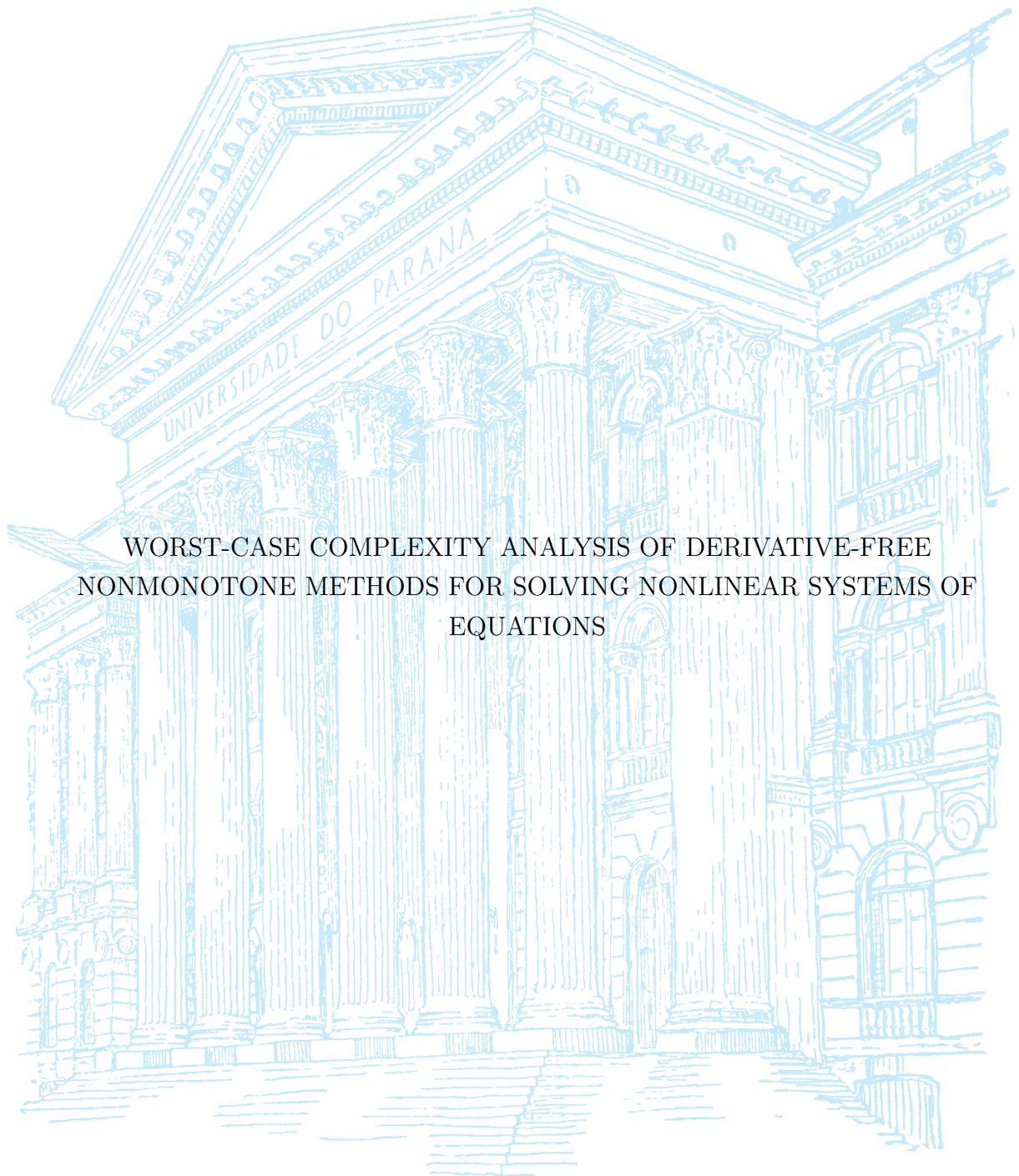


UNIVERSIDADE FEDERAL DO PARANÁ
FLÁVIA CHOROBURA



WORST-CASE COMPLEXITY ANALYSIS OF DERIVATIVE-FREE
NONMONOTONE METHODS FOR SOLVING NONLINEAR SYSTEMS OF
EQUATIONS

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FLÁVIA CHOROBURA

WORST-CASE COMPLEXITY ANALYSIS OF DERIVATIVE-FREE
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EQUATIONS

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Orientador: Prof. Dr. Geovani Nunes Grapiglia.

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A outorga do título de mestre está sujeita à homologação pelo colegiado, ao atendimento de todas as indicações e correções solicitadas pela banca e ao pleno atendimento das demandas regimentais do Programa de Pós-Graduação.

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RESUMO

Nesta dissertação estudamos uma classe geral de métodos não-monótonos sem derivadas para solução de sistemas de equações não-lineares, incluindo o método N-DF-SANE proposto em (IMA J. Numer. Anal. 29: 814–825, 2009). Esses métodos correspondem à métodos de otimização sem derivadas aplicados à minimização de uma função mérito conveniente. O comportamento não-monótono é controlado por duas sequências de parâmetros que definem os procedimentos de busca linear. Supondo que a função que define as equações não-lineares possui Jacobiana Lipschitz, mostramos que os métodos da referida classe precisam de no máximo $\mathcal{O}(|\log(\epsilon)|\epsilon^{-2})$ avaliações da função para gerarem um ponto estacionário da função mérito com precisão $\epsilon > 0$. A generalidade da nossa análise permite mais liberdade para o desenvolvimento de novos métodos em termos das escolhas para as sequências que controlam o comportamento não-monótono dos valores da função mérito. Essa característica é ilustrada por experimentos numéricos preliminares incluindo novas variantes do método N-DF-SANE.

Palavras-chave: *sistemas não-lineares de grande porte, métodos não-monótonos, métodos sem derivadas, complexidade de pior caso*

ABSTRACT

In this dissertation we study a wide class of derivative-free nonmonotone methods for solving nonlinear systems of equations, covering the method N-DF-SANE proposed in (IMA J. Numer. Anal. 29: 814–825, 2009). These methods correspond to derivative-free optimization methods applied to the minimization of a suitable merit function. The non-monotonicity is controlled by two sequences of parameters that define the line-search procedure. Assuming that the mapping defining the nonlinear equations has Lipschitz continuous Jacobian, we show that the methods in the referred class need at most $\mathcal{O}(|\log(\epsilon)|\epsilon^{-2})$ function evaluations to generate an ϵ -approximate stationary point of the merit function. The generality of our analysis allows more freedom for the design of new methods in terms of the choices for the sequences that control the nonmonotone behavior of the merit function values. This feature is illustrated by preliminary numerical experiments including new variants of the method N-DF-SANE.

