Mahdi Dodangeh

WORST CASE COMPLEXITY OF DIRECT SEARCH UNDER CONVEXITY

Tese de Programa Inter-Universitário de Doutoramento em Matemática, orientada pelo Professor Luís Nunes Vicente e apresentada ao Departamento de Matemática da Faculdade de Ciências e Tecnologia da Universidade de Coimbra.

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UNIVERSIDADE DE COIMBRA

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Abstract

In this thesis we prove that the broad class of direct-search methods of directional type, based on imposing sufficient decrease to accept new iterates, exhibits the same worst case complexity bound and global rate of the gradient method for the unconstrained minimization of a convex and smooth function without using derivatives.

More precisely, it will be shown that the number of iterations needed to reduce the norm of the gradient of the objective function below a certain threshold is at most proportional to the inverse of the threshold. It will be also shown that the absolute error in the function values decay at a sub-linear rate proportional to the inverse of the iteration counter.

In addition, we prove that the sequences of absolute errors of function values and iterates converge r-linearly in the uniformly/strongly convex case.

A second open problem is solved in this thesis regarding the worst case complexity of direct search for smooth functions. It is proved that the factor consisting of the dimension of the problem squared that appears in the bounds for the worst number of function evaluations is optimal, in the sense that no better power of the problem dimension is attainable.

Resumo

Nesta dissertação, provamos que a abrangente classe de métodos de procura directa do tipo direccional, que tem por base aceitar novas iteradas recorrendo a uma condição de decréscimo suficiente, exibe o mesmo limite superior de complexidade, no pior dos casos, que o método do gradiente para a minimização de uma função convexa e suave sem recurso a derivadas.

Mais precisamente, será demonstrado que o número de iterações necessárias para reduzir a norma do gradiente da função objectivo abaixo de um determinado valor é, no máximo, proporcional ao inverso desse valor. Será também mostrado que o erro absoluto nos valores da função decresce a uma taxa sub-linear, proporcional ao inverso do contador das iterações.

Demonstramos, igualmente, que as sucessões de erros absolutos, no valor da função e nas iteradas, convergem r-linearmente no caso uniformemente/fortemente convexo.

É resolvido ainda um segundo problema em aberto na complexidade no pior dos casos da procura directa para funções suaves. É provado que o factor da dimensão do problema ao quadrado, presente nos limites superiores para o pior número de avaliações da função, é óptimo no sentido em que não é possível alcançar uma melhor potência na dimensão do problema.

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Chapter 1

Introduction

In this thesis we focus on direct-search methods of directional type applied to the minimization of a real-valued, convex, and continuously differentiable objective function f, without constraints,

$$\min_{x \in \mathbb{R}^n} \; f(x). \tag{1.1}$$

In direct-search methods, the objective function is evaluated, at each iteration, at a finite number of points. No derivatives are required. The action of declaring an iteration successful (moving into a point of lower objective function value) or unsuccessful (staying at the same iterate) is based on objective function value comparisons. Some of these methods are directional in the sense of moving along predefined directions along which the objective function will eventually decrease for sufficiently small step sizes ([24], [13, Chapter 9]). Those of simplicial type (see, e.g., [13, Chapter 8]), such as the Nelder-Mead method [27], are not considered here. There are essentially two ways of globalizing direct-search methods (of directional type), meaning making them convergent to stationary points independently of the starting point: (i) by integer lattices, insisting on generating points in grids or meshes (which refine only with the decrease of the step size), or (ii) by imposing a sufficient decrease condition, involving the size of the steps, on the acceptance of new iterates. Although we derive our results for the latter strategy, we recall that both share the essentials of this class of direct-search methods: the directional feature for the displacements, and, as in any other direct-search technique, the fact that decisions in each iteration are taken solely by comparison of objective function values.

The analyzes of global convergence of algorithms can be complemented or refined by deriving worst case complexity (WCC) bounds for the number of iterations or number of function evaluations, an information which becomes valuable in many instances. In terms of the derivation of WCC bounds, Nesterov [28, Page 29] first showed that the steepest descent or gradient method for unconstrained optimization takes at most $\mathcal{O}(\epsilon^{-2})$ iterations (or gradient evaluations) to drive the norm of the gradient of the objective function below $\epsilon \in (0, 1)$. Such a bound has been proved sharp or tight by Cartis, Gould, and Toint [10]. There has been quite an amount of research on WCC bounds for several other classes of algorithms in the non-convex case (see, e.g., [11, 22, 31]).

Derivative-free or zero-order methods have also been recently analyzed with the purpose of establishing their WCC bounds. It has been shown in [38] a WCC bound of $\mathcal{O}(\epsilon^{-2})$ for the number of iterations of direct-search methods (of directional type, when imposing sufficient decrease, and applied to a smooth, possibly non-convex function), which translates to $\mathcal{O}(n^2\epsilon^{-2})$ in terms of the number of function evaluations. Cartis, Gould, and Toint [12] have derived a WCC bound of $\mathcal{O}(n^2\epsilon^{-3/2})$ for their adaptive cubic overestimation algorithm when using finite differences to approximate derivatives. (By a smooth function we always mean that the gradient is Lipschitz continuous.) In the non-smooth case, using smoothing techniques, both Garmanjani and Vicente [20] and Nesterov [30] established a WCC bound of approximately $\mathcal{O}(\epsilon^{-3})$ iterations (and $\mathcal{O}(n^3\epsilon^{-3})$ function evaluations) for their zero-order methods, where the threshold ϵ refers now to the gradient of a smoothed version of the original function. Nesterov [30] random Gaussian approach sees its worst case cost in terms of function evaluations reduced to $\mathcal{O}(n^2\epsilon^{-2})$ in the non-convex smooth case.

Nesterov [28, Section 2.1.5] has also shown that the gradient method achieves an improved WCC bound of $\mathcal{O}(\epsilon^{-1})$ if the objective function is convex. For derivative-free optimization, Nesterov [30] proved that his random Gaussian approach also attains the $\mathcal{O}(\epsilon^{-1})$ in the convex (smooth) case. It is thus natural to ask if one can achieve a similar bound for deterministic zero-order methods, and direct search offers a simple and instructive setting to answer such a question. In this thesis, we will show that direct search can indeed achieve a bound of $\mathcal{O}(\epsilon^{-1})$ under the presence of convexity. The derived WCC bound measures the maximum number of iterations required to find a point where norm of the gradient of the objective function is below ϵ, and, once again, it is proved for directional direct-search methods when a sufficient decrease condition based on the size of the steps is imposed to accept new iterates. As in the non-convex case, the corresponding maximum number of objective function evaluations becomes $\mathcal{O}(n^2\epsilon^{-1})$ (matching Nesterov's random Gaussian derivative-free approach [30]).

In the convex case it is also possible to derive global rates for the absolute error in function values when the solutions set is non-empty. Such an error is known to decay at a sub-linear rate of $1/k$ for the gradient method when the function is convex. The rate is global since no assumption on the starting point is made. We derive in this thesis a similar rate for direct search. As in the gradient method, we also go one step further and show that the absolute error in function values as well as in the iterates converges globally and r-linearly when the function is uniformly/strongly convex. These results have been reported in a paper submitted for publication [18]. Such a rate applies to the whole sequence of iterates and its derivation does not require a monotone non-increase of the step size (as it is the case of a similar r-linear rate derived for direct search globalized using integer lattices by Dolan, Lewis, and Torczon [19]).

Our results are derived for convex functions where the longest distance from the initial level set to the solutions set is finite. Such property is satisfied when the solutions set is bounded (including uniformly/strongly convexity as a particular case), but it is also met in several instances where the solutions sets are unbounded.

We tested direct-search methods numerically in the context of convex functions. In our experiments, the computational expense was always well below the WCC bounds derived in this dissertation, even if the longest distance mentioned above is infinity.

The WCC bounds derived in this dissertation depend on the number of directions used in each iteration. When the objective function is smooth, such a set of directions is typically chosen as a positive spanning set (PSS), since PSSs are known to contain at least one descent direction. In the smooth non-convex case [38], the dependency of the WCC bound $\mathcal{O}(n^2\epsilon^{-2})$ for function evaluations on the usage of PSSs is expressed by the order of n^2. Such a result was obtained using the PSS $D_\oplus$ formed by the coordinate vectors and their negatives. In this dissertation we will prove that indeed $D_\oplus$ is optimal in the sense that it minimizes the order n^2 (on the dimension n) in the WCC bounds for the number of function evaluations.

The structure of the thesis is as follows. In Chapter 2, we start by reviewing basic properties of convex functions and then briefly comment on the worst case complexity (WCC) bounds and global rates of the gradient or steepest descent method. In Chapter 3, we describe the class of direct search under consideration and provide the known results (global asymptotics and WCC bounds) for the smooth and non-convex case. Then, in Chapter 4, we derive the global rate and WCC bound for such direct-search methods in the also smooth but now convex case. The uniformly/strongly convex is covered in Chapter 5. Our numerical experience with direct search in the context of convex functions is reported in Chapter 6. In Chapter 7, we show that the WCC bounds for the number of function evaluations of $\mathcal{O}(n^2\epsilon^{-2})$ or $\mathcal{O}(n^2\epsilon^{-1})$ (respectively, non-convex or convex cases) are optimal in the order of the power of n. In Chapter 8 we draw some concluding remarks based on the specifics of the material covered during the thesis.

We note that the notation $\mathcal{O}(A)$ has meant and will mean a multiple of A, where the constant multiplying A does not depend on the iteration counter k of the method under analysis (thus depending only on f or on algorithmic constants which are set at the initialization of the method). The dependence of A on the dimension n of the problem will be made explicit whenever appropriate. The notation $\mathbb{R}^n$ will denote the n-dimensional Euclidean space. When $n = 1$ we simply write $\mathbb{R}$. The inner product $\langle \cdot, \cdot \rangle$ is also the Euclidean one, i.e., $\langle x, y \rangle = x^\top y$, for $x, y \in \mathbb{R}^n$. The vector norms will be the ℓ_2 ones. The notation $|D|$ refers to the number of elements in the set D.

Chapter 2

WCC of gradient-type methods

In this thesis, we make use of the terms sub-linear rate and linear or r-linear rate of convergence. We briefly describe here what we mean by this terminology. Let $\{x_k\}_{k\geq 0}$ be a sequence in $\mathbb{R}^n$ converging to x_*. The rate of convergence is linear or q-linear (where the q stands for quotient [33, Chapter 9]) when there exists $\theta \in (0,1)$ such that

$$\frac{\|x_{k+1} - x_*\|}{\|x_k - x_*\|} \;\leq\; \theta \quad \text{for all } k \text{ sufficiently large.}$$

The rate is super-linear when this ratio converges to 0 and sub-linear when it converges to 1. The rates are prefixed by an r (like r-linear where the r stands for root [33, Chapter 9]) when $\{x_k\}_{k\geq 0}$ is bounded by another sequence $\{y_k\}_{k\geq 0}$, typically in $\mathbb{R}$, that converges in the normal or q sense. As examples $\{1/\sqrt{k}\}_{k\geq 0}$ and $\{1/k\}_{k\geq 0}$ converge sub-linearly to zero.

In this chapter, we briefly review the worst case complexity of gradient-type methods. First, in order to be precise, let us define the classes of real functions in $\mathbb{R}^n$ that we will address in this dissertation.

2.1 Basic definitions of convexity

To define a convex function there is no need to assume any kind of smoothness, even continuity.

Definition 2.1.1 *A function f is said to be convex in a convex set Ω if for any $x, y \in \Omega$,*

$$f(\lambda x + (1-\lambda)y) \;\leq\; \lambda f(x) + (1-\lambda) f(y), \quad \forall \lambda \in [0,1]. \tag{2.1}$$

If inequality (2.1) always holds strictly unless $x = y$ or $\lambda(1-\lambda) = 0$, we say that the function is strictly convex.

A convex function f is uniformly convex in $\mathbb{R}^n$ (with constant μ) if there exists a constant $\mu > 0$ such that, for any $x, y \in \mathbb{R}^n$ and $\lambda \in [0, 1]$,

$$f(\lambda x + (1-\lambda)y) \;\le\; \lambda f(x) + (1-\lambda)f(y) - \frac{1}{2}\lambda(1-\lambda)\mu\|x-y\|^2. \tag{2.2}$$

We use the notation $\mathcal{F}(\Omega)$ to represent the set of convex functions defined in a convex set Ω and $\mathcal{F}_\mu(\mathbb{R}^n)$ to denote the sub-class of uniformly convex functions.

Note that all the uniformly convex functions are strictly convex. But, there exist strictly convex functions which are not uniformly convex. For instance, the exponential function $\exp(x)$ ($x \in \mathbb{R}$).

Convex functions are interesting in optimization since any local minimizer of a convex function is also a global minimizer (see, e.g., [23, Theorem VI.2.2.1]). Also, a strictly convex function has at most one global minimizer (see, e.g., [23, Proposition VI.6.1.3]). Existence of a minimizer is assured by uniform convexity. In fact, a continuous uniformly convex function has a unique minimizer in a convex and closed set (see, e.g., [25, Corollary 8.4.12]).

The class of continuously differentiable functions (notation $\mathcal{C}^1(\Omega)$, where Ω is an open subset of $\mathbb{R}^n$) is present nearly everywhere in this dissertation. We refer to the sub-class of continuously differentiable convex functions by $\mathcal{F}^1(\Omega)$, where Ω is open and convex. The following theorem characterizes the functions in $\mathcal{F}^1(\Omega)$.

Theorem 2.1.1 *([23, Theorems IV.4.1.1 and IV.4.1.4]) A function f belongs to $\mathcal{F}^1(\Omega)$ if and only if it is continuously differentiable and for all $x, y \in \Omega$,*

$$f(y) \;\ge\; f(x) + \langle \nabla f(x), y - x\rangle, \tag{2.3}$$

or, equivalently,

$$\langle \nabla f(x) - \nabla f(y), x - y\rangle \;\ge\; 0. \tag{2.4}$$

Moreover, the inequalities above hold strictly for distinct x and y if and only if f is strictly convex.

Strongly convex functions (defined below) guarantee a reasonable rate of convergence to a unique minimizer to most first order algorithms.

Definition 2.1.2 *A continuously differentiable function f is said to be strongly convex in $\mathbb{R}^n$ (with constant μ, notation $f \in \mathcal{F}^1_\mu(\mathbb{R}^n)$) if there exists a constant $\mu > 0$ such that, for any $x, y \in \mathbb{R}^n$,*

$$f(x) \;\ge\; f(y) + \langle \nabla f(y), x - y\rangle + \frac{\mu}{2}\|x-y\|^2. \tag{2.5}$$

The inequality above strengthens inequality (2.3) in Theorem 2.1.1. It has an equivalent version that strengthens, in turn, inequality (2.4). When f is continuously differentiable, strong convexity and uniform convexity are equivalent.

Theorem 2.1.2 *([28, Theorem 2.1.9]) A function f belongs to $\mathcal{F}^1_\mu(\mathbb{R}^n)$ if and only if it is continuously differentiable and equation (2.2) holds for any $x, y \in \mathbb{R}^n$ and $\lambda \in [0, 1]$.*

Since our functions will always be assumed continuously differentiable, uniform and strong convexity are thus equivalent notions, and from now on we will talk only about strongly convex functions. Strongly convex functions are continuous and uniformly convex and thus have a unique minimizer in $\mathbb{R}^n$ (see, again, [25, Corollary 8.4.12]).

Theorem 2.1.3 *([28, Theorem 2.1.9]) A function f is in $\mathcal{F}^1_\mu(\mathbb{R}^n)$ if and only if it is continuously differentiable and for $x, y \in \mathbb{R}^n$,*

$$\langle \nabla f(x) - \nabla f(y), x - y \rangle \;\geq\; \mu \|x - y\|^2. \tag{2.6}$$

The following theorem introduces two more inequalities which hold for strongly convex functions.

Theorem 2.1.4 *([28, Theorem 2.1.10]) If $f \in \mathcal{F}^1_\mu(\mathbb{R}^n)$, then for any x and y in $\mathbb{R}^n$ one has*

$$f(x) \;\leq\; f(y) + \langle \nabla f(y), x - y \rangle + \frac{1}{2\mu} \|\nabla f(x) - \nabla f(y)\|^2 \tag{2.7}$$

and

$$\langle \nabla f(x) - \nabla f(y), x - y \rangle \;\leq\; \frac{1}{\mu} \|\nabla f(x) - \nabla f(y)\|^2. \tag{2.8}$$

Proof. The proof is given since the result will be used later in our theory. Given $x \in \mathbb{R}^n$, the function

$$h(y) \;=\; f(y) - \langle \nabla f(x), y \rangle$$

belongs also to $\mathcal{F}^1_\mu(\mathbb{R}^n)$ (see [28, Lemma 2.1.4]). Note that $\nabla h(x) = 0$. Hence the unique minimizer of h is x.

