New York University

Master's Thesis

A Large-Scale Constrained Optimizer for NonSmooth Functions

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Declaration of Authorship

I, Wilmer Henao, declare that this thesis titled, 'A Large-Scale Constrained Optimizer for NonSmooth Functions' and the work presented in it are my own. I confirm that:

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Abstract

Faculty Name
Department of Mathematics

Master of Science in Scientific Computing

A Large-Scale Constrained Optimizer for NonSmooth Functions

by Wilmer Henao

The Thesis Abstract is written here ...

Acknowledgements

I would like to than my advisor Michael Overton for all the hours of hard work and for all the great recommendations and changes that suggested for the creation of this thesis.

I also would like to thank Allan Kaku and Anders Skaaja for earlier contributions to other versions of the code. . . .

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Abbreviations

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

Physical Constants

Speed of Light $c = 2.997\ 924\ 58 \times 10^8\ \mathrm{ms}^{-\mathrm{S}}$ (exact)

Symbols

a	distance	m
P	power	W (Js^{-1})
ω	angular frequency	$rads^{-1}$

For/Dedicated to/To my...

Chapter 1

Introduction

The goal in this thesis is to find a solution 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 $f \colon \mathbb{R}^n \to \mathbb{R}$, n is a very large but finite number. And l_i and $u_i \in \mathbb{R}$

Larger problems not only mean that the problem will take a longer time to solve compared to a similar problem. But storing and calculating a Hessian matrix is prohibitively expensive. There a few techniques that have already been developed for the case when n is very large and this is what we know as large scale optimization. Also, Several techniques have already been developed to handle this type of problems as long as the function f is smooth.

In this thesis $f(x)$ is a nonsmooth function.

For the particular case when n is a small number, several methods that solve optimization problems of nondifferentiable functions in lower dimensions [2] have been developed. In the case of smooth functions, it is possible to use Newton iteration algorithms and achieve quadratic convergence, the problem with Newton algorithms is that they require second derivatives to be provided[1]. In the 1950's and several years after that, several quasi-newton methods were proposed where the second derivative Hessian matrix is "approximated" step by step [1]. These approximations or "updates" are calculated after every iteration and the way in which this update is found defines a new method

[1] the main issue with the second derivative is that it requires a total of $n \times n$ partial derivatives. Which is impractical for medium and for some small-size problems

depending on the particular needs. This thesis will only be concerned with the $BFGS$. [2] which can achieve super linear convergence, has proven to work in most practical purposes and posseses very nice self correcting features [3]. In other words, it doesn't matter that one update incorrectly estimates the curvature in the objective function, $BFGS$ will always correct itself in just a few steps. This self-correcting property is very desired in the nonsmooth case, since changes in curvature could be large near the optimal point. $BFGS$ is not the right tool for large scale optimization and therefore an $L-BFGS$ adaptation is needed to solve the problem obtained on 1.1

A final assumption in this thesis is that the Hessian matrix is not sparse. In this case, there are other algorithms that may be more suitable [5, 6], some of them have even been implemented in fortran [7].

This thesis builds upon the original $L-BFGS-B$ code [**?**] that solves smooth problems of f. There were three main changes in the code. The first one is the line search conditions which required a small change in order to satisfy the different structure that a nonsmooth function requires. The second one is the line search methodology which was changed from a cubic interpolation to a bisection algorithm and last change in the thesis was the termination condition.

Nocedal's original algorithm consists of 2 steps. In the first step most of the dimensions in the problem should be removed, making the problem a lot simpler. And in the second step there is some fine tuning to guarantee better than just linear speed of convergence.

[2] BFGS stands for the last names of its authors Broyden, Fletcher, Goldfarb and Shanno

Chapter 2

Original algorithm

The original algorithm [12] has an accompanying software written on *FORTRAN* [**?**] and this thesis builds upon that software by making sufficient changes to make it applied to the nonsmooth case.

The original algorithm was created for the case when n is large and f is nonsmooth. The method is based on a gradient projection method similar to the one outlined in [13, 14] which is used to determine an active set corresponding to those variables that are bound at each step.