Keywords: *large scale nonlinear systems, nonmonotone methods, derivative-free methods, worst-case complexity*

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Introduction

In this dissertation we study methods to solve nonlinear equations of the form

$$F(x) = 0, \tag{1}$$

where $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a continuously differentiable mapping. Several problems in Engineering, Statistics, Economy and Chemistry can be reduced to the solution of nonlinear equations [4]. Moreover, nonlinear equations also arise in the numerical solution of certain differential equations [7, 10, 15].

The main iterative scheme for solving (1) is Newton's method [14]. Its advantage is that it converges very fast starting from a good initial guess. However, when the dimension n is very large, Newton's method becomes very expensive since its execution requires the computation and storage of the Jacobian matrix of $F(\cdot)$, and also the solution of a large-scale linear system at each iteration. Thus, in this work, we are interested in derivative-free methods for solving (1), that is, methods that do not require the use of the Jacobians of $F(\cdot)$ neither the solution of linear systems. Specifically, we focus on derivative-free nonmonotone spectral methods [2, 8].

The Spectral Approach for Nonlinear Equations (SANE) was introduced by La Cruz and Raydan [9]. Subsequently, La Cruz, Martínez and Raydan [8] presented a derivative-free version of SANE, which they called DF-SANE. The latter method uses a derivative-free version of the nonmonotone line-search proposed by Grippo, Lampariello and Lucidi [6]. Another derivative-free variant of SANE, called N-DF-SANE, was proposed by Cheng and Li [2], in which they use a derivative-free version of the nonmonotone line-search proposed by Zhang and Hager [17]. Numerical experiments reported in [2] indicated that N-DF-SANE was often better than DF-SANE in terms of the number of function evaluations and the CPU time.

Motivated by these observations, in this dissertation we study a class of derivative-free nonmonotone methods for solving (1) that includes the N-DF-SANE method. More specifically, we analyze the worst-case complexity of these methods. In the context of derivative-based methods¹, worst-case complexity bounds of $\mathcal{O}(\epsilon^{-2})$ or $\mathcal{O}(|\log(\epsilon)|\epsilon^{-2})$

¹By *derivative-based* methods we mean methods that make explicit use of the Jacobian matrix of $F(\cdot)$ or its product with some vector.

have been obtained in [16, 18, 11, 1]. Under the assumption that the Jacobian of $F(\cdot)$ is Lipschitz continuous, we show that the methods in the referred class need at most $\mathcal{O}(|\log(\epsilon)|\epsilon^{-2})$ function evaluations to generate an ϵ -approximate stationary point of the merit function $f(x) = (1/2)\|F(x)\|_2^2$.

In the methods analyzed, the nonmonotonicity is controlled by two sequences of parameters that define the line-search procedure. The generality of our analysis allows more freedom for the design of new methods in terms of the choices for these sequences. This feature is illustrated by preliminary numerical experiments including new variants of the method N-DF-SANE applied to a subset of the Moré-Garbow-Hillstom [12] test problems.

This dissertation is organized as follows. In Chapter 1, we analyze the worst-case complexity of a general class of derivative-free non-monotone method. In Chapter 2, we present a particular case that englobes N-DF-SANE method. In Chapter 3, we present the numerical experiments.

Chapter 1

General Class of Nonmonotone Algorithms

In what follows, we will consider the merit function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ defined by

$$f(x) = \frac{1}{2} \|F(x)\|_2^2. \quad (1.1)$$

Our analysis will be carried out for the general algorithm described below.

Algorithm 1. (General Nonmonotone Method)

Step 0. Given a starting point $x_0 \in \mathbb{R}^n$ and constants $\beta \in (0, 1)$ and $\rho > 0$, choose a sequence $\{\theta_k\}_{k \geq 0}$ of positive numbers satisfying

$$\sum_{k=0}^{+\infty} \theta_k \leq \theta < +\infty, \quad (1.2)$$

and set $k := 0$.

Step 1. Compute $\sigma_k \neq 0$ such that $|\sigma_k| \in [\sigma_{min}, \sigma_{max}]$, with $0 < \sigma_{min} \leq \sigma_{max} < +\infty$.

Step 2.1. Set $\ell := 0$ and choose $\nu_k \geq 0$.

Step 2.2. If

$$f(x_k - \beta^\ell \sigma_k F(x_k)) \leq f(x_k) + \nu_k + \theta_k - \rho (\beta^\ell)^2 f(x_k), \quad (1.3)$$

then, set $\ell_k = \ell$, $\alpha_k = \beta^{\ell_k}$, $d_k = -\sigma_k F(x_k)$ and go to Step 3. Otherwise, go to Step 2.3.

Step 2.3. If

$$f(x_k + \beta^\ell \sigma_k F(x_k)) \leq f(x_k) + \nu_k + \theta_k - \rho (\beta^\ell)^2 f(x_k), \quad (1.4)$$

then set $\ell_k = \ell$, $\alpha_k = \beta^{\ell_k}$, $d_k = \sigma_k F(x_k)$ and go to Step 3. Otherwise, set $\ell := \ell + 1$, and go to Step 2.2.

Step 3. Set $x_{k+1} = x_k + \alpha_k d_k$, $k := k + 1$ and go to Step 1.

Let us define the stationarity measure

$$\psi(x) = \begin{cases} \min \left\{ \|F(x)\|, \frac{|\langle \nabla f(x), F(x) \rangle|}{\|F(x)\|} \right\}, & \text{whenever } F(x) \neq 0, \\ 0, & \text{otherwise.} \end{cases} \quad (1.5)$$

In Algorithm 1, we want to find x^* such that $\psi(x^*) = 0$.

Remark 1.1. If $F(x^*) = 0$ then, by (1.5) we have $\psi(x^*) = 0$. However, the converse is not necessarily true, since we may have $\langle \nabla f(x^*), F(x^*) \rangle = 0$ with $F(x^*) \neq 0$ and $\nabla f(x^*) \neq 0$. For example, consider $F(z) = F(x, y) = (\sin^2 x, y - 1)$. We have

$$J(z) = \begin{pmatrix} 2 \sin(x) \cos(x) & 0 \\ 0 & 1 \end{pmatrix}.$$

At the point $z^* = \left(\frac{3\pi}{4}, \frac{3}{2}\right)$, we have that $F(z^*) = \left(\frac{1}{2}, \frac{1}{2}\right)$,

$$J(z^*) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

and $\nabla f(z^*) = J(z^*)^T F(z^*) = \left(-\frac{1}{2}, \frac{1}{2}\right)$. This implies that $\langle \nabla f(z^*), F(z^*) \rangle = 0$, hence $\psi(z^*) = 0$ but $F(z^*) \neq 0$ and $\nabla f(z^*) \neq 0$.

Let us consider the following assumptions:

A1 The mapping $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is continuously differentiable and its Jacobian $J : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}$ is L_J -Lipschitz continuous.

A2 $\sum_{k=0}^{+\infty} \nu_k \leq \nu < +\infty$.