Now, using inequality (2.5) for any $y = v \in \mathbb{R}^n$, we have that

$$\begin{aligned} h(x) = \min_{v \in \mathbb{R}^n} h(v) \;&\geq\; \min_{v \in \mathbb{R}^n} \left\{ h(y) + \langle \nabla h(y), v - y \rangle + \frac{\mu}{2} \|v - y\|^2 \right\} \\ &=\; h(y) - \frac{1}{2\mu} \|\nabla h(y)\|^2, \end{aligned}$$

which is exactly (2.7) (recall the definition of h). By adding two copies of (2.7) with x and y interchanged, we obtain (2.8). □

In Chapter 5, with the help of inequality (2.7), we will derive an r-linear convergence rate for direct search.

Given an open subset Ω of $\mathbb{R}^n$, we denote by $\mathcal{C}^1_\nu(\Omega)$ the set of continuously differentiable functions in Ω with Lipschitz continuous gradient in Ω, where ν is the Lipschitz constant of the gradient. The intersection of $\mathcal{F}^1(\Omega)$ and $\mathcal{C}^1_\nu(\Omega)$ is denoted by $\mathcal{F}^1_\nu(\Omega)$, where Ω is open and convex. The following theorem is important in convex optimization, and it characterizes functions in $\mathcal{F}^1_\nu(\Omega)$.

Theorem 2.1.5 *([28, Theorem 2.1.5]) Let $f \in \mathcal{C}^1(\Omega)$, where Ω is open and convex. Then each of the following conditions, holding for all $x, y \in \Omega$, are equivalent to the fact that $f \in \mathcal{F}^1_\nu(\Omega)$ (in other words to the fact that f is convex with Lipschitz continuous gradient),*

$$0 \;\leq\; f(y) - f(x) - \langle \nabla f(x), y - x\rangle \;\leq\; \frac{\nu}{2}\|x - y\|^2, \tag{2.9}$$

$$f(y) \;\geq\; f(x) + \langle \nabla f(x), y - x\rangle + \frac{1}{2\nu}\|\nabla f(x) - \nabla f(y)\|^2, \tag{2.10}$$

$$\langle \nabla f(x) - \nabla f(y), x - y\rangle \;\geq\; \frac{1}{\nu}\|\nabla f(x) - \nabla f(y)\|^2. \tag{2.11}$$

Proof. The proof is given since the result will be used later in our theory. If we suppose that $f \in \mathcal{F}^1_\nu(\Omega)$ (and thus convex), then for any $x, y \in \Omega$ we have (see Theorem 2.1.1),

$$0 \;\leq\; f(y) - f(x) - \langle \nabla f(x), y - x\rangle.$$

Now, by the integral form of the Mean Value Theorem we obtain

$$\begin{aligned} 0 \;\leq\; f(y) - f(x) - \langle \nabla f(x), y - x\rangle \;&=\; \int_0^1 \langle \nabla f(x + t(y - x)) - \nabla f(x), y - x\rangle \, dt \\ &\leq\; \int_0^1 |\langle \nabla f(x + t(y - x)) - \nabla f(x), y - x\rangle| \, dt \\ &\leq\; \int_0^1 \|\nabla f(x + t(y - x)) - \nabla f(x)\| \|y - x\| \, dt \\ &\leq\; \nu\|y - x\|^2 \int_0^1 t \, dt \;=\; \frac{\nu}{2}\|y - x\|^2, \end{aligned} \tag{2.12}$$

where the last inequality follows from Lipschitz continuity of the gradient of f. So, (2.9) holds for any x, y in Ω when $f \in \mathcal{F}^1_\nu(\Omega)$.

Now, let (2.9) hold for any x, y in Ω. By adding two copies of (2.9) with x and y interchanged, we obtain that

$$\langle \nabla f(x) - \nabla f(y), x - y\rangle \;\leq\; \nu\|x - y\|^2, \quad \forall x, y \in \Omega. \tag{2.13}$$

From Theorem 2.1.1, one knows that f is convex. Given $x \in \Omega$, define

$$h(y) \;=\; f(y) - \langle \nabla f(x), y\rangle, \quad y \in \Omega.$$

It is obvious that h is convex and in $\mathcal{C}^1(\Omega)$. One can then use (2.13) to rederive (2.12) and prove that h also satisfies (2.9). Note that $x_* = x$ is a minimizer of h (see, e.g., [28, Theorem 2.1.1]). Then, by re-writing (2.9) in terms of h for the pair $y, y - 1/\nu\nabla h(y)$, we have

$$\begin{aligned} h(x) &\leq h(y - 1/\nu\nabla h(y)) \\ &\leq h(y) + \langle \nabla h(y), -\frac{1}{\nu}\nabla h(y)\rangle + \frac{\nu}{2}\left\|\frac{1}{\nu}\nabla h(y)\right\|^2 \\ &= h(y) - \frac{1}{2\nu}\|\nabla h(y)\|^2. \end{aligned}$$

Taking into account the definition of h, the above inequality implies

$$\begin{aligned} f(x) - \langle \nabla f(x), x\rangle &= h(x) \\ &\leq f(y) - \langle \nabla f(x), y\rangle - \frac{1}{2\nu}\|\nabla h(y)\|^2 \\ &= f(y) - \langle \nabla f(x), y\rangle - \frac{1}{2\nu}\|\nabla f(y) - \nabla f(x)\|^2, \end{aligned}$$

which is (2.10).

Now, let (2.10) hold for any $x, y \in \Omega$. Then, we have

$$f(y) \geq f(x) + \langle \nabla f(x), y - x\rangle + \frac{1}{2\nu}\|\nabla f(x) - \nabla f(y)\|^2$$

and

$$f(x) \geq f(y) + \langle \nabla f(y), x - y\rangle + \frac{1}{2\nu}\|\nabla f(y) - \nabla f(x)\|^2.$$

By summing up these two inequalities, we obtain

$$f(y) + f(x) \geq f(x) + f(y) + \langle \nabla f(x) - \nabla f(y), y - x\rangle + \frac{1}{\nu}\|\nabla f(x) - \nabla f(y)\|^2,$$

which is equivalent to (2.11).

Finally, due to Theorem 2.1.1, from (2.11) we conclude that f is convex. Using Cauchy-Schwartz, inequality (2.11) implies Lipschitz continuity of the gradient of f. So, (2.11) implies $f \in \mathcal{F}_\nu^1(\Omega)$. The proof is then completed. □

Note that equations (2.10) and (2.11) strengthen equations (2.3) and (2.4) in Theorem 2.1.1, respectively.

The notation $\mathcal{F}_{\nu,\mu}^1(\Omega)$ will denote the intersection of $\mathcal{C}_\nu^1(\Omega)$ and $\mathcal{F}_\mu^1(\Omega)$. For functions in $\mathcal{F}_{\nu,\mu}^1(\Omega)$, we have an inequality stronger than both (2.6) and (2.11) as presented in the following theorem.

Theorem 2.1.6 *([28, Theorem 2.1.12]) Let $f \in \mathcal{F}^1_{\nu,\mu}(\mathbb{R}^n)$. Then for any $x, y \in \mathbb{R}^n$ one has*

$$\langle \nabla f(x) - \nabla f(y), x - y \rangle \ \geq \ \frac{\mu\nu}{\mu + \nu}\|x - y\|^2 + \frac{1}{\mu + \nu}\|\nabla f(x) - \nabla f(y)\|^2. \tag{2.14}$$

Due to the strong convexity of f (Theorem 2.1.3) and the Lipschitz continuity of $\nabla f(x)$, we have

$$\|\nabla f(x) - \nabla f(y)\| \ \geq \ \mu\|x - y\|$$

and

$$\|x - y\| \ \geq \ \nu^{-1}\|\nabla f(x) - \nabla f(y)\|$$

respectively. Hence it is easy to see that (2.14) implies both (2.6) and (2.11).

The last theorem is important for deriving an r-linear convergence rate of gradient-type methods for functions in $\mathcal{F}^1_{\nu,\mu}(\Omega)$.

2.2 Results for non-convex functions

Given a starting point $x_0 \in \mathbb{R}^n$, the gradient or steepest descent method takes the form

$$x_{k+1} = x_k - h_k \nabla f(x_k),$$

where $h_k > 0$ defines the step size. The algorithm can be applied whenever the function f is continuously differentiable, and the well-known fact that $-\nabla f(x_k)$ is a descent direction provides the basis for the convergence properties of the method. The update of the step size h_k is also a crucial point in this class of minimization algorithms. There are improper choices of the step size that make such gradient-type algorithms diverge [32, Chapter 3]. The proper update of the step size is thus central in achieving global convergence (see, e.g., [28, 32]).

For a number of the well-known strategies to update the step size, it is possible to prove that, when $f \in \mathcal{C}^1_\nu(\mathbb{R}^n)$, there is a constant $C = C(\nu) > 0$ such

$$f(x_k) - f(x_{k+1}) \ \geq \ C(\nu)\|\nabla f(x_k)\|^2, \tag{2.15}$$

where $C(\nu)$ is essentially a multiple of $1/\nu$, with ν the Lipschitz constant of the gradient of f, (being the multiple dependent on the parameters involved in the update of the step size; in [28, Page 26], for instance, $C(\nu) = 1/(2\nu)$ for $h_k = 1/\nu$). In such cases, assuming that f is also bounded from below in $\mathbb{R}^n$, one can easily see from (2.15) that the gradient method takes at most $\mathcal{O}(\epsilon^{-2})$ iterations to reduce the gradient below $\epsilon \in (0, 1)$ (see [28, Page 29]), to be more specific

$$\left(\frac{f(x_0) - f_{low}}{C(\nu)}\right)\frac{1}{\epsilon^2}.$$

The constant multiplying ϵ^{-2} depends thus only on ν, on the parameters involved in the update of the step size, and on the lower bound f_{low} for f in

$$L_f(x_0) \;=\; \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}.$$

It is also easy to prove from (2.15) that the gradient decays at a sub-linear rate of $1/\sqrt{k}$.

2.3 Results for convex functions

If, additionally, f is assumed convex, i.e., $f \in \mathcal{F}^1_\nu(\mathbb{R}^n)$, then Nesterov [28, Section 2.1.5] showed that one can achieve a better WCC bound in terms of the negative power of ϵ. First, based on the geometric properties of smooth convex functions (essentially equation (2.10)), he proved, for simplicity using $h_k = 1/\nu$, that the absolute error in function values decays at a sub-linear rate of $1/k$

$$f(x_k) - f_* \;\leq\; \frac{2\nu\|x_0 - x_*\|^2}{k+4}, \tag{2.16}$$

where f_* is the value of the function at a (global) minimizer (see [28, Corollary 2.1.2]), assumed to exist. But then one can easily see, by repeatedly applying (2.15), that

$$\frac{2\nu\|x_0 - x_*\|^2}{k+4} \;\geq\; C(\nu)\sum_{\ell=k}^{2k}\|\nabla f(x_\ell)\|^2.$$

The gradient method is then proved to only take at most $\mathcal{O}(\epsilon^{-1})$ iterations to achieve a threshold of ϵ on the norm of the gradient. The constant multiplying ϵ^{-1} is essentially a multiple of $\nu\|x_0 - x_*\|$.

Note that assuming $h_k = 1/\nu$ was just for convenience. This result can be extended to the general case of $0 < h_k \leq 2/\nu$ (see [28, Theorem 2.1.14]). In practice we do not have any knowledge about the Lipschitz constant of the gradient, and hence the constant step size strategy in gradient-type methods is not practical. A workaround is to approximate the Lipschitz constant by a back-tracking procedure in the course of algorithm and improve the approximation at each iteration. It is possible to prove that gradient-type methods with back-tracking strategies comply with the same global rate and WCC bound (see, e.g., [4, 29]).

2.4 Results for strongly convex functions

For an objective function $f \in \mathcal{F}^1_{\mu,\nu}$, Nesterov [28, Theorem 2.1.14] shows that the gradient-type method with constant step size $h_k = h \leq 2/(\mu+\nu)$ generates a sequence $\{x_k\}$ such that

$$\|x_k - x_*\|^2 \;\leq\; \left(1 - \frac{2h\mu\nu}{\mu+\nu}\right)^k \|x_0 - x_*\|^2,$$

where x_* is the minimizer of function f.

The proof of above inequality is based on $\nabla f(x_*) = 0$ and inequality (2.14). In fact,

$$\begin{aligned}
\|x_{k+1} - x_*\|^2 &= \|x_k - x_* - h\nabla f(x_k)\|^2 \\
&= \|x_k - x_*\|^2 - 2h\langle \nabla f(x_k), x_k - x_*\rangle + h^2\|\nabla f(x_k)\|^2 \\
&\le \|x_k - x_*\|^2 - \frac{2h\mu\nu}{\mu+\nu}\|x_k - x_*\|^2 - \frac{2h}{\mu+\nu}\|\nabla f(x_k)\|^2 + h^2\|\nabla f(x_k)\|^2 \\
&= \left(1 - \frac{2h\mu\nu}{\mu+\nu}\right)\|x_k - x_*\|^2 + h\left(h - \frac{2}{\mu+\nu}\right)\|\nabla f(x_k)\|^2 \\
&\le \left(1 - \frac{2h\mu\nu}{\mu+\nu}\right)\|x_k - x_*\|^2,
\end{aligned}$$

where the first inequality follows from inequality (2.14) and $\nabla f(x_*) = 0$, and the last one is due to the assumption that $h \le 2/(\mu + \nu)$.

By choosing the maximum available step size $h = 2/(\mu + \nu)$ at each iteration, which is the greediest, we obtain the following global r-linear convergence rate

$$\|x_k - x_*\| \;\le\; \left(\frac{Q_f - 1}{Q_f + 1}\right)^k \|x_0 - x_*\|.$$

where $Q_f = \nu/\mu$. Then, by using (2.9),

$$f(x_k) - f_* \;\le\; \frac{\nu}{2}\left(\frac{Q_f - 1}{Q_f + 1}\right)^{2k} \|x_0 - x_*\|^2.$$

For gradient-type methods with a back-tracking procedure, it is also possible to establish an r-linear convergence rate when the objective function is strongly convex (see, e.g., [29]).

One could also choose the step size to be the global minimizer of $g(h) = f(x_k - h\nabla f(x_k))$, $h > 0$. The procedure to find this step size is called exact line search (for more details see [32, Chapter 3]).

Luenberger [26] analyzes the global rate of the gradient-type method with exact line search when the objective function is quadratic. He also shows an r-linear rate for the algorithm in this case. To give an idea, let f be the following quadratic function in $\mathbb{R}^n$,

$$f(x) \;=\; \frac{1}{2}\langle x, Qx\rangle - \langle b, x\rangle, \tag{2.17}$$

where Q is a symmetric and positive definite matrix. Then, the gradient at the point x is $\nabla f(x) = Qx - b$. Therefore, the unique minimizer of f is $x_* = Q^{-1}b$.

In order to find the exact minimizer of f at each iteration of gradient-type methods, we need to solve exactly the following one-dimensional minimization problem

$$\min_{h>0} g(h) = f(x_k - h\nabla f(x_k)),$$

which in the quadratic case is,

$$\min_{h>0}\ g(h) \ = \ \min_{h>0}\left\{\frac{1}{2}\big\langle x_k - h\nabla f(x_k), Q(x_k - h\nabla f(x_k))\big\rangle \ + \ \big\langle b, x_k - h\nabla f(x_k)\big\rangle\right\}.$$

By differentiating function g respect to h, and setting the derivative to zero, we obtain

$$h_k \ = \ \frac{\big\langle \nabla f(x_k), \nabla f(x_k)\big\rangle}{\big\langle \nabla f(x_k), Q\nabla f(x_k)\big\rangle}.$$

So, the k-th iteration will be

$$x_{k+1} \ = \ x_k - h_k\nabla f(x_k). \tag{2.18}$$

Now, since $Qx_* = b$, we have

$$\begin{aligned}
\frac{1}{2}\big\langle x - x_*, Q(x - x_*)\big\rangle \ &= \ \frac{1}{2}\big\langle x, Qx\big\rangle - \big\langle x_*, Qx\big\rangle + \frac{1}{2}\big\langle x_*, Qx_*\big\rangle \\
&= \ \frac{1}{2}\big\langle x, Qx\big\rangle - \big\langle b, x\big\rangle + \frac{1}{2}\big\langle x_*, Qx_*\big\rangle \\
&= \ f(x) - \Big(\frac{1}{2}\big\langle x_*, Qx_*\big\rangle - \big\langle b, x_*\big\rangle\Big) \\
&= \ f(x) - f(x_*).
\end{aligned}$$

Then, the difference between the current objective value and the optimal value is equal to the distance between x_k and x_* in the Q-norm, which is defined by $\|y\|_Q^2 = \big\langle y, Qy\big\rangle$.

