New York University

Master's Thesis

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

Author:
Wilmer Henao

Supervisor:
Michael L. Overton

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Declaration of Authorship

I, Wilmer Henao, declare that this thesis titled, 'An L-BFGS-B 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

Faculty Name
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Master of Science in Scientific Computing

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

by Wilmer Henao

The Thesis Abstract is written here ...

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I also would like to thank Allan Kaku and Anders Skaaja for earlier contributions to other versions of the code and Ariana Promessi for contributing to the language in the final version.

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Contents

List of Figures

LAH **L**ist **A**bbreviations **H**ere

Dedicated to my mother, my brother and Dr. Ian Malcolm

Chapter 1

Introduction

The problem addressed is to find a local minimizer of the nonsmooth minimization problem

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

where $f : \mathbb{R}^n \to \mathbb{R}$, is continuous but not differentiable everywhere and n is a very large but finite number.

The $L-BFGS-B$ algorithm [1] is a standard method for solving large instances of 1.1 when f is a smooth function. The original name of $BFGS$ stands for Broyden, Fletcher, Goldfarb and Shanno, the authors of the original "BFGS" quasi-Newton algorithm for unconstrained optimization discovered and published independently by them in 1970 [2] [3] [4] [5]. This method requires storing and updating a matrix which approximates the inverse of the Hessian matrix $\nabla^2 f(x)$ and hence requires $\mathcal{O}(n^2)$ operations per iteration. The $L-BFGS$ variant [6] where the L stands for "Large", is based on $BFGS$ but requires only $\mathcal{O}(mn)$ operations per iteration. And not only it requires less FLOPS, but it also requires much less memory. Instead of storing the $n \times n$ hessian approximations, $L-BFGS$ stores only m vectors of dimension n, where m is 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 1.1. The $L-BFGS-B$ algorithm is implemented in a well known Fortransoftware package by the same name [7]

In this thesis, there is a brief description of the $L-BFGS-B$ algorithm at a high level and then an explanation of how the modified algorithm is more suitable for functions f which may not be differentiable at their local or global optimizers. 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 [8] 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 nonsmooth 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 at a very high level [7]. The original software is intended to work well with smooth functions. This thesis discusses how to modify the algorithm for Non-Smooth functions. The original FORTRAN code contains as well some documentation [9] about how the software was built

2.1 BFGS

$BFGS$ is a standard tool for optimization of smooth functions.[10] It is a line search method and its goal is to find a search direction starting from its current position x. The search direction is of type $d = -B_k \nabla f$ [1] where B_k is the k^{th} approximation to the inverse Hessian. [2] This k^{th} step approximation is calculated via the $BFGS$ formula

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

where $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$ and $s_k = x_{k+1} - x_k$ and where the first approximation of B_0 is assumed to be the the identity matrix I in this thesis [3]. $BFGS$ exhibits superlinear convergence but it also requires $\mathcal{O}(n^2)$ operations per iteration. [10]

In the case of Non-Smooth functions. $BFGS$ typically succeeds in finding a local minimizer. This however requires some modifications of the line search conditions. This line search conditions are known as the Armijo and weak Wolfe line search conditions and

[1] Notice that when B is the identity, this is the same direction as steepest descent. Another common line search method of optimization

[2] When 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 single step.

[3] a different starting matrix is suggested in Nocedal's book [10]

they are a set of inequalities for computing an appropriate step length that reduces the objective function "sufficiently". These inequalities will be explained later in 3.1

2.2 L-BFGS

$L-BFGS$ stands for Limited-memory $BFGS$. This algorithm approximates $BFGS$ using only a limited amout of computer memory to approximate the inverse of the Hessian B. 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 according to the problem at hand.[4] It is for this reason that during the first m iterations, $BFGS$ and $L-BFGS$ produce exactly the same search directions.

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

2.3 L-BFGS-B

Finally $L-BFGS-B$ comes naturally as 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 at bound at the optimum thus reducing the initial dimensionality of the problem and the number of iterations and running time. After this *gradient projection* comes the second step or *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 during the search step phase the step length is restricted as much as necessary in order to remain within the box defined by 1.1.

2.3.1 Gradient Projection

The original algorithm was created for the case when n is large and f is smooth. Its first step is a gradient projection similar to the one outlined in [11, 12] which is used to

[4] In 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

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:

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

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. At least a number $\mathcal{B}$ 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 approximation model:

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

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 piecewise linear segment starts on the current point x_k in the direction $-\nabla f(x_k)$. Whenever this direction encounters one of the constraints, the line segment turns corners in order to remain feasible. The path is nothing but the feasible piecewise projection of the negative gradient direction on the constraint box determined by the values $\overrightarrow{l}$ and $\overrightarrow{u}$. At the end of this stage, the value of x that minimizes $m_k(x)$ restricted to this piecewise gradient projection path is known as the "Cauchy point" x^c.

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 or 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 idea at a higher level is to solve the constrained problem 2.3, but only on those dimensions that are free. The starting point for this new stage will be the previously found Cauchy point x^c, the $L - BFGS$ algorithm provides a new search direction $\hat{d}^u$ that takes implicit advantage of second order approximations of the Hessian matrix.

