi(t)$ is Lipschitz continuous at $t = 0$.

The second derivative provides a bit more of information.

$$\frac{d^2}{dt^2}\phi(t) = p(p-1)|t|^{p-2} \quad (4.3)$$

If $p \geq 2$ the function is smooth. However if $p < 2$, the second derivative becomes $\frac{p(p-1)}{|t|^q}$, where $q = 2 - p > 0$ and this second derivative blows up as $|t| \rightarrow 0$. The special case $p = 1$ has second derivative equal to zero since $p(p-1) = 0$ except at $t = 0$ where it is undefined.

Having explained the characteristics of the function, the next thing that needs to be defined is the region to be tested. We chose the region to be defined by the “box” with boundaries

$$x_i = \begin{cases} [-100, 100] & \text{if } i \in \text{even numbers} \\ [10, 100] & \text{if } i \in \text{odd numbers} \end{cases} \quad (4.4)$$

The initial point was chosen to be the midpoint of the box, plus a different small perturbation for each dimension, chosen so that the line search does not reach the boundary of several dimensions in one step.

$$x_i = \frac{u_i + l_i}{2} - (1 - 2^{1-i}) \quad (4.5)$$

The problem is twice continuously differentiable for values of $p \geq 2$, but as the values of p approach 1, the original L-BFGS-B optimizer should start to have problems. We tested the original L-BFGS-B optimizer on the modified Rosenbrock function with p varying between 2 and 1.

4.2.1 Performance of L-BFGS-B

For a value of $p = 2$, the original L-BFGS-B yields good results as seen on the resulting table [4.1](#).

This exercise tested three different values of m , where m stands for the memory of L-BFGS. The values that were tested are 5, 10 and 20. The number of dimensions in this exercise ranges from 2 to 1000. The column *nfg* stands for the number of function

m	n	p	nfq	f	proj. gradient	Final Message
5	2	2	2	81	0	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	2	2	2	81	0	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	2	2	2	81	0	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	4	2	16	9305.933478101	3.56736524480539E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	4	2	16	9305.933478101	6.07144989004382E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	4	2	16	9305.933478101	6.07144989004382E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	6	2	16	18531.1434970151	0.0004915995	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	6	2	16	18531.1434970151	0.0001894185	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	6	2	16	18531.1434970151	0.0001894185	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	8	2	19	27756.3535159291	0.0004019183	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	8	2	20	27756.3535159291	2.37577273765055E-006	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	8	2	20	27756.3535159291	2.60957631326164E-006	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	10	2	21	36981.5635348431	3.91524008875876E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	10	2	21	36981.5635348431	8.6504593070913E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	10	2	21	36981.5635348431	0.0001417493	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	20	2	21	83107.6136294132	1.41428957078915E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	20	2	21	83107.6136294132	3.35955473929061E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	20	2	21	83107.6136294131	7.1452743526379E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	50	2	17	221485.763913123	4.44565693129562E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	50	2	17	221485.763913123	2.13216261073512E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	50	2	17	221485.763913123	2.13216261073512E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	100	2	21	452116.014385974	0.0001450164	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	100	2	21	452116.014385974	0.0003285038	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	100	2	21	452116.014385974	0.0006095352	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	200	2	22	913376.515331672	0.0001644781	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	200	2	22	913376.515331672	0.0003509085	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	200	2	22	913376.515331672	0.0006814536	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
5	1000	2	24	4603460.52289722	0.00004037	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
10	1000	2	22	4603460.52289722	0.0003237067	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL
20	1000	2	30	4603460.52289721	1.18303889848903E-005	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT <= PGTOL

FIGURE 4.1: Satisfactory results for the original algorithm L-BFGS-B applied to the Modified Rosenbrock function with $p = 2$

and gradient evaluations taken and f stands for the optimal value that was achieved by the optimization. The last two columns show the norm of the final projected gradient and the final message when the algorithm finished. The termination tolerance for the projected gradients was 10^{-3}

In all cases this test was satisfied.

The overall conclusion from this exercise is that the original L-BFGS-B optimizer works well for the smooth modified Rosenbrock case.

On the other hand, the value of $p = 1$ leads to an abnormal line search termination for L-BFGS-B in most of the cases presented. This is to be expected as the function is non-smooth.

In this exercise, the memory length m of L-BFGS, does not have an impact on the final value f of the optimization, but this is because all cases crashed before the 5th iteration and therefore all different cases of m end up looking exactly the same in this table.

Several other values of p were also tested, among others 1.5, 1.1, 1.01, 1.001, ... , 1.000000001, 1. As expected, those values where p is closer to 1 are the most difficult for the original algorithm. When $p = 1$ the algorithm does not work⁵. It is important to point out that the two dimensional case is successful because in this particular case the function is smooth inside its bounding box.