A3 The level set $\mathcal{L}_f(x_0) := \{x \in \mathbb{R}^n : f(x) \leq f(x_0) + \nu + \theta\}$ is bounded as follows

$$\sup \{\|x - x_0\| : x \in \mathcal{L}_f(x_0)\} \equiv D_0 < +\infty.$$

Remark 1.2. Under A3, if $\bar{x} \in \text{co}(\mathcal{L}_f(x_0))$ (i.e., if $\bar{x}$ belongs to the convex hull of $\mathcal{L}_f(x_0)$) then $\|\bar{x} - x_0\| \leq D_0$.

Remark 1.3. Combining (1.3), (1.4), (1.2) and A2, if $\{x_k\}_{k=0}^N$ is well-defined, then

$$f(x_k) \leq f(x_0) + \sum_{i=0}^{k-1} \nu_i + \sum_{i=0}^{k-1} \theta_i \leq f(x_0) + \nu + \theta,$$

for all $k \in \{1, \dots, N\}$. Thus, we have $\{x_k\}_{k=0}^N \subset \mathcal{L}_f(x_0)$ and so, under A3, $\|x_k - x_0\| \leq D_0$ for all $k \geq 0$.

Lemma 1.1. *Suppose that A1-A3 hold. Then, for function $f(\cdot)$ in (1.1) we have*

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \leq \frac{L}{2} \|y - x\|^2, \quad \forall x, y \in \mathcal{L}_f(x_0), \quad (1.6)$$

where

$$L = (L_J D_0 + \|J(x_0)\|)^2 + L_J [(L_J D_0 + \|J(x_0)\|) D_0 + \|F(x_0)\|]. \quad (1.7)$$

Proof. To obtain (1.6), it is enough to show that $\nabla f(\cdot)$ is L -Lipschitz continuous on $\text{co}(\mathcal{L}_f(x_0))$. Given $x, y \in \text{co}(\mathcal{L}_f(x_0))$,

$$\begin{aligned} \|\nabla f(x) - \nabla f(y)\| &= \|J(x)^T F(x) - J(y)^T F(y)\| \\ &\leq \|J(x)^T F(x) - J(x)^T F(y)\| + \|J(x)^T F(y) - J(y)^T F(y)\| \\ &\leq \|J(x)\| \|F(x) - F(y)\| + \|J(x) - J(y)\| \|F(y)\|. \end{aligned} \quad (1.8)$$

From A1 and Remark 1.2, we get

$$\begin{aligned} \|J(\bar{x})\| &\leq \|J(\bar{x}) - J(x_0)\| + \|J(x_0)\| \leq L_J \|\bar{x} - x_0\| + \|J(x_0)\| \\ &\leq L_J D_0 + \|J(x_0)\|, \quad \forall \bar{x} \in \text{co}(\mathcal{L}_f(x_0)). \end{aligned} \quad (1.9)$$

Thus, by the Mean Value Inequality and A3, we have

$$\|F(x) - F(y)\| \leq (L_J D_0 + \|J(x_0)\|) \|x - y\|, \quad (1.10)$$

and

$$\|F(y)\| \leq \|F(y) - F(x_0)\| + \|F(x_0)\| \leq (L_J D_0 + \|J(x_0)\|) D_0 + \|F(x_0)\|. \quad (1.11)$$

Finally, combining (1.8)-(1.11) and A1, we obtain

$$\begin{aligned} \|\nabla f(x) - \nabla f(y)\| &\leq (L_J D_0 + \|J(x_0)\|)^2 \|x - y\| \\ &\quad + L_J [(L_J D_0 + \|J(x_0)\|) D_0 + \|F(x_0)\|] \|x - y\|, \end{aligned}$$

and so, (1.6) holds for L given in (1.7). □

The next lemma guarantees that the iterates of Algorithm 1 are well-defined.

Lemma 1.2. *Suppose that A1-A3 hold and let x_k ($k \geq 0$) be an iterate in Algorithm 1. If $\langle \nabla f(x_k), F(x_k) \rangle \neq 0$ and*

$$0 < \alpha \leq \frac{2|\langle \nabla f(x_k), \sigma_k F(x_k) \rangle|}{(\rho + L\sigma_{max}^2) \|F(x_k)\|^2}, \quad (1.12)$$

with L defined in the Lemma 1.1, then

$$\min \{f(x_k + \alpha \sigma_k F(x_k)), f(x_k - \alpha \sigma_k F(x_k))\} \leq f(x_k) + \nu_k + \theta_k - \rho \alpha^2 f(x_k). \quad (1.13)$$

Proof. Let us divide the proof in two cases.

Case I: $\langle \nabla f(x_k), \sigma_k F(x_k) \rangle < 0$.

In this case, we will show that

$$f(x_k + \alpha \sigma_k F(x_k)) \leq f(x_k) + \nu_k + \theta_k - \rho \alpha^2 f(x_k). \quad (1.14)$$

For that, assume by contradiction that (1.14) is not true, that is,

$$f(x_k + \alpha \sigma_k F(x_k)) > f(x_k) + \nu_k + \theta_k - \rho \alpha^2 f(x_k). \quad (1.15)$$

Let us define

$$\xi_1(t) := f(x_k + t \sigma_k F(x_k)) - [f(x_k) + \nu_k + \theta_k - \rho t^2 f(x_k)].$$

Then, by (1.15), we have $\xi_1(0) = -\nu_k - \theta_k < 0 < \xi_1(\alpha)$. Consequently, by the Intermediate Value Theorem, there exists $\hat{\alpha} \in (0, \alpha)$ such that $\xi_1(\hat{\alpha}) = 0$, that is,

$$f(x_k + \hat{\alpha} \sigma_k F(x_k)) = f(x_k) + \nu_k + \theta_k - \rho(\hat{\alpha})^2 f(x_k). \quad (1.16)$$

By Remark 1.3 and (1.16), we have $x_k, x_k + \hat{\alpha} \sigma_k F(x_k) \in \mathcal{L}_f(x_0)$. Then, combining (1.16) and Lemma 1.1, it follows that

$$\begin{aligned} -\rho(\hat{\alpha})^2 f(x_k) &\leq f(x_k + \hat{\alpha} \sigma_k F(x_k)) - f(x_k) \\ &\leq \hat{\alpha} \langle \nabla f(x_k), \sigma_k F(x_k) \rangle + \frac{L(\hat{\alpha})^2}{2} \|\sigma_k F(x_k)\|^2 \\ \implies -\rho \hat{\alpha} f(x_k) &\leq \langle \nabla f(x_k), \sigma_k F(x_k) \rangle + \frac{L \hat{\alpha} \sigma_{max}^2}{2} \|F(x_k)\|^2 \\ \implies -\langle \nabla f(x_k), \sigma_k F(x_k) \rangle &\leq \hat{\alpha} \left(\frac{\rho + L \sigma_{max}^2}{2} \right) \|F(x_k)\|^2 \\ \implies \hat{\alpha} &\geq -\frac{2 \langle \nabla f(x_k), \sigma_k F(x_k) \rangle}{(\rho + L \sigma_{max}^2) \|F(x_k)\|^2} = \frac{2 |\langle \nabla f(x_k), \sigma_k F(x_k) \rangle|}{(\rho + L \sigma_{max}^2) \|F(x_k)\|^2}. \end{aligned}$$

Since $\alpha > \hat{\alpha}$, it follows that

$$\alpha > \frac{2 |\langle \nabla f(x_k), \sigma_k F(x_k) \rangle|}{(\rho + L \sigma_{max}^2) \|F(x_k)\|^2},$$

contradicting (1.12). Thus, (1.14) must be true.