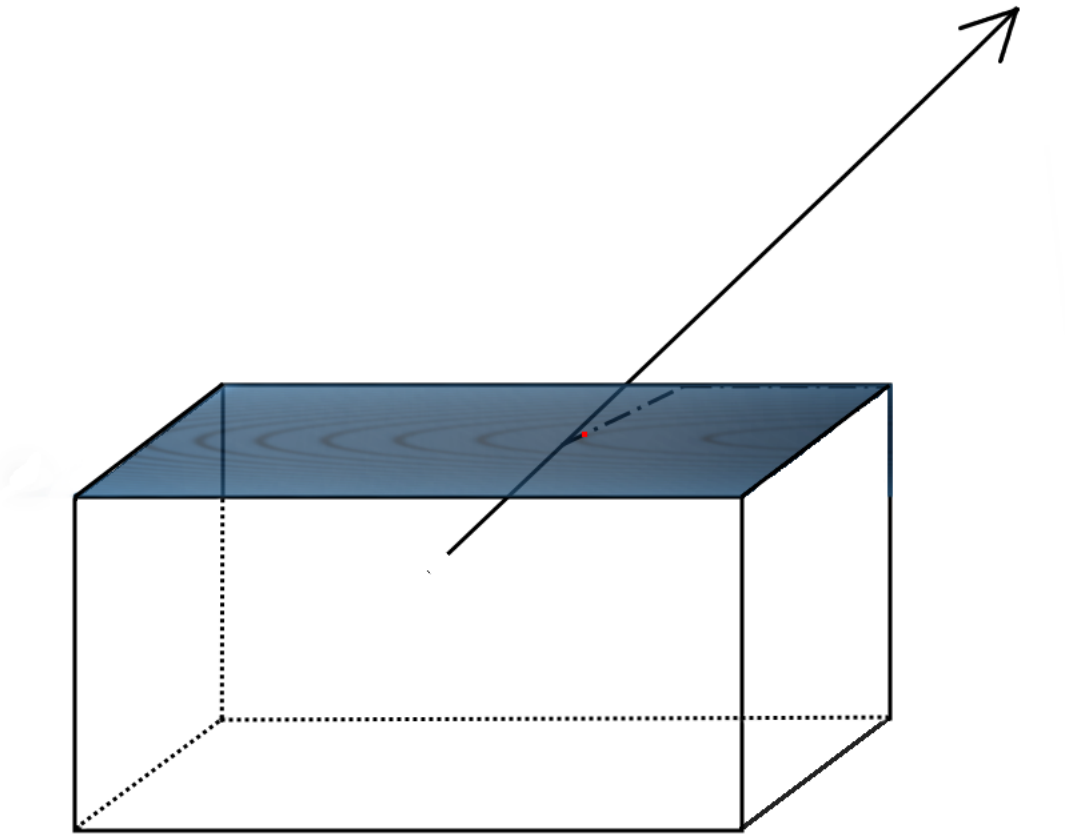


FIGURE 2.1: The arrow represents the direction of the gradient. The dotted path represents the projected gradient path from the gradient and onto the box. The region represents the level sets of the model. The optimal point (in red) is the Cauchy point x^c

The algorithm will move in the direction $\hat{d}^* = \alpha^* \hat{d}^u$ where α^* (the step length) is chosen so that the new point $\bar{x}_i$ satisfies Armijo and weak wolfe descent and curvature conditions, A third restriction on the step length is added so that the next iteration stays feasible. Once this step is finished, the next and final step will be the termination condition. If the termination condition fails, a new gradient projection and subspace minimization will be needed.

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

Probably the most important change made to the original code was the change in the curvature condition. It is accepted that the Armijo and Wolfe conditions work very well whenever the function f is smooth [13]. The Armijo condition, also known as the sufficient decrease requirement in the direction d_k is defined as

$$f(x_k + \alpha_p d_k) \leq f(x_k) + c_1 \alpha_k d_k^T \nabla f(x_k) \tag{3.1}$$

where $0 < c_1 < 1$ is a constant usually $c_1 = 10^{-4}$[10]. This condition guarantees that the function continues decreasing and eventually reaches the optimum. 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 and the one that was actually changed, is the curvature condition, of which the most popular version is the "strong Wolfe" curvature condition:

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

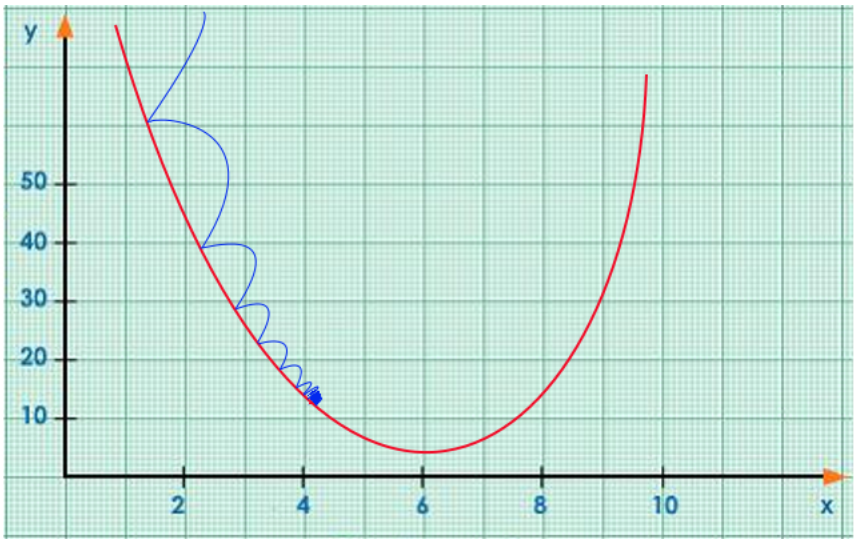


FIGURE 3.1: In this figure, the iterations always reduce the value of the function a little bit, but never enough to go below 12

Where d_k represents the search direction and c_2 is a constant such that $0 < c_1 < c_2 < 1$ and is usually $c_2 = 0.9$[10]. The strong Wolfe condition is a natural choice for optimization 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

$$d_k^T \nabla f(x_k + \alpha_k d_k) \geq c_2 d_k^T \nabla f(x_k) \tag{3.3}$$

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 [14]. This weak version is suited for the problems in this thesis. It was changed inside of the line search algorithm explained in the next section.

