The method and the trajectory of Levenberg-Marquardt

PhD Thesis by
Roger Behling

Supervisor
Alfredo Noel Iusem
Co-Supervisor
Andreas Fischer

IMPA - Instituto Nacional de Matemática Pura e Aplicada
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Mut ohne Klugheit ist Unfug,
und Klugheit ohne Mut ist Quatsch!
Erich Kästner

Dedicated to Nina

Agradecimentos

Eu tinha cerca de dez anos de idade quando fui pela primeira vez a uma feira de matemática apresentar um trabalho. A professora que nos acompanhou me ensina valores e outras coisas importantes da vida até hoje. Formalmente, Dona Marilise não é mais minha professora, mas continua sendo minha mãe. Não posso dizer que com a Matemática foi amor à primeira vista, como foi com o Rock n' Roll. Essa paixão foi surgindo devagarzinho na minha vida. Aos sete eu queria ter uma banda de rock, ser soldado ou cientista. Eu tinha meu toca fitas que não parava de tocar Guns n' Roses, meu próprio laboratório de química e um arsenal de espadas no rancho dos meus pais. Contribuí para que ali a população de lagartixas não crescesse descontroladamente, já que minhas experiências exigiam muitos dos seus ovos. Apesar dessa minha passagem pela química, foi meu irmão e melhor amigo Ronan que seguiu na área. Ele também começou cedo, testando tintas metálicas em cães.

Muitas vezes alunos se apegam a professores. Comigo não foi diferente, e tudo começou já no jardim de infância. Ao longo dos anos, vários educadores passaram e permanecem em minha vida. Sou grato a eles pelo incentivo, ações e palavras. Há uma época em que achamos que podemos tudo, que somos indestrutíveis, mas essa fase vai passando e como diz Oscar Wilde "não sou mais jovem o suficiente para saber tudo". Na sétima série eu me interessava pela engenharia civil e meu sonho era construir em Pomerode uma réplica do castelo Moritzburg. Sabe, depois de tanto tempo, o quadro desse castelo na casa dos meus pais continua me fascinando. O fato é que não me tornei engenheiro civil e por enquanto também não tenho condições de construir um castelo, mas acabei me casando com uma linda arquiteta e morando com ela por um ano em Dresden, a poucos quilômetros de Moritzburg.

Ainda na sétima série uma outra carreira foi que me chamou a atenção. O professor Marcos era um cara bacana que andava de Fiat 147. Se não me engano, ele tinha acabado de perder o emprego numa empresa e foi parar em meio às montanhas em Testo Alto para dar aula de PPT (preparação para o trabalho) na escola Amadeu da Luz. Apesar de ser do tipo tranquilo ele era um pouco polêmico. Ele disse que queria que fizéssemos as coisas direito, não importando se fôssemos ladrões, ou o que quer que seja, desde que mostrássemos dedicação e competência. Mas foi o que ele fez num dos primeiros dias de aula, todo despojado sentado em cima da mesa, que me marcou profundamente. O trato era o seguinte: os alunos que assistissem o filme que passaria naquele mesmo dia, as 23:30h num dado canal da TV aberta, passariam de ano sem ter que fazer absolutamente nada pelo resto do período letivo. Os que não o assistissem teriam que se dedicar normalmente as aulas. Se todos os professores que tive me passassem de ano só pelo fato de assistir "Sociedade dos poetas mortos" eu já seria doutor a mais tempo. Devo dizer contudo, que essa foi a melhor lição de casa que eu já tive e muito mais séria e instrutiva do que eu imaginava... "Capitão, meu capitão!!".

Dizem que na vida existem altos e baixos. Eu nunca fiz parte dos mais altos, mas a professora Maike disse que eu poderia me tornar um grande homem. "Mas por

quantos caminhos um homem deve andar antes de podermos chamá-lo de homem?" Isso eu ainda não sei, e pelo visto Bob Dylan também não respondeu a essa pergunta até hoje. Alguns acreditam em predestinação e dizem que já está tudo escrito, mas eu vi que isso não é totalmente verdade na hora de redigir minha tese. O fato é que de uma ou de outra maneira eu fui realizando meus sonhos de menino. O doutorado no IMPA, por exemplo, me dará o título de Doutor em Ciências, o que tecnicamente me faz um cientista. Minha idéia é de continuar nesse ramo da alquimia que é a matemática, em que transformamos cafés em teoremas, como dizia Paul Erdös. Roqueiro eu sempre fui e sempre vou ser. Na New Rose, minha própria banda de rock, já faço barulho desde 2004. Então, duas das minhas aspirações de infância foram quitadas. Só me resta a tarefa de me tornar soldado. Talvez eu me torne um Rambo da educação, quem sabe, isso certamente seria útil à sociedade.

As lembranças são ótimas, mas é hora de fazer agradecimentos precisos. Até o ensino médio passei pelas escolas Bonifácio Cunha, Amadeu da Luz e Dr. Blumenau e os professores que mais me marcaram foram Simone, Elcina, Marilise, Elmo, Arão, Jeane, Maike, Terezinha, Joana e Wilson. A eles meu muito obrigado. Na graduação foram Vladimir, Elisa e Pinho. Também não posso me esquecer das lições incomuns deixadas pelo professor Andrzej, como dizer que matemáticos deviam ler romances ("só não vale Sabrina!") e nos fazer refletir sobre o quadro de Magritte, intitulado "Isto não é um cachimbo", ilustrado a seguir.

Cinco nomes próprios, de sete letras cada, formam o alicerce docente do meu mestrado e doutorado: Alfredo, Fischer, Gonzaga, Solodov e Svaiter.

Eu tive o privilégio de morar em cidades muito bonitas no decorrer da minha vida e dos meus estudos, e conhecer pessoas inteligentíssimas. O que me levou de Pomerode a Florianópolis foi acima de tudo o amor da minha vida, Rose Anne Meinicke Behling, mais conhecida como Nina. Com grande ajuda do Professor Clóvis C. Gonzaga migrei da UFSC para o IMPA. Ao chegar ao Rio de Janeiro fiquei maravilhado, olhando para a estátua do Cristo Redentor e vendo como seu braço direito se enverga sobre a floresta, bem próximo ao IMPA, e dei minha própria interpretação à frase de Gauss "Deus faz Aritmética". Foi uma honra fazer parte desse instituto de excelência por esses quatro anos, bem como ser orientado pelo Professor Alfredo Noel Iusem e co-orientado em Dresden pelo Professor Andreas Fischer. Uma tia avó de Nina esteve na cidade de Erich Kästner em meio a um dos bombardeios mais questionados da História, no dia

13 de fevereiro de 1945. Apesar do odor amargo de guerra que passou por Dresden, eu só pude sentir o perfume de sua primavera, que, aliás, foi a melhor primavera que alguém poderia me dar. Ao DAAD sou grato pelo curso de alemão no Instituto Goethe e ao CNPQ pelo financiamento do meu programa de doutorado, inclusive da bolsa de doutorado sanduíche na TU Dresden. Voltando ao IMPA, eu agradeço aos professores, funcionários, amigos, colegas e ainda em especial a professora de inglês Mariluce, que trouxe cultura, diversão e informação às nossas aulas. Agradeço também aos Professores membros de minha banca de defesa Alfredo Noel Iusem, Andreas Fischer, Clóvis C. Gonzaga, Mikhail V. Solodov, Susana Scheimberg de Makler e Rolando Gárciga Otero.

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Seja **A** o conjunto de pessoas a quem agradeço. Os que lerem esses agradecimentos provavelmente pertencem pelo menos ao fecho de **A**. Existem pessoas que sequer vão passar perto dessas palavras, mas que pertencem definitivamente ao interior de **A**. Logicamente, meu "conjunto família" está calorosamente contido nesse interior. Agradeço ao meu pai Hans Behling por me mostrar que o trabalho dignifica o homem e a minha mãe Marilise pelo incentivo à educação. Além de nomes como Behling, Krüger e Meinicke, muitos outros estão no coração de **A**. A todos, minha sincera gratidão.