The active set at x^*:

$$\mathcal{A}(x^*) = \{i \in \{1 \dots n\} | x_i^* = l_i \vee x_i^* = u_i\} \tag{2.1}$$

It seems like working on this active set is efficient in large problems and according to previous research its properties are theoretically good [4]. The most important reason in theory is that the gradient projection step is able to find most of the active set variables in a single stroke. Usually, while performing quadratic optimizations, the active set changes by one variable at a time during the line search step [1]. So, if 1 million constraints are active at the nondenerage solution, at least 1 million iterations will be needed. Gradient projection gets rid of that problem, diminishing the number of iterations, and at the same reducing the number of variables for the next step.

[Try to introduce a graphic of gradient projection here]

[1] the line search is cut short immediately after the first bound is hit, so only one active constraint will change at every step... that is, unless the line search hits several constraints at the same time by coincidence, which is very unlikely

Just like its unconstrained counterparty $L-BFGS$, $L-BFGS-B$ does not require a Hessian matrix to be provided and instead the Hessian is approximated. Following some simple computational techniques that will all be explained, the number of computations and the storage required, are all kept in the order of n.

2.1 Overview of the Algorithm

At the beginning of the k^{th} step, the function $f(x)$ is approximated by a second-order Taylor expansion around x_k. This approximation will be refered to as "the model".

$$m_k(x) = f(x_k) + \nabla f(x_k)^T(x - x_k) + \frac{(x - x_k)^T B_k(x - x_k)}{2} \tag{2.2}$$

In this model it is important to point out that the gradient ∇f is provided, however B_k will be a $L-BFGS-B$ approximation to the Hessian $\nabla^2 f$ and will not be calculated explicitly. The algorithm assumes that the function is similar to the quadratic model at least in a neighborhood of k, therefore, the first step will be to try and minimize the model 2.2 subject to the constraints $l_i < x_{k,i} < u_i$ via the gradient projection method.

On each iteration of the gradient projection algorithm there will be two stages, a cauchy point computation and a subspace minimization. In the first stage the algorithm starts on the current point x_k searching on the direction of $-\nabla f(x_k)$. Now, whenever this search direction encounters one of the constraints, the search direction turns on the boundaries in order to remain feasible. The path is nothing but the feasible piecewise projection of the steepest descent search direction on the contraint "box" determined by the values $\overrightarrow{l}$ and $\overrightarrow{u}$. At the end of this stage, the value of x that minimizes $m_k(x)$ on this piecewise gradient projection path is known as the "Cauchy point" x^c.

For stage two, define the working set as the active set defined on the cauchy point $\mathcal{A}(x^c)$. In order to do this, solve the quadratic subproblem in which all values of the working set $\mathcal{A}(x^c)$ are fixed at the values corresponding to x^c

2.1.1 Generalized Cauchy Point Calculation

The generalized cauchy point that minimizes 2.2 and lies along the gradient projection path can be calculated by a simple algorithm. First of all, any point on the space can be projected on the feasible region by the following formula:

$$\mathcal{P}(x,\vec{l},\vec{u}) = \begin{cases} l_i, & \text{if } x_i < l_i \\ x_i, & \text{if } x_i \in [l_i, u_i] \\ u_i, & \text{if } x_i > u_i \end{cases} \tag{2.3}$$

The piecewise linear path that starts on x_k and goes on the projected direction of the negative gradient at x_k can be parameterized by t as:

$$x(t) = \mathcal{P}(x_k - t\nabla f(x_k), \vec{l}, \vec{u}) \tag{2.4}$$

With this definition the k^{th} Generalized Cauchy point is the first local minimizer of the function $m_k(x(t))$ where $t > 0$. The minimizer is obtained by examining each of the different segments one by one in order. In order to do this, it is important to find out the elements at which the breakpoints occur. These elements are characteristized disorderly by:

$$\hat{t_i} = \begin{cases} \frac{x_{i,k}-u_i}{\nabla f(x_k)_i}, & \text{if } \nabla f(x_k)_i < 0 \\ \frac{x_{i,k}-l_i}{\nabla f(x_k)_i}, & \text{if } \nabla f(x_k)_i > 0 \\ \infty, & \text{otherwise} \end{cases} \tag{2.5}$$

where $x_{i,k}$ represents the i^{th} coordinate of x_k and $\nabla f(x_k)_i$ stands for the i^{th} coordinate of the gradient. It is therefore very important to find a piecewise representation of the components of $x(t)$ which is piecewise defined as

$$x_i(t) = \begin{cases} x_{i,k} - t\nabla f(x_k)_i, & \text{if } t \leq \hat{t_i} \\ x_{i,k} - \hat{t_i}\nabla f(x_k)_i, & \text{otherwise} \end{cases} \tag{2.6}$$

Now, in order to iterate in order through the different $\hat{t_i}$ values. It is necessary to sort the values with a heapsort algorithm [2] which can do the job in $O(n \log(n))$. Eliminating repeated and zero values of $\hat{t_i}$, this ordering defines the intervals $[0, t_1]$, $[t_1, t_2]$, ... [3].