Case II: $\langle \nabla f(x_k), \sigma_k F(x_k) \rangle > 0$.

In this case, we will show that

$$f(x_k - \alpha \sigma_k F(x_k)) \leq f(x_k) + \nu_k + \theta_k - \rho \alpha^2 f(x_k). \quad (1.17)$$

For that, assume by contradiction that (1.17) is not true, that is,

$$f(x_k - \alpha \sigma_k F(x_k)) > f(x_k) + \nu_k + \theta_k - \rho \alpha^2 f(x_k). \quad (1.18)$$

Let us define

$$\xi_2(t) := f(x_k - t \sigma_k F(x_k)) - [f(x_k) + \nu_k + \theta_k - \rho t^2 f(x_k)].$$

Then, by (1.18), we have $\xi_2(0) = -\nu_k - \theta_k < 0 < \xi_2(\alpha)$. Consequently, by the Intermediate Value Theorem, there exists $\bar{\alpha} \in (0, \alpha)$ such that $\xi_2(\bar{\alpha}) = 0$, that is,

$$f(x_k - \bar{\alpha} \sigma_k F(x_k)) = f(x_k) + \nu_k + \theta_k - \rho(\bar{\alpha})^2 f(x_k). \quad (1.19)$$

As in Case I, by Remark 1.3, (1.19) and Lemma 1.1, we obtain

$$\begin{aligned} -\rho(\bar{\alpha})^2 f(x_k) &\leq f(x_k - \bar{\alpha} \sigma_k F(x_k)) - f(x_k) \\ &\leq -\bar{\alpha} \langle \nabla f(x_k), \sigma_k F(x_k) \rangle + \frac{L(\bar{\alpha})^2}{2} \|\sigma_k F(x_k)\|^2 \\ \implies -\rho \bar{\alpha} f(x_k) &\leq -\langle \nabla f(x_k), \sigma_k F(x_k) \rangle + \frac{L \bar{\alpha} \sigma_{max}^2}{2} \|F(x_k)\|^2 \\ \implies \langle \nabla f(x_k), \sigma_k F(x_k) \rangle &\leq \bar{\alpha} \left(\frac{\rho + L \sigma_{max}^2}{2} \right) \|F(x_k)\|^2 \\ \implies \bar{\alpha} &\geq \frac{2 \langle \nabla f(x_k), \sigma_k F(x_k) \rangle}{(\rho + L \sigma_{max}^2) \|F(x_k)\|^2} = \frac{2 |\langle \nabla f(x_k), \sigma_k F(x_k) \rangle|}{(\rho + L \sigma_{max}^2) \|F(x_k)\|^2}. \end{aligned}$$

Since $\alpha > \bar{\alpha}$, it follows that

$$\alpha > \frac{2 |\langle \nabla f(x_k), \sigma_k F(x_k) \rangle|}{(\rho + L \sigma_{max}^2) \|F(x_k)\|^2},$$

contradicting (1.12). Thus, (1.17) must be true. $\square$

From Lemma 1.2, we can obtain a lower bound for α_k in Algorithm 1.

Lemma 1.3. *Suppose that A1-A3 hold and let x_k be an iterate in Algorithm 1. If $\langle \nabla f(x_k), F(x_k) \rangle \neq 0$, then*

$$\alpha_k \geq \min \left\{ 1, \frac{2\beta \sigma_{min} |\langle \nabla f(x_k), F(x_k) \rangle|}{(\rho + L \sigma_{max}^2) \|F(x_k)\|^2} \right\}. \quad (1.20)$$

Proof. If $\ell_k = 0$, then $\alpha_k = 1$ and (1.20) holds. If $\ell_k > 0$, it follows from Step 2 of Algorithm 1 that

$$\min \{f(x_k + \beta^{\ell_k-1} \sigma_k F(x_k)), f(x_k - \beta^{\ell_k-1} \sigma_k F(x_k))\} > f(x_k) + \nu_k + \theta_k - \rho (\beta^{\ell_k-1})^2 f(x_k).$$

In view of Lemma 1.2, we must have

$$\beta^{\ell_k-1} > \frac{2|\langle \nabla f(x_k), \sigma_k F(x_k) \rangle|}{(\rho + L\sigma_{max}^2) \|F(x_k)\|^2}$$

and so

$$\alpha_k = \beta^{\ell_k-1} \beta > \frac{2\beta |\langle \nabla f(x_k), \sigma_k F(x_k) \rangle|}{(\rho + L\sigma_{max}^2) \|F(x_k)\|^2}.$$

In this case, the conclusion (1.20) follows from the inequality above and $|\sigma_k| \geq \sigma_{min}$. $\square$

The theorem below establishes that, given $\epsilon > 0$, Algorithm 1 takes at most $\mathcal{O}(\epsilon^{-2})$ iterations to generate x_k such that $\psi(x_k) \leq \epsilon$.

Theorem 1.1. *Suppose that A1-A3 hold and let $\{x_k\}_{k \geq 0}$ be generated by Algorithm 1. Given $\epsilon > 0$, the number of elements of the set*

$$\Omega(\epsilon) = \{k : \psi(x_k) > \epsilon\} \tag{1.21}$$

is bounded as follows

$$|\Omega(\epsilon)| \leq \frac{2(f(x_0) + \nu + \theta)}{\rho \min \left\{ 1, \frac{2\beta\sigma_{min}}{\rho + L\sigma_{max}^2} \right\}^2} \epsilon^{-2}. \tag{1.22}$$