Die Gelegenheit in Deutschland zu wohnen konnte, und habe ich auch nicht verpasst. Diese Erfahrung an der Elbe war sicherlich die größte und beste meines Lebens, die ich in meiner Meinung auch ganz gut genoßen habe. Ich konnte endlich mal sehen aus welchem Land meine Vorfahren gekommen sind. Und wie es im Lied "So ein Tag" gesungen wird, "diese Tage dürften ja nie vergehen". Sie werden auch nie vergehen, mindestens nicht in meinem Herz. Zu guter Letzt bedanke ich mich bei meinen Kollegen der TU Dresden und des Goethe Instituts, den Mitarbeiten und Professoren des Instituts für Numerische Mathematik, hauptsächlich meinem Betreuer Professor Fischer, und auch den Komilitonen und Freunden die ich jetzt in Deutschland habe.

Abstract

In this thesis we study both the method and the trajectory of Levenberg-Marquardt, which stem from the forties and sixties. Recently, the method turned out to be a valuable tool for solving systems of nonlinear equations subject to convex constraints, even in the presence of non-isolated solutions. We consider basically a projected and an inexact constrained version of a Levenberg-Marquardt type method in order to solve such systems of equations. Our results unify and extend several recent ones on the local convergence of Levenberg-Marquardt and Gauss-Newton methods. They were carried out under a regularity condition called calmness, which is also called upper-Lipschitz continuity and is described by an error bound. This hypothesis became quite popular in the last decade, since it generalizes the classical regularity condition that implies that solutions are isolated. In this direction, one of the most interesting results in this work states that the solution set of a calm problem must be locally a differentiable manifold.

We have also obtained primal-dual relations between the central path and the Levenberg-Marquardt trajectory. These results are directly applicable in convex programming and path following methods.

Keywords. Calmness, upper-Lipschitz continuity, nonlinear equations, error bound, Levenberg-Marquardt, Gauss-Newton, central path, interiors points, constrained equation, convergence rate, inexactness, non-isolated solution.

Resumo

Nesta tese estudamos o método e a trajetória de Levenberg-Marquardt, que foram desenvolvidos na década de quarenta e sessenta. Recentemente, provou-se que o método é uma ferramenta eficiente para resolver sistemas de equações não lineares sujeitos a restrições convexas, mesmo na presença de soluções não isoladas. Nós consideremos basicamente métodos de Levenberg-Marquardt projetados e inexatos restritos para resolver tais sistemas de equações. Nossos resultados estendem e unificam diversas análises recentes relacionadas à convergência local de métodos de Levenberg-Marquardt e Gauss-Newton. Tomamos como hipótese uma condição de regularidade chamada calmaria, ou continuidade Lipschitz superior, que é caracterizada por uma cota de erro local. Essa hipótese se tornou bastante popular recentemente já que generaliza a condição clássica de regularidade que implica que as soluções são isoladas. Nesse sentido, um dos resultados mais interessantes do nosso trabalho diz que o conjunto solução de um problema calmo deve ser localmente uma variedade diferenciável.

Obtivemos também propriedades relacionadas à trajetória de Levenberg-Marquardt. Provamos que ela possui relações primais e duais com a trajetória central. Esses resultados são diretamente aplicáveis a problemas de programação convexa e métodos interiores baseados em trajetória central.

Palavras chave. Levenberg-Marquardt, continuidade Lipschitz superior, equações não lineares, Gauss-Newton, trajetória central, pontos interiores, taxa de convergência, solução não isolada.

Contents

Chapter 1

Introduction

Some of our mathematical contributions are related to the nonlinear system of equations

$$H(x) = 0, \tag{1.1}$$

with $H : \mathbb{R}^n \to \mathbb{R}^m$.

The classical concept of regularity for Problem 1.1 at a solution x^* in the smooth and square case, i.e. with $m = n$, is the nonsingularity of the Jacobian matrix $\nabla H(x^*)$. For regular problems, a large array of iterative methods have been developed, studied and implemented. One of them, is the well known Newton method, whose subproblems are given by linear systems of equations such as

$$\nabla H(s)^\top (x - s) = -H(s), \tag{1.2}$$

where $s \in \mathbb{R}^n$ denotes a current iterate. The Newton method is well defined in a neighborhood of a solution x^* if H is differentiable and x^* is a regular point. If ∇H is continuous, the method possesses local superlinear convergence. The convergence is quadratic when the Jacobian is in addition locally Lipschitz continuous. When a solution x^* is a regular point in the classical sense, it is necessarily an isolated solution. For details we refer the reader to the books [8, 66]. A condition that extends the classical concept of a regular problem in this direction is a notion named calmness in the book by Rockafellar and Wets [69].

We say that Problem 1.1 is calm at $x^* \in X^*$, where $X^* := \{x \in \mathbb{R}^n | H(x) = 0\}$, if there exist $\omega > 0$ and $\delta > 0$ so that

$$\omega \operatorname{dist}[x, X^*] \leq \|H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \delta)$, where $\operatorname{dist}[a, A]$ denotes the Euclidean distance from a point a to a set $A \subset \mathbb{R}^n$ and $\| \cdot \|$ is the Euclidean norm.

It is easy to see that when $n = m$ and x^* is an isolated solution, the classic regularity and the calmness conditions coincide. Besides its applicability to nonsmooth and rectangular systems, the notion of calmness encompasses situations with non-isolated solutions. In the particular case of smooth systems with $m = 1$, calmness implies that directional derivatives in directions normal to the solution set are nonnull. At the same time, the notion of calmness is powerful enough as to allow the extension of a large array of results which were previously known to hold only for regular systems in the classical sense, and hence it became quite popular. This condition, that is also called upper-Lipschitz continuity (e.g. [68]), is described, as we have seen, by a local error bound. Roughly speaking, this error bound says that in a neighborhood of a solution the distance of a point $x \in \mathbb{R}^n$ to the solution set is proportional to $\|H(x)\|$. For understanding this better, consider for instance $H : \mathbb{R}^2 \to \mathbb{R}^1$, with $H(x_1, x_2) := x_1^2 + x_2^2 - 1$. Then, one can easily verify that Problem 1.1 is calm around any solution. This is in some sense expected, due to the geometric structure of the graphic of H, which is illustrated next.

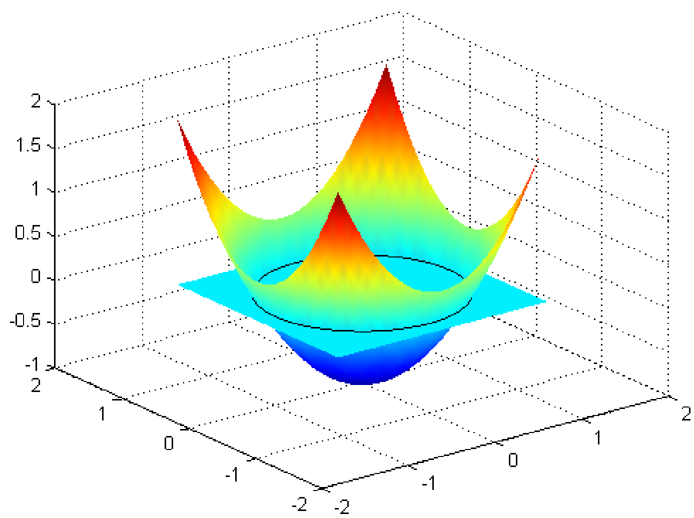

Figure 1.1: Illustration of a calm problem

If H is affine, Hoffmmann's Lemma (see [39]) guarantees that the error bound always holds and is global. Calmness also has implications in connection with constraint qualifications, Karush-Kuhn-Tucker systems and second order optimality conditions (see [41]).