3.2 The line search methodology

The original FORTRAN software[7] contains a line search subroutine. This subroutine originally consisted of three steps. This line search consists of finding a step length that satisfies a decrease and a curvature condition (the Armijo and Wolfe conditions from the

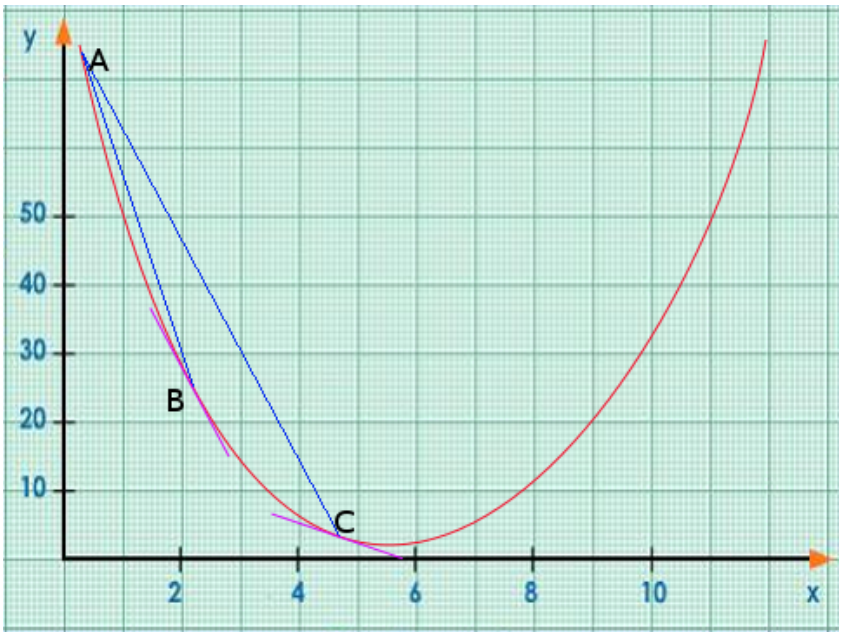


FIGURE 3.2: The logic of Wolfe conditions is this. Starting at point A. Point B is a step in the right direction, however, point C offers a "flatter" tangent and should be closer to the optimum which has a tangent of zero (Smooth case)

previous section). This subprocedure was completely changed for the purpose of this thesis. The old version of the code was not removed, it was left commented out and is only explained here with the purpose of showing why it needed to be modified. It was called on line 2662 A.1 of `lbfgsbnomessages.f90` which is a file within the github repository[8].

First the line search requires a maximum step. This maximum step is such that it guarantees that the step length stays within the bounding box delimited by l and u, as such, this is a unique feature of the bounded algorithm$L-BFGS-B$. In the original FORTRAN code, this part of the line search was not changed.

Second an interval for α_k is chosen so that it contains a minimizer of the modified function,

$$\Psi(\alpha_k) = f(x_k + \alpha_k d_k) - f(x_k) - c_1 \alpha_k d_k^T \nabla f(x_k) \tag{3.4}$$

which is nothing but a modification of the Armijo condition3.1. If $\Psi(\alpha_k) < 0$ and $\alpha_k d_k^T \nabla f(x_k) > 0$. The interval contains a minimizer of f and the subroutine can continue to the next step. This first stage took place in the subroutine *dcsrch*; specifically on lines 3687 and 3709A.2.

Third stage is the typical line search[10]. It was called on line 3713 of `lbfgsbnomessages.f90` and its mission was to find the step that satisfied Armijo and "Strong" Wolfe conditions on the original function f. Both steps 2 and step 3 are called on the subroutine *dcstep*. The subroutine still exists on file `lbfgsbnomessages.f90` for illustration. Although it is only commented out and never called in this thesis.

Those three steps make up the original subroutine. But there is a problem with the function *dcstep* on the third step as it concerns this thesis. It turns out that function *dcstep* was designed to work only with smooth functions in mind. The algorithm takes advantage of quadratic and cubic approximations to the function in order to calculate the next points that satisfy Armijo and Wolfe conditions. Unfortunately, these second and third order approximations do not work in the Non-Smooth case, and the optimizer crashes under the line search as it is. Function *dcstep* starts on line 3779 and a sample of the approximations is shown in between lines 3881 and 3902 A.3 of `lbfgsbnomessages.f90`.

The solution to this particular issue is to use a line search similar to the one implemented in hanso [15]. The HANSO approach is to double the step length while the Armijo condition is violated. And once the interval has been bracketed, to do a bisection until both Armijo and Wolfe conditions are satisfied. The only difference with the HANSO approach in this thesis is that the line search in HANSO can double its step length up to 30 times [1]. Whereas in this thesis, the step length can double only as long as the step length is less than the maximum value that guarantees feasibility of the solution (the maximum stablished in the first step of the original line search). This version of the bisection and expansion is found in between lines 4425 and 4456 of `lbfgsbnomessages.f90`A.4

3.3 The Termination Condition

One important requirement of an algorithm is that it ends in a finite time. In the case of smooth functions, $L-BFGS-B$'s way to check whether the algorithm has converged, is by using 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[2] the algorithm has converged. In the case of Non-Smooth functions however, this is not necessarily true and the function at the minimum may have a wedge. In this wedge the projected gradient may not vanish. Furthermore, if there is a sequence of points that approaches the optimum x from the right, the projected gradients corresponding to this

[1] for all practical purposes this is considered a good limit of iterations
[2] smaller than some tiny $\epsilon > 0$

sequence of points might be completely different from the projected gradients associated to a sequence of points that approach the optimum x from the left.