Finally, due to fact that $\nabla f(x_k) = Q(x_k - x_*)$, we have

$$\begin{aligned}
\|x_{k+1} - x_*\|_Q^2 \ &= \ \|x_k - x_* - h_k\nabla f(x_k)\|_Q^2 \\
&= \ \|x_k - x_*\|_Q^2 - 2h_k\big\langle x_k - x_*, Q\nabla f(x_k)\big\rangle + h_k^2\big\langle \nabla f(x_k), Q\nabla f(x_k)\big\rangle \\
&= \ \|x_k - x_*\|_Q^2 - 2h_k\big\langle \nabla f(x_k), \nabla f(x_k)\big\rangle + h_k^2\big\langle \nabla f(x_k), Q\nabla f(x_k)\big\rangle \\
&= \ \|x_k - x_*\|_Q^2 - \frac{\Big[\big\langle \nabla f(x_k), \nabla f(x_k)\big\rangle\Big]^2}{\big\langle \nabla f(x_k), Q\nabla f(x_k)\big\rangle} \\
&= \ \left(1 - \frac{\Big[\big\langle \nabla f(x_k), \nabla f(x_k)\big\rangle\Big]^2}{\big\langle \nabla f(x_k), Q\nabla f(x_k)\big\rangle\big\langle \nabla f(x_k), Q^{-1}\nabla f(x_k)\big\rangle}\right)\|x_k - x_*\|_Q^2,
\end{aligned}$$

where the last equality follows from

$$\begin{aligned} \|x_k - x_*\|_Q^2 &= \big\langle x_k - x_*, Q(x_k - x_*)\big\rangle \\ &= \big\langle x_k - x_*, \nabla f(x_k)\big\rangle \\ &= \big\langle \nabla f(x_k), Q^{-1}\nabla f(x_k)\big\rangle. \end{aligned}$$

To conclude the argument, we need to recall a well-known fact about symmetric positive definite matrices.

Lemma 2.4.1 *(Kantorovich Inequality [26]) Let Q be a symmetric positive definite matrix. Then for any non-zero vector x, we have*

$$\frac{\Big(\big\langle x, x\big\rangle\Big)^2}{\big\langle x, Qx\big\rangle\big\langle x, Q^{-1}x\big\rangle} \;\geq\; \frac{4\lambda_1\lambda_n}{(\lambda_1+\lambda_n)^2}, \tag{2.19}$$

where λ_1 and λ_n are the smallest and largest eigenvalues of Q, respectively.

Now one can see that the following theorem holds.

Theorem 2.4.1 *([26]) Applied to the strongly convex quadratic function (2.17), the gradient-type method with exact line search (2.18) generates a sequence $\{x_k\}_{k\geq 0}$ of iterates such that*

$$\|x_k - x_*\|_Q \;\leq\; \Big(\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}\Big)^k \|x_0 - x_*\|_Q,$$

where λ_1 and λ_n are the smallest and largest eigenvalues of Q, respectively.

Chapter 3

WCC of direct search

In direct-search methods, the objective function is evaluated, at each iteration, at a finite number of points. No derivatives or approximation thereof are required. As we mentioned before, in this dissertation we study direct-search methods of directional type [13]. Those of simplicial type (see, e.g., [13, Chapter 8]), such as the Nelder-Mead method [27], are not considered here.

In this chapter, we will start by reviewing some basic concepts of (directional) direct-search methods for smooth functions. Then we will describe an algorithm based on imposing the sufficient decrease condition. We will present the global convergence properties of this algorithm when applied to smooth functions as well as an analysis of worst case complexity. More detailed explanations can be found in [13, Chapters 2 and 7] and in [38].

3.1 Basic definitions and the algorithm

At each iteration, direct search considers a set of directions which in the smooth case are required to include a descent one. A direction d is descent at a point x if there exists $\overline{\alpha} > 0$ such that

$$f(x + \alpha d) \; < \; f(x), \quad \forall \alpha \in (0, \overline{\alpha}].$$

When f is continuously differentiable at a point x, any direction which makes an acute angle with the negative gradient $-\nabla f(x)$ at x is a descent direction [32]. So, it is sufficient that at least one of the directions used at each iteration makes an acute angle with $-\nabla f(x)$.

To fulfill this condition we recall the concept of a positive spanning set (PSS) introduced by Davis [17]. By positive span or convex cone of a set of directions we mean the set of all finite linear combinations of the directions with non-negative coefficients.

Definition 3.1.1 *A positive spanning set in $\mathbb{R}^n$ is a set of vectors whose positive span is $\mathbb{R}^n$.*

The minimum number of directions to form a PSS in $\mathbb{R}^n$ is $n+1$ (see [17, Theorem 3.7]).

It is then well known (see [17, Theorem 3.3] or [13, Theorem 2.3]) that at least one of the directions in a PSS makes an acute angle with $-\nabla f(x)$.

To describe PSSs further we recall the definition of positive basis (PB). We say that D is positively dependent if there exist a direction in D which is in the positive span of other directions in D; otherwise we say that D is positively independent. A positive basis (PB) in $\mathbb{R}^n$ is a PSS which is positively independent.

It is also known that the minimum number of directions to form a PB in $\mathbb{R}^n$ is $n+1$ (see [17, Theorem 3.8]), and the maximum is $2n$ (see [1] and [13]). PBs with $n+1$ and $2n$ directions are called minimal PBs and maximal PBs, respectively.

If D is a PB and W is an invertible matrix, then WD is also a PB (see [13, Theorem 2.4] and [36]). It is easy to prove that $D = [I \; -\mathbf{1}_n]$ and $D_\oplus = [I \; -I]$ are minimal and maximal PBs, respectively, where I is the identity matrix and $\mathbf{1}_n = (1, \ldots, 1)^\top \in \mathbb{R}^n$. Thus $[W \; -W\mathbf{1}_n]$ and $[W \; -W]$ are also minimal and maximal PBs, respectively, if W is invertible.

The direct-search method under analysis is described in Algorithm 3.1.1, following the presentation in [13, Chapter 7]. The directional feature is presented in the poll step, where points of the form $x_k + \alpha_k d$, for directions d belonging to the PSS D_k, are tested for sufficient decrease. For this purpose, following the terminology in [24],

$$\rho : (0, \infty) \to (0, \infty)$$

will represent a forcing function, i.e., a non-decreasing (typically continuous) function satisfying

$$\lim_{t \downarrow 0} \frac{\rho(t)}{t} = 0.$$

Typical examples of forcing functions are $\rho(t) = \mathcal{C}t^p$, for $p > 1$ and $\mathcal{C} > 0$.

The poll step is successful if the value of the objective function is sufficiently decreased relatively to the step size α_k, in the sense of

$$f(x_k + \alpha_k d_k) \; < \; f(x_k) - \rho(\alpha_k),$$

in which case the step size is possibly increased.

The algorithm opportunistically moves to the first of such points found. Failure in doing so defines an unsuccessful iteration, and the step size is decreased by a factor strictly less than 1 that changes between two bounds which need to be fixed during the course of the iterations.

The search step is purposely left open since it does not interfere in any of the convergence properties of the algorithm, and it is solely used to improve the practical performance of the overall algorithm. For the purposes of counting function evaluations, we assume throughout this thesis that the search step, whenever applied, does not exceed the maximum number of function evaluations taken by the poll step.

Algorithm 3.1.1 (Directional direct-search method)

Initialization

Choose x_0 with $f(x_0) < +\infty$, $\alpha_0 > 0$, $0 < \beta_1 \leq \beta_2 < 1$, and $\gamma \geq 1$.

For $k = 0, 1, 2, \ldots$

1. **Search step:** Try to compute a point with $f(x) < f(x_k) - \rho(\alpha_k)$ by evaluating the function f at a finite number of points. If such a point is found, then set $x_{k+1} = x$, declare the iteration and the search step successful, and skip the poll step.
2. **Poll step:** Choose a positive spanning set D_k. Order the set of poll points $P_k = \{x_k + \alpha_k d : d \in D_k\}$. Start evaluating f at the poll points following the chosen order. If a poll point $x_k + \alpha_k d_k$ is found such that $f(x_k + \alpha_k d_k) < f(x_k) - \rho(\alpha_k)$, then stop polling, set $x_{k+1} = x_k + \alpha_k d_k$, and declare the iteration and the poll step successful. Otherwise, declare the iteration (and the poll step) unsuccessful and set $x_{k+1} = x_k$.
3. **Mesh parameter update:** If the iteration was successful, then maintain or increase the step size parameter: $\alpha_{k+1} \in [\alpha_k, \gamma\alpha_k]$. Otherwise, decrease the step size parameter: $\alpha_{k+1} \in [\beta_1\alpha_k, \beta_2\alpha_k]$.

When the objective function is bounded from below one can prove that there exists a subsequence of unsuccessful iterates driving the step size parameter to zero (see [24] or [13, Theorems 7.1 and 7.11 and Corollary 7.2]).

Lemma 3.1.1 *Let f be bounded from below on $L_f(x_0) = \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$. Then Algorithm 3.1.1 generates an infinite subsequence K of unsuccessful iterates for which* $\lim_{k \in K} \alpha_k = 0$.

Note that when the function f is convex and has a minimizer, it is necessarily bounded from below (see, e.g., [28, Theorem 2.1.1]).

To continue towards the global properties (asymptotic convergence and rates) for this class of direct search, one must look at the key feature of a positive spanning set, its cosine measure [24].

Definition 3.1.2 *Given a positive spanning set D (with non-zero vectors), its cosine measure is given by*

$$\mathrm{cm}(D) \;=\; \min_{0\neq v\in\mathbb{R}^n}\max_{d\in D}\frac{\langle v,d\rangle}{\|v\|\|d\|}.$$

Due to Definitions 3.1.1 and 3.1.2, any PSS with non-zero vectors has a positive cosine measure. There are a few PSSs with known cosine measures. Such instances are $D_\oplus = [I\ -I]$ ([36, Lemma 6.2]) and the minimal PB with uniform angles (among all directions), say U ([13, Corollary 2.6 and Exercise 2.7.7]),

$$\mathrm{cm}(D_\oplus) \;=\; \frac{1}{\sqrt{n}}, \qquad \mathrm{cm}(U) \;=\; \frac{1}{n}.$$

Given a non-zero vector $v\in\mathbb{R}^n$ and a PSS D (always assumed here with a finite number of directions), there exists a direction $\bar{d}$ in D such that

$$\max_{d\in D}\frac{\langle v,d\rangle}{\|v\|\|d\|} \;=\; \frac{\langle v,\bar{d}\rangle}{\|v\|\|\bar{d}\|}.$$

This fact implies that for any non-zero vector, in particular the negative gradient at a given point, there is at least one direction in D making an acute angle with it, since

$$0 \;<\; \mathrm{cm}(D)\|\nabla f(x)\|\|\bar{d}\| \;\leq\; -\langle\nabla f(x),\bar{d}\rangle.$$

Such a property enables us to derive that the norm of the gradient is of the order of the step size when an unsuccessful iteration occurs [19, 24] (see also [13, Theorem 2.4 and Equation (7.14)]).

Theorem 3.1.1 *([19, 24]) Let D_k be a positive spanning set and $\alpha_k > 0$ be given. Assume that ∇f is Lipschitz continuous (with constant $\nu > 0$) in an open set containing all the poll points in P_k. If $f(x_k) \leq f(x_k+\alpha_k d)+\rho(\alpha_k)$, for all $d\in D_k$, i.e., the iteration k is unsuccessful, then*

$$\|\nabla f(x_k)\| \;\leq\; \mathrm{cm}(D_k)^{-1}\left(\frac{\nu}{2}\alpha_k\max_{d\in D_k}\|d\| + \frac{\rho(\alpha_k)}{\alpha_k\min\limits_{d\in D_k}\|d\|}\right). \tag{3.1}$$

Proof. The proof is given for completion since we will use this result later in our theory. Given $0\neq v\in\mathbb{R}^n$, as we said before the theorem, there exists a $\bar{d}_k$ in D_k such that

$$\max_{d\in D_k}\frac{\langle v,d\rangle}{\|v\|\|d\|} \;=\; \frac{\langle v,\bar{d}_k\rangle}{\|v\|\|\bar{d}_k\|}.$$

As we also said before, by setting v equal to the negative gradient of f at x_k, the vector $\bar{d}_k \in D_k$ satisfies

$$\mathrm{cm}(D_k)\|\nabla f(x_k)\|\|\bar{d}_k\| \;\leq\; -\big\langle \nabla f(x_k), \bar{d}_k \big\rangle. \tag{3.2}$$

On the other hand, since $f(x_k) \leq f(x_k + \alpha_k d) + \rho(\alpha_k)$, for all $d \in D_k$, from the integral form of the Mean Value Theorem we obtain that

$$0 \;\leq\; f(x_k + \alpha_k \bar{d}_k) - f(x_k) + \rho(\alpha_k) \;=\; \int_0^1 \langle \nabla f(x + t\alpha_k \bar{d}_k), \alpha_k \bar{d}_k \rangle \, dt + \rho(\alpha_k).$$

By multiplying inequality (3.2) by α_k and adding it to the above inequality, we arrive at

$$\begin{aligned} \mathrm{cm}(D_k)\|\nabla f(x_k)\|\|\bar{d}_k\|\alpha_k \;&\leq\; \int_0^1 \langle \nabla f(x + t\alpha_k \bar{d}_k) - \nabla f(x_k), \alpha_k \bar{d}_k \rangle \, dt + \rho(\alpha_k) \\ &\leq\; \int_0^1 \|\nabla f(x + t\alpha_k \bar{d}_k) - \nabla f(x_k)\| \|\alpha_k \bar{d}_k\| \, dt + \rho(\alpha_k) \\ &\leq\; \alpha_k^2 \nu \|\bar{d}_k\|^2 \int_0^1 t \, dt + \rho(\alpha_k) \;=\; \frac{1}{2}\alpha_k^2 \nu \|\bar{d}_k\|^2 + \rho(\alpha_k), \end{aligned}$$

where the second inequality follows from the Cauchy-Schwartz inequality and the last inequality follows from the Lipschitz continuity of the gradient. Thus, the following upper bound holds

$$\|\nabla f(x_k)\| \;\leq\; \mathrm{cm}(D_k)^{-1} \left(\frac{\nu}{2}\alpha_k \|\bar{d}_k\| + \frac{\rho(\alpha_k)}{\alpha_k \|\bar{d}_k\|} \right).$$

Now, since $\min_{d \in D_k} \|d\| \leq \|\bar{d}_k\| \leq \max_{d \in D_k} \|d\|$, the proof is completed. $\square$

It becomes then obvious that one needs to avoid degenerate PSSs.

Assumption 3.1.1 *All positive spanning sets D_k used for polling (for all k) must satisfy $\mathrm{cm}(D_k) \geq \mathrm{cm}_{\min}$ and $d_{\min} \leq \|d\| \leq d_{max}$ for all $d \in D_k$ (where $\mathrm{cm}_{\min} > 0$ and $0 < d_{\min} \leq d_{\max}$ are constants). The PSSs D_k are all finite and there exists $d_\# > 0$ so that $|D_k| \leq d_\#$ for all k.*

A first global asymptotic result is then easily obtained by combining Lemma 3.1.1 and Theorem 3.1.1 (under Assumption 3.1.1), and assures the convergence to zero of the gradient at a subsequence of unsuccessful iterates. Asymptotic global convergence is not, however, a topic of this thesis.

3.2 WCC of direct search

As promised before, we will briefly review the recent development in the study of the worst case complexity of direct search for smooth possibly non-convex functions. We know that each iteration of Algorithm 3.1.1 is either successful or unsuccessful. Therefore, in order to derive an upper bound on the total number of iterations, it is enough to derive separately upper bounds on the numbers of successful and unsuccessful iterations.

In this manner, it was presented in [38, Theorem 3.1] an upper bound on the number of successful iterations after the first unsuccessful iteration. It was also showed that the number of unsuccessful iterations is proportional to that of successful iterations [38, Theorem 3.2]. In the last part of the derivation in [38] it is derived an upper bound on the number of successful iterations to achieve an unsuccessful iteration. It was then concluded the following result.