We have studied the influence of calmness on the solution set of systems of equations (1.1) when H is continuously differentiable. Under these hypotheses the main result in Chapter 3, maybe the most important of the whole thesis, states that the rank of the Jacobian of H must be constant on the solution set of (1.1). We also conclude that X^* must be locally a differentiable manifold. Further properties, examples, and algorithmic implications are presented too.

One area where the notion of calmness turned out to be quite useful is the study of the convergence properties of iterative methods for solving systems of nonlinear equations, e.g. Levenberg-Marquardt type methods. The algorithm of Levenberg-Marquardt is one of the main subjects in this thesis. It was first published by Kenneth Levenberg in 1944 (see [52]) and rediscovered in 1963 by the statistician Donald Marquardt, who developed his algorithm in [56] to solve fitting nonlinear chemical models to laboratory data. The method is still popular and being used for solving real world problems. This is the case in [10], where it is implement for image processing.

Among the papers which use the notion of calmness for solving nonlinear equations applying Levenberg-Marquardt type methods we mention [14, 22, 23, 24, 28, 29, 46, 76, 77, 78]. For the first result in this direction see the paper [76], published by Yamashita and Fukushima in 2001. In [20, 28, 46] applications of Levenberg-Marquardt techniques to other problems are dealt with. Related globalization technics were suggested in [7, 30, 46, 55, 78]. For semismooth problems Levenberg-Marquardt type algorithms have been developed in [21, 44, 45]. However, the conditions used for proving their local superlinear convergence imply the local uniqueness of the solution.

Levenberg-Marquardt type methods were recently also adapted for problems like (1.1) where in addition, feasibility with respect to a closed convex set Ω is required. Projected methods were suggested in [46] and constrained ones in [46] and [77] (the latter for nonnegative constraints only). In two chapters of the present thesis we consider the following system of nonlinear equations subject to constraints

$$H(x) = 0, \quad x \in \Omega, \tag{1.3}$$

where $H : \mathbb{R}^n \to \mathbb{R}^m$ is a sufficiently smooth mapping and $\Omega \subseteq \mathbb{R}^n$ is a given closed convex set.

Let us now define iterations of Levenberg-Marquardt type methods in order to explain what has happened in the field in the last decade. We firstly address Problem 1.1, which is the same as Problem 1.3 without constraints, i.e., when $\Omega = \mathbb{R}^n$. Then, the Levenberg-Marquardt subproblem reads as follows

$$\min_{x\in\mathbb{R}^n} \frac{1}{2}\|H(s) + \nabla H(s)^\top (x-s)\|^2 + \frac{1}{2}\alpha(s)\|x-s\|^2 + \pi(s)^\top (x-s) \tag{1.4}$$

where $s \in \mathbb{R}^n$ is the current iterate, $\alpha(s)$ is a positive number called Levenberg-Marquardt regularization parameter and $\pi(s) \in \mathbb{R}^n$ formally denotes inexactness within the subproblems. When $\alpha(s)$ and $\pi(s)$ are set equal to zero the method reduces to the classical Gauss-Newton method.

The unconstrained Levenberg-Marquardt method generates a sequence $\{x^k\} \subset \mathbb{R}^n$ where x^{k+1} is precisely the unique solution of the quadratic program (1.4) with $s := x^k$. The resulting algorithm is well defined, since (1.4) consists of a minimization of a strongly convex function. Now if we set $\pi \equiv 0$ we recover the pure method; otherwise, we get a so called inexact Levenberg-Marquardt method. Such inexact versions were investigated in [14, 23, 29]. Under the local error bound condition implied by calmness, a well known theory for the level of inexactness in Newton's method exists [17].

The first order necessary optimality conditions correspondent to (1.4), which are also sufficient due to convexity, are given by

$$(\nabla H(s)\nabla H(s)^\top + \alpha(s)I)(x-s) + \nabla H(s)H(s) = -\pi(s). \tag{1.5}$$

This linear system of equations clarifies why $\pi(s)$ describes an inexactness within subproblems. Note that $-\pi(s)$ is a residual in (1.5). This residual might be the result of approximate data, truncated solution algorithms, or numerical errors.

Convergence properties of Levenberg-Marquardt methods strongly depend on the choice of the parameter $\alpha(s)$. If $\alpha(s)$ is chosen as $\|H(s)\|^\beta$ with $\beta \in [1,2]$ and H is continuously differentiable with a locally Lipschitz continuous Jacobian, the exact unconstrained Levenberg-Marquardt method is known to achieve local quadratic convergence [76]. These results were extended to projected Levenberg-Marquardt method for solving (1.3) when Ω is a proper set of $\mathbb{R}^n$ (see [29] and [46]). An iteration of the projected method is divided in two phases. Firstly, one solves the unconstrained subproblem (1.4). The second phase consists then of projecting the solution of (1.4) onto Ω. It is known that the projected methods can be regarded as inexact unconstrained ones. These similarities follow from the fact that the same calmness assumption, which does not take constraints into account, is taken for both the projected and the unconstrained Levenberg-Marquardt methods. See the details in [29].

The subproblems of constrained Levenberg-Marquardt methods consist of minimizing the objective function from (1.4) subject to Ω. A property of the constrained method is that, for its local fast convergence, one needs the error bound described by calmness to hold just in the intersection of a neighborhood of a solution with Ω. Before our work, its local quadratic convergence was only known for the particular choice $\beta = 2$ [46]. Part of this thesis is destined to extend this result for β in the interval $[1,2]$. This is done in Chapter 5 for an inexact constrained version of a Levenberg-Marquardt method with a sharp level of inexactness. The relevance of our generalizations lie mainly on the fact that with particular choices of the exponent β one is able to get simultaneously robustness of subproblems and a large level of inexactness that preserves the rate of convergence of the exact method. In the table next, the letters U, P, C stand for unconstrained, projected and constrained, respectively. In it, we describe the level of inexactness, that maintains the rate of convergence of the exact method, obtained in the literature and in our work.

Reference	LM type method	$\alpha(s)$	$\|\pi(s)\|$
[14]	U	$\|H(s)\|^2$	$\|H(s)\|^4$
[23]	U	$\|H(s)\|^1$	$\|H(s)\|^3$
[29]	U,P	$\|H(s)\|^1$	$\|H(s)\|^2$
Our work	U,P,C	$\|H(s)\|^\beta$	$\|H(s)\|^{\beta+1}$

Table 1.1: Results from the literature

Our theorem in Chapter 5 says that when $\beta \in (0, 2]$, the local rate of convergence of the unconstrained, projected and constrained Levenberg-Marquardt method is $\tau := 1 + \min\{\beta, 1\}$, and that our level of inexactness, as in the previous table, does not destroy this rate and is sharp. It seemed that nothing was known on the behavior of inexact versions of the constrained Levenberg-Marquardt method. The reason for this may lay in the fact that it was not even clear whether a quadratic rate was possible if the value $\|H(s)\|$ were used for the regularization parameter $\alpha(s)$. In this sense the result in [29] served as a benchmark for us when considering constraints. Our study on constrained Levenberg-Marquardt methods improve or extend previous results, in particular those in [14, 23, 29, 46, 77].

In this thesis we are particularly interested in the relation between the Levenberg-Marquardt regularization parameter and quadratic convergence of the method. We will see in Chapter 4 that when the positive singular values of the Jacobian matrix $\nabla H(s)$ remain larger than a constant times $\|H(s)\|$, the regularization parameter is not needed in unconstrained and projected Levenberg-Marquardt methods in order to get local quadratic convergence. Still in Chapter 4, we present examples that show that in general one does not have quadratic convergence if $\alpha(s) := \|H(s)\|^\beta$ with $\beta \in (3, \infty)$.