Proof. By Steps 2 and 3 of Algorithm 1 and Lemma 1.3, if $k \in \Omega(\epsilon)$, we have

$$\begin{aligned} \theta_k + \nu_k + f(x_k) - f(x_{k+1}) &\geq \rho \alpha_k^2 f(x_k) \\ &\geq \rho \min \left\{ 1, \left(\frac{2\beta\sigma_{min}}{\rho + L\sigma_{max}^2} \right)^2 \frac{|\langle \nabla f(x_k), F(x_k) \rangle|^2}{\|F(x_k)\|^4} \right\} f(x_k) \\ &= \rho \min \left\{ \frac{1}{2} \|F(x_k)\|^2, \left(\frac{2\beta\sigma_{min}}{\rho + L\sigma_{max}^2} \right)^2 \frac{|\langle \nabla f(x_k), F(x_k) \rangle|^2}{2\|F(x_k)\|^2} \right\} \\ &\geq \frac{\rho}{2} \min \left\{ 1, \left(\frac{2\beta\sigma_{min}}{\rho + L\sigma_{max}^2} \right)^2 \right\} \min \left\{ \|F(x_k)\|, \frac{|\langle \nabla f(x_k), F(x_k) \rangle|}{\|F(x_k)\|} \right\}^2 \\ &= \frac{\rho}{2} \min \left\{ 1, \left(\frac{2\beta\sigma_{min}}{\rho + L\sigma_{max}^2} \right)^2 \right\} \psi(x_k)^2 \\ &> \frac{\rho}{2} \min \left\{ 1, \left(\frac{2\beta\sigma_{min}}{\rho + L\sigma_{max}^2} \right)^2 \right\} \epsilon^2. \end{aligned} \tag{1.23}$$

Then, combining (1.23), (1.2) and A2, it follows that

$$\begin{aligned}
\frac{\rho}{2} \min \left\{ 1, \left(\frac{2\beta\sigma_{\min}}{\rho + L\sigma_{\max}^2} \right)^2 \right\} \epsilon^2 |\Omega(\epsilon)| &= \sum_{k \in \Omega(\epsilon)} \frac{\rho}{2} \min \left\{ 1, \left(\frac{2\beta\sigma_{\min}}{\rho + L\sigma_{\max}^2} \right)^2 \right\} \epsilon^2 \\
&\leq \sum_{k=0}^{+\infty} (f(x_k) - f(x_{k+1}) + \nu_k + \theta_k) \\
&\leq f(x_0) + \sum_{k=0}^{+\infty} \nu_k + \sum_{k=0}^{+\infty} \theta_k \\
&\leq f(x_0) + \nu + \theta.
\end{aligned}$$

Therefore, $\Omega(\epsilon)$ satisfies (1.22). $\square$

Remark 1.4. Let N_k be the number of function evaluations at the k -th iteration of Algorithm 1. Note that $N_k \leq 2(\ell_k + 1)$. If $\psi(x_k) > \epsilon$ with $\epsilon \in (0, 1)$, then, by Lemma 1.3 and (1.11), we have

$$\begin{aligned}
\alpha_k &= \beta^{l_k} \geq \min \left\{ 1, \frac{2\beta\sigma_{\min} |\langle \nabla f(x_k), F(x_k) \rangle|}{(\rho + L\sigma_{\max}^2) \|F(x_k)\|^2} \right\} \\
&\geq \min \left\{ 1, \frac{2\beta\sigma_{\min}}{(\rho + L\sigma_{\max}^2) [(L_J D_0 + \|J(x_0)\|) D_0 + \|F(x_0)\|]} \frac{|\langle \nabla f(x_k), F(x_k) \rangle|}{\|F(x_k)\|} \right\} \\
&> \min \left\{ 1, \frac{2\beta\sigma_{\min}\epsilon}{(\rho + L\sigma_{\max}^2) [(L_J D_0 + \|J(x_0)\|) D_0 + \|F(x_0)\|]} \right\} \\
&\geq \min \left\{ 1, \frac{2\beta\sigma_{\min}}{(\rho + L\sigma_{\max}^2) [(L_J D_0 + \|J(x_0)\|) D_0 + \|F(x_0)\|]} \right\} \epsilon \equiv \kappa_c \epsilon.
\end{aligned}$$

Consequently,

$$N_k \leq 2(\ell_k + 1) \leq 2 + \frac{2 \log(\kappa_c \epsilon)}{\log(\beta)}.$$

Combining this result with Theorem 1.1 it follows that Algorithm 1 performs at most $\mathcal{O}(|\log(\epsilon)|\epsilon^{-2})$ evaluations of $f(\cdot)$ to generate the first iterate x_k for which $\psi(x_k) \leq \epsilon$.

Corollary 1.1. Suppose that A1-A3 hold and let $\{x_k\}_{k \geq 0}$ be generated by Algorithm 1. Then $\{x_k\}$ has a limit point x^* such that $\psi(x^*) = 0$.

Proof. First, let us show that

$$\lim_{k \rightarrow +\infty} \psi(x_k) = 0. \quad (1.24)$$

Indeed, if we assume that (1.24) does not hold, then there exist $\epsilon > 0$ and a subsequence $\{x_{k_j}\}_{j \in \mathbb{N}}$ of $\{x_k\}$ such that

$$\psi(x_{k_j}) > \epsilon, \quad \forall j \in \mathbb{N}.$$

Consequently, for this ϵ , we would have $|\Omega(\epsilon)| = +\infty$, contradicting Theorem 1.1. Therefore, (1.24) is true. Since $\{x_k\} \subset \mathcal{L}_f(x_0)$, it follows from A3 that $\{x_k\}_{k \in \mathbb{N}}$ is bounded.

Thus, $\{x_k\}$ possess a subsequence $\{x_{k_\ell}\}_{\ell \in \mathbb{N}}$ that is convergent, let us say

$$\lim_{\ell \rightarrow +\infty} x_{k_\ell} = x^*. \quad (1.25)$$

Notice that $\psi(\cdot)$ is continuous. Hence, combining (1.24) and (1.25) we conclude that $\psi(x^*) = 0$. $\square$

Remark 1.5. Notice that if the mapping F is strictly monotone, then $J(x)$ is positive-definite and so

$$\begin{aligned} \psi(x^*) = 0 &\Rightarrow F(x^*) = 0 \text{ or } \langle \nabla f(x^*), F(x^*) \rangle = 0 \\ &\Rightarrow F(x^*) = 0 \text{ or } F(x^*)^T J(x^*) F(x^*) = 0 \\ &\Rightarrow F(x^*) = 0. \end{aligned}$$

Therefore, when F is strictly monotone, at least one limit point of any sequence $\{x_k\}_{k \geq 0}$ generated by Algorithm 1 is a zero of F .

Chapter 2

A Subclass of Nonmonotone Algorithms

Let us consider now the following algorithmic framework:

Algorithm 2.

Step 0. Given a starting point $x_0 \in \mathbb{R}^n$ and constants $\delta_{min}, \beta \in (0, 1)$ and $\rho > 0$, choose a sequence $\{\theta_k\}_{k \geq 0}$ of positive numbers satisfying $\sum_{k=0}^{+\infty} \theta_k \leq \theta < +\infty$, set $C_0 = f(x_0)$ and $k := 0$.