Theorem 3.2.1 *([38]) Consider the application of Algorithm 3.1.1 when $\rho(\alpha) = \mathcal{C}\alpha^p$, $p > 1$, $\mathcal{C} > 0$, and D_k satisfies Assumption 3.1.1. Let f be bounded from below in $L_f(x_0)$ and $f \in \mathcal{C}^1_\nu(\Omega)$ where Ω is an open set containing $L_f(x_0)$.*

Under these assumptions, to reduce the gradient below $\epsilon \in (0,1)$, Algorithm 3.1.1 takes at most

$$\lceil \eta_1 \epsilon^{-\hat{p}} + \eta_2 \rceil$$

iterations, and at most

$$d_\# \lceil \eta_1 \epsilon^{-\hat{p}} + \eta_2 \rceil$$

function evaluations, where $\hat{p} = p/\min(1, p-1)$,

$$\begin{aligned}
\eta_1 &= (1 - \log_{\beta_2}(\gamma)) \frac{f(x_{k_0}) - f_{low}}{C\beta_1^p L_1^p} - \log_{\beta_2}(\exp(1)), \\
\eta_2 &= \log_{\beta_2}\Big(\frac{\beta_1 L_1 \exp(1)}{\alpha_{k_0}}\Big) + \frac{f(x_0) - f_{low}}{C\alpha_0^p}, \\
L_1 &= \min\Big(1, L_2^{-\frac{1}{\min(1,p-1)}}\Big), \quad \textit{and} \ \ L_2 = \mathrm{cm}_{\min}^{-1}(\nu d_{\max}/2 + d_{\min}^{-1} C).
\end{aligned}$$

One can easily see that $p = 2$ is the optimal choice in the power $\epsilon^{-\hat{p}}$. When $p = 2$, the constant η_1 becomes

$$\eta_1 \; = \; (1 - \log_{\beta_2}(\gamma)) \frac{f(x_{k_0}) - f_{low}}{C\beta_1^2 \min(1, \mathrm{cm}_{\min}^2 (\nu d_{\max}/2 + d_{\min}^{-1} C)^{-2})} - \log_{\beta_2}(\exp(1)).$$

In this case, one sees that the maximum number of iterations is $\mathcal{O}(\mathrm{cm}_{\min}^{-2}\, \epsilon^{-2})$ and the maximum number of function evaluations is $\mathcal{O}(d_\#\, \mathrm{cm}_{\min}^{-2}\, \epsilon^{-2})$. In [38] it was suggested to use $D_\oplus$ at each iteration, which, from $\mathrm{cm}(D_\oplus) = 1/\sqrt{n}$ and $|D_\oplus| = 2n$, implies an $\mathcal{O}(n^2\epsilon^{-2})$ for the

Model:	Unconstrained minimization $f \in \mathcal{C}^1_\nu(\mathbb{R}^n)$ f bounded below
Oracle:	Zero order oracle (evaluation of f)
ϵ-solution:	$f(x_*^{appr}) \leq f(x_0), \|\nabla f(x_*^{appr})\| \leq \epsilon$

Table 3.1: Summary of an unconstrained problem class for zero order algorithms. In the table, $\nu > 0$ is the Lipschitz constant of the gradient of the function, x_*^{appr} is the approximated solution, and x_0 is the starting point given to the method.

number of function evaluations. In Chapter 7 we will show that this upper bound is optimal with respect to the order of the power of n.

As mentioned in [38], and following what Nesterov [28, Page 29] states for first order oracles, it is then possible to ensure an upper complexity bound for the problem class given in Table 3.1, where one can only evaluate the objective function f and not its derivatives and where f is assumed smooth. The WCC bound described in this section says thus that the number of calls of the oracle is $\mathcal{O}(n^2\epsilon^{-2})$, and thus it establishes an upper complexity bound for the problem class of Table 3.1. When we later consider convex and strongly convex functions, similar upper complexity bounds can be derived for the corresponding problem classes.

Chapter 4

WCC of direct search for convex functions

In the previous chapter we reviewed direct-search methods of directional type for smooth functions and their global asymptotic convergence and worst case complexity properties. In this chapter, we will analyze the WCC of direct search for a broad class of convex functions.

4.1 Assumption on the step size

How the step size α_k is updated impacts in several ways the WCC bounds given in Chapter 3 for Algorithm 3.1.1. In fact, the choice of $\mathcal{C}$ in the forcing function and the choice of the parameters β_1, β_2, and γ in the step size updating formulas influence the constant in the bound (3.1). Increasing $\mathcal{C}$, for instance, will decrease the number of successful iterations [38, Theorem 3.1], possibly leading to more unnecessary unsuccessful iterations and consequently more unnecessary function evaluations.

Increasing the value of the expansion factor $\gamma \geq 1$ will increase the maximum number of unsuccessful iterations compared to the number of successful ones (see Theorem 3.2.1), again possibly leading to more unnecessary unsuccessful iterations and consequently more unnecessary function evaluations. Setting $\gamma = 1$ leads to an optimal choice in this respect. One practical strategy to accommodate $\gamma > 1$ is by considering an upper bound for the step size itself.

Assumption 4.1.1 *There is a positive constant M such that $\alpha_k \leq M$ for $\forall k \geq 0$.*

Under this assumption Theorem 3.1.1 simplifies to the following:

Corollary 4.1.1 *Consider $\rho(\alpha_k) = \mathcal{C}\alpha_k^p$, $p > 1$, $\mathcal{C} > 0$. Under the assumptions of Theorem 3.1.1 and Assumptions 3.1.1 and 4.1.1, if $f(x_k) \leq f(x_k + \alpha_k d) + \rho(\alpha_k)$, for all $d \in D_k$,* *i.e., the iteration k is unsuccessful, then*

$$\|\nabla f(x_k)\| \;\leq\; \mathrm{cm}_{\min}^{-1} \frac{\frac{\nu}{2} d_{\max} M + \mathcal{C} d_{\min}^{-1} M^{p-1}}{M^{\min(1,p-1)}} {\alpha_k}^{\min(1,p-1)}. \tag{4.1}$$

The step size upper bound M will appear thus in the upper bound for the gradient in unsuccessful iterations. When $p = 2$, the upper bound on the gradient does not depends on M,

$$\|\nabla f(x_k)\| \;\leq\; \mathrm{cm}_{\min}^{-1} \left(\frac{\nu}{2} d_{\max} + \mathcal{C} d_{\min}^{-1}\right) \alpha_k.$$

The analysis of worst case complexity for the convex case when $p \neq 2$ (the non-optimal case) will, however, depend on the upper bound M for the step size.

4.2 Assumption on the function

We will derive a global rate and a WCC bound when the objective function is smooth and convex under the following additional assumption.

Assumption 4.2.1 *The solutions set $X_*^f = \{x_* \in \mathbb{R}^n : x_* \text{ is a minimizer of } f\}$ for problem (1.1) is non-empty. The level set $L_f(x) = \{y \in \mathbb{R}^n : f(y) \leq f(x)\}$ is bounded for some x or, if that is not the case, $\sup_{y \in L_f(x_0)} \mathrm{dist}(y, X_*^f)$ is still finite.*

If $L_f(x_0)$ is bounded, then $\sup_{y \in L_f(x_0)} \mathrm{dist}(y, X_*^f)$ is trivially finite.

Furthermore, it is known that for a (proper and closed or semi-continuous) convex function (see [34, Corollary 8.7.1]) that if $\{x \in \mathbb{R}^n : f(x) \leq \alpha\}$ is non-empty and bounded for some α, then it is bounded for all α. In particular, since we assume that X_*^f is non-empty, $X_*^f = L_f(x_*)$ for some x_*, and if X_*^f is bounded so is $L_f(x_0)$. Moreover, a (finite, thus continuous) strongly convex function in $\mathbb{R}^n$ has a unique minimizer x_*, which then makes X_*^f non-empty and bounded.

In conclusion, and generally speaking, strong convexity of f and boundedness of either X_*^f or $L_f(x_0)$ fulfill the above assumption and make $\sup_{y \in L_f(x_0)} \mathrm{dist}(y, X_*^f)$ finite. For what comes next, let

$$R \;=\; \sup_{y \in L_f(x_0)} \mathrm{dist}(y, X_*^f).$$

Note that there are convex functions f such that $\sup_{y \in L_f(x_0)} \mathrm{dist}(y, X_*^f)$ is finite but neither f is strongly convex nor $L_f(x)$ is bounded for any x, being such an instance the two-dimensional function $f(x, y) = y^2$.

There are however some rare pathological instances where Assumption 4.2.1 does not hold. An example is the following two-dimensional convex function

$$f(x,y) \;=\; \sqrt{x^2+y^2}-x.$$

The minimum of f is equal to zero and the solutions set is $X_*^f = \{(x,0) : x \geq 0\}$. Let $\varsigma = f(x_0,y_0) > 0$ be given for some (x_0,y_0). Then

$$f^{-1}(\{\varsigma\}) \;=\; \{z \in \mathbb{R}^2 : f(z) = \varsigma\} \;=\; \{((t^2-\varsigma^2)/2\varsigma, t)\}_{t\in\mathbb{R}}.$$

Thus, for $z = ((t^2-\varsigma^2)/2\varsigma, t) \in f^{-1}(\{\varsigma\})$, one has $\mathrm{dist}(z, X_*^f) \geq |t|$, which implies

$$\sup_{z\in L_f(x_0,y_0)} \mathrm{dist}(z,X_*^f) \;\geq\; \sup_{z\in f^{-1}(\{\varsigma\})} \mathrm{dist}(z,X_*^f) \;\geq\; \sup_{t\in\mathbb{R}} |t| \;=\; +\infty.$$

Notice that this function is not continuously differentiable at the origin but an alternative, smoothed version (by squaring it) could be instead considered.

Note also that assuming finiteness of the longest distance from the initial level set to the solutions set is unnecessary in the gradient method since it can be proved that for a constant step size smaller than $2/\nu$ the iterates satisfy $\|x_k - x_*\| \leq \|x_0 - x_*\|$ (see Nesterov [28, Theorem 2.1.13]). As we mentioned before, in the context of gradient-type methods, the constant step size is not practical and the Lipschitz constant has to be approximated by a back-tracking procedure in the course of algorithm. It is possible to prove that gradient-type methods with back-tracking strategies generate iterations such that the first iterate has the largest distance to the solutions set (see, e.g., [4, 29]). The lack of knowledge of the gradient makes the control of the longest distance to the solutions set harder in direct search.

To avoid repeating the several assumptions in the statements of the results of this chapter we will combine them in the following one.

Assumption 4.2.2 *Consider the application of Algorithm 3.1.1 when $\rho(t) = \mathcal{C}\, t^p$, $p > 1$, $\mathcal{C} > 0$, and D_k satisfies Assumption 3.1.1. Let $f \in \mathcal{F}_\nu^1(\Omega)$, where Ω is an open and convex set containing $L_f(x_0)$. Let Assumption 4.1.1 (when $p \neq 2$) and Assumption 4.2.1 also hold.*

We will make extensive use of the sets $\mathcal{S}(k_0,j)$ and $\mathcal{U}(k_0,j)$ to represent the indices of successful and unsuccessful iterations, respectively, between k_0 (including it) and j (excluding it).

4.3 Global rate on function values

We will start by measuring the decrease obtained in the objective function until a given iteration as a function of the number of successful iterations occurred until then. Recall that $f_* = f(x_*)$ for some $x_* \in X_*^f$ and $\hat{p} = p/\min(1, p-1) \geq 2$ for $p > 1$.

Lemma 4.3.1 *Let Assumptions 4.2.2 hold. Let k_0 be the index of the first unsuccessful iteration (which must exist from Lemma 3.1.1). Then Algorithm 3.1.1 generates a sequence $\{x_k\}_{k\geq k_0}$ such that*

$$(f(x_k) - f_*)^{\hat{p}-1} \; < \; \frac{R^{\hat{p}}}{\omega|\mathcal{S}(k_0,k)|}, \tag{4.2}$$

where

$$\omega \; = \; \omega_g^{\hat{p}}\beta_1^p\mathcal{C}, \quad \omega_g \; = \; \frac{2\,\mathrm{cm}_{\min}\,M^{\min(1,p-1)}}{\nu d_{\max}M + 2\mathcal{C}d_{\min}^{-1}M^{p-1}}, \tag{4.3}$$

and $|\mathcal{S}(k_0,k)|$ is the number of successful iterations between k_0 (including it) and k.

Proof. Let $\mathcal{U}(k_0,k) = \{k_i\}_{i=0}^m$ represent the set of unsuccessful iterations which occur between iteration k_0, inclusively, and iteration k. One has $|\mathcal{S}(k_0,k)| = k - k_0 - m - 1$.

Since all iterations between k_m and k are successful and k_m is unsuccessful, we have that

$$\begin{aligned} f(x_k) \; &< \; f(x_{k-1}) - \mathcal{C}\alpha_{k-1}^p \\ &\;\;\vdots \\ &< \; f(x_{k_m+1}) - \mathcal{C}\sum_{j=k_m+1}^{k-1}\alpha_j^p \\ &\leq \; f(x_{k_m+1}) - \mathcal{C}(k-k_m-1)\alpha_{k_m+1}^p \\ &\leq \; f(x_{k_m}) - \beta_1^p\mathcal{C}(k-k_m-1)\alpha_{k_m}^p. \end{aligned}$$

Now, by Corollary 4.1.1,

$$f(x_k) \; < \; f(x_{k_m}) - (k-k_m-1)\omega\|\nabla f(x_{k_m})\|^{\hat{p}}. \tag{4.4}$$

By applying a similar argument, but now starting from x_{k_i}, $i = m,\ldots,1$, we deduce that

$$f(x_{k_i}) \; < \; f(x_{k_{i-1}}) - (k_i - k_{i-1} - 1)\omega\|\nabla f(x_{k_{i-1}})\|^{\hat{p}}. \tag{4.5}$$

Denote $\Delta f_i = f(x_{k_i}) - f_*$, for $i = 0,\ldots,m$ and $\Delta f_{m+1} = f(x_k) - f_*$. Then, using the property stated in equation (2.11) for $f \in \mathcal{F}_\nu^1(\Omega)$,

$$\begin{aligned} f_* \; &= \; f(x_*^i) \\ &\geq \; f(x_{k_i}) + \langle\nabla f(x_{k_i}), x_*^i - x_{k_i}\rangle + \frac{1}{2\nu}\|\nabla f(x_*^i) - \nabla f(x_{k_i})\|^2 \\ &\geq \; f(x_{k_i}) + \langle\nabla f(x_{k_i}), x_*^i - x_{k_i}\rangle, \end{aligned}$$

where, for $i = 0, \ldots, m$, x_*^i is the projection of x_{k_i} onto the solutions set X_*^f (which is convex and closed since f is convex and continuous). Thus, using Assumption 4.2.1,

$$\begin{aligned} \Delta f_i &\leq \langle \nabla f(x_{k_i}), x_{k_i} - x_*^i \rangle \\ &\leq \|\nabla f(x_{k_i})\| \|x_{k_i} - x_*^i\| \\ &\leq R\|\nabla f(x_{k_i})\|, \quad i = 0, \ldots, m. \end{aligned} \tag{4.6}$$

By combining inequalities (4.4), (4.5), and (4.6) and setting here for simplicity $k_{m+1} = k$, we obtain, for $i = 1, \ldots, m, m+1$,

$$\Delta f_i \;\leq\; \Delta f_{i-1} - \frac{\omega}{R^{\hat{p}}}(k_i - k_{i-1} - 1)\Delta f_{i-1}^{\hat{p}} \;\leq\; \Delta f_{i-1}. \tag{4.7}$$

Hence, $\Delta f_{i-1}/\Delta f_i \geq 1$, $i = 1, \ldots, m, m+1$. Now we divide the first inequality in (4.7) by $\Delta f_i \Delta f_{i-1}$, then use $\hat{p} \geq 2$ and $\Delta f_{i-1} \geq \Delta f_{m+1}$, and later $\Delta f_{i-1}/\Delta f_i \geq 1$,

$$\begin{aligned} \frac{1}{\Delta f_i} &\geq \frac{1}{\Delta f_{i-1}} + \frac{\omega}{R^{\hat{p}}}(k_i - k_{i-1} - 1)\frac{\Delta f_{i-1}^{\hat{p}-1}}{\Delta f_i} \\ &\geq \frac{1}{\Delta f_{i-1}} + \frac{\omega \Delta f_{m+1}^{\hat{p}-2}}{R^{\hat{p}}}(k_i - k_{i-1} - 1)\frac{\Delta f_{i-1}}{\Delta f_i} \\ &\geq \frac{1}{\Delta f_{i-1}} + \frac{\omega \Delta f_{m+1}^{\hat{p}-2}}{R^{\hat{p}}}(k_i - k_{i-1} - 1). \end{aligned} \tag{4.8}$$

By summing the inequality (4.8) for $i = 1, \ldots, m, m+1$, we arrive at

$$\begin{aligned} \frac{1}{\Delta f_{m+1}} &\geq \frac{1}{\Delta f_0} + \frac{\omega \Delta f_{m+1}^{\hat{p}-2}}{R^{\hat{p}}}(k_{m+1} - k_0 - m - 1) \\ &\geq \frac{\omega \Delta f_{m+1}^{\hat{p}-2}}{R^{\hat{p}}}(k_{m+1} - k_0 - m - 1), \end{aligned}$$

or, equivalently,

$$\begin{aligned} (f(x_k) - f^*)^{\hat{p}-1} &= \Delta f_{m+1}^{\hat{p}-1} \\ &\leq \frac{R^{\hat{p}}}{\omega(k_{m+1} - k_0 - m - 1)} \\ &= \frac{R^{\hat{p}}}{\omega(k - k_0 - m - 1)}, \end{aligned}$$

as we wanted to prove (since, remember, $|\mathcal{S}(k_0, k)| = k - k_0 - m - 1$). □

Following [38, Theorem 3.2], one can also guarantee that the number of unsuccessful iterations is of the same order as the number of successful ones.