In the last part of the thesis, namely in Chapter 6, we derive some results with respect to the trajectory of Levenberg-Marquardt. This trajectory is based on a penalization of type $\frac{1}{2}\|\cdot\|^2$, as in the subproblems of Levenberg-Marquardt type methods, therefore its name. We compare the Levenberg-Marquardt trajectory with the primal-dual central path correspondent to a convex problem in a region close to the analytic center of the feasible set.

Logarithmic type penalizations stem from the work by Frish [31], who in the fifties, used for the first time the logarithmic barrier function in optimization. But it was in the last twenty years, due to the success of interior point methods, that the barrier methods, which apply internal penalty technics, had a massive development, even in nonlinear programming, see [12, 16, 50, 60, 65, 70, 74]. A motivation for the development of interior point methods were the polynomial time algorithms by Khachiyan [49], Karmarkar [48], De Ghellinck and Vial [15] and Renegar [67]. For a general penalization approach we refer the book by Fiacco and McCormick [26] and the work by Auslender et al. [2].

In the eighties, the penalty approaches [59, 58, 10] led to a precise definition of the so called central path, a path described by optimizers of logarithmic type penalization problems, that depend on a positive parameter. Ever since, several papers studied the limiting behavior of the central path such as its good definition for different kinds of convex programs [1, 4, 19, 38, 40, 64]. Nevertheless, the central path is not necessarily well defined for general convex problems, as shown in [32]. In our work, we deal with a convex problem, where the feasible set is given by linear equalities and nonnegative constraints. Moreover, we assume the existence of an analytic center [71]. Then, due to [38], these conditions are sufficient for the good definition of the central path. Our theorem provides primal-dual interior feasible points based on a Levenberg-Marquardt trajectory. Algorithmically, this can be useful for path following methods.

Now, let us outline the thesis. In Chapter 2 we collect results from the literature which will be used in sequel. This preliminary material is presented for the sake of self containment and to separate known mathematical facts from our contributions. Chapters 3 is based on our paper [6], where we study the influence of calmness on the solution set of nonlinear equations. Chapter 4 consists of a convergence analysis of projected Gauss-Newton and Levenberg-Marquardt methods. In Chapter 5 we present the results on constrained inexact Levenberg-Marquardt methods that we developed in [5]. In Chapter 6, the just mentioned primal dual relations between the Levenberg-Marquardt trajectory and the central path with applications are given. As far as we know, the content of Chapters 3-6 consists basically of original contributions.

Notation

- $\mathbb{R}^n$, the n-dimensional Euclidian space.
- $\|\cdot\|$, the Euclidean norm or the associated matrix norm.
- $\mathrm{dist}[a, A]$, the Euclidean distance from a point a to a set $A \subset \mathbb{R}^n$.
- $\mathcal{B}(x, \delta)$, the closed ball centered at $x \in \mathbb{R}^n$ with radius $\delta > 0$.
- $\mathcal{B}$ denotes the unit ball $\mathcal{B}(0, 1)$.
- $\nabla H(x) \in \mathbb{R}^{n\times m}$ denotes the Jacobian matrix associated to $H : \mathbb{R}^n \to \mathbb{R}^m$, evaluated at the point $x \in \mathbb{R}^n$.
- e, the n-vector of ones.
- log, the natural logarithmic function.
- exp, the exponential function.
- $x^\top s$, the scalar product between $x \in \mathbb{R}^n$ and $s \in \mathbb{R}^n$.
- $A^\top$, the transposed of the matrix A.
- $x \cdot s := (x_1 s_1, ..., x_n s_n) \in \mathbb{R}^n$, the Hadamard product.
- $\mathbb{R}_+ := [0, \infty)$, $\mathbb{R}_{++} := (0, \infty)$, $\mathbb{R}^n_+ := \{x \in \mathbb{R}^n | x_i \in \mathbb{R}_+ \text{ for all } i = 1, ..., n\}$ and $\mathbb{R}^n_{++} := \{x \in \mathbb{R}^n | x_i \in \mathbb{R}_{++} \text{ for all } i = 1, ..., n\}$.
- For a given matrix $A \in \mathbb{R}^{n\times m}$ we define $\mathrm{Kernel}(A) := \{x \in \mathbb{R}^n | Ax = 0\}$.
- $\frac{\partial f}{\partial x_i}(x)$, the partial derivative of $f : \mathbb{R}^n \to \mathbb{R}$ with respect to the variable x_i.
- $\nabla^2 f(x)$, the Hessian matrix associated to $f : \mathbb{R}^n \to \mathbb{R}$ evaluated at the point $x \in \mathbb{R}^n$.

Chapter 2

Background material and preliminaries

In this chapter we collect some mathematical definitions, theorems and present results from the literature, for the sake of self containment of the thesis or in view of their later use.

2.1 Some technical results

Lemma 2.1. *Let $H : \mathbb{R}^n \to \mathbb{R}^m$ be a continuously differentiable function with a locally Lipschitz Jacobian $\nabla H : \mathbb{R}^n \to \mathbb{R}^{n \times m}$ and $x^* \in \mathbb{R}^n$ an arbitrary, but fixed point. Then, there exist $L > 0$ and $\delta > 0$ such that for all $x, s \in \mathcal{B}(x^*, \delta)$ the following inequalities are satisfied:*

$$\|H(x)\| \leq L; \tag{2.1}$$

$$\|\nabla H(x)\| \leq L; \tag{2.2}$$

$$\|H(x) - H(s)\| \leq L\|x - s\|; \tag{2.3}$$

$$\|\nabla H(x) - \nabla H(s)\| \leq L\|x - s\|; \tag{2.4}$$

$$\|H(x) - H(s) - \nabla H(s)^\top (x - s)\| \leq L\|x - s\|^2. \tag{2.5}$$

Proof. The existence of some $L_0 > 0$ so that (2.1)-(2.4) hold, follows from the definition of H and the fact that $\mathcal{B}(x^*, \delta)$ is compact. Therefore, we only need to prove (2.5). The Mean Value Theorem (see [53]) implies that

$$H(x) - H(s) = \int_0^1 \nabla H(x + t(x - s))^\top (x - s) dt.$$

Then, using (2.4) with a Lipschitz constant $L_0 > 0$, we get

$$\begin{aligned}\|H(x) - H(s) - \nabla H(s)^\top (x-s)\| &= \left\| \int_0^1 \left(\nabla H(x + t(x-s) - \nabla H(s))\right)^\top (x-s)dt \right\| \\ &\le \max_{t\in[0,1]} \|\nabla H(x+t(x-s) - \nabla H(s))\| \|x-s\| \\ &\le \max_{t\in[0,1]} L_0 \|x + t(x-s) - s\| \|x-s\| \\ &= 2L_0 \|x-s\|^2.\end{aligned}$$

Thefore, the statements hold with $L := 2L_0$. □

Assuming $H : \mathbb{R}^n \to \mathbb{R}^m$ to be a continuously differentiable function we are able to express its Jacobian $\nabla H(\cdot)$, evaluated at the point $x \in \mathbb{R}^n$, in terms of the following singular value decomposition (SVD)

$$\nabla H(x)^\top = U_x \Sigma_x V_x^\top,$$

where $U_x \in \mathbb{R}^{m\times m}$ and $V_x \in \mathbb{R}^{n\times n}$ are orthogonal and Σ_x is the m by n diagonal matrix $\mathrm{diag}(\sigma_1(x), \sigma_2(x), ..., \sigma_{r_x}(x), 0, ..., 0)$ with positive singular values $\sigma_1(x) \ge \sigma_2(x) \ge ... \ge \sigma_{r_x}(x) > 0$. We recall that these singular values are the nonzero eigenvalues of the matrix $\nabla H(x)\nabla H(x)^\top$. Note that $r_x \ge 0$ indicates the rank of $\nabla H(x)$ (the rank is 0 when all singular values are null). Such decomposition can be obtained for any matrix with real entries (see [18], p. 109, or [37]). By the well known results of the perturbations theory for linear operators ([51], [73], [48], for instance), we get the following lemma.