When this algorithm is run, the intervals are analysed one by one starting with $[0, t_1]$. If the optimal is found in this interval, the algorithm stops. If it has not been found the algorithm continues to the next interval and so on. Assuming that the algorithm has

[2] several algorithms can be chosen in this situation

[3] Notice that the $\hat{at}$ represents the unordered breakpoints, whereas the lack of represents the ordered breakpoints

not found a solution until t_{j-1}, and the point $x(t_{j-1})$ has been found and the direction of the projected gradient is given by

$$d_i^{j-1} = \begin{cases} -\nabla f(x_k)_i, & \text{if } t_{j-1} < \hat{t}_i \\ 0, & \text{otherwise} \end{cases} \tag{2.7}$$

the model 2.2 on the next line segment will be

$$\begin{aligned} m_k(x) = f(x_k) + \nabla f(x_k)^T (x_{j-1} - x_k + \Delta t d^{j-1}) + \\ \frac{(x_{j-1} - x_k + \Delta t d^{j-1})^T B_k (x_{j-1} - x_k + \Delta t d^{j-1})}{2} \end{aligned} \tag{2.8}$$

where

$$\Delta t = t - t^{j-1}$$

With this equation it is now possible to obtain a formula for the optimal Δt. All there is to do is to group the terms in powers of Δt, derive, equate to zero and obtain the optimal values. Grouping the terms from 2.8

$$\begin{aligned} m_k(x) = f(x_k) + \nabla f(x_k)^T (x_{j-1} - x_k) + \frac{1}{2}(x_{j-1} - x_k)^T B_k (x_{j-1} - x_k) + \\ \left(\nabla f(x_k)^T d^{j-1} + {d^{j-1}}^T B_k (x_{j-1} - x_k) \right) \Delta t + \\ \left(\frac{{d^{j-1}}^T B_k d^{j-1}}{2} \right) \Delta t^2 \end{aligned} \tag{2.9}$$

And defining the corresponding terms to be

$$f_{j-1} := f(x_k) + \nabla f(x_k)^T (x_{j-1} - x_k) + \frac{1}{2}(x_{j-1} - x_k)^T B_k (x_{j-1} - x_k) \tag{2.10}$$

$$f'_{j-1} := \nabla f(x_k)^T d^{j-1} + {d^{j-1}}^T B_k (x_{j-1} - x_k) \tag{2.11}$$

$$f''_{j-1} := {d^{j-1}}^T B_k d^{j-1} \tag{2.12}$$

The optimal value will be $\Delta t^* = \frac{-f'_{j-1}}{f''_{j-1}}$ as long as this Δt^* is located within the interval $[0, t_j - t_{j-1}]$. If it is not, there are two other alternatives. Either $f'_{j-1} \geq 0$ in which case the optimal cauchy point is located right at the breakpoint x_{j-1}, or $f'_{j-1} < 0$ in

which case the solution is not in the current interval, or finishes at t_j if this was the last interval analysed, or it moves over to the interval $[t_j, t_{j+1}]$, replacing

$$x_j = x_{j-1} + \Delta t^{j-1} d^{j-1}, \text{ where} \Delta t^{j-1} = \hat{t_j} - \hat{t_{j-1}} \tag{2.13}$$

and of course, replacing the search direction d^j by cancelling the corresponding coordinate to 0 zero. That is,

$$d^j = d^{j-1} + \nabla f(x_k)_b e_b \tag{2.14}$$

Where b represents the variable that becomes active at $\hat{t_j}$

A more surprising result [12] not demonstrated here is that it is possible to calculate f_j' and f_j'' using the $L-BFGS$ formulae recursively as