Lemma 4.3.2 *Let Assumptions 4.2.2 hold. Let k_0 be the index of the first unsuccessful iteration (which must exist from Lemma 3.1.1). Then Algorithm 3.1.1 generates a sequence $\{x_k\}_{k \geq k_0}$ such that*

$$|\mathcal{U}(k_0, k)| \;\leq\; \left\lceil \omega_1 |\mathcal{S}(k_0, k)| + \omega_2 + \frac{1}{\min(1, p-1)} \log_{\beta_2} \left(\frac{\omega_g}{R} (f(x_k) - f_*) \right) \right\rceil, \tag{4.9}$$

where

$$\omega_1 \;=\; -\log_{\beta_2}(\gamma), \quad \omega_2 \;=\; \log_{\beta_2}(\beta_1/\alpha_{k_0}), \tag{4.10}$$

ω_g is given in (4.3), and $|\mathcal{S}(k_0, k)|$ and $|\mathcal{U}(k_0, k)|$ are the number of successful and unsuccessful iterations between k_0 (including it) and k, respectively.

Proof. Since $f \in \mathcal{F}^1_\nu(\Omega)$ and X^f_* is non-empty, one has for each unsuccessful iteration k_i (with $k_0 \leq k_i \leq k$)

$$f(x_k) - f_* \;\leq\; f(x_{k_i}) - f_* \;\leq\; \langle \nabla f(x_{k_i}), x_{k_i} - x^i_* \rangle,$$

where x^i_* is the projection of x_{k_i} onto the solutions set X^f_* (which, again, is convex and closed since f is convex and continuous). Then, using Assumption 4.2.1,

$$\frac{1}{R}(f(x_k) - f_*) \;\leq\; \|\nabla f(x_{k_i})\|. \tag{4.11}$$

From Corollary 4.1.1 and the definition of ω_g in (4.3), we have, for each unsuccessful iteration k_i, that

$$\|\nabla f(x_{k_i})\| \;\leq\; \omega_g^{-1} \alpha_{k_i}^{\min(1,p-1)}. \tag{4.12}$$

As before, we can back-track from any iteration j after k_0 to the nearest unsuccessful iteration (say k_ℓ, with $k_\ell \geq k_0$) and, due to the step size updating rules, (4.12) implies then

$$\alpha_j \;\geq\; \beta_1 (\omega_g \|\nabla f(x_{k_\ell})\|)^{\frac{1}{\min(1,p-1)}}, \quad j = k_0, k_0+1, \ldots, k$$

(which holds trivially from (4.12) if j is itself unsuccessful). Combining the above inequality with (4.11) gives a lower bound for each step size α_j

$$\alpha_j \;\geq\; \beta_1 \left(\frac{\omega_g}{R} (f(x_k) - f_*) \right)^{\frac{1}{\min(1,p-1)}}, \quad j = k_0, k_0+1, \ldots, k.$$

On the other hand, one knows that either $\alpha_j \leq \beta_2 \alpha_{j-1}$ or $\alpha_j \leq \gamma \alpha_{j-1}$. Hence, by induction,

$$\alpha_k \;\leq\; \alpha_{k_0} \gamma^{|\mathcal{S}(k_0,k)|} \beta_2^{|\mathcal{U}(k_0,k)|}.$$

In conclusion one has

$$\beta_1 \left(\frac{\omega_g}{R} (f(x_k) - f_*) \right)^{\frac{1}{\min(1,p-1)}} \leq \alpha_k \leq \alpha_{k_0} \gamma^{|\mathcal{S}(k_0,k))|} \beta_2^{|\mathcal{U}(k_0,k)|},$$

from which we conclude,

$$f(x_k) - f_* \leq \frac{R}{\omega_g} \left(\frac{\alpha_{k_0}}{\beta_1} \gamma^{|\mathcal{S}(k_0,k)|} \beta_2^{|\mathcal{U}(k_0,k)|} \right)^{\min(1,p-1)}.$$

Now, since $\beta_2 < 1$, the function $\log_{\beta_2}(\cdot)$ is monotonically decreasing, and one obtains (the coefficient ω_1 is nonnegative due to $\gamma \geq 1$)

$$|\mathcal{U}(k_0, k)| \leq \omega_1 |\mathcal{S}(k_0, k)| + \omega_2 + \frac{1}{\min(1, p-1)} \log_{\beta_2} \left(\frac{\omega_g}{R} (f(x_k) - f_*) \right).$$

□

Lemmas 4.3.1 and 4.3.2 lead to a sub-linear global convergence rate for the absolute error in the function values after the first unsuccessful iteration.

Theorem 4.3.1 *Let Assumptions 4.2.2 hold. Let k_0 be the index of the first unsuccessful iteration (which must exist from Lemma 3.1.1). Then Algorithm 3.1.1 generates a sequence $\{x_k\}_{k \geq k_0}$ such that*

$$(f(x_k) - f_*)^{\hat{p}-1} < \frac{\kappa_1}{k - \kappa_2}, \quad \forall k > \kappa_2,$$

where

$$\begin{aligned} \kappa_1 &= (1 - \log_{\beta_2}(\gamma)) \frac{R^{\hat{p}}}{\omega} - \log_{\beta_2}(\exp(1)), \\ \kappa_2 &= \frac{f(x_0) - f_*}{\mathcal{C}\alpha_0^p} + \log_{\beta_2} \left(\frac{\beta_1}{\alpha_{k_0}} \right) + \frac{1}{\min(1, p-1)} \log_{\beta_2} \left(\frac{\omega_g}{R} [f(x_0) - f_*]^{1-(\hat{p}-1)\min(1,p-1)} \right), \end{aligned}$$

and ω and ω_g are given in (4.3).

Proof. Due to the definition of k_0 and the step size updating rules one has

$$k_0 \mathcal{C}\alpha_0^p \leq \sum_{j=0}^{k_0-1} \mathcal{C}\alpha_j^p < \sum_{j=0}^{k_0-1} f(x_j) - f(x_{j+1}) = f(x_0) - f(x_{k_0})$$

and so

$$k_0 < \frac{f(x_0) - f_*}{\mathcal{C}\alpha_0^p}. \tag{4.13}$$

By applying Lemmas 4.3.1 and 4.3.2 and inequality (4.13) one has

$$\begin{aligned}
k - \frac{f(x_0) - f_*}{\mathcal{C}\alpha_0^p} &< k - k_0 \\
&= |\mathcal{U}_k(k_0)| + |\mathcal{S}_k(k_0)| \\
&\leq (1 - \log_{\beta_2}(\gamma))|\mathcal{S}_k(k_0)| + \log_{\beta_2}(\beta_1/\alpha_{k_0}) \\
&\quad + \frac{1}{\min(1, p-1)} \log_{\beta_2}\left(\frac{\omega_g}{R}(f(x_k) - f_*)\right) \\
&\leq (1 - \log_{\beta_2}(\gamma))\frac{R^{\hat{p}}}{\omega}\frac{1}{(f(x_k) - f_*)^{\hat{p}-1}} + \log_{\beta_2}(\beta_1/\alpha_{k_0}) \\
&\quad + \frac{1}{\min(1, p-1)} \log_{\beta_2}\left(\frac{\omega_g}{R}(f(x_k) - f_*)\right) \\
&= (1 - \log_{\beta_2}(\gamma))\frac{R^{\hat{p}}}{\omega}\frac{1}{(f(x_{k_0}) - f_*)^{\hat{p}-1}} + \log_{\beta_2}(\beta_1/\alpha_{k_0}) \\
&\quad + \frac{1}{\min(1, p-1)} \log_{\beta_2}\left(\frac{\omega_g}{R}(f(x_{k_0}) - f_*)\right) \\
&\quad + \frac{1}{\min(1, p-1)} \log_{\beta_2}\left(\frac{f(x_k) - f_*}{f(x_{k_0}) - f_*}\right). \qquad (4.14)
\end{aligned}$$

Note that for any $p > 1$, $\hat{p}$ is bigger than 2 and so $\hat{p} - 1 \geq 1$. Since $1/\min(1, p-1)$ is equal to $\hat{p} - 1$ when $1 < p \leq 2$ and to 1 when $p > 2$, it holds $1/\min(1, p-1) \leq \hat{p} - 1$. From $(f(x_k) - f_*)/(f(x_{k_0}) - f_*) \leq 1$ and $\beta_2 < 1$, one has $\log_{\beta_2}((f(x_k) - f_*)/(f(x_{k_0}) - f_*)) \geq 0$. So, from (4.14)

$$\begin{aligned}
k - \frac{f(x_0) - f_*}{\mathcal{C}\alpha_0^p} &< (1 - \log_{\beta_2}(\gamma))\frac{R^{\hat{p}}}{\omega}\frac{1}{(f(x_{k_0}) - f_*)^{\hat{p}-1}} + \log_{\beta_2}(\beta_1/\alpha_{k_0}) \\
&\quad + \frac{1}{\min(1, p-1)} \log_{\beta_2}\left(\frac{\omega_g}{R}[f(x_{k_0}) - f_*]^{1-(\hat{p}-1)\min(1,p-1)}\right) \\
&\quad + (\hat{p} - 1)\log_{\beta_2}(f(x_k) - f_*). \qquad (4.15)
\end{aligned}$$

Now, given $\bar{\epsilon} \in (0, \infty)$,

$$\begin{aligned}
(\hat{p} - 1)\log_{\beta_2}(\bar{\epsilon}) &= -\log_{\beta_2}(\bar{\epsilon}^{(1-\hat{p})}) \\
&= -\log_{\beta_2}(\exp(1))\log(\bar{\epsilon}^{(1-\hat{p})}) \\
&\leq -\log_{\beta_2}(\exp(1))\bar{\epsilon}^{(1-\hat{p})}, \qquad (4.16)
\end{aligned}$$

where the last inequality follows from $\log(x) \leq x$, $x > 0$.

Then, from (4.16) with $\bar{\epsilon} = f(x_k) - f_*$, one has

$$(\hat{p} - 1)\log_{\beta_2}(f(x_k) - f_*) \leq -\log_{\beta_2}(\exp(1))\frac{1}{(f(x_k) - f_*)^{\hat{p}-1}}$$

and the proof is concluded by plugging this inequality in (4.15) and using $k > \kappa_2$. $\square$

4.4 WCC bounds

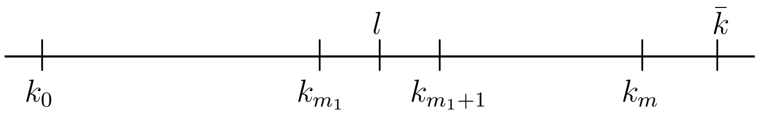
In the following lemma, by using the result of Lemma 4.3.1, we will derive an upper bound for the number of successful iterations after t he first unsuccessful one needed to achieve an iterate for which the norm of the gradient is below a given threshold.

Lemma 4.4.1 *Let Assumptions 4.2.2 hold. Let k_0 be the index of the first unsuccessful iteration (which must exist from Lemma 3.1.1). Given any $\epsilon \in (0,1)$, assume that $\|\nabla f(x_{k_0})\| > \epsilon$ and let $\bar{k}$ be the first iteration after k_0 such that $\|\nabla f(x_{\bar{k}})\| \leq \epsilon$. Then, to achieve $\|\nabla f(x_{\bar{k}})\| \leq \epsilon$, starting from k_0, Algorithm 3.1.1 takes at most $|\mathcal{S}(k_0, \bar{k})|$ successful iterations, where*

$$|\mathcal{S}(k_0,\bar{k})| \;\leq\; \left\lceil 2\frac{R}{\omega}\epsilon^{1-\hat{p}} + 1 \right\rceil \tag{4.17}$$

and ω is given in (4.3).

Proof. Let l, with $k_0 < l < \bar{k}$, be the index of a successful iteration occurring before $\bar{k}$, $m = |\mathcal{U}(k_0,\bar{k})|$ be number of unsuccessful iterations between k_0 (including it) and $\bar{k}$, m_1 be the number of unsuccessful iterations between k_0 and l, and $k_1, k_2, \ldots, k_m$ be the sequence of unsuccessful iterations between k_0 and $\bar{k}$.



Let us assume first that there are unsuccessful iterations between l and $\bar{k}$ (like in the figure above). Exactly as in the derivation of inequalities (4.4)–(4.5), applying also Corollary 4.1.1 and the step size updating rules, we have

$$f(x_{\bar{k}}) \;<\; f(x_{k_m}) - (\bar{k} - k_m - 1)\omega\|\nabla f(x_{k_m})\|^{\hat{p}}$$

and,

$$\begin{aligned} f(x_{k_i}) \;&<\; f(x_{k_{i-1}}) - (k_i - k_{i-1} - 1)\omega\|\nabla f(x_{k_{i-1}})\|^{\hat{p}}, \quad m_1 + 2 \leq i \leq m, \\ f(x_{k_{m_1+1}}) \;&<\; f(x_l) - (k_{m_1+1} - l)\omega\|\nabla f(x_{k_{m_1}})\|^{\hat{p}}. \end{aligned}$$

Summing up these inequalities and considering $\|\nabla f(x_k)\| > \epsilon$ for $k < \bar{k}$ lead us to

$$f(x_l) \;>\; f(x_{\bar{k}}) + (\bar{k} - l - m + m_1)\omega\epsilon^{\hat{p}}.$$

If there are no unsuccessful iterations between l and $\bar{k}$, $m = m_1$ and this inequality is also true by a similar argument. On the other hand, by Lemma 4.3.1

$$(f(x_l) - f_*)^{\hat{p}-1} \;\leq\; \frac{R^{\hat{p}}}{\omega(l - k_0 - m_1 - 1)}.$$

So, in conclusion

$$\begin{aligned}(\bar{k} - l - m + m_1)\omega\epsilon^{\hat{p}} &\leq (\bar{k} - l - m + m_1)\omega\epsilon^{\hat{p}} + f(x_{\bar{k}}) - f_* \\ &\leq f(x_l) - f_* \\ &\leq \left(\frac{R^{\hat{p}}}{\omega(l - k_0 - m_1 - 1)}\right)^{\frac{1}{\hat{p}-1}}. \end{aligned} \tag{4.18}$$

Now we choose l such that the number of successful iterations after l is at most one times higher than the number of successful iterations until l. To explicitly describe l we divide the number of successful iterations into two parts $(\bar{k} - k_0 - m - 1)/2$, then add the number m_1 of unsuccessful iterations until the middle point, and finally shift by k_0. Hence l is given by

$$l \;=\; \left\lfloor \frac{\bar{k} - k_0 - m - 1}{2} \right\rfloor + k_0 + m_1 + 1.$$

With such a choice of l, the number κ of successful iterations between k_0 and l is

$$\kappa \;=\; l - k_0 - m_1 - 1$$

and a simple argument shows that

$$\kappa \;=\; l - k_0 - m_1 - 1 \;\leq\; \bar{k} - l - m + m_1 \;\leq\; \kappa + 1, \tag{4.19}$$

as expected.

Now, from (4.18),

$$\begin{aligned}(\omega\kappa)^{\frac{\hat{p}}{\hat{p}-1}} &\leq \omega(\bar{k} - l - m + m_1)[\omega(l - k_0 - m_1 - 1)]^{\frac{1}{\hat{p}-1}} \\ &\leq R^{\frac{\hat{p}}{\hat{p}-1}}\epsilon^{-\hat{p}},\end{aligned}$$

and

$$\kappa \;\leq\; \frac{R}{\omega}\epsilon^{1-\hat{p}}. \tag{4.20}$$

But due to equation (4.19), $2\kappa+1$ is bigger than the number of successful iterations between k_0 and k,

$$\begin{aligned}2\kappa + 1 &= \kappa + 1 + \kappa \\ &\geq (\bar{k} - l - m + m_1) + (l - k_0 - m_1 - 1) \\ &= \bar{k} - k_0 - m - 1,\end{aligned}$$

which finishes the proof. $\square$

One can also guarantee that the number of unsuccessful iterations is of the same order as the number of successful ones.