Lemma 2.2. *If $H : \mathbb{R}^n \to \mathbb{R}^m$ is a continuously differentiable function it holds that*

$$\|\Sigma_y - \Sigma_x\| \le \|\nabla H(y) - \nabla H(x)\|.$$

In the following, we recall the terminology used for the rate of convergence of sequences.

We say that a sequence $\{w^k\} \subset \mathbb{R}^n$ converges to $\hat{w} \in \mathbb{R}^n$ with Q-order of at least τ, when $w^k \to \hat{w}$ and there exists $C \ge 0$ so that

$$\limsup_{w^k \to \hat{w}} \frac{\|w^{k+1} - \hat{w}\|}{\|w^k - \hat{w}\|^\tau} \le C.$$

Quadratic convergence correspondents to Q-order convergence with $\tau := 2$. The convergence is called linear when the limit above with $\tau := 1$ is smaller than 1 and superlinear if it is 0.

Next, we present Lemma 2.9 from [29] and reproduce its proof.

Lemma 2.3. *Let $\{w^k\} \subset \mathbb{R}^n$, $r_k \subset [0, \infty)$ be sequences, and $r \in [0, 1)$, $R > 0$ numbers so that, for $k = 0, 1, 2, \ldots$,*

$$\|w^k - w^0\| \le r_0 \frac{R}{1-r} \tag{2.6}$$

implies

$$r_{k+1} \leq r\, r_k \quad \textit{and} \quad \|w^{k+1} - w^k\| \leq R r_k. \tag{2.7}$$

Then, the following assertions hold

(a) $\{r^k\}$ *converges to* 0 *and* $\{w^k\}$ *converges to some* $\hat{w} \in \mathbb{R}^n$.

(b) *If, for some* $t > 1$ *and* $c > 0$,

$$r_{k+1} \leq c r_k^t \quad \textit{and} \quad \|\hat{w} - w^k\| \geq r_k \tag{2.8}$$

is satisfied for $k = 0, 1, 2, \ldots$ *then* $\{w^k\}$ *converges to* $\hat{w}$ *with the Q-order of* t. *In particular,*

$$\|w^{k+1} - \hat{w}\| \leq \frac{cR}{1-r} \|w^k - \hat{w}\|^\tau$$

is valid for all $k = 0, 1, 2, \ldots$.

Proof. (a) We first show by induction that Equations (5.22) and (5.23) hold for all $k \geq 0$. Obviously, (5.22) is valid for $k = 0$. Let us now assume that for some k, inequality (5.22) is satisfied for $\nu = 1, ..., k$. Then, by assumption, the inequalities in (5.23) are valid for $\nu = 0, ..., k$ and we have that for ν, ℓ with $k + 1 \geq \nu > \ell \geq 0$

$$r_\nu \leq r r_{\nu-1} \leq r_\ell r^{\nu-\ell} \tag{2.9}$$

and

$$\|w^\nu - w^\ell\| \leq \sum_{i=0}^{\nu-\ell-1} \|w^{\ell+i+1} - w^\ell + i\| \leq R \sum_{i=0}^{\nu-\ell-1} r_{\ell+i} \leq R r_\ell \sum_{i=0}^{\nu-\ell-1} r^i. \tag{2.10}$$

By $0 \leq r < 1$, (2.9) implies

$$\|w^\nu - w^\ell\| < r_\ell \frac{R}{1-r} \tag{2.11}$$

for ν, ℓ with $k + 1 \geq \nu \geq l \geq 0$. Taking $\nu = k + 1$ and $l = 0$ in (2.11) is valid for $\nu = 0, ..., k + 1$. By induction it follows that (5.22) and (5.23) hold for all $k \geq 0$, and that (2.9), (2.10) and (2.11) hold for arbitrary integers ν, ℓ with $\nu \geq \ell \geq 0$. Hence, by $0 \leq r < 1$ and by (2.9), the sequence $\{r_k\}$ must converge to 0. Furthermore, with (2.11) we then conclude that w^k is a Cauchy sequence and, thus, converges to some $\hat{w} \in \mathbb{R}^n$.

(b) For $\nu > \ell := k + 1$ we obtain from (2.11) and the first inequality in (2.9) that

$$\|w^\nu - w^{k+1}\| r_{k+1} \frac{R}{1-r} \leq r_k^\tau \frac{R}{1-r}.$$

Passing to the limit for $\nu \to \infty$ and using the second inequality in (2.9) yields

$$\frac{\|\bar{w} - w^{k+1}\|}{\|\bar{w} - w^{k+1}\|} \leq \frac{cR}{1-r} < \infty$$

for $k = 0, 1, 2, ...$ Hence, the sequence $\{w^k\}$ converges to $\bar{w}$ with the Q-order of τ. □

2.2 Optimality conditions

Lemma 2.4. *Let $\Omega \in \mathbb{R}^n$ be a closed convex set and $f : \mathbb{R}^n \to \mathbb{R}$ a differentiable function at the point $\bar{x} \in \Omega$. If $\bar{x}$ is a local minimizer of f in Ω, then $-\nabla f(\bar{x})$ belongs to the normal cone*

$$\mathrm{N}_\Omega(\bar{x}) := \{y \in \mathbb{R}^n \,|\, y^\top (z - \bar{x}) \leq 0 \text{ for all } z \in \Omega\}.$$

Or equivalently,

$$0 \in \nabla f(x) + \mathrm{N}_\Omega(\bar{x}).$$

Proof. If $\bar{x}$ is a local minimizer of f in Ω, Theorem 3.2.5 in [42] says that

$$P_\Omega(\bar{x} - \alpha \nabla f(\bar{x})) = \bar{x},$$

for all $\alpha \geq 0$. On the other hand, using the Projection Theorem from [42] and taking $\alpha := 1$, we get

$$(\bar{x} - \nabla f(\bar{x}) - \bar{x})^\top (z - \bar{x}) \leq 0,$$

for all $z \in \Omega$. This proves the lemma. □

Consider the optimization problem

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & h(x) = 0 \\ & g(x) \leq 0, \end{array} \tag{2.12}$$

with $f : \mathbb{R}^n \to \mathbb{R}$, $h : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^n \to \mathbb{R}^\ell$. We say that x is a Karush-Kuhn-Tucker point associated to (2.12) if there exist multipliers $\lambda \in \mathbb{R}^m$ and $s \in \mathbb{R}^\ell_+$ so that

$$\nabla f(x) + \nabla h(x)\lambda + \nabla g(x)s = 0; \tag{2.13}$$

$$h(x) = 0, \;\; g(x) \leq 0; \tag{2.14}$$

$$s \cdot g(x) = 0. \tag{2.15}$$

where $s \cdot g(x) := (s_1 g_1(x), ..., s_\ell g_\ell(x)) \in \mathbb{R}^\ell$.

Remember that the optimization problem (2.12) is called convex if f is convex, h is affine and all the component functions of g are convex.

Theorem 2.1. *Suppose that (2.12) is a convex problem and that the Slater condition holds, i.e., there exists $\bar{x} \in \mathbb{R}^n$ so that $h(\bar{x}) = 0$ and $g(\bar{x}) < 0$. Then, a point x is a minimizer (global) of (2.12) if, and only if, x is a Karush-Kuhn-Tucker point associated to (2.12).*

Proof. Theorem 4.2.1 in [42]. □

2.3 Some results on Levenberg-Marquardt methods

2.3.1 The trajectory of Levenberg-Marquardt

Assume $q : \mathbb{R}^n \to \mathbb{R}$ to be a convex quadratic function bounded bellow and $\Omega \subset \mathbb{R}^n$ a nonempty closed convex set. In order to define a Levenberg-Marquardt type trajectory let us consider the optimization problem

$$\begin{array}{ll} \min & q(x) + \frac{1}{2}\alpha\|x\|^2 \\ \text{s.t.} & x \in \Omega \end{array} \tag{2.16}$$

The objective function in this problem is strongly convex for each $\alpha > 0$, and thus, 2.16 has a unique minimizer in which we will denote by $x_{LM}(\alpha)$. Then, the Levenberg-Marquardt trajectory corresponding to q and Ω is given by

$$\{x_{LM}(\alpha) | \alpha > 0\}.$$

Denote by $\mathbf{S}$ the solution set of Problem 2.16 with $\alpha := 0$. Note that $\mathbf{S}$ is nonempty, closed and convex. Therefore, the problem

$$\begin{array}{ll} \min & \frac{1}{2}\alpha\|x\|^2 \\ \text{s.t.} & x \in \mathbf{S} \end{array}$$

has the unique solution that we denote by $x_{LM}(0)$ or simply by x_{GN}, where GN stands for Gauss-Newton.