Given this set of conditions, there is a need for a special set of rules to establish the finalization of the optimization, these rules have already been established in some works before[14] [16].

3.3.1 Description of the Solution

Overton and Lewis formulate an algorithm that gives a practical solution to this problem on section 6.3 [14] The best practical methodology should be to calculate wheter zero 0 or a very small number is the norm of a vector that is part of the convex hull of gradients evaluated at points near the optimum candidate x. In order to make sure that the gradient zero $\vec{0}$ or a vector with a very small norm smaller than a very tiny tolerance $\tau_d > 0$ is part of the convex hull calculated near a neighbourhood of the optimum, the algorithm keeps a record of the latest gradient vectors in this small neighbourhood of the point where it is suspected that the optimum is located. The neighborhood is defined as those points with a distance to x smaller than a small tolerance $\tau_x > 0$ and no more than $J \in \mathbb{N}$ iterations back. This list of gradients is referred to as the set $\mathcal{G}$ [14]

With this list $\mathcal{G}$ of gradients at hand. The next step is to solve a quadratic program that locates the vector with the minimal norm that lives in the convex hull of these gradients. If the norm of this vector has a norm smaller than τ_d , the algorithm ends with a message of convergence success. If the minimum such norm is larger than the tolerance, the algorithm must continue to the following iteration and not terminate.

Every vector in the convex hull can be expressed as a nonnegative linear 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 $\sum_{i=1}^{n} z_i = 1$ 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

$$\begin{aligned} \min \quad & q(z) = ||Gz||_2^2 = z^T G^T G z \\ \text{s.t.} \quad & \sum_{i=1}^{J} z_i = 1 \\ & z_i >= 0. \end{aligned} \tag{3.5}$$

The solution to this problem z^* has the associated vector Gz^*. And if $||Gz^*||_2 < \tau_d$ the algorithm converges.

3.3.2 The Solution of the Quadratic Program

The solution of 3.5 was implemented with a practical primal-dual methodology. This methodology is the same methodology implemented by Skajaa [16] in his thesis. His code qpspecial was implemented in FORTRAN for this thesis and is part of `lbfgsbnomessages.f90`. His algorithm solution is a typical Mehrotra's Predictor-Corrector algorithm implementation applied to quadratic programming.

This algorithm initially tries to solve the Karush-Kuhn-Tucker KKT conditions. The KKT is a system of equations whose solution characterizes the solution of the original optimization problem. In 3.5, the Karush Kuhn Tucker equations are:

$$\begin{aligned} G^T G z - e^T s &= 0 \\ \sum_{i=1}^{J} x - 1 &= 0 \\ z_i s_i &= 0; \quad i = 1, 2, \ldots, J \\ (s, z) &\geq 0 \end{aligned} \tag{3.6}$$

Where s is the variable that represents the dual problem.

In order to solve this system of equations a variant of Newton's method is used. Thmethod provides a search direction which requires a corresponding step length. Since this is an interior point method, it approaches the solution following a path inside the convex interior of the feasible set. In the best of cases, it would be nice to approach the solution through a *central path* where the third equation in 3.6 is allowed to take more relaxed values $z_i s_i = \tau$, where $\tau \geq 0$. If the solution is approached through this *central path*. The convergence will require fewer iterations [3].

The problem is that a pure Newton's method solution is not close to this central path. The step length is usually very small because of the nature of the third and fourth equations. If the step length is too large, the condition of $z > 0$ or $s > 0$ will be violated and unfortunately, the pure method as it is does not allow reasonable step sizes in practice. The method approaches the solution very close to the boundaries of the feasible set and far away from the *central path* where the step lengths could be larger and the convergence therefore would be faster. It is for this reason that a *centering* of the path is performed. This first step is known as the "predictor" step.

Besides the centering; Mehrotra proposed a "correction" stage which pushes the solution closer to the *central path* by taking into account its curvature. This second stage is also

[3] The reason why the central path is so convenient is more thoroughly explained in Nocedal's text chapter 14[10]

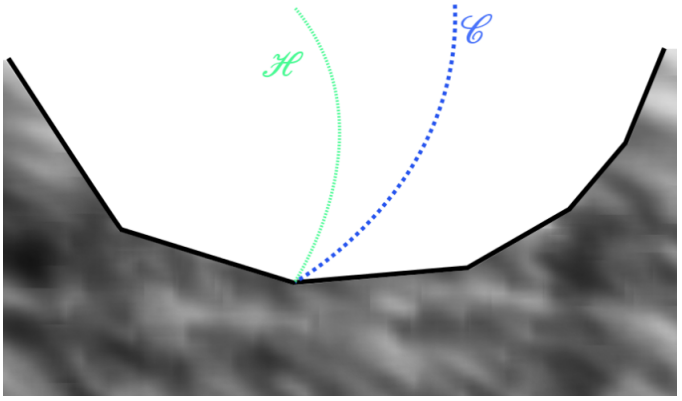


FIGURE 3.3: The central path $\mathcal{C}$ is approached from a current and noncentral point on the tangent path $\mathcal{H}$

used to calibrate some of the parameters used during the centering in the "predictor" stage[4]. The second stage is similar to the first stage in that it requires the solution of a new system of equations.