Lemma 4.4.2 *Let Assumptions 4.2.2 hold. Let k_0 be the index of the first unsuccessful iteration (which must exist from Lemma 3.1.1). Given any $\epsilon \in (0,1)$, assume that $\|\nabla f(x_{k_0})\| > \epsilon$ and let $\bar{k}$ be the first iteration after k_0 such that $\|\nabla f(x_{\bar{k}})\| \leq \epsilon$. Then, to achieve $\|\nabla f(x_{\bar{k}})\| \leq \epsilon$, starting from k_0, Algorithm 3.1.1 takes at most $|\mathcal{U}(k_0,\bar{k})|$ unsuccessful iterations, where*

$$|\mathcal{U}(k_0,\bar{k})| \;\leq\; \left\lceil \omega_1 |\mathcal{S}(k_0,\bar{k})| + \omega_2 + \frac{1}{\min(p-1,1)} \log_{\beta_2}(\omega_g \epsilon) \right\rceil,$$

ω_g is given in (4.3), and ω_1 and ω_2 are given in (4.10).

Proof. The proof is similar to the one of Lemma 4.3.2 using $\bar{k}-1$ instead of k and ϵ instead of $(f(x_k)-f_*)/R$. The bound will then be on $|\mathcal{U}(k_0,\bar{k}-1)|$ but $|\mathcal{U}(k_0,\bar{k})| = |\mathcal{U}(k_0,\bar{k}-1)|$ since $\bar{k}-1$ is successful (and in the notation $\mathcal{U}(k_0,j)$ one is not counting j). $\square$

We are finally ready to state the WCC bound for Algorithm 3.1.1 when the objective function is convex. To do that we combine Lemmas 4.4.1 and 4.4.2 and bound the number of successful iterations until the first unsuccessful one. By doing so we show below that direct search takes at most $\mathcal{O}(\epsilon^{1-\hat{p}})$ iterations after the first unsuccessful one to bring the norm of the gradient below $\epsilon \in (0,1)$.

Theorem 4.4.1 *Let Assumptions 4.2.2 hold. To reduce the gradient below $\epsilon \in (0,1)$, Algorithm 3.1.1 takes at most*

$$\lceil \kappa_3 \epsilon^{1-\hat{p}} + \kappa_4 \rceil$$

iterations, and at most

$$d_{\#}\lceil \kappa_3 \epsilon^{1-\hat{p}} + \kappa_4 \rceil$$

function evaluations, where $\hat{p} = p/\min(1,1-p)$,

$$\begin{aligned}
\kappa_3 &= 2(1-\log_{\beta_2}(\gamma))\frac{R}{\omega} - \log_{\beta_2}(\exp(1)),\\
\kappa_4 &= \log_{\beta_2}\left(\frac{\beta_1}{\alpha_{k_0}}\right) + \log_{\beta_2}\left(\frac{\beta_2}{\gamma}\omega_g^{\frac{1}{\min(1,p-1)}}\right) + \frac{f(x_0)-f_*}{\mathcal{C}\alpha_0^p},
\end{aligned}$$

and ω and ω_g are given in (4.3).

Proof. One can now use Lemmas 4.4.1 and 4.4.2

$$\begin{aligned}\bar{k} - k_0 &= |\mathcal{S}(k_0, \bar{k})| + |\mathcal{U}(k_0, \bar{k})| \\ &\leq (1 - \log_{\beta_2}(\gamma))|\mathcal{S}(k_0, \bar{k})| + \log_{\beta_2}(\beta_1/\alpha_{k_0}) \\ &\quad + \frac{1}{\min(1, p-1)} \log_{\beta_2}(\omega_g \epsilon) \\ &\leq (1 - \log_{\beta_2}(\gamma)) \left(2\frac{R}{\omega}\epsilon^{1-\hat{p}} + 1 \right) + \log_{\beta_2}(\beta_1/\alpha_{k_0}) \\ &\quad + \frac{1}{\min(1, p-1)} \log_{\beta_2}(\omega_g \epsilon).\end{aligned}$$

From $1/\min(1, p-1) \leq \hat{p} - 1$ (see the proof of Theorem 4.3.1) and the derivation (4.16) with $\bar{\epsilon} = \epsilon$,

$$\frac{1}{\min(1, p-1)} \log_{\beta_2}(\omega_g \epsilon) \;\leq\; (\hat{p} - 1) \log_{\beta_2}(\omega_g \epsilon).$$

The proof is then completed by using $1 - \log_{\beta_2}(\gamma) = \log_{\beta_2}(\beta_2/\gamma)$ and then by applying the bound (4.13) on k_0. □

The optimal choice of p in $\epsilon^{1-\hat{p}}$ is $p = 2$. When $p = 2$, one can see from the expression for κ_3 that the maximum number of iterations is $\mathcal{O}(\mathrm{cm}_{\min}^{-2}\, \epsilon^{-1})$ and that the maximum number of function evaluations is $\mathcal{O}(d_\# \,\mathrm{cm}_{\min}^{-2}\, \epsilon^{-1})$, where, recall, $\mathrm{cm}_{\min}$ is a lower bound for the cosine measure of D_k and $d_\#$ is an upper bound for $|D_k|$ (for all k).

The WCC bound $\mathcal{O}(d_\# \,\mathrm{cm}_{\min}^{-2}\, \epsilon^{-1})$ depends on n only in $d_\#$ and $\mathrm{cm}_{\min}$. In [38] (see Theorem 3.2.1 and the discussion afterwards), it was suggested to use $D_\oplus = [I \; -I]$ across all iterations. Since $\mathrm{cm}(D_\oplus) = 1/\sqrt{n}$ and $|D_\oplus| = 2n$, the bound $\mathcal{O}(d_\# \,\mathrm{cm}_{\min}^{-2}\, \epsilon^{-1})$ becomes then $\mathcal{O}(n^2\epsilon^{-1})$. In Chapter 7 we will show that $D_\oplus$ (or any rotation of $D_\oplus$) is an optimal choice for the WCC bound for the number of function evaluations in terms of the power n^2.

For our reference, we summarize in the following corollary the main result of this chapter.

Corollary 4.4.1 *Let Assumptions 4.2.2 hold. Let* $\mathrm{cm}_{\min}$ *be at least a multiple of* $1/\sqrt{n}$ *and the number of function evaluations per iteration be at most a multiple of* n*. To reduce the gradient below* $\epsilon \in (0,1)$*, Algorithm 3.1.1 takes at most*

$$\mathcal{O}\left(n^{\frac{\hat{p}+2}{2}} \epsilon^{1-\hat{p}} \right)$$

function evaluations. When $p = 2$*, this number is of* $\mathcal{O}(n^2\epsilon^{-1})$*.*

Chapter 5

Global rate of direct search under strong convexity

Let us recall the definition of a strongly convex functions (Definition 2.1.2). From (2.7), one can see that strong convexity implies

$$f(x) - f_* \;\leq\; \frac{1}{2\mu}\|\nabla f(x)\|^2, \quad \forall x \in \mathbb{R}^n, \tag{5.1}$$

where $f_* = f(x_*)$ and x_* is the unique minimizer of f (and thus $\nabla f(x_*) = 0$). Also due to $\nabla f(x_*) = 0$, inequality (2.5) implies

$$f(x) - \; f_* \;\geq\; \frac{1}{2}\mu\|x - x_*\|^2, \quad \forall x \in \mathbb{R}^n. \tag{5.2}$$

We will also make use of inequality (2.9) for $f \in \mathcal{F}^1_{\nu,\mu}(\Omega)$ (meaning when f is strongly convex and ∇f is Lipschitz continuous with constant $\nu > 0$).

We are thus prepared to prove that the rate of convergence of function values and iterates for strongly convex functions is linear when $p = 2$.

To avoid repeating the several assumptions in the statements of the results of this chapter we will combine them in the following one.

Assumption 5.1.1 *Consider the application of Algorithm 3.1.1 when $\rho(t) = \mathcal{C}\, t^2$ $(p = 2)$, $\mathcal{C} > 0$, and D_k satisfies Assumption 3.1.1. Let $f \in \mathcal{F}^1_{\nu,\mu}(\mathbb{R}^n)$.*

As usual, we will start by considering first the case of the successful iterations.

Lemma 5.1.3 *Let Assumptions 5.1.1 hold. Let k_0 be the index of the first unsuccessful iteration (which must exist from Lemma 3.1.1). Then Algorithm 3.1.1 generates a sequence $\{x_k\}_{k\geq k_0}$ such that*

$$f(x_k) - f_* \;<\; (1 - 2\omega\mu)^{|\mathcal{S}(k_0,k)|}(f(x_{k_0}) - f_*), \tag{5.3}$$

$$\|x_k - x_*\| \ < \ \sqrt{\frac{\nu}{\mu}}(1-2\mu\omega)^{\frac{1}{2}|\mathcal{S}(k_0,k)|}\|x_{k_0} - x_*\|, \tag{5.4}$$

where ω is given in (4.3) and $|\mathcal{S}(k_0,k)|$ is the number of successful iterations between k_0 (including it) and k.

Proof. Let j (with $k_0 < j \leq k$) be index of a successful iteration generated by Algorithm 3.1.1. Again, we can back-track to nearest unsuccessful iteration k_ℓ (with $k_\ell \geq k_0$), and using the sufficient decrease condition, the step size updating rules, Corollary 4.1.1, and the definition of ω in (4.3), we obtain

$$\begin{aligned} f(x_j) - f(x_{j+1}) &> \mathcal{C}\alpha_j^2 \\ &\geq \mathcal{C}\beta_1^2\alpha_{k_\ell}^2 \\ &\geq \omega\|\nabla f(x_{k_\ell})\|^2 \\ &\geq 2\omega\mu(f(x_{k_\ell}) - f_*) \\ &> 2\omega\mu(f(k_\ell) - f_*), \end{aligned}$$

where the fourth inequality follows from inequality (5.1). Hence,

$$f(x_{j+1}) - f_* \ < \ (1-2\omega\mu)(f(x_j) - f_*).$$

A repeatedly application of the above inequality will lead us to (5.3). (From this we also see that $1 - 2\omega\mu \in (0,1)$.)

Now, the application of inequalities (5.2), (5.3), and (2.9) with $y = x_{k_0}$ and $x = x_*$ gives us

$$\begin{aligned} \frac{\mu}{2}\|x_k - x_*\|^2 &\leq f(x_k) - f_* \\ &< (1-2\mu\omega)^{|\mathcal{S}(k_0,k)|}(f(x_{k_0}) - f_*) \\ &\leq (1-2\mu\omega)^{|\mathcal{S}(k_0,k)|}\frac{\nu}{2}\|x_{k_0} - x_*\|^2, \end{aligned}$$

yielding (5.4). □

Note that the inequality

$$f(x_{k+1}) - f_* \ < \ (1-2\omega\mu)(f(x_k) - f_*), \quad \forall k \geq k_0 \tag{5.5}$$

implies that the distance from the current iteration to the minimizer is less than all the previous iterations up to the constant $\sqrt{\nu/\mu}$. In fact, from (5.1) and the above inequality for any $j < k$ we have

$$\begin{aligned}\frac{\mu}{2}\|x_{k+1} - x_*\|^2 &\le f(x_{k+1}) - f_* \\ &< (1-2\mu\omega)^{|\mathcal{S}(J,k+1)|}(f(x_j) - f_*) \\ &= (1-2\mu\omega)^{|\mathcal{S}(J,k+1)|}(f(x) - f_*), \quad \forall x \in f^{-1}(f(x_j)) \\ &\le (1-2\mu\omega)^{|\mathcal{S}(J,k+1)|}\frac{\nu}{2}\|x - x_*\|^2, \quad \forall x \in f^{-1}(f(x_j)),\end{aligned}$$

where $|\mathcal{S}(J, k+1)|$ is the number of successful iterations from iteration $J = \max(k_0, j)$ until iteration $k+1$. Now, since the last inequality is valid for any $x \in f^{-1}(f(x_j))$, by minimizing the right-hand side we will end up with

$$\|x_{k+1} - x_*\|^2 \le \frac{\nu}{\mu}(1-2\mu\omega)^{|\mathcal{S}(J,k+1)|} \min_{x\in f^{-1}(f(x_j))} \|x - x_*\|^2, \quad \forall k \ge J.$$

Applying the above argument to the left-hand side of inequality (5.5), we obtain that

$$\begin{aligned}\max_{x\in f^{-1}(f(x_{k+1}))} \|x - x_*\|^2 &< \frac{\nu}{\mu}(1-2\mu\omega)^{|\mathcal{S}(J,k+1)|} \min_{x\in f^{-1}(f(x_j))} \|x - x_*\|^2 \\ &< \frac{\nu}{\mu} \min_{x\in f^{-1}(f(x_j))} \|x - x_*\|^2.\end{aligned}$$

Note that the min and max above are attained since we are optimizing a continuous function on bounded and closed subsets (see, again, [34, Corollary 8.7.1]).

Now we need to take care of the number of unsuccessful iterations. The assumption of strongly convexity will lead to a bound better than (4.9).

Lemma 5.1.4 *Let Assumptions 5.1.1 hold. Let k_0 be the index of the first unsuccessful iteration (which must exist from Lemma 3.1.1). Then Algorithm 3.1.1 generates a sequence $\{x_k\}_{k\ge k_0}$ such that*

$$|\mathcal{U}(k_0, k)| \le \left\lceil \omega_1|\mathcal{S}(k_0,k)| + \omega_2 + \log_{\beta_2}(\omega_g\sqrt{2\mu(f(x_k) - f_*)}) \right\rceil, \tag{5.6}$$

$$|\mathcal{U}(k_0, k)| \le \left\lceil \omega_1|\mathcal{S}(k_0,k)| + \omega_2 + \log_{\beta_2}(\mu\omega_g\|x_k - x_*\|) \right\rceil, \tag{5.7}$$

where ω_g is given in (4.3), ω_1 and ω_2 are given in (4.10), and $|\mathcal{S}(k_0, k)|$ and $|\mathcal{U}(k_0, k)|$ are the number of successful and unsuccessful iterations between k_0 (including it) and k, respectively.

Proof. From inequality (5.1), one has for each unsuccessful iteration k_i (with $k_0 \le k_i \le k$)

$$\|\nabla f(x_{k_i})\|^2 \ge 2\mu(f(x_{k_i}) - f_*) \ge 2\mu(f(x_k) - f_*).$$

Now, by an argument like in the proof of the Lemma 4.3.2, but using $\sqrt{2\mu(f(x_k)-f_*)}$ instead of $(f(x_k)-f_*)/R$, one obtains

$$f(x_k)-f_* \;\leq\; \frac{1}{2\mu\omega_g^2}\left(\frac{\alpha_{k_0}}{\beta_1}\gamma^{|\mathcal{S}(k_0,k)|}\beta_2^{|\mathcal{U}(k_0,k)|}\right)^2.$$

In turn, this inequality and (5.2) imply

$$\|x_k-x_*\| \;\leq\; \frac{1}{\mu\omega_g}\left(\frac{\alpha_{k_0}}{\beta_1}\gamma^{|\mathcal{S}(k_0,k)|}\beta_2^{|\mathcal{U}(k_0,k)|}\right),$$

and the proof can be finished by applying $\log_{\beta_2}$ and noting that $\beta_2<1$ and $\omega_1\geq 0$. □

Lemmas 5.1.3 and 5.1.4 result in a (global) linear convergence rate (when $p=2$) for the absolute error in function values and iterates after the first unsuccessful iteration.

Theorem 5.1.2 *Let Assumptions 5.1.1 hold. Let k_0 be the index of the first unsuccessful iteration (which must exist from Lemma 3.1.1). Then Algorithm 3.1.1 generates a sequence $\{x_k\}_{k\geq k_0}$ such that*

$$f(x_k)-f_* \;<\; \beta^{\frac{1}{\kappa_5}(k-\kappa_6)},$$

$$\|x_k-x_*\| \;<\; \beta^{\frac{1}{2\kappa_5}(k-\kappa_7)},$$

where

$$\begin{aligned}
\kappa_5 &= (1+\omega_1)\log_{1-2\omega\mu}(\beta)+\log_{\beta_2}(\sqrt{\beta}), \quad \beta \;=\; \min(\beta_2,1-2\mu\omega),\\
\kappa_6 &= \frac{f(x_0)-f_*}{\mathcal{C}\alpha_0^2}-(1+\omega_1)\log_{1-2\omega\mu}(f(x_{k_0})-f_*)+\omega_2+\log_{\beta_2}(\omega_g\sqrt{2\mu}),\\
\kappa_7 &= \frac{\nu\|x_0-x_*\|^2}{2\mathcal{C}\alpha_0^2}-(1+\omega_1)\log_{1-2\omega\mu}\left(\frac{\nu}{\mu}\|x_{k_0}-x_*\|^2\right)+\omega_2+\log_{\beta_2}(\omega_g\mu),
\end{aligned}$$

ω and ω_g are given in (4.3), and ω_1 and ω_2 are given in (4.10).