$$\begin{aligned} f_j' &= f_{j-1}' + \Delta t^{j-1} f_{j-1}'' + (\nabla f(x_k)_b)^2 + \theta \nabla f(x_k)_b (x_j - x_k)_b - \\ &\quad \nabla f(x_k)_b w_b^T M W^T (x_j - x_k) \\ f_j'' &= f_{j-1}'' + 2\theta \nabla f(x_k)_b^2 - 2\nabla f(x_k) w_b^T M W^T d^{j-1} + \theta (\nabla f(x_k)_b)^2 - \\ &\quad \nabla f(x_k)_b^2 w_b^T M w_b \end{aligned} \tag{2.15}$$

which is very cheap to calculate since it only implies an $O(n)$ calculations, coming from the the matrix products $W^T(x_j - x_k)$ and $W^T d^j$. Looking closely however, these values are updated everytime just one iteration. So it makes sense to store the vectors and update them everytime.

$$p_j := W^T d^j = W^T (d^{j-1} + \nabla f(x_k)_b e_b) = p_{j-1} + \nabla f(x_k)_b w_b \tag{2.16}$$

$$c_j := W^T (x_j - x_k) = W^T (x_{j-1} - x_k + \Delta t^{j-1} d^{j-1}) = c_{j-1} + \Delta t^{j-1} p_{j-1} \tag{2.17}$$

which brings the order of calculation updates down to $O(m^2)$. Since only the first iteration requires a total calculation of the order of $O(n)$, the algorithm is very cheap to calculate

In synthesis the algorithm works like this, there is an initialization phase that works for the first segment and an iteration phase that works for the other segments.

Algorithm 1: Generalized Cauchy Point

Data: x, $\vec{l}$, $\vec{u}$, $\nabla f(x_k)$, and B_k

Result: The Generalized Cauchy Point

for $i \in 1, \ldots, n$ **do**
  Calculate $\vec{t_i}$ according to 2.5;
  Calculate d_i based on $\vec{t_i}$;
end
initialization;
$\mathcal{F} := \{i : \vec{t_i} > 0\}$;
$p := W^T d$;
$c := 0$;
$f' := -d^T d$;
$f'' := -\theta f' - p^T M p$;
$\Delta t^* := \frac{-f'}{f''}$;
$t_{old} := 0$;
$t := min\{t_i : i \in \mathcal{F}\}$;
$b := i$ s.t. $t_i = t$ the boundary just hit;
remove b from $\mathcal{F}$;
$\Delta t := t - 0$;
Subsequent;
while $\Delta t^* \geq \Delta t$ **do**
  $x_b^{cp} := u_b$ or l_b Depending on what boundary was hit;
  $z_b := x_b^{cp} - x_b$;
  $c := c + \Delta t p$;
  $f' := f' + \Delta t f'' + (\nabla f_b)^2 + \theta \nabla f_b z_b - \nabla f_b w_b^T M c$;
  $f'' := f'' - \theta(\nabla f_b)^2 - 2\nabla f_b w_b^T M p - (\nabla f_b)^2 w_b^T M w_b$;
  $p := p + \nabla f_b w_b$;
  $d_b := 0$;
  $\Delta t^* := -frac f' f''$;
  $t_{old} := t$;
  $t := min\{t_i : i \in \mathcal{F}\}$;
  $b := i$ s.t. $t_i = t$;
  $\Delta t := t - t_{old}$;
end
$\Delta t^* := \max\{\Delta t^*, 0\}$;
$t_{old} := t_{old} + \Delta t^*$;
$x_i^{cp} := x_i + t_{old} d_i$, whenever $t_i \geq t$;
$\forall i \in \mathcal{F}$ with t_i remove i from the set $\mathcal{F}$;
$c := c + \Delta t^* p$;

Overall, the major cost of the algorithm is the heapsort step for t_i, which is run in $O(n \log(n)$

2.1.2 Subspace Minimization

The final step on this alrorithm is the subspace minimization. Once the gradient direction step has been taken, several dimensions in the problem will have been removed. Here, the algorithm takes advantage of this situation and solves the quadratic model 2.2 restricted to the simple constraints. In order to do this, a new search direction is proposed. And the step length is such that it stays within the bounds stablished in the problem.

The idea at a higher level is to solve the constrained problem, but only on those dimensions that are free (not at bound). In the notation set forth in the previous algorithm. $\mathcal{F}$ represents the set of indices corresponding to the t free variables. Z_k is the matrix formed by the t unit vector columns that span the dimensions of the free variables and A_k is the corresponding matrix that represents the active constraint gradient (also unit vectors). The dimension of Z_k would be $n \times t$ and the dimension of A_k $n \times (n - t)$.