Step 1. Compute $\sigma_k \neq 0$ such that $|\sigma_k| \in [\sigma_{min}, \sigma_{max}]$, with $0 < \sigma_{min} \leq \sigma_{max} < +\infty$.

Step 2.1. Set $\ell := 0$.

Step 2.2. If

$$f(x_k - \beta^\ell \sigma_k F(x_k)) \leq C_k + \theta_k - \rho (\beta^\ell)^2 f(x_k), \quad (2.1)$$

then set $\ell_k = \ell$, $\alpha_k = \beta^{\ell_k}$, $d_k = -\sigma_k F(x_k)$ and go to Step 3. Otherwise, go to Step 2.3.

Step 2.3. If

$$f(x_k + \beta^\ell \sigma_k F(x_k)) \leq C_k + \theta_k - \rho (\beta^\ell)^2 f(x_k), \quad (2.2)$$

then set $\ell_k = \ell$, $\alpha_k = \beta^{\ell_k}$, $d_k = \sigma_k F(x_k)$ and go to Step 3. Otherwise, set $\ell := \ell + 1$ and go to Step 2.2.

Step 3. Set $x_{k+1} = x_k + \alpha_k d_k$, compute $\delta_{k+1} \in [\delta_{min}, 1]$, set

$$C_{k+1} = (1 - \delta_{k+1})(C_k + \theta_k) + \delta_{k+1} f(x_{k+1}), \quad (2.3)$$

$k := k + 1$ and go to Step 1.

In Algorithm 2, different choices for δ_{k+1} , give different nonmonotone terms C_k and,

consequently, different nonmonotone algorithms. For example, consider the choice

$$\delta_{k+1} = \frac{1}{\eta_k Q_k + 1},$$

where $Q_0 = 1$, $Q_{k+1} = \eta_k Q_k + 1$ and $\eta_k \in [\eta_{\min}, \eta_{\max}]$ with $0 \leq \eta_{\min} \leq \eta_{\max} < 1$. In this case we have

$$\begin{aligned} Q_0 &= 1 \\ Q_1 &= 1 + \eta_0 \\ Q_2 &= 1 + \eta_1 Q_1 = 1 + \eta_1 + \eta_1 \eta_0 \\ Q_3 &= 1 + \eta_2 Q_2 = 1 + \eta_2 + \eta_2 \eta_1 + \eta_2 \eta_1 \eta_0 \\ &\vdots \\ Q_{k+1} &= 1 + \sum_{j=0}^k \prod_{i=0}^j \eta_{k-i}. \end{aligned}$$

Since $\eta_k \in [0, \eta_{\max}]$ for all k , it follows that

$$\begin{aligned} Q_{k+1} &\leq 1 + \sum_{j=0}^k \prod_{i=0}^j \eta_{\max} \\ &\leq 1 + \sum_{j=0}^k \eta_{\max}^{j+1} \\ &\leq \sum_{j=0}^{+\infty} \eta_{\max}^j \\ &= \frac{1}{1 - \eta_{\max}}. \end{aligned}$$

which gives

$$\delta_{k+1} = \frac{1}{Q_{k+1}} \geq 1 - \eta_{\max} \equiv \delta_{\min}.$$

Moreover, the corresponding updating rule for the nonmonotone terms is

$$\begin{aligned} C_{k+1} &= (1 - \delta_{k+1})(C_k + \theta_k) + \delta_{k+1} f(x_{k+1}) \\ &= \frac{\eta_k Q_k}{\eta_k Q_k + 1} (C_k + \theta_k) + \frac{f(x_{k+1})}{\eta_k Q_k + 1} \\ &= \frac{\eta_k Q_k (C_k + \theta_k) + f(x_{k+1})}{Q_{k+1}}. \end{aligned}$$

This is exactly how the nonmonotone terms are defined in the Algorithm N-DF-SANE proposed by Cheng and Li [2]. Therefore, N-DF-SANE is a particular instance of Algo-

rithm 2.

Our next lemma establishes that Algorithm 2 is a particular case of Algorithm 1 with the corresponding sequence $\{\nu_k\}$ satisfying A2. The proof is an adaptation of the proof of Theorem 4 in [5]

Lemma 2.1. *Let $\{C_k\}_{k \geq 0}$ be generated by Algorithm 2. Then,*

$$C_k = f(x_k) + \nu_k, \quad \forall k, \quad (2.4)$$

with

$$\nu_0 = 0 \quad \text{and} \quad \nu_{k+1} = (1 - \delta_{k+1})(f(x_k) + \nu_k + \theta_k) + (\delta_{k+1} - 1)f(x_{k+1}). \quad (2.5)$$

Moreover, the sequence $\{\nu_k\}_{k \geq 0}$ defined in (2.5) satisfies

$$\sum_{k=0}^{+\infty} \nu_k \leq \left(\frac{1 - \delta_{\min}}{\delta_{\min}} \right) (f(x_0) + \theta) \equiv \nu. \quad (2.6)$$

Proof. Since

$$C_0 = f(x_0) = f(x_0) + \nu_0,$$

it follows that (2.4) holds for $k = 0$. Assume that (2.4) is true for some $k \geq 0$. Then, by the induction assumption and (2.5) we have

$$\begin{aligned} C_{k+1} &= (1 - \delta_{k+1})(C_k + \theta_k) + \delta_{k+1}f(x_{k+1}) \\ &= (1 - \delta_{k+1})(f(x_k) + \nu_k + \theta_k) + \delta_{k+1}f(x_{k+1}) \\ &= f(x_{k+1}) + [(1 - \delta_{k+1})(f(x_k) + \nu_k + \theta_k) + (\delta_{k+1} - 1)f(x_{k+1})] \\ &= f(x_{k+1}) + \nu_{k+1}, \end{aligned}$$

that is, (2.4) also holds for $k + 1$. Therefore, (2.4) is true.

On the other hand, since

$$f(x_{k+1}) + \nu_{k+1} = C_{k+1} = f(x_k) + \nu_k + \theta_k - \delta_{k+1} [f(x_k) + \nu_k + \theta_k - f(x_{k+1})]$$

we have

$$\delta_{k+1} [f(x_k) + \nu_k + \theta_k - f(x_{k+1})] = (f(x_k) + \nu_k + \theta_k) - (f(x_{k+1}) + \nu_{k+1}).$$

Then, summing up the above equalities for $k = 0, \dots, N$ and using $f(x_{N+1}) \geq 0$ and

$\sum_{k=0}^{+\infty} \theta_k \leq \theta$, we obtain

$$\begin{aligned}
\sum_{k=0}^N \delta_{k+1} [f(x_k) + \nu_k + \theta_k - f(x_{k+1})] &\leq \sum_{k=0}^N f(x_k) - f(x_{k+1}) + \sum_{k=0}^N \theta_k \\
&\quad + \sum_{k=0}^N \nu_k - \nu_{k+1} \\
&= f(x_0) - f(x_{N+1}) + \sum_{k=0}^N \theta_k + \nu_0 - \nu_{N+1} \\
&\leq f(x_0) + \sum_{k=0}^{+\infty} \theta_k \\
&\leq f(x_0) + \theta.
\end{aligned} \tag{2.7}$$