Hence, it seems that one has to solve two minimization problems to obtain the Gauss-Newton point, but this is not entirely true. Indeed, there are iterative methods that naturally, tend to find solutions of minimum norm. It is the case of the conjugate gradient method (CG), quite popular for solving unconstrained quadratics programs and linear least squares problems in general. For more details, see [43], for instance.

Levenberg-Marquardt type methods generate sequences of quadratic subproblems where in each iteration a point on a Levenberg-Marquardt trajectory is chosen and set as the next iterate or some intermediate step.

The next result states well known properties of the Levenberg-Marquardt trajectory.

Lemma 2.5. *For all $\alpha \geq 0$ it holds that:*

(a) $x_{LM}(\alpha)$ minimizes f in the convex trust region $\{x \in \Omega | \|x\| \leq \|x_{LM}(\alpha))\|\}$ and $\alpha \geq 0 \mapsto \|x_{LM}(\alpha)\|$ is a nonincreasing function;

(b) the trajectory $\{x_{LM}(\alpha) \in \mathbb{R}^n | \alpha \geq 0\}$ is well defined and $\lim_{\alpha\to 0} x_{LM}(\alpha) = x_{GN}$.

Proof. Item (a) can be obtained by means of Lemma 6.3, given in Chapter 6. Therefore, we omit its proof. Item (b) follows elementarily using (a) and the definition of x_{GN}. □

2.3.2 Recent results for Levenberg-Marquardt methods

As we have already mentioned, Levenberg-Marquardt methods turned out to be a valuable tool for solving nonlinear systems of equations under the condition of calmness in the last decade. In this subsection we present some assumptions and recent results on the local convergence of Levenberg-Marquardt type methods for solving the following system of nonlinear equations subject to convex constraints

$$H(x) = 0, \quad x \in \Omega, \tag{2.17}$$

where $H : \mathbb{R}^n \to \mathbb{R}^m$ is a continuously differentiable mapping and $\Omega \subseteq \mathbb{R}^n$ a closed convex set. We assume that the solution set $X^* := \{x \in \Omega | H(x) = 0\}$ is nonempty and consider from now on, the arbitrary, but fixed solution $x^* \in X^*$.

Projected Levenberg-Marquardt methods for solving Problem 2.17 use the following calmness condition around x^*.

Assumption 2.1. *There exist $\omega_1 > 0$ and $\delta_1 \in (0, 1]$ so that*

$$\omega_1 \text{dist}[x, X^*] \le \|H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \delta_1)$.

We will deal with this condition in Chapters 3 and 4.

In constrained Levenberg-Marquardt type methods this condition is assumed to hold in the intersection with Ω, i.e., they require the following regularity condition.

Assumption 2.2. *There exist $\omega_2 > 0$ and $\delta_2 \in (0, 1]$ so that*

$$\omega_2 \text{dist}[x, X^*] \le \|H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \delta_2) \cap \Omega$.

In the unconstrained case, i.e., when $\Omega := \mathbb{R}^n$, the assumptions above are equivalent. When Ω is a proper set of $\mathbb{R}^n$ Assumption 2.2 is clearly more general than Assumption 2.1. Nevertheless, it is a sufficient condition for local fast convergence of the constrained, but not for the projected Levenberg-Marquardt method as we will see in Chapter 5. In fact, it was proved that projected methods can be regarded as inexact unconstrained ones under Assumption 2.1. This is shown in [29].

Let us now define the first order model of H at a point $s \in \Omega$ used in Levenberg-Marquardt subproblems.

Consider the function $\psi : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ given by

$$\psi(x, s) := \frac{1}{2}\|H(s) + \nabla H(s)^\top (x - s)\|^2 + \frac{1}{2}\alpha(s)\|x - s\|^2 + \pi(s)^\top (x - s), \tag{2.18}$$

where $\alpha(s)$ is the Levenberg-Marquardt parameter and $\pi(s) \in \mathbb{R}^n$ denotes a perturbation that enables inexactness within subproblems.

In the sequel, we present the projected and the constrained Levenberg-Marquardt methods.

Algorithm 2.1. Projected Levenberg-Marquardt method
Step 0. Choose $x^0 \in \Omega$ and $\beta > 0$.
Step 1. If $H(x^k) = 0$, stop. Otherwise, set $s := x^k$ and compute the solution $\tilde{x}^{k+1}$ of

$$\min \quad \psi(x, s)$$

with $\pi(s) \equiv 0$ and $\alpha(s) := \|H(s)\|^\beta$.
Step 2. Compute the projection $x^{k+1} := P_\Omega(\tilde{x}^{k+1})$.
Step 3. Set $k := k + 1$ and go to Step 1.
End

The projected Levenberg-Marquardt method was introduced in [46]. There, its local quadratic convergence is proved, for the choice $\alpha(s) := \|H(s)\|^2$. In the unconstrained case, inexact versions of the Levenberg-Marquardt method were considered for the first time in [14], where the level of inexactness was required to satisfy

$$\frac{\|\pi(s)\|}{\alpha(s)} \sim \|H(s)\|^2.$$

It is mentioned in [14] that this result could probably not be improved. What we are going to do in Chapter 5, is to show that a level of inexactness satisfying

$$\frac{\|\pi(s)\|}{\alpha(s)} \sim \|H(s)\|, \tag{2.19}$$

does not worsen the convergence rate of the pure method. Furthermore, we extend this result to constrained Levenberg-Marquardt methods and show that this level of inexactness is sharp. The relation between $\pi(s)$ and $\alpha(s)$, given by 2.19, was already used in [29] for the unconstrained method with the choice $\alpha := \|H(s)\|$.

Next, we present the constrained Levenberg-Marquardt method.

Algorithm 2.2. Constrained Levenberg-Marquardt method
Step 0. Choose $x^0 \in \Omega$ and $\beta > 0$.
Step 1. If $H(x^k) = 0$, stop. Otherwise, set $s := x^k$ and compute the solution x^{k+1} of

$$\begin{array}{ll} \min & \psi(x, s) \\ \text{s.t.} & x \in \Omega, \end{array}$$

with $\pi(s) \equiv 0$ and $\alpha := \|H(s)\|^\beta$.
Step 2. Set $k := k + 1$ and go to Step 1.
End

Our article [5] is the first work that considers inexact constrained Levenberg-Marquardt methods.

The Gauss-Newton method (projected or constrained) we are going to deal with, is based on the definition of the Gauss-Newton point presented in the previous subsection.

One sets $\alpha(s) := 0$ and considers the closest solution of the quadratic subproblem to the current iterate s.

The next result plays a crucial role in Chapter 3 and is also a particular case of Lemma 5.1, which we present in Chapter 5.

Lemma 2.6. *Let Assumption 2.1 be satisfied. Then, there exist* $\bar{\delta} > 0$ *and* $\bar{\omega} > 0$ *so that*

$$\bar{\omega}\,\mathrm{dist}[x, X^*] \leq \|\nabla H(x) H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \bar{\delta})$.

Proof. Corollary 2 in [27]. □

The proof of the following lemma can be found in [46].