The starting point for this new problem will be the previously found cauchy point x^c, and the algorithm only moves in a direction that lives in the space generated by the columns of Z_k. In other words, if $\hat{d}$ is the t-dimensional search direction,

$$x = x^c + Z_k \hat{d} \tag{2.18}$$

Under this equation and replacing in 2.2, it's obtained

$$m_k(x) = \hat{d}^T \hat{r}^c + \frac{1}{2} \hat{d}^T \hat{B}_k \hat{d} + \gamma \tag{2.19}$$

where γ is a constant and $\hat{B}_k = Z_k^T B_k Z_k$, or the Hessian restricted to the "free" dimensions in the problem. $\hat{r}^c = Z_k^T (g_k + B_k(x^c - x_k))$ is the corrected gradient restricted to the same "free" dimensions. Which restates the problem as

$$\begin{aligned} \min_{\hat{d} \in \mathbb{R}^t} \quad & \hat{m}_k(\hat{d}) = \hat{d}^T \hat{r}^c + \frac{1}{2} \hat{d}^T \hat{B}_k \hat{d} + \gamma \\ \text{s.t.} \quad & l_i - x_i^c \leq \hat{d}_i \leq u_i - x_i^c, \\ & i \in \mathcal{F} \end{aligned} \tag{2.20}$$

And the solution is simply $\hat{d}^u = -\hat{B}_k^{-1}\hat{r}^c$[4]. Now the step length should be $\hat{d}^* = \alpha^*\hat{d}^u$ where α^* is chosen so that the new point $\bar{x}_i$ stays within the constraints originally imposed.

[4]Notice that this implies the inversion of $\hat{B}_k$. However there is a numerical trick explained in [4], that makes this operation trivial, since $\hat{B}_k$ is a small-rank correction of a diagonal matrix and its inverse can be computed by the Sherman-Morrison-Woodbury formula

Chapter 3

Modifications to the original algorithm

3.1 Convex Hull and termination conditions

The most important requirement of a practical algorithm is that it ends in a finite time. For the case of smooth functions, the formal way to do this is to check whether the gradient has dimension zero 0 wherever the constraints are not at bound. In the case of nonsmooth functions however, this is not necessarily true and the function at the minimum, may have a kink. In this kink the gradient may not vanish. Furthermore, if there is a sequence of points that approaches the optimum x from the right, the gradients corresponding to this sequence of points might be completely different from the gradients associated to a sequence gradients associated to a sequence of points that approaches the optimum from the left. In other cases, the optimum might be located right at one of the boundaries, In this case the gradient does not necessarily vanish.

Given this set of conditions, there is the need for a special set of rules to establish the finalization of each optimization.

Since BFGS approximations typically converge to Clarke-Stationary points. The right methodology is to calculate the subgradient. One particular methodology that guarantees an end to the algorithm is suggested in [15]. In order to make sure that the gradient zero $\vec{0}$ is part of the subgradient calculated over a neighbourhood of the optimum. The algorithm keeps a record of the latest gradient vectors in a small neighbourhood of the point that we suspect is the optimum, This collection is called G_k in [15], This collection of gradients spans an associated convex hull of gradients. If this convex hull contains at least one vector of dimension smaller than a tiny number τ_k, the algorithm ends.

Of course the best way to find a vector with such properties is to find the vector with the minimal norm that resides in the convex hull generated by G_k

3.1.0.1 minimization of the quadratic program

This solution is guarantees to end up at a local optimum. However, one subalgorithm needs to be solved. This algorithm is a practical primal-dual algorithm. In this case in particular the best solution is to implement a variation of Mehrotra's Predictor-Corrector algorithm applied to quadratic programming. The primal dual method requires the solution of a system in order to calculate the search direction. The most expensive part of this solution is the calculation of the cholesky decomposition. Mehrotra's algorithm uses the same cholesky decomposition to calculate both directions. the predictor, and the corrector.

Currently there is not a theoretical calculation of the complexity of this algorithm but it is very used in practice. The implementation here is exactly the one on [**?**]. It was implemented in fortran as part of the optimizer.

3.2 cubic interpolation replaced with line search

The original software by Nocedal[**?**], included a cubic line search. The idea of a cubic interpolation line search is to take advantage of the smooth properties of functions and take advantage of the curvature properties. It is debatable to see which one works better whether a simple line search or a cubic interpolation. However, In the case of nonsmooth functions, this line search does not serve our purpose and therefore a more typical line search that implements a bisection was used.