And this is very important, because both steps require a solution of a system of equations and part of this solution can be recycled. Mehrotra's algorithm requires only one Cholesky factorization for the first stage. This factorization is reused during the second stage. By reusing the factorization, the performance is improved.

[4]These are some parameters that calibrate the speed at which the tangent path is pushed into the central path. This is also explained in chapter 14[10]

Chapter 4

Solution Tests

The 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 files using a PBS generator script B.1. This script generator created PBS files which in turn run bash scripts B.2. 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. The original $L-BFGS-B$ optimizer displays different messages depending on the initial condition that triggered the exit.

4.1 Exit Conditions

The following is a list of some of the other most common exit messages in the original $L-BFGS-B$ optimizer.

- 'ABNORMAL_TERMINATION_IN_LNSRCH' This message means that there was a problem and a premature exit was required. It is typically found in Non-Smooth functions where the cubic interpolation is impossible. But the message is also 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 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 instead3.3.

- '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.
- 'ERROR: N .LE. 0': This is one of many error checks performed at the beginning of the execution.
- 'ERROR: NO FEASIBLE SOLUTION': An error condition for those cases when the solution is not feasible. This is because the original $L-BFGS-B$ optimizer allows oppen boxes of type $[l, \infty[$, $]-\infty, u]$ and $]-\infty, \infty[$
- 'WARNING: ROUNDING ERRORS PREVENT PROGRESS': If there is a rounding error issue

on top of these messages, $L-BFGS-B-NS$ introduced a new message for a succesful exit from its termination condition3.3

- 'CONVERGENCE: ZERO_GRAD_IN_CONV_HULL' What this means is that all termination conditions3.3 were satisfied[1].

4.2 Modified Rosenbrock Function

With those tools in hand, it is possible to run a few tests of the algorithm. Several functions were evaluated. One of them is a modified version of the Rosenbrock function problem[2]:

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

Here, the properties of the function depend on the value of p[3]. This function can be proven to be locally lipschitz continuous whenever $p \geq 1$. In particular it is Locally Lipschitz continuous if restricted to a finite domain of the type l, u, similar to the one defined on1.1.

The region to be tested is defined by the "box" with boundaries

[1] This does not mean that the resulting vector is exactly equal to zero 0, but it is small enough to finish the execution of the algorithm

[2] rosenbrock

[3] The original Rosenbrock function would have a value of $p = 2$

$$x_i = \begin{cases} [-100, 100] & \text{if } i \in \text{ even numbers} \\ [10, 100] & \text{if } i \in \text{ odd numbers} \end{cases} \tag{4.2}$$

And the initial point was chosen to be the midpoint of the box, plus a small perturbation chosen so that the search direction does not reach the boundary of several dimensions in one stroke.

$$x_i = \frac{u_i - l_i}{2} - (1 - 2^{1-i}) \tag{4.3}$$

The problem is smooth for values of p close to 2, but as the values of p approach 1, the original $L - BFGS - B$ optimizer should start to have problems. In order to check for that, we plug the Modified Rosenbrock function into the original $L - BFGS - B$ optimizer with p parameters varying between 2 and 1.

For a value of $p = 2$, the original $L - BFGS - B$ optimizer does not have too many problems and it yields good results as seen on the resulting table4.1.

This exercise tested three different values of m, where m stands for the steps in memory of $L - BFGS$. The steps that were tested are 5, 10 and 20, because they cover more or less the set of recommended values. The number of dimensions in this exercise in particular ranges from 2 to 1000 and covering many values in between. The column nfg stands for the number of iterations taken in order to finish the algorithm and f stands for the optimal value that was achieved during the optimization. The two last columns stand for the norm of the projected gradient and the final message when the algorithm finished.

In all cases the projected gradient has a very small norm. When this norm is tiniest the convergence is achieved because the norm of the projected gradient is smaller than the threshold. In other cases, the program exits succesfully after a relative reduction in the size of the function. In other cases, an abnormal termination message is sent to the output.

Notice that in 4.1 the program sometimes sends a warning message even though the function has converged to a value that more or less is very close to the optimal expected value. This is because the Rosenbrock function is designed to be very difficult to solve. Its minimum is located in a banana shaped valley. This valley is very flat and causes a lot of trouble to even the best optimizers.

m	n	p	nfg	f	proj gradient	Final message
5	2	2	2	81.00	0	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL
10	2	2	2	81.00	0	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL
20	2	2	2	81.00	0	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL
5	4	2	56	9305.93	3.56737E-005	ABNORMAL_TERMINATION_IN_LNSRCH
10	4	2	17	9305.93	4.33747E-007	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
20	4	2	17	9305.93	4.33747E-007	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
5	6	2	18	18531.14	0.000000058	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
10	6	2	17	18531.14	3.57280E-006	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
20	6	2	17	18531.14	3.57280E-006	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
5	8	2	22	27756.35	2.14264E-008	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
10	8	2	21	27756.35	2.07683E-008	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
20	8	2	28	27756.35	2.60729E-006	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
5	10	2	22	36981.56	5.36315E-006	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
10	10	2	22	36981.56	1.70055E-006	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
20	10	2	23	36981.56	3.42189E-008	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
5	20	2	26	83107.61	7.82706E-008	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
10	20	2	43	83107.61	3.26243E-005	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
20	20	2	22	83107.61	3.80408E-006	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
5	50	2	18	221485.76	7.93769E-007	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
10	50	2	63	221485.76	2.12629E-005	ABNORMAL_TERMINATION_IN_LNSRCH
20	50	2	63	221485.76	2.12629E-005	ABNORMAL_TERMINATION_IN_LNSRCH
5	100	2	22	452116.01	2.51616E-005	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
10	100	2	38	452116.01	4.04381E-006	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
20	100	2	22	452116.01	1.96281E-005	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
5	200	2	63	913376.52	2.85871E-005	ABNORMAL_TERMINATION_IN_LNSRCH
10	200	2	32	913376.52	0.0003494976	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
20	200	2	54	913376.52	0.0006327763	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
5	1000	2	48	4603460.52	3.01364E-005	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
10	1000	2	36	4603460.52	0.0003236833	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
20	1000	2	70	4603460.52	1.18304E-005	ABNORMAL_TERMINATION_IN_LNSRCH