Combining (2.7) and $\delta_{k+1} \geq \delta_{\min}$, it follows that

$$\begin{aligned}
\sum_{k=0}^N \nu_k = \sum_{k=0}^{N-1} \nu_{k+1} &\leq \sum_{k=0}^{N-1} \left(\frac{1 - \delta_{k+1}}{\delta_{k+1}} \right) \delta_{k+1} [f(x_k) + \nu_k + \theta_k - f(x_{k+1})] \\
&\leq \left(\frac{1 - \delta_{\min}}{\delta_{\min}} \right) \sum_{k=0}^{N-1} \delta_{k+1} [f(x_k) + \nu_k + \theta_k - f(x_{k+1})] \\
&\leq \left(\frac{1 - \delta_{\min}}{\delta_{\min}} \right) (f(x_0) + \theta).
\end{aligned}$$

Because $N \geq 0$ is arbitrary, we conclude that $\sum_{k=0}^{+\infty} \nu_k \leq \left(\frac{1 - \delta_{\min}}{\delta_{\min}} \right) (f(x_0) + \theta)$. $\square$

By Lemma 2.1, Algorithm 2 is a particular case of Algorithm 1 with $\{\nu_k\}$ satisfying A2. Combining this fact with Theorem 1.1 and Remark 1.4 we obtain the following result.

Theorem 2.1. *Suppose that A1 holds. If A3 holds for ν given in (2.6) then, given $\epsilon > 0$, Algorithm 2 needs at most $\mathcal{O}(|\log(\epsilon)|\epsilon^{-2})$ evaluations of $f(\cdot)$ to generate the first x_k such that $\psi(x_k) \leq \epsilon$.*

Chapter 3

Illustrative Numerical Results

In order to investigate the numerical performance of Algorithms 1 and 2, we performed some numerical numerical experiments comparing the following four MATLAB codes:

- **DF-SANE**: the nonmonotone algorithm in [8] that corresponds to Algorithm 1 with $\theta_k = \frac{\|F(x_0)\|}{(1+k)^2}$ and

$$\nu_k = \max_{0 \leq j \leq m(k)} [f(x_{k-j})] - f(x_k),$$

where $m(0) = 0$ and $m(k) = \min \{m(k-1) + 1, 10\}$. Note that this method is not covered by our theory.

- **N-DF-SANE**: the nonmonotone algorithm in [2] that corresponds to Algorithm 2 with $\theta_k = \frac{\|F(x_0)\|}{(1+k)^2}$ and

$$\delta_{k+1} = \frac{1}{\eta_k Q_k + 1},$$

where $Q_0 = 1$, $Q_{k+1} = \eta_k Q_k + 1$ and $\eta_k = 0.85$.

- **NM1**: Algorithm 2 with $\theta_k = \frac{\|F(x_0)\|}{(1+k)^2}$ and

$$\delta_{k+1} = 10^{-3}.$$

This choice of δ_{k+1} is inspired by [3]

- **NM2**: Algorithm 2 with $\theta_k = 0.8^{(k+1)}(k+1)^8 \|F(x_0)\|^2$ and

$$\delta_{k+1} = \max \left\{ 10^{-3}, \frac{\|F(x_k)\|^2}{\|F(x_k)\|^2 + 1} \right\}.$$

In all implementations we consider parameters $\sigma_{min} = 10^{-1}$, $\sigma_{max} = 10^{10}$, $\sigma_0 = 1$, $\beta = 0.5$ and $\rho = 10^{-4}$. The spectral stepsize σ_k is computed as in [8]. Specifically, let

$$\tilde{\sigma}_k = \frac{\langle s_k, s_k \rangle}{\langle s_k, y_k \rangle},$$

where $s_k = x_k - x_{k-1}$ and $y_k = F(x_k) - F(x_{k-1})$. We set $\sigma_k = \tilde{\sigma}_k$ whenever $|\tilde{\sigma}_k| \in [\sigma_{min}, \sigma_{max}]$. Otherwise, we set

$$\sigma_k = \begin{cases} 1, & \text{if } \|F(x_k)\| > 1, \\ \|F(x_k)\|^{-1}, & \text{if } 10^{-5} \leq \|F(x_k)\| \leq 1, \\ 10^5, & \text{if } \|F(x_k)\| < 10^{-5}. \end{cases}$$

The codes were applied to a set of 30 nonconvex test problems of unconstrained minimization [12], most of them highly nonlinear. In our tests, we applied the codes to find zeros of the gradients of these problems. We used the stopping rules

$$\frac{\|F(x_k)\|_2}{\|F(x_0)\|_2} \leq \epsilon, \quad \epsilon = 10^{-4},$$

and

$$k = k_{max} \equiv 2000.$$

Table 3.1 shows the number of function evaluations required by the codes for solving each test problem. An entry “F” indicates that the maximum number of 2000 iterations was reached. Table 3.2 contains a summary with the number of problems solved by each code and the number of problems in which each code was strictly better than the others in terms of function evaluations. As we can see, NM1 and NM2 (the new variants of N-DF-SANE covered by our theory) outperformed N-DF-SANE and DF-SANE.

For a complementary assessment of the codes, we also used the data profiles proposed in [13]. The convergence test for the codes is:

$$f(x_0) - f(x) \geq (1 - \tau)(f(x_0) - f_L), \quad (3.1)$$

where $\tau > 0$ is a tolerance, x_0 is the starting point for the problem, and f_L is computed for each problem as the smallest value of $f(\cdot)$ obtained by any solver within a given number of function evaluations. Let $t_{p,s}$ be the number of function evaluations required by solver s to satisfy the above convergence test for problem p . For each solver s we plot the graph of the corresponding *data profile* $d_s(\cdot)$ defined by

$$d_s(\alpha) = \frac{\text{number of problems for which } t_{p,s} \leq \alpha}{\text{total number of test problems}}.$$

Note that $d_s(\alpha)$ is the percentage of problems solved by solver s with α function evalua-

tions.

Specifically, we considered $\tau \in \{10^{-3}, 10^{-5}\}$ and a budget of 1000 function evaluations. The results in Figure 3.1 confirm the good performance of NM2.