Lemma 2.7. *Let Assumption 2.1 be satisfied and* $x_{PLM}(s)$ *denote the unique minimizer of* $\psi(\cdot, s)$*, with* ψ *as in (2.18) so that* $\pi(s) \equiv 0$ *and*

$$\alpha(s) := \begin{cases} \|H(s)\|^2, & \text{if } H(s) \neq 0; \\ 1, & \text{otherwise.} \end{cases}$$

Then, there exist $\delta_{PLM} > 0$ *and* $C_{PLM} > 0$ *so that*

$$\|x_{PLM}(s) - s\| \leq C_{CLM} \mathrm{dist}[s, X^*]$$

for all $s \in \mathcal{B}(x^*, \delta_{PLM})$.

2.4 The central path

Consider the optimization problem

$$\begin{array}{rl} \min & f(x) \\ \text{s.t.} & Ax = b \\ & x \geq 0, \end{array} \tag{2.20}$$

with $f : \mathbb{R}^n \to \mathbb{R}$ convex and differentiable, $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. The central path associated to (2.20) is defined in terms of the following problem

$$\begin{array}{rl} \min & f(x) - \mu \sum_{i=1}^{n} \log(x_i) \\ \text{s.t.} & Ax = b \\ & x > 0, \end{array}$$

where $\mu > 0$ is the barrier penalty parameter. The unique solution of this penalized problem (if it exists) is characterized by the Karush-Kuhn-Tucker conditions

$$P_{\mathcal{K}(A)}\left(\nabla f(x) - s\right) = 0;$$

$$Ax = b,\ x > 0;$$
$$x \cdot s = \mu e;$$
$$s > 0,$$

and will be denoted by $(x(\mu), s(\mu)) \in \mathbb{R}^n \times \mathbb{R}^n$ and called primal-dual central point correspondent to $\mu > 0$. The primal-dual central path is then given by

$$\{(x(\mu), s(\mu)) | \mu > 0\}.$$

We define now the set of primal-dual feasible points associated to Problem 2.20.

$$\Gamma := \{(x, s) \in \mathbb{R}^n_+ \times \mathbb{R}^n_+ | Ax = b,\ P_{\mathcal{K}(A)}(\nabla f(x) - s) = 0\}.$$

The points from Γ that lie in the strictly positive octant describe the set of interior feasible primal-dual points associated to Problem 2.20, which is denoted by

$$\Gamma^\circ := \{(x, s) \in \mathbb{R}^n_{++} \times \mathbb{R}^n_{++} | Ax = b,\ P_{\mathcal{K}(A)}(\nabla f(x) - s) = 0\}.$$

Note that central points belong to Γ°.

The following result is related to the good definition of central points and the central path.

Theorem 2.2. *Assume that there exists an interior feasible point $\tilde{x} \in \mathbb{R}^n$, i.e., $A\tilde{x} = b$ and $\tilde{x} > 0$. Then, the following conditions are equivalent:*

(a) *The solution set of Problem 2.20 is nonempty and bounded;*

(b) *the central path $\{(x(\mu), s(\mu)) | \mu > 0\}$ is well defined;*

(c) *for some $\mu_0 > 0$, the central point $(x(\mu_0), s(\mu_0))$ is well defined;*

(d) *there exists an interior feasible primal-dual point $(\bar{x}, \bar{s}) \in \Gamma^\circ$.*

Proof. See Theorem 2.1 in [38]. □

We present now the definition of analytic center and make some comments on the behavior of the central path when $\mu \to 0^+$.

Let us consider the convex problem

$$\begin{array}{ll} \min & -\sum_{i=1}^{n} \log(x_i) \\ \text{s.t.} & Ax = b \\ & x > 0. \end{array} \tag{2.21}$$

The strictly convexity of the objective function guarantees the uniqueness of solution of Problem 2.21. If the solution exists, it is called the analytic center of $\Omega := \{x \in \mathbb{R}^n | x \geq 0 \text{ and } Ax = b\}$. Observe that when Ω is bounded and has a nonempty relative interior (i.e., there exists an interior feasible point $\tilde{x} \in \mathbb{R}^n$), its analytic center is well defined.

We end up this subsection giving some references on the convergence of the central path. From Theorem 4.1 in [38] it is known that under the existence of an interior feasible point, the primal central path $\{x(\mu)|\mu > 0\}$ converges to the analytic center of the solution set of Problem 2.20 as $\mu \to 0^+$, if in addition f is twice continuously differentiable. For convex problems in which the central path does not have such nice properties see [32]. For primal-dual convergence properties of central paths we refer the reader to [64]. This will not be a subject in this thesis, since we will be more interested in the features of the central path close to the analytic center. Roughly speaking, the analytic center is the point where the central path starts. Indeed, it is the limit of the primal central path $\{x(\mu)\}$ as $\mu \to \infty$, see [71]. For features of the central path in linear programming such as their role in the complexity of algorithms see Gonzaga [33] and the book by Wright [75].

2.4.1 Neighborhoods of the central path

Sequences generated by path following algorithms ([33, 34, 35, 62, 63, 61]) remain close enough to the central path along the iterates in the sense described by proximity measures. The proximity measure we are going to use in this work is characterized by the function $\sigma : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}_{++} \to \mathbb{R}_+$, given by

$$\sigma(x, s, \mu) := \left\| \frac{x \cdot s}{\mu} - e \right\|. \tag{2.22}$$

Note that if for some pair $(\tilde{x}, \tilde{s}) \in \Gamma^\circ$ and a parameter $\tilde{\mu} > 0$ we have $\delta(\tilde{x}, \tilde{s}, \tilde{\mu}) = 0$, then $(\tilde{x}, \tilde{s}) = (x(\tilde{\mu}), s(\tilde{\mu}))$ (the central point correspondent to $\tilde{\mu} > 0$). Path following algorithms do not necessarily calculate points on the central path, since this task may be as difficult as solving the main problem itself. Nevertheless, one might be able to compute steps so that the iterates remain in a certain neighborhood of the central path. Commonly, this is done by computing points in a region like

$$\mathcal{N}(\rho) := \{(x, s) \in \Gamma^\circ | \sigma(x, s, \mu) \leq \rho, \text{ with } \rho > 0\}.$$

Proximity measures that might encompass larger regions of feasible points are presented in [36].

2.4.2 Rewriting a quadratic program

In this subsection we show how one can rewrite a certain quadratic program, that may arise from trust region methods, into the standard format we are going to deal with in Chapter 6.

Consider the convex quadratic program

$$\begin{array}{ll} \min & \frac{1}{2}(\bar{z}+d)^\top Q_0(\bar{z}+d) + c_0^\top(\bar{z}+d) \\ \text{s.t.} & A_0 d = 0 \\ & -u \le d \le u, \end{array} \tag{2.23}$$

where $Q_0 \in \mathbb{R}^{n\times n}$ is symmetric and positive semidefinite, $c_0 \in \mathbb{R}^n$, $u \in \mathbb{R}^n_{++}$ and $A_0 \in \mathbb{R}^{m\times n}$. This problem might be interpreted as a subproblem of a trust region method. The objective function could be a second order model of a Lagrange function centered in $\bar{z} \in \mathbb{R}^n$, $A_0 d = 0$ a tangent space related to equality constraints and the box $[-u, u] := \{d \in \mathbb{R}^n | -u \le d \le u\}$ could represent the trust region itself.