* Sometimes the message output reads "ABNORMAL_TERMINATION_IN_LNSRCH". However, the function converges to the right value

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

The overall conclusion from this exercise is that the original $L-BFGS-B$ optimizer works well, for the smooth Rosenbrock case[4].

On the other hand, the value of $p=1$ has an abnormal line search termination in all of the cases presented. The projected gradient values are always far away from zero. The memory length m of $L-BFGS$, does not have an impact in the final value f of the optimization, but this is because all cases crashed before the 5^{th} iteration and therefore all different cases of m end up looking exactly the same in this table.

By the same token 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 give the most

[4]The original algorithm solves a modified version of this function 4.1, so it is to be expected that the performance is good

m	n	p	nfg	f	proj gradient	Final message
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 $p = 1$

problems to the original algorithm. When $p = 1$ the algorithm does not work as seen in 4.2[5].

For intermediate values, the new changes seem to provide better values of f. Here is a simple comparison of the algorithm running on $m = 5, 10$ for selected values of p 4.3

These are typical values of optimizations for intermediate values of p. In the bar graph it is possible to see that values generated via $L-BFGS-B-NS$ are a little better for values of p closer to 1.

[5]This is expected because the algorithm is originally designed to handle only smooth functions

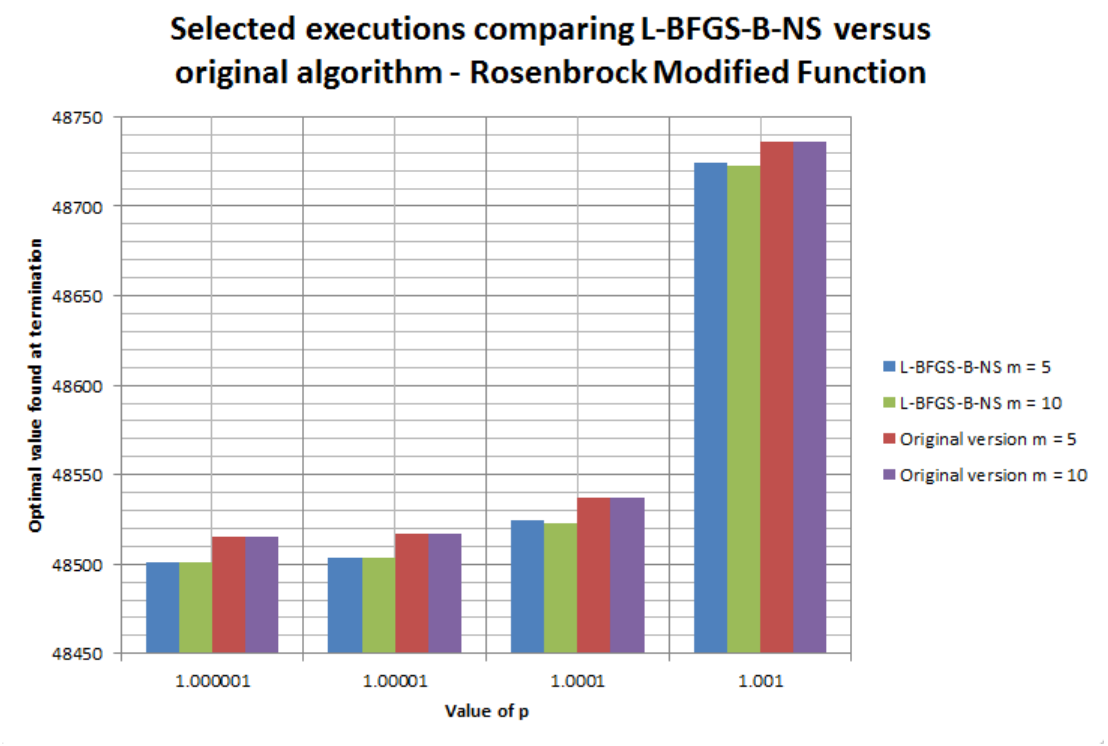


FIGURE 4.3: Comparison of the performance of $L-BFGS-B-NS$ vs. the Original version of $L-BFGS-B$ applied to the Modified Rosenbrock function with selected values of p in 1.000 dimensions

4.3 Nesterov's Chebyshev-Rosenbrock Modified function

This function is a Non-Smooth variation of `NCR-NS1` which was first introduced in the thesis by Kaku[17]. The function is defined very similar to 4.1.

$$f(x) = \frac{(x_1 - 1)^2}{4} + \sum_{i=1}^{n-1} |x_{i+1} - 2x_i^2 + 1|^p \tag{4.4}$$

Where the p is also assigned as a control variable for the Lipschitz Continuity of the function. The problem as stated in Kaku's thesis, is that the manifold defined by the term inside the sum, also known as:

$$M = \{x : x_{i+1} - 2x_i^2 + 1 = 0, i = 1, \ldots, n-1\} \tag{4.5}$$

is highly oscillatory in nature, and therefore $BFGS$ methods require many iterations to converge. In particular, the next table tries to slice the number of iterations required to finish the algorithm given different combinations of p and n, the number of dimensions4.4.