Proof. From inequalities (5.3) and (5.6) one has

$$\begin{aligned}
k-k_0 &= |\mathcal{U}(k_0,k)|+|\mathcal{S}(k_0,k)|\\
&\leq (1+\omega_1)|\mathcal{S}(k_0,k)|+\omega_2+\log_{\beta_2}\left(\omega_g\sqrt{2\mu(f(x_k)-f_*)}\right)\\
&\leq (1+\omega_1)\log_{1-2\omega\mu}\left(\frac{f(x_k)-f_*}{f(x_{k_0})-f_*}\right)+\omega_2+\log_{\beta_2}\left(\omega_g\sqrt{2\mu(f(x_k)-f_*)}\right)\\
&= \left[(1+\omega_1)\log_{1-2\omega\mu}(\beta)+\log_{\beta_2}(\sqrt{\beta})\right]\log_\beta(f(x_k)-f_*)\\
&\quad -(1+\omega_1)\log_{1-2\omega\mu}(f(x_{k_0})-f_*)+\;\omega_2+\log_{\beta_2}(\omega_g\sqrt{2\mu}).
\end{aligned}$$

Then, from inequality (4.13), one obtains

$$\begin{aligned} k &- \left[\frac{f(x_0)-f_*}{\mathcal{C}\alpha_0^2} - (1+\omega_1)\log_{1-2\omega\mu}(f(x_{k_0})-f_*) + \omega_2 + \log_{\beta_2}(\omega_g\sqrt{2\mu})\right] \\ &< \left[(1+\omega_1)\log_{1-2\omega\mu}(\beta) + \log_{\beta_2}(\sqrt{\beta})\right]\ \log_\beta(f(x_k)-f_*) \end{aligned}$$

which proves the first part of the theorem.

By similar arguments, but using now inequalities (5.4) and (5.7), it results that

$$\begin{aligned} k - k_0 &= |\mathcal{U}(k_0,k)| + |\mathcal{S}(k_0,k)| \\ &\le (1+\omega_1)|\mathcal{S}(k_0,k)| + \omega_2 + \log_{\beta_2}(\omega_g\mu\|x_k-x_*\|) \\ &\le (1+\omega_1)\log_{1-2\omega\mu}\left(\frac{\mu}{\nu}\frac{\|x_k-x_*\|^2}{\|x_{k_0}-x_*\|^2}\right) + \omega_2 + \log_{\beta_2}(\omega_g\mu\|x_k-x_*\|) \\ &= \left[2(1+\omega_1)\log_{1-2\omega\mu}(\beta) + \log_{\beta_2}(\beta)\right]\log_\beta(\|x_k-x_*\|) \\ &\quad - (1+\omega_1)\log_{1-2\omega\mu}\left(\frac{\nu}{\mu}\|x_{k_0}-x_*\|^2\right) + \omega_2 + \log_{\beta_2}(\omega_g\mu). \end{aligned}$$

Again using inequality (4.13), but now followed by (2.9) with $x = x_0$ and $y = x_*$, yields

$$\begin{aligned} k &- \left[\frac{\nu\|x_0-x_*\|^2}{2\mathcal{C}\alpha_0^2} - (1+\omega_1)\log_{1-2\omega\mu}\left(\frac{\nu}{\mu}\|x_{k_0}-x_*\|^2\right) + \omega_2 + \log_{\beta_2}(\omega_g\mu)\right] \\ &\le \left[2(1+\omega_1)\log_{1-2\omega\mu}(\beta) + \log_{\beta_2}(\beta)\right]\log_\beta(\|x_{\bar{k}}-x_*\|), \end{aligned}$$

which proves the second part. □

The result of Theorem 5.1.2 improves significantly what has been known for direct search. In fact, it was proved in [19] that the absolute error for unsuccessful iterates exhibits an r-linear rate of convergence under the following assumptions: α_k is monotonically non-increasing and x_k is sufficiently close to a point x_* for which $\nabla f(x_*) = 0$ and $\nabla^2 f(x)$ is positive definite around x_*.

Our result is therefore stronger since (i) the r-linear rate is over the all sequence $\|x_k - x_*\|$, whether k is successful or not, (ii) only first order continuously differentiability is assumed, and (iii) α_k can be increased at successful iterations.

Chapter 6

Numerical illustration

In the previous chapters, we have studied the worst case complexity of direct search when the objective function is convex. Now we apply Algorithm 3.1.1 to convex functions and observe the numerical behavior of the algorithm. We use the software developed in [14, 15].

Assumption 4.2.1 was convenient for our theoretical analysis. The goal of Section 6.2 is to find out how direct search may behave if this assumption is not satisfied. We will see that the performance of Algorithm 3.1.1 is not necessarily severely affected for problems where Assumption 4.2.1 is not met.

Although only a sub-linear rate is established under convexity (and Assumption 4.2.1), direct search does achieve an r-linear global rate when the objective function is strongly convex, as shown in Chapter 5. The purpose of Section 6.3 is to illustrate the performance of Algorithm 3.1.1 on convex functions with and without strong convexity. We will observe that the algorithm does not always work more efficiently when the objective function is strongly convex.

As seen in Corollary 4.4.1 and Theorem 5.1.2, the Lipschitz constant ν and the strong convexity constant μ (when applicable) appear in the worst case complexity bounds of direct search. Small values of ν and large values of μ are considered favorable to the performance of the algorithm in terms of WCC bounds. But this is not always the case in practice, and we will show this phenomenon by some examples in Section 6.4.

6.1 Description of the experiments

In the experiments of this chapter, we used a fixed maximal positive basis $D_\oplus = [I \ -I]$ as the set of poll directions. The step size α_k was kept unchanged after a successful iteration, and contracted by a factor of 1/2 after an unsuccessful one. The forcing function $\rho(t)$ was $10^{-3}t^2$. Regarding the order of the function evaluations in the poll step, three polling strategies were tested, namely

- Dynamic Polling: moving the poll direction that led to success to the beginning of the list of directions for the next poll step [2],
- Random: the poll directions are ordered randomly at each iteration,
- Consecutive, Cycling: the poll directions are evaluated at each iteration in the same consecutive order as originally stored, starting a new poll step in the direction appearing after the last one used (consecutive) and moving from the last one in $D_\oplus$ to the first when necessary (cycling).

The algorithm runs were stopped when the error in terms of function value was less than 10^{-6}. All the figures reported in the tables of results are averages of 10 runs made for 10 starting points, randomly generated in the hypercube $[-10, 10]^4$. We use $f_{\bar{k}}$ and f_* to denote the function value obtained at the final iteration $\bar{k}$ and the accurate minimum function value, respectively.

The objective functions used are reported in tables where the columns are organized as follows:

- the first column is for problem number, `#P`,
- the second column is for objective function,
- the third column corresponds to strong convexity, namely to the `constant` μ,
- the fourth column corresponds to Lipschitz continuity of gradient, namely to the `constant` ν.

One knows that calculating the Lipschitz constant ν and the strong convexity constant μ is very difficult in practice. We approximated these constants based on the initial points. For each problem, we computed the Hessian of the objective function f at the initial points x_0, and took maximum and minimum eigenvalues of $\nabla^2 f(x_0)$ as approximations for ν and μ.

6.2 A numerical study of Assumption 4.2.1

In this section we test Algorithm 3.1.1 with some problems that do not satisfy Assumption 4.2.1.

By convention, let us define the distance between any point and the empty set is as infinity. Consequently,

$$\sup_{y \in L_f(x_0)} \operatorname{dist}(y, X_f^*) = \infty \quad \text{if} \quad X_f^* = \emptyset. \tag{6.1}$$

We then tried Algorithm 3.1.1 on two sets of objective functions in $\mathbb{R}^4$:

- Set 1, a set of functions without minimizers (because the infimums are not attainable), as presented in Table 6.1,
- Set 2, a set of functions with minimizers, but for which the supremum in (6.1) is still infinity, as presented in Table 6.2.

`#P`	`objective function`	`constant` μ	`constant` ν
01	$\sum_{i=1}^{3}(x_i + x_{i+1})^2 + exp(x_4)$	-	+1.948e+03
02	$\sum_{i=1}^{3}(10^{-\frac{1}{2}}x_i + 10^{\frac{1}{2}}x_{i+1})^2 + exp(x_4)$	-	+1.948e+03
03	$\sum_{i=1}^{3}(10^{-1}x_i + 10x_{i+1})^2 + exp(x_4)$	-	+1.948e+03

Table 6.1: Functions in **Set 1**.

`#P`	`objective function`	`constant` μ	`constant` ν
04	$(\sum_{i=1}^{4} x_i^2)^{\frac{1}{2}} - x_1$	-	+1.539e-01
05	$[(\sum_{i=1}^{4} x_i^2)^{\frac{1}{2}} - x_1]^2$	-	+1.452e+01
06	$[(\sum_{i=1}^{4} x_i^2)^{\frac{1}{2}} - x_1]^4$	-	+1.538e+04

Table 6.2: Functions in **Set 2**.

The results are reported in Tables 6.3–6.4, where the columns are organized as follows:

- the first column is for problem number, `#P`,
- the second column is for polling strategy, `order option`,
- the third column is for number of iterations, `#iter`,
- the fourth column is for number of successful iterations, `#isuc`,
- the fifth column is for number of function evaluations, `#feval`,
- the sixth column is for error in terms of function value, $f_{\bar{k}} - f_*$,
- the seventh column is for error in terms of norm of gradient, $\|\nabla f(x_{\bar{k}})\|$.

#P	order option	#iter	#isuc	#fevals	$f_{\bar{k}} - f_*$	$\|\nabla f(x_{\bar{k}})\|$
01	Dynamic Polling	1773	1759	1960	+9.694e-07	+4.665e-04
02		2750	2736	2941	+8.354e-07	+1.527e-03
03		5282	5267	5477	+5.470e-07	+3.286e-03
01	Random	1557	1543	7007	+9.981e-07	+3.526e-04
02		1860	1846	8356	+9.268e-07	+9.641e-04
03		3683	3668	16590	+7.333e-07	+4.067e-03
01	Consecutive, Cycling	1557	1543	12330	+9.981e-07	+3.526e-04
02		1780	1767	14113	+9.268e-07	+8.616e-04
03		3683	3668	29339	+7.334e-07	+4.067e-03

Table 6.3: Number of function evaluations for **Set 1**.

#P	order option	#iter	#isuc	#fevals	$f_{\bar{k}} - f_*$	$\|\nabla f(x_{\bar{k}})\|$
04	Dynamic Polling	29	20	136	+3.132e-07	+1.849e-04
05		63	53	162	+9.765e-07	+1.199e-05
06		260	249	361	+9.101e-07	+2.213e-06
04	Random	26	17	135	+3.986e-07	+3.201e-04
05		31	22	150	+9.249e-07	+1.852e-05
06		53	43	237	+9.452e-007	+4.002e-06
04	Consecutive, Cycling	25	16	127	+4.424e-07	+3.606e-04
05		26	17	143	+8.716e-07	+1.998e-05
06		58	47	323	+9.866e-07	+4.596e-06

Table 6.4: Number of function evaluations for **Set 2**.

We observe that, even though Assumption 4.2.1 is not true for the testing functions here, Algorithm 3.1.1 still drove the function value to a satisfying level using a reasonable amount of function evaluations. Actually, all the numbers of function evaluations were below the worst case complexity bound given in Theorem 4.3.1 and Corollary 4.4.1, where Assumption 4.2.1 is required. Thus Assumption 4.2.1 does not seem critical to the practical performance of Algorithm 3.1.1. This suggests that it may be possible to extend our theory to the most general convex case.

6.3 Convex v.s. strongly convex

In Chapter 5 we saw that Algorithm 3.1.1 converges r-linearly when the objective function is strongly convex, while only a sub-linear rate is guaranteed without strong convexity (see Theorem 4.3.1). So, the theory indicates that Algorithm 3.1.1 should perform better on strongly convex functions than on general convex functions. But in practice this is not necessarily always the case. To illustrate this, we tested Algorithm 3.1.1 on the following two sets of functions:

- Set 3, a set of functions that are convex but not strongly convex, as presented in Table 6.5,
- Set 4, a set of strongly convex functions as presented in Table 6.6.

#P	objective function	constant μ	constant ν
07	$\sum_{i=1}^{4}(x_i + x_{i+1})^2$	-	+6.828e+00
08	$\sum_{i=1}^{4}(10^{-1}x_i + 10x_{i+1})^2$	-	+2.028e+02
09	$\sum_{i=1}^{4}(10^{-2}x_i + 10^2x_{i+1})^2$	-	+2.000e+04

Table 6.5: Functions in **Set 3**.

#P	objective function	constant μ	constant ν
10	$(x_1 + x_2)^2 + \sum_{i=2}^{4} x_i^2$	+7.639e-01	+5.236e+00
11	$(10^{-\frac{1}{2}}x_1 + 10^{\frac{1}{2}}x_2)^2 + \sum_{i=2}^{4} x_i^2$	+1.803e-02	+2.218e+01
12	$(10^{-1}x_1 + 10x_2)^2 + \sum_{i=2}^{4} x_i^2$	+1.980e-04	+2.020e+02

Table 6.6: Functions in **Set 4**.

The results are presented in Tables 6.7–6.8, which are organized in the same way as in Table 6.3. We observe that, for these testing problems, strong convexity did not lead to a better performance of Algorithm 3.1.1.

#P	order option	#iter	#isuc	#fevals	$f_{\bar{k}} - f_*$	$\|\nabla f(x_{\bar{k}})\|$
07	Dynamic Polling	36	23	202	+6.166e-07	+2.102e-03
08		104	89	301	+4.073e-07	+1.165e-02
09		6864	6846	7094	+4.970e-07	+1.363e-01
07	Random	36	23	181	+6.461e-07	+2.216e-03
08		60	44	299	+5.425e-07	+1.367e-02
09		2218	2200	10056	+3.801e-07	+1.095e-01
07	Consecutive, Cycling	35	22	164	+6.246e-07	+2.142e-03
08		60	45	352	+6.016e-07	+1.460e-02
09		2218	2199	17595	+3.503e-07	+1.054e-01

Table 6.7: Number of function evaluations for **Set 3**.

#P	order option	#iter	#isuc	#fevals	$f_{\bar{k}} - f_*$	$\|\nabla f(x_{\bar{k}})\|$
10	Dynamic Polling	43	30	234	+5.922e-07	+1.715e-03
11		712	696	1267	+9.788e-07	+6.939e-04
12		61505	61486	65378	+9.994e-07	+5.890e-04
10	Random	38	25	197	+6.362e-07	+1.676e-03
11		480	465	2139	+9.174e-07	+1.316e-03
12		40591	40574	182064	+9.139e-07	+1.282e-03
10	Consecutive, Cycling	42	29	182	+6.517e-07	+1.730e-03
11		484	469	3400	+9.134e-07	+1.271e-03
12		40593	40576	321389	+9.135e-07	+1.273e-03

Table 6.8: Number of function evaluations for **Set 4**.

6.4 The Lipschitz constant and the strong convexity constant

As shown in Theorems 4.3.1 and 5.1.2 and Corollary 4.4.1, the worst case complexity bounds are monotonically increasing with respect to the Lipschitz constant ν and monotonically decreasing with respect to the strong convexity constant μ. Hence, generally speaking, one may expect direct search to work more efficiently if ν is smaller and if μ (when applicable) is larger. But we noticed in our numerical experiments that the opposite can also happen. We illustrate this phenomenon by the following two sets of testing functions:

- Set 5, a set of functions with moderate Lipschitz constants and decreasing strong convexity constants, as presented in Table 6.9,

- Set 6, a set of functions with large Lipschitz constants and decreasing strong convexity constants, as presented in Table 6.10.

#P	objective function	constant μ	constant ν
13	$\sum_{i=1}^{3}(x_i + x_{i+1})^2 + x_4^2$	+2.412e-01	+7.064e+00
14	$\sum_{i=1}^{3}(10^{-\frac{1}{8}}x_i + 10^{\frac{1}{8}}x_{i+1})^2 + 10^{\frac{1}{4}}x_4^2$	+3.399e-02	+8.586e+00
15	$\sum_{i=1}^{3}(10^{-\frac{1}{4}}x_i + 10^{\frac{1}{4}}x_{i+1})^2 + 10^{\frac{1}{2}}x_4^2$	+2.704e-03	+1.335e+01

Table 6.9: Functions in **Set 5**.