Problem (n,m)	DF-SANE	N-DF-SANE	NM1	NM2
1. Rosenbrock (2,2)	123	F	741	460
2. Freudenstein-Roth (2,2)	339	240	114	69
3. Powell badly scaled (2,2)	56	56	56	56
4. Brown badly scaled (2,3)	F	F	F	F
5. Beale (2,3)	42	39	F	57
6. Jennrich-Sampson (2,10)	1	1	1	1
7. Helical valley (3,3)	348	207	76	109
8. Bard (3,15)	127	162	123	31
9. Gaussian (3,15)	7	7	7	9
10. Meyer (3,16)	40	40	40	40
11. Gulf (3,3)	1	1	1	1
12. Box (3,3)	28	27	27	27
13. Powell singular (4,4)	97	81	64	64
14. Wood (4,6)	64	62	62	62
15. Kowalik-Osborne (4,11)	516	442	225	59
16. Brown-Dennis (4,20)	87	94	76	69
17. Osborne 1 (5,33)	F	F	87	92
18. Biggs EXP6 (6,6)	898	399	333	30
19. Osborne 2 (11,65)	F	F	1234	97
20. Watson (31,31)	F	F	253	F
21. Extended Rosen (4,4)	123	F	82	467
22. Extended Powell sing. (4,4)	97	81	64	64
23. Penalty I (6,7)	25	25	25	25
24. Penalty II (5,10)	50	35	50	44
25. Variably dimensioned (10,12)	56	56	56	56
26. Trigonometric (10,10)	57	57	57	57
27. Discrete bound. value (4,4)	38	50	36	37
28. Discrete int. equation (20,20)	7	7	7	7
29. Broyden tridiagonal (20,20)	29	29	29	95
30. Broyden banded (10,10)	38	38	38	41

Table 3.1: Number of function evaluations for the test problems from [12].

Code	Succeeded	Better than others codes
DF-SANE	26	1
N-DF-SANE	24	2
NM1	28	5
NM2	28	6

Table 3.2: Number of problems solved by each code and the number of problems in which each code was strictly better than the others in terms of function evaluations.

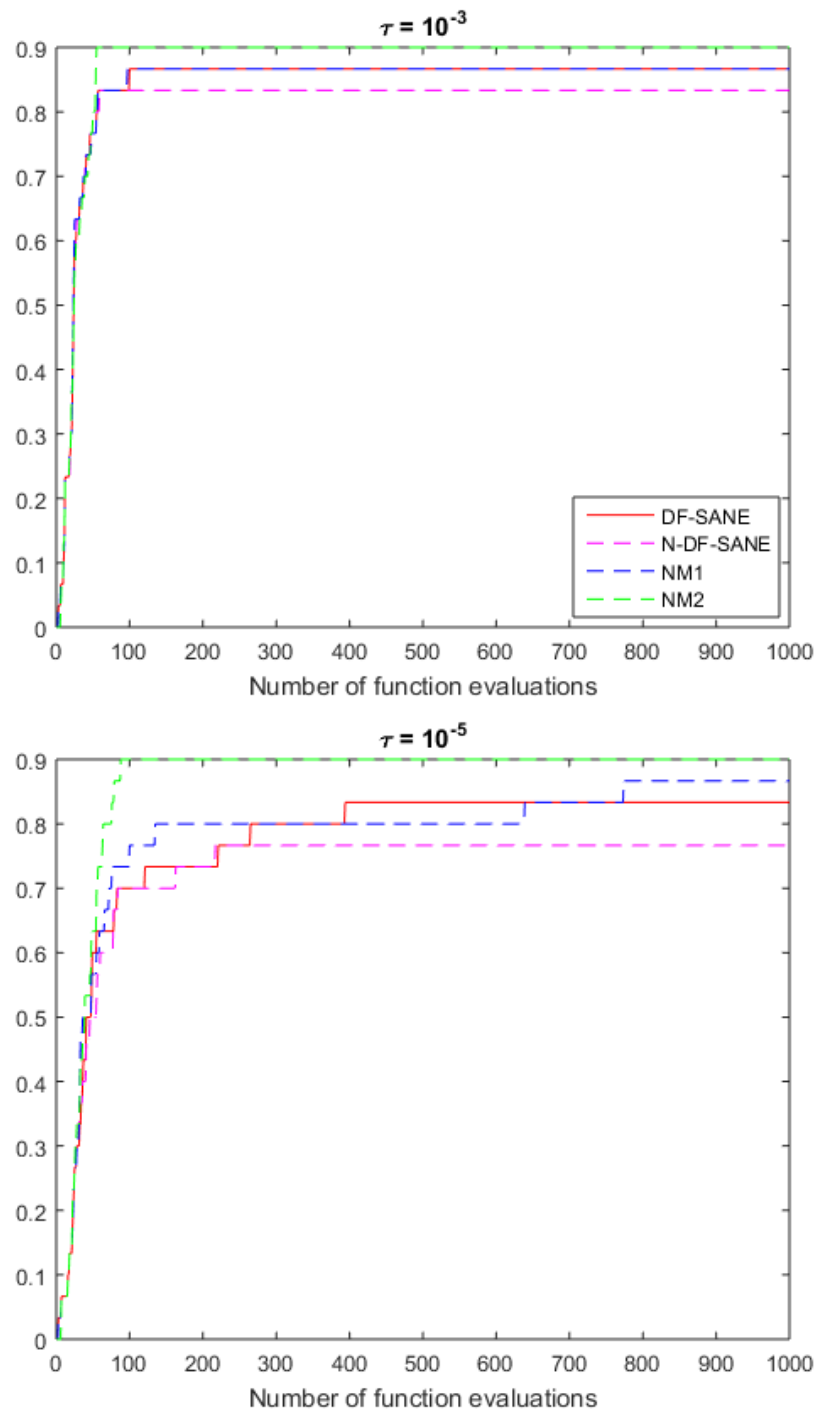


Figure 3.1: Data Profile, with tolerance $\tau = 10^{-3}$ and $\tau = 10^{-5}$

Conclusion

In this dissertation we studied the worst-case complexity of a class of derivative-free nonmonotone methods for nonlinear equations that includes the N-DF-SANE method [2]. For this class of methods, we proved that if the Jacobian of the mapping $F(\cdot)$ is Lipschitz continuous, the methods take at most $\mathcal{O}(\epsilon^{-2})$ iterations to generate x_k such that $\psi(x_k) \leq \epsilon$, where $\psi(\cdot)$ is a stationarity measure for the merit function $f(x) = (1/2)\|F(x)\|_2^2$. From this iteration-complexity bound we obtained a lim-type global complexity result and also an evaluation-complexity bound of $\mathcal{O}(|\log(\epsilon)|\epsilon^{-2})$. In our preliminary numerical experiments, the implementation of a new variant of N-DF-SANE (referred to as NM2) outperformed N-DF-SANE and also DF-SANE [8] on a subset of 30 problems from the Moré-Garbow-Hillstom collection [12]. As a future work, we plan to study the worst-case complexity of the same class of methods applied to the problem of finding zeros of strongly monotone mappings. In this case, an improved evaluation-complexity bound of $\mathcal{O}(|\log(\epsilon)|)$ is expected.

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