Average number of Iterations given p and n (yurirosen function)

n \ p	1	1.000000001	1.00000001	1.0000001	1.000001	1.00001	1.0001	1.001	1.01	1.1	2
2	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	1.00
4	19.33	19.33	26.33	24.00	29.67	40.00	32.67	31.67	33.00	38.33	17.00
6	812.67	830.67	965.00	2480.67	2884.67	977.00	14.33	68.33	653.67	52.33	17.67
8	60.00	63.67	60.00	79.00	216.67	1072.00	97.33	74.33	121.33	67.33	22.67
10	80.00	107.33	79.33	61.67	51.33	242.67	108.33	111.00	90.67	83.33	24.00
20	129.00	130.33	127.00	124.33	124.67	125.00	116.67	113.67	158.67	137.67	18.00
50	156.00	185.67	199.33	189.33	201.33	181.00	197.00	152.33	151.00	195.00	19.67

*Average of m = 5; 10; 20

FIGURE 4.4: Comparison of the number of iterations in order to converge for the Modified NCR-NS1 functions sliced by the number of dimensions n and the p parameter that controls the Smoothness of the function

Average number of Iterations given m and n (yurirosen function)

n \ m	5	10	20
2	1.92	1.92	1.92
4	33.67	25.42	25.25
6	502.50	1234.08	909.83
8	64.75	94.67	337.50
10	75.58	120.25	84.75
20	110.50	109.42	138.83
50	215.00	139.75	147.00

* For values of p = 2; 1.1; 1.01; 1.001; 1.0001; 1.00001; 1.000001; 1

FIGURE 4.5: Comparison of the number of iterations in order to converge for the Modified NCR-NS1 functions sliced by the number of dimensions n and the memory lag m

The results show that the number of iterations increases significatively with smaller values of p, and in general with larger values of the dimension n.

This table was also sliced with the parameters n and m in figure 4.5.

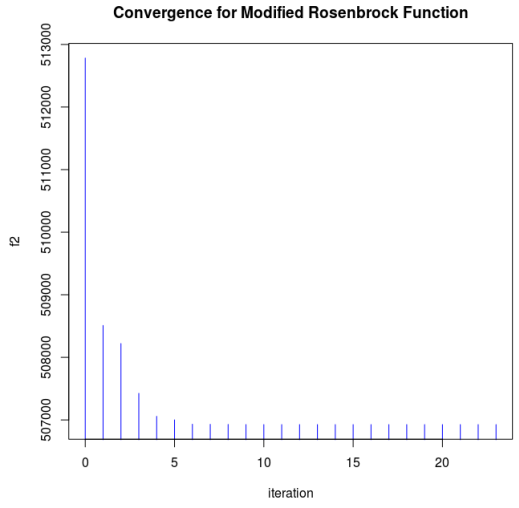
Chapter 5

Conclusions

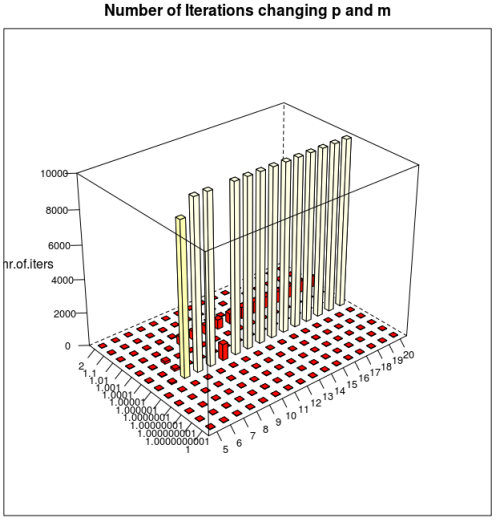
and in fact, whenever the function is restricted to a finite domain this function will be lipschitz continuous for $p > 1$. Whenever $p > 1$ the function $f(z) = |z|^p$ is zero 0 around zero because the derivative $p|z|^{p-1}$ is zero whenever z tends to zero from the right. (this is also the case from the left because it is an even function). However the second derivative will not be as nice.

For the case when $p \leq 1$ the second derivative tends to infinity. $\lim_{x \to 0^+} f' = \infty$. Which is already well known given the "heavyside" look of $f(z) = |z|$.

The convergence of the algorithm smoothly descends to the objective



The converge is adversely affected by the selection of p as one would expect. Values of p descending to 1 make the function less "smooth" and have the adverse effect of making the convergence much more difficult. In this exercise it is noticeable how slow the convergence becomes for a few specific values of p. In particular for 1.0001



$$f(x_k + \alpha_k p_k) \leq f(x_k) + c_1 \alpha_k p_k^T \nabla f(x_k) \tag{5.1}$$

Appendix A

Samples of Code

A.1 Ignoring old code

All the code is available on [8] . This is also true for the code that is not being used anymore. Here the old function dcsrch is commented out. lineww is replacing it instead

```
2607
2608 !     call dcsrch(f,gd,stp,ftol,gtol,xtol,zero,stpmx,csave,isave,dsave)
2609       call lineww(f,gd,stp,ftol,gtol,xtol,zero,stpmx,csave,isave,dsave)
```