⁵This is expected because the algorithm was originally designed to handle only smooth functions.

m	n	p	nfg	f	proj gradie	Final message
5	2	1	2	81.00	0.00	CONVERGEN
10	2	1	2	81.00	0.00	CONVERGEN
20	2	1	2	81.00	0.00	CONVERGEN
5	4	1	68	274.68	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
10	4	1	68	274.68	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
20	4	1	68	274.68	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
5	6	1	57	371.80	96.81	ABNORMAL_TERMINATION_IN_LNSRCH
10	6	1	57	371.80	96.81	ABNORMAL_TERMINATION_IN_LNSRCH
20	6	1	57	371.80	96.81	ABNORMAL_TERMINATION_IN_LNSRCH
5	8	1	59	468.38	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
10	8	1	59	468.38	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
20	8	1	59	468.38	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
5	10	1	59	565.28	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
10	10	1	59	565.28	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
20	10	1	59	565.28	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
5	20	1	69	1049.37	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
10	20	1	69	1049.37	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
20	20	1	69	1049.37	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
5	50	1	55	2502.10	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
10	50	1	55	2502.10	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
20	50	1	55	2502.10	96.84	ABNORMAL_TERMINATION_IN_LNSRCH
5	100	1	55	4923.83	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
10	100	1	55	4923.83	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
20	100	1	55	4923.83	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
5	200	1	55	9767.31	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
10	200	1	55	9767.31	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
20	200	1	55	9767.31	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
5	1000	1	55	48515.21	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
10	1000	1	55	48515.21	96.83	ABNORMAL_TERMINATION_IN_LNSRCH
20	1000	1	55	48515.21	96.83	ABNORMAL_TERMINATION_IN_LNSRCH

FIGURE 4.2: Unsatisfactory results for the original algorithm L-BFGS-B applied to the Modified Rosenbrock function with $p = 1$, notice however that the two-dimensional case is successful. This is because the function is smooth in this particular case.

4.2.2 Performance of L-BFGS-B-NS

For intermediate values, the new changes seem to provide better values of f . Values generated via L-BFGS-B-NS are a little better whenever p is closer to 1, since the function is “less” smooth.

On table (4.3). The parameter p changes and all other things are held constant, this makes the problem more difficult to solve. Here the termination conditions is the one seen on (3.3). Under this condition and for the same values of τ_{u_d} The number of iterations taken in order to finish seems to grow until a certain point. Roughly the cases where p is smaller than $1 + 10^{-8}$ look the same, this due to the effects of machine epsilon.

And the final table (4.4). Shows a collection of runs with very different values for the dimension n . The software shows that it is possible to run Large Scale problems. In all cases the criterion for convergence used was the termination criterion outlined in section (3.3)

p	Iterations	Value of f	Smallest norm of projected gradient	Final Message
2	8	41,116,905.61	1.88E-03	CONVERGENCE: ZERO_GRAD_IN_CONVEX_HULL
1.1	24	764,853.32	1.72E-06	CONVERGENCE: ZERO_GRAD_IN_CONVEX_HULL

TABLE 4.1: Table taken from

p	iterations	value of f	Norm projected gradient	Final Message
2	8	46,116,905.61	1.88E-03	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.1	24	764,853.32	1.72E-06	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.0001	27	484,394.49	1.91E-08	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.00001	84	484,195.01	1.06E-06	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.0000001	21	484,173.43	1.77E-08	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.000000009999999	20	484,172.80	6.98E-03	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.000000001	19	484,172.78	6.98E-03	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.0000000001	21	484,172.84	8.26E-08	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.00000000001	22	484,172.78	1.77E-08	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.0000000000001	20	484,172.84	1.77E-08	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.000000000000009	20	484,172.86	1.77E-08	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.000000000000001	20	484,172.86	1.77E-08	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.0000000000000001	20	484,172.85	1.77E-08	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1.00000000000000001	42	484,172.77	6.07E-05	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL

FIGURE 4.3: This is the number of algorithm iterations for different values of p . The value of the projected gradient is presented as well. This exercise in particular was run with an $n = 10.000$, $m = 10$ and $\tau_d = 10^{-3}$

n	p	iterations	nfg	f	projected gradient	Final Message
1000	1	17	163	48403.02345	0.00000017	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
100000	2	14	21	461251356.5	0.0045109424	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
100000	1.1	28	72	7649181.041	0.0003342748	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
100000	1.0000000001	20	137	4841870.573	5.58223998490572E-008	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
100000	1	20	139	4841870.448	4.65621336225627E-007	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1000000	2	13	21	4612595865	0.0019350335	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL
1000000	1.0000000001	27	196	48418845.6	2.12665317407389E-006	CONVERGENCE: ZERO_GRAD_IN_CONV_HULL

FIGURE 4.4: This is a collection of selected runs that achieved convergence using the methodology from section (3.3) $m = 10$ and $\tau_d = 10^{-3}$

Chapter 5

Conclusions

In the case of Non-Smooth functions, a few changes were proposed in this thesis. Implementing the changes proposed to the original L-BFGS-B software provides the capability to run optimizations on Non-Smooth functions on simply restricted domains. With the new L-BFGS-B-NS tool, it is possible to run optimizations of problems in large dimensions for some complicated tests.

The conclusion overall is that there is not a good rule of thumb to choose parameter m , and that the parameter p in the Modified Rosenbrock test function has a big impact on the number of iterations that need to be performed in order to achieve convergence.

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