#P	objective function	constant μ	constant ν
16	$\sum_{i=1}^{2}(x_i + x_{i+1})^2 + \exp([\sum_{i=3}^{4} x_i^2 + 1]^{\frac{1}{2}})$	+5.049e-01	+6.307e+04
17	$\sum_{i=1}^{2}(10^{-\frac{1}{8}}x_i + 10^{\frac{1}{8}}x_{i+1})^2 + \exp([\sum_{i=3}^{4} x_i^2 + 1]^{\frac{1}{2}})$	+1.188e-01	+6.307e+04
18	$\sum_{i=1}^{2}(10^{-\frac{1}{4}}x_i + 10^{\frac{1}{4}}x_{i+1})^2 + \exp([\sum_{i=3}^{4} x_i^2 + 1]^{\frac{1}{2}})$	+1.944e-02	+6.307e+04

Table 6.10: Functions in **Set 6**.

The numerical results on these problems are presented in Tables 6.11–6.12, which are organized in the same way as Table 6.3. One sees clearly from Tables 6.11–6.12 that the algorithm performed better on Set 6 than on Set 5, even though in the former set the functions have bigger condition numbers (seen as the ratio ν/μ).

#P	order option	#iter	#isuc	#fevals	$f_{\bar{k}} - f_*$	$\|\nabla f(x_{\bar{k}})\|$
13		99	85	477	+9.026e-07	+1.614e-03
14	Dynamic Polling	727	711	2530	+9.866e-07	+0.000e+00
15		6623	6606	17070	+9.983e-07	+0.000e+00
13		98	84	404	+8.861e-07	+0.000e+00
14	Random	570	554	2162	+9.503e-07	+0.000e+00
15		4533	4516	17845	+9.697e-07	+0.000e+00
13		110	96	362	+8.971e-07	+0.000e+00
14	Consecutive, Cycling	574	558	2419	+9.510e-07	+0.000e+00
15		4538	4521	25411	+9.789e-07	+0.000e+00

Table 6.11: Number of function evaluations for **Set 5**.

#P	order option	#iter	#isuc	#fevals	$f_{\bar{k}} - f_*$	$\|\nabla f(x_{\bar{k}})\|$
16		52	39	275	+6.648e-07	+1.649e-03
17	Dynamic Polling	180	165	683	+9.192e-07	+4.094e-03
18		1033	1016	2740	+9.787e-07	+2.690e-03
16		50	36	236	+6.847e-07	+1.627e-03
17	Random	172	158	733	+9.082e-07	+4.024e-03
18		728	712	3009	+8.267e-07	+2.187e-03
16		54	41	222	+6.243e-07	+1.554e-03
17	Consecutive, Cycling	139	125	643	+7.728e-07	+3.531e-03
18		727	712	4165	+8.377e-07	+2.325e-03

Table 6.12: Number of function evaluations for **Set 6**.

6.5 Relevance of variable separability

In practice we noticed that the separability of the objective function is one of the key structures that influences the performance of Algorithm 3.1.1. As an illustration, we tested the algorithm on Set 7, which is a set of separable functions listed in Table 6.13. The organization of Table 6.13 is the same as that of Table 6.1.

#P	objective function	constant μ	constant ν
19	$\sum_{i=1}^{4} \exp(\sqrt{x_i^2+1})$	+2.719e+00	+4.164e+04
20	$\sum_{i=1}^{4} i \exp(\sqrt{10^{\frac{1}{4}} x_i^2+1})$	+4.839e+00	+5.226e+06
21	$\sum_{i=1}^{4} i^2 \exp(\sqrt{10^{\frac{1}{2}} x_i^2+1})$	+9.938e+00	+5.972e+09

Table 6.13: Functions in **Set 7**.

In this experiment, the settings of Algorithm 3.1.1 were the same as in Section 6.2, except that the directions set was set to be $D = [Q\ -Q]$, where Q was an orthonormal matrix generated randomly at the beginning of the experiment (see [39]). The initial points were also generated in the same way as in Section 6.2. The results displayed show that, for these problems, the performance of Algorithm 3.1.1 did not change significantly when the Lipschitz constant increased considerably.

#P	order option	#iter	#isuc	#fevals	$f_{\bar{k}} - f_*$	$\|\nabla f(x_{\bar{k}})\|$
19	Dynamic Polling	40	27	232	+6.181e-07	+1.783e-03
20		49	35	275	+6.686e-07	+4.306e-03
21		59	43	311	+5.931e-07	+8.897e-03
19	Random	40	27	194	+6.364e-07	+1.813e-03
20		47	33	226	+5.843e-07	+3.819e-03
21		56	40	264	+6.366e-07	+8.719e-03
19	Consecutive, Cycling	40	27	167	+5.657e-07	+1.697e-03
20		48	34	189	+6.226e-07	+4.020e-03
21		59	43	234	+5.654e-07	+8.441e-03

Table 6.14: Number of function evaluations for **Set 7**.

The testing problems in this chapter were chosen as simple illustrations. In any case, the observations encourage us to do further theoretical research, in order to extend the results to general convex functions, and also to obtain more specific results for functions with a special structure.

Chapter 7

Sharpness of the WCC bounds in terms of function evaluations

The worst case complexity (WCC) bounds derived for direct search depend on the properties of the positive spanning sets (PSSs) used in the poll step. Let us consider Algorithm 3.1.1 with a search step empty and a forcing function using $p = 2$. In fact, the bound derived in [38] for the smooth and non-convex case is of the $\mathcal{O}(\mathrm{cm}_{\min}^{-2}\,\nu^2\epsilon^{-2})$ (for iterations) and of the $\mathcal{O}(d_\#\,\mathrm{cm}_{\min}^{-2}\,\nu^2\epsilon^{-2})$ (for function evaluations), where $d_\#$ is the maximum number of directions in any PSS used during the course of the iterations and $\mathrm{cm}_{\min}$ is a lower bound on their cosine measures (see the discussion after Theorem 3.2.1). For the smooth and convex case, we have shown in Chapter 4 a similar dependence, being the difference just the order of ϵ: $\mathcal{O}(\mathrm{cm}_{\min}^{-2}\,\nu^2\epsilon^{-1})$ (for iterations) and $\mathcal{O}(d_\#\,\mathrm{cm}_{\min}^{-2}\,\nu^2\epsilon^{-1})$ (for function evaluations), see the discussion after Theorem 4.4.1. As we have also mentioned, if in all iterations we use the positive basis $D_\oplus$ (formed by the coordinate vectors and their negatives for which $|D_\oplus| = 2n$ and $\mathrm{cm}(D_\oplus) = 1/\sqrt{n}$), one has $\mathrm{cm}_{\min}^{-2} = n$ and $d_\# = 2n$ and thus $d_\#\,\mathrm{cm}_{\min}^{-2} = 2n^2$. In this chapter we will prove that such an order of n^2 is indeed optimal in the WCC bounds for the number of function evaluations.

It is obvious that adding directions to a PSS will increase its cosine measure (see Definition 3.1.2). So, by using more polling directions, one can increase the cosine measure, which is favorable in terms of number of iterations. However, such a strategy will increase the number of function evaluations in each iteration. So, there is a trade-off in the number of directions to use in the PSSs when we consider the bound for the number of function evaluations.

Let us clarify this trade-off with a few examples. We know that a minimal positive basis with uniform angles in $\mathbb{R}^n$ has $n + 1$ directions and a cosine measure of $1/n$ [13, Corollary 2.6 and Exercise 2.7.7]. If we apply this PSS to Algorithm 3.1.1 (with $p = 2$ in the forcing function), then the WCC bound for the number of function evaluations will become $\mathcal{O}(n^3\epsilon^{-1})$. But if we use $D_\oplus$, the bound is $\mathcal{O}(n^2\epsilon^{-1})$. In this case, increasing the number of directions improves the WCC bound. This is not always true. For example, if we use a PSS with n^4 directions, then the bound will become at least $\mathcal{O}(n^4\epsilon^{-1})$.

To find the PSS that leads to the optimal WCC bound for the number of function evaluations in terms of the power of the n, we need to solve the following problem

$$\min_{D\in\mathcal{D}} \frac{|D|}{\mathrm{cm}(D)^2}, \tag{7.1}$$

where $\mathcal{D}$ is the set of all PSSs in $\mathbb{R}^n$. In two dimensions, problem (7.1) is not difficult. One can easily prove that the PSSs with five directions and uniform $2\pi/5$ angles are optimal for problem (7.1). When we go to higher dimensions, determining the optimal PSSs for problem (7.1) is not that easy. It is not clear what are the solutions to this problem when $n \geq 3$. But we are able to show that $D_\oplus$ is 'almost optimal' for problem (7.1) in the sense of that

$$\min_{D\in\mathcal{D}} \frac{|D|}{\mathrm{cm}(D)^2} \;\geq\; c\,\frac{|D_\oplus|}{\mathrm{cm}(D_\oplus)^2}, \tag{7.2}$$

for some constant $c > 0$ not depending on n or on any specific PSS. In fact, we will prove the following result.

Theorem 7.1.1 *For every PSS D in $\mathbb{R}^n$, there exists a constant $C > 0$ not depending on n and D such that*

$$\frac{|D|}{\mathrm{cm}(D)^2} \;\geq\; C\,n^2.$$

Inequality (7.2) will then follow directly from Theorem 7.1.1 and the properties of $D_\oplus$.

To prove Theorem 7.1.1, we observe first a connection between the cosine measure and sphere covering, which is presented in Lemma 7.1.1 below. Before stating this result, let us define

$$\mathbb{C}(x,\phi) = \left\{y \in \mathbb{S}^{n-1} : \mathrm{d}(y,x) \leq \phi\right\}, \tag{7.3}$$

where $\mathbb{S}^{n-1}$ is the unit sphere in $\mathbb{R}^n$, x is a fixed point on $\mathbb{S}^{n-1}$, ϕ is a constant in $[0,\pi]$, and $\mathrm{d}(\cdot,\cdot)$ is the geodesic distance on $\mathbb{S}^{n-1}$. We will call $\mathbb{C}(x,\phi)$ a spherical cap centered at x with geodesic radius ϕ.

Lemma 7.1.1 *Suppose that $D = [d_1 \cdots d_m]$ is a PSS in $\mathbb{R}^n$ consisting of unit vectors. If* $\mathrm{cm}(D) = \kappa$*, then*

$$\mathbb{S}^{n-1} \;\subseteq\; \bigcup_{i=1}^{m} \mathbb{C}(d_i, \arccos(\kappa)). \tag{7.4}$$

In other words, $\mathbb{S}^{n-1}$ is covered by the spherical caps centered at d_i ($i = 1,2,\ldots,m$) with geodesic radius $\arccos(\kappa)$*.*

Proof. According to Definition 3.1.2, for any $v \in \mathbb{S}^{n-1}$, there exists an $i \in \{1, 2, \ldots, m\}$ such that

$$v^\top d_i \;\geq\; \mathrm{cm}(D) \;=\; \kappa. \tag{7.5}$$

Since the radius of the sphere is 1, the geodesic distance between v and d_i is equal to the angle between them. Hence inequality (7.5) implies that

$$\mathrm{d}(v, d_i) \;\leq\; \arccos(\kappa), \tag{7.6}$$

which is equivalent to

$$v \;\in\; \mathbb{C}(d_i, \arccos(\kappa)). \tag{7.7}$$

This is sufficient to conclude the proof as v is arbitrary. □

To prove Theorem 7.1.1, we need an upper bound for the cosine measure $\mathrm{cm}(D)$ in terms of the dimension n and the number of directions in $|D|$. In light of Lemma 7.1.1, it is desirable to have a lower bound for ϕ (or, equivalently, an upper bound for $\cos(\phi)$) in terms of n and m when $\mathbb{S}^{n-1}$ is covered by m equal spherical caps with geodesic radius ϕ. Such a bound is fortunately already established in the research community of *Discrete Geometry.* The conclusion of the following lemma is given in Tikhomirov [35] for $n+1 \leq m \leq 2n$. The case $m \geq 2n$ was established much earlier (for more details see [3], [5, Chapter 6], [7], [8, Corollary 9.5], [9], [21] and [35])[1].

Lemma 7.1.2 *([35]) Any covering of $\mathbb{S}^{n-1}$ by $m \geq n+1$ spherical caps of geodesic radius ϕ satisfies*

$$\cos(\phi) \;\leq\; \zeta\sqrt{n^{-1}\log(n^{-1}m)}, \tag{7.8}$$

for some constant $\zeta > 0$ not depending on n and m.

With the help of Lemmas 7.1.1 and 7.1.2, we obtain the desired upper bound for the cosine measure.

Lemma 7.1.3 *Any PSS D in $\mathbb{R}^n$ satisfies*

$$\mathrm{cm}(D) \;\leq\; \zeta\,\sqrt{n^{-1}\log(n^{-1}|D|)}, \tag{7.9}$$

for the same constant ζ as in Lemma 7.1.2.

Proof. Without loss of generality, we assume that all the directions in D are normalized. Then inequality (7.9) follows immediately from Lemmas 7.1.1 and 7.1.2. □

Then, Theorem 7.1.1 is a straightforward consequence of this bound, since

$$\sqrt{n^{-1}\log(n^{-1}|D|)} \;\leq\; \sqrt{n^{-1}(n^{-1}|D|-1)} \;\leq\; n^{-1}|D|^{\frac{1}{2}}. \tag{7.10}$$

From Theorem 7.1.1, the WCC bounds of $\mathcal{O}(n^2\epsilon^{-2})$ (derived in [38] for smooth, non-convex functions) and of $\mathcal{O}(n^2\epsilon^{-1})$ (derived in Chapter 4 for smooth, convex functions) are optimal in the power of n^2, in the sense that no PSS will provide a better power than $D_\oplus$.

[1]We are grateful to Professor Károly Böröczky, Jr. for drawing our attention to these references.

Chapter 8

Concluding remarks

To our knowledge it is the second time that a derivative-free method is shown to exhibit a worst case complexity (WCC) bound of $\mathcal{O}(\epsilon^{-1})$ in the convex case, following the random Gaussian approach [30], but the first time for a deterministic approach. In fact we have proved that a maximum of $\mathcal{O}(\epsilon^{-1})$ iterations and $\mathcal{O}(n^2\epsilon^{-1})$ function evaluations are required to compute a point for which the norm of the gradient of the objective function f is smaller than $\epsilon \in (0,1)$ (see Theorem 4.4.1 and Corollary 4.4.1 when $p = 2$ in the forcing function).

In addition we proved that the absolute error $f(x_k) - f_*$ decreases at a sub-linear rate of $1/k$ (see Theorem 4.3.1). Such results are global in the sense of not depending on the proximity of the initial iterate to the solutions set.

These WCC bounds and global rates were proved when the solutions set is bounded or, when that is not the case, when the longest distance from the initial level set to the solutions set is bounded (Assumption 4.2.1). A particular case is strong convexity where the solution set is a singleton. In such a case, we went a step further (when $p = 2$ in the forcing function) and showed that $f(x_k) - f_*$ decreases r-linearly and so does $\|x_k - x_*\|$ (see Theorem 5.1.2).

In Chapter 6 we tested Algorithm 3.1.1 on some specific convex examples. In our experiments, the actual number of function evaluations was far below the theoretical WCC bound when Assumption 4.2.1 was violated. This encourages us to extend the results of this dissertation to an even weaker version of Assumption 4.2.1, possibly by controlling the step size in the algorithm so that the distance of the current iterate to the starting point is better monitored.

We also observed that although the WCC bounds become worse by changing some problem parameters, the actual performance of the algorithm does not follow the same trend. In fact the structure of the objective function does influence the performance of the algorithm heavily. This observation suggests that we could refine the theory for problems with special structure like separability or partial separability.

In Chapter 7, we proved the optimality of $D_\oplus$ in the sense of minimizing the order n^2 in the WCC bound for the number of function evaluations. We did this by establishing a lower bound for the value of problem (7.1), but this problem is itself still open. A closely related problem is

$$\max_{D \in \mathcal{D}(m)} \operatorname{cm}(D), \tag{8.1}$$

where $\mathcal{D}(m)$ is the set of all the PSSs consisting of m directions ($m \geq n+1$). This problem is also widely open. In the language of sphere covering, problem (8.1) is: find the most 'economical' covering of the sphere by m equal spherical caps. In the special case of $m = 2n$, it is intuitive to conjecture that $D_\oplus$ is the solution to problem (8.1). This is clear when $n = 2$, but it becomes non-trivial when $n \geq 3$. The optimality of $D_\oplus$ for the case $m = 2n$ is already proved when $n = 3$ (see [37, Theorem 5.4.1]), and $n = 4$ (see [16, Theorem 6.7.1]), but it is open when $n \geq 5$ according to [5, Page 194], [6], and [7, Conjecture 1.3].

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