A.2 Old Stage 1 of the line search

Stage 1 of the line search[7] . This stage is not being run in lbfgsbNS. But is kept there for comparisson. For the new line search that replaces it A.4

```
3687        if (stage .eq. 1 .and. f .le. fx .and. f .gt. ftest) then
3688
3689 !  Here we define the modified function and derivative values.
3690 !  This line search will only aim to satisfy the condition in (3.3) modified
        Armijo
3691           fm = f - stp*gtest
3692           fxm = fx - stx*gtest
3693           fym = fy - sty*gtest
3694           gm = g - gtest
3695           gxm = gx - gtest
3696           gym = gy - gtest
3697
3698 !  Call dcstep to update stx, sty, and to compute the new step.
3699 !
3700           call dcstep(stx,fxm,gxm,sty,fym,gym,stp,fm,gm,brackt,stmin,stmax)
3701
3702 !         Reset the function and derivative values for f
3703
```

```
3704          fx = fxm + stx*gtest
3705          fy = fym + sty*gtest
3706          gx = gxm + gtest
3707          gy = gym + gtest
3708
3709       else
```

A.3 Cubic and Quadratic line search sample

This part of the code does not work in the case when the function is Non-Smooth . For this reason it was eliminated from execution on lbfgsbNS and replaced with A.4. stx in this case is a variable that represents the step with the minimum value so far.

```
3881  !     First case: A higher function value. The minimum is bracketed.
3882  !     If the cubic step is closer to stx than the quadratic step, the
3883  !     cubic step is taken, otherwise the average of the cubic and
3884  !     quadratic steps is taken.
3885    ! theta, three, gamma are parameters
3886        if (fp .gt. fx) then
3887           theta = three*(fx - fp)/(stp - stx) + dx + dp
3888           s = max(abs(theta),abs(dx),abs(dp))
3889           gamma = s*sqrt((theta/s)**2 - (dx/s)*(dp/s))
3890           if (stp .lt. stx) gamma = -gamma
3891           p = (gamma - dx) + theta
3892           q = ((gamma - dx) + gamma) + dp
3893           r = p/q
3894           stpc = stx + r*(stp - stx) !quadratic step
3895           stpq = stx + ((dx/((fx - fp)/(stp - stx) + dx))/two)* &
3896                                                          (stp - stx) !The
     cubic step
3897           if (abs(stpc-stx) .lt. abs(stpq-stx)) then
3898              stpf = stpc
3899           else
3900              stpf = stpc + (stpq - stpc)/two
3901           endif
3902           brackt = .true.
```

A.4 Line Search Enforcing Weak Wolfe Conditions

This is the implementation of the line search that enforces the weak Wolfe conditions. Bisections and expansions (as long as it doesn't mean leaving the bounding box) of the step length. This version tries to be as similar as possible to the interior of the while loop in qpspecial.m at hanso [15]

```
4425        if (fp .ge. ftest) then
4426          sty = stp
```

```
4427            fy = fp
4428            dy = dp
4429            brackt = .true.
4430         else
4431 !       if second condition is violated not gone far enough (Wolfe)
4432            if (-dp .ge. gtol*(-ginit)) then
4433               stx = stp
4434               fx = fp
4435               dx = dp
4436            else
4437               return
4438            endif
4439         endif
4440
4441         !Bisection and expansion
4442         if (brackt) then
4443            stp = (sty + stx)/two
4444         else
4445            if (two * stp .le. stpmax) then !Remain within boundaries
4446               ! Still in expansion mode
4447               stp = two * stp
4448            else
4449               brackt = .true.
4450               sty = stp
4451               fy = fp
4452               dy = dp
4453            endif
4454         endif
4455         return
4456         end
```

Appendix B

Automation

This appendix includes some of the files that were used to run examples in parallel at the High Performance Clusters at NYU. All of these files can be found in the repository [8]

B.1 Script Generator

This is a sample of the script generator that creates pbs files to be sent to the High Performance Machines. The value "i" creates a different set of files, in this case one file for each value of p that we want to test. To see a result of running this script look at B.2.

```
#!/bin/bash

for i in {0..20}
do
  cat > pbs.script.rosenbrock.$i <<EOF
#!/bin/bash

#PBS -l nodes=1:ppn=8,walltime=48:00:00
#PBS -m abe
#PBS -M weh227@nyu.edu
#PBS -N rosenbrockHD$((i))

module load gcc/4.7.3

cd /scratch/weh227/rosenbrock/
p=$(bc -l <<< "1+10 ^(-$((i)))")
for n in 1000 100000 1000000 10000000 100000000
do
   echo 10 \$n \$p
   ~/Documents/thesis/lbfgsfortran/./rosenbrockp 10 \$n \$p >> outputrosenbrock$
    ((i)).txt
```

```
21 done
22
23 exit 0;
24
25 EOF
26 done
```

After they are created I could fire all of the runs at once by using the command

for i in 0..20; do qsub pbs.script.rosenbrock.$$i$; done

B.2 PBS File Sample

This is a sample file general with B.1. It runs a special value p. These are the ones that get started with the the qsub command.

Lines 4 to 5 provide the user with emails and critical information while running the process. Line 13 defines a run for different sizes of n. Line 16 is the actual run that will be sent to an output file. In this case "outputrosenbrock9.txt"

```
1
2 #!/bin/bash
3
4 #PBS -l nodes=1:ppn=8,walltime=48:00:00
5 #PBS -m abe
6 #PBS -M weh227@nyu.edu
7 #PBS -N rosenbrockHD9
8
9 module load gcc/4.7.3
10
11 cd /scratch/weh227/rosenbrock/
12 p=1.00000000100000000000
13 for n in 1000 100000 1000000 10000000 100000000
14 do
15    echo 10 $n $p
16    ~/Documents/thesis/lbfgsfortran/./rosenbrockp 10 $n $p >> outputrosenbrock9.
       txt
17 done
18
19 exit 0;
```

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