In general, a step length is selected. If this step length does not satisfy the sufficient decrease and curvature conditions, then a step length of half or double the size is selected. the algorithm is guaranteed to converge under a careful selection of the parameters, however, in case this does not happen, the software will stop with a warning.

3.3 the functions to be tested

In order to make some tests, a few functions will be evaluated. The most important function to test this non-smooth optimizer is a modified version of rosenbrock's:

$$f(x) = (x_1 - 1)^2 + \sum_{i=2}^{n} |x_i - x_{i-1}^2|^p \tag{3.1}$$

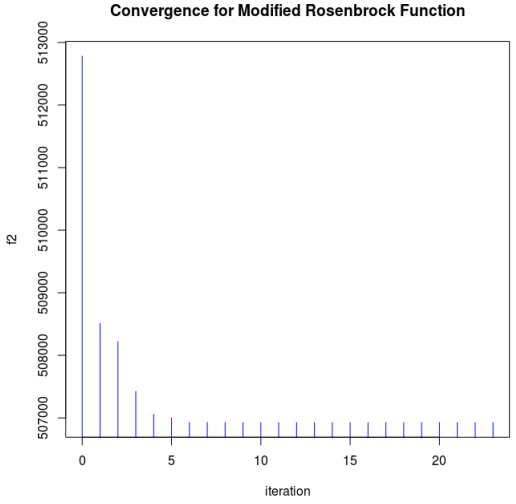
Where the value of p changes the behaviour of the optimizer. This function can be proven to be lipschitz continuous whenever $p > 1$ if restricted to the domain defined by

$$x_i = \begin{cases} [-100, 100] & \text{if } i \in \text{ even numbers} \\ [10, 100] & \text{if } i \in \text{ odd numbers} \end{cases} \tag{3.2}$$

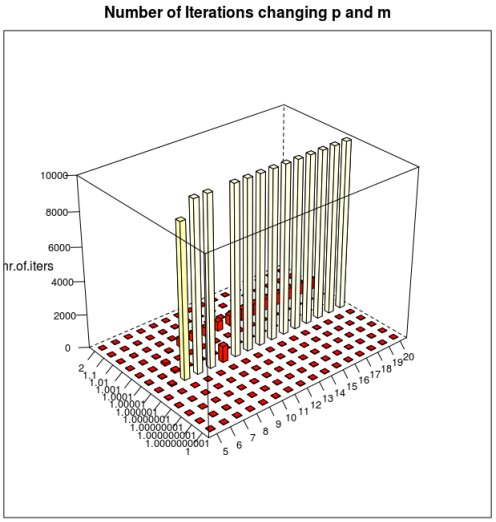
and in fact, whenever the function is restricted to a finite domain. Because whenever $p > 1$ we have that the function $f(z) = |z|^p$ is zero 0 around zero because the derivative $p|z|^{p-1}$ is zero whenever z tends to zero from the right. (from the left also because it is an even function). However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

For the case when $p \leq 1$ we have that 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



3.4 Weak wolfe conditions

Probably the most important change made to the original code was the change in the curvature condition. Originally there are two Wolfe conditions, one of them is the Armijo condition, also known as the sufficient decrease conditions.

$$f(x_k + \alpha_k p_k) \leq f(x_k) + c_1 \alpha_k p_k^T \nabla f(x_k) \tag{3.3}$$

and the other one is the curvature condition, of which the most popular version is the strong wolfe curvature condition:

$$|p_k^T \nabla f(x_k + \alpha_k p_k)| \leq |p_k^T \nabla f(x_k)| \tag{3.4}$$

The strong wolfe is a more natural way to see and achieve convergence, but the problem is that it does not work well for the nonsmooth case. This is because near the minimal points, there maybe abrupt changes in curvature, in these cases there is no other option but to relax the curvature condition as long as the sufficient decrease condition is satisfied. The suggested new decrease condition is this.

$$p_k^T \nabla f(x_k + \alpha_k p_k) \geq p_k^T \nabla f(x_k) \tag{3.5}$$

It is noticeable that with this new condition the algorithm does not crash, as opposed to when the hard wolfe condition is used.

Appendix A

Appendix Title Here

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