The following reformulation of Problem (2.23) is based on the change and addition of variables $z := u + d$ and $w := u - d$.

$$\begin{array}{ll} \min & 1/2 z^\top Q_0 z + (c_0 + Q_0(\bar{z}-u))^\top z \\ \text{s.t.} & \begin{bmatrix} A_0 & 0 \\ I & I \end{bmatrix} \begin{bmatrix} z \\ w \end{bmatrix} = \begin{bmatrix} A_0 u \\ 2u \end{bmatrix} \\ & z, w \ge 0. \end{array} \tag{2.24}$$

Defining $U := \operatorname{diag}(u)$ and $x := (U^{-1}z, U^{-1}w) \in \mathbb{R}^{2n}$ we rewrite Problem (2.24) as

$$\begin{array}{ll} \min & \frac{1}{2}x^\top Q x + c^\top x \\ \text{s.t.} & Ax = b \\ & x \ge 0, \end{array} \tag{2.25}$$

where $Q := \begin{bmatrix} U^{-2}Q_0 & 0 \\ 0 & 0 \end{bmatrix}$, $c := \begin{bmatrix} U^{-1}(c + Q_0(\bar{z}-u)) \\ 0 \end{bmatrix}$, $A := \begin{bmatrix} U^{-1}A_0 & 0 \\ U^{-1} & U^{-1} \end{bmatrix}$ and $b := \begin{bmatrix} Au \\ 2u \end{bmatrix}$.

One can easily check that (2.25) inherits the convexity of (2.23) and that these problems are in an obvious correspondence with respect to optimality, due to our change of variables. Moreover, we have that $e \in \mathbb{R}^{2n}$ is the analytic center of the compact polyhedron $\Omega := \{x \in \mathbb{R}^{2n} | Ax = b \text{ and } x \ge 0\}$.

Chapter 3

The effect of calmness on the solution set of nonlinear equations

We address the problem of solving a continuously differentiable nonlinear system of equations under the condition of calmness. This property, also called upper Lipschitz-continuity in the literature, can be described by a local error bound and is being widely used as a regularity condition in optimization. Indeed, it is known to be significantly weaker than classical regularity assumptions that imply that solutions are isolated. We prove in this chapter that under this condition, the rank of the Jacobian of the function that defines the system of equations must be locally constant on the solution set. As a consequence, As a consequence, we prove that locally, the solution set must be a differentiable manifold. The results in this chapter are illustrated by examples and discussed in terms of their theoretical relevance and algorithmic implications.

3.1 Introduction

Let us consider the following system of nonlinear equations

$$H(x) = 0, \tag{3.1}$$

where $H : \mathbb{R}^n \to \mathbb{R}^m$ is a continuously differentiable function. We denote by X^* the set of solutions of (3.1) and suppose it is nonempty.

We will deal with the notion of *calmness* of the system (3.1), introduced in Chapter 2. Let us formally recall the definition of a calm problem.

Definition 3.1. *We say that Problem* (3.1) *is calm at $x^* \in X^*$ if there exist $\omega > 0$ and $\delta > 0$ so that*

$$\omega \operatorname{dist}[x, X^*] \leq \|H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \delta)$.

For equivalent definitions of calm problems see [69]. Thanks to the Implicit Function Theorem we know that full rank systems are calm. We will see in this chapter that in some sense, calm problems do not go that much beyond systems of equations with full rank Jacobians. We will establish that the local error bound described by calmness, together with the continuous differentiability of H, imply that the rank of the Jacobian is locally constant on the solution set of system (3.1).

The chapter is organized as follows. In Section 3.2 we prove our main result. In Section 3.3 we present some related results and examples. We end up with some remarks on the algorithmical relevance of our theorem in Section 3.4.

3.2 Our main result

We assume from now on that H is continuously differentiable. Before proving our main theorem, we recall a result by Fischer, presented in Chapter 2, that will play a crucial role in our proof.

Lemma 2.6. *Assume that Problem (3.1) is calm at x^*. Then, there exist $\bar{\delta} > 0$ and $\bar{w} > 0$ so that*

$$\bar{\omega}\,\mathrm{dist}[x, X^*] \leq \|\nabla H(x) H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \bar{\delta})$.

This lemma says that the problem $\nabla H(x)H(x) = 0$ inherits the calmness of $H(x) = 0$, and also that these systems must be equivalent in a neighborhood of x^*.

We now arrive at the main result of this chapter.

Theorem 3.1. *Assume that Problem (3.1) is calm at x^*. Then, there exists $\delta^\diamond > 0$ so that* $\mathrm{rank}(\nabla H(x)) = \mathrm{rank}(\nabla H(x^*))$ *for all $x \in \mathcal{B}(x^*, \delta^\diamond) \cap X^*$.*

Proof. Suppose that there exists a sequence $\{x^k\} \subset X^*$ with $x^k \to x^*$ so that

$$\mathrm{rank}\left(\nabla H(x^k)\right) \neq \mathrm{rank}\left(\nabla H(x^*)\right),$$

for all k. From the continuity of the Jacobian we can assume, without loss of generality, that

$$\mathrm{rank}\left(\nabla H(x^k)\right) > \mathrm{rank}\left(\nabla H(x^*)\right).$$

Let us consider now the singular value decomposition of $\nabla H(x)$ (see Chapter 2, p.8),

$$\nabla H(x)^\top = U_x \Sigma_x V_x^\top,$$

where $U_x \in \mathbb{R}^{m \times m}$ and $V_x \in \mathbb{R}^{n \times n}$ are orthogonal and Σ_x is the m by n diagonal matrix $\mathrm{diag}(\sigma_1(x), \sigma_2(x), ..., \sigma_{r_x}(x), 0, ..., 0)$ with positive singular values $\sigma_1(x) \geq \sigma_2(x) \geq ... \geq \sigma_{r_x}(x) > 0$. Note that $r_x \geq 0$ indicates the rank of $\nabla H(x)$. According to these definitions we have that $r_{x^*} < r_{x^k}$. In order to facilitate the notation we omit x in some manipulations and set $r := r_{x^*}$ and $r_k := r_{x^k}$. Now define $v^k := V_k e_{r+1}$, where

$$e_{r+1} := (0, ..., 0, \underbrace{1}_{r+1}, 0, ..., 0) \in \mathbb{R}^n.$$

Then, for all k we have that $\|v^k\| = 1$ and

$$v^k \perp \text{Kernel}\left(\nabla H(x^k)^\top\right) = \text{Span}\{V_k e_{r_k+1}, ..., V_k e_n\}. \tag{3.2}$$

We introduce now an auxiliary operator. Let $\Sigma_* := \Sigma_{x^*}$ and define $T : \mathbb{R}^n \to \mathbb{R}^{n\times m}$ as

$$T(x) := V_x \Sigma_*^\top U_x^\top.$$

Using the notation $U_k := U_{x^k}$, $V_k := V_{x^k}$ and $\Sigma_k := \Sigma_{x^k}$, we get, for all k,

$$T(x^k)\nabla H(x^k)^\top v^k = V_k\Sigma_*^\top U_k^\top U_k \Sigma_k V_k^\top v^k = V_k \Sigma_*^\top \Sigma_k e_{r+1} = V_k \Sigma_k^\top \Sigma_* e_{r+1} = 0. \tag{3.3}$$

Using Lemma 2.6 we conclude that

$$\begin{aligned}\text{dist}[x, X^*] &\leq \bar{\omega}\|\nabla H(x)H(x)\| \\ &\leq \bar{\omega}\|\left(\nabla H(x) - T(x^k)\right) H(x)\| + \bar{\omega}\|T(x^k)H(x)\| \\ &\leq \bar{\omega}\|\nabla H(x) - T(x^k)\|\|H(x)\| + \bar{\omega}\|T(x^k)H(x)\|. \end{aligned} \tag{3.4}$$

From the differentiability of H we know that there exist $\check{\delta} > 0$ and a Lipschitz constant $L > 0$ so that

$$\|H(x) - H(y)\| \leq L\|x - y\|,$$

for all $x, y \in \mathcal{B}(x^*, \check{\delta})$. Let $\bar{x} \in X^*$ denote a solution that satisfies $\|x - \bar{x}\| = \text{dist}[x, X^*]$ for an arbitrary point x. Then, there exists a positive constant $\bar{\delta} \leq \check{\delta}$ so that for all $x \in \mathcal{B}(x^*, \bar{\delta})$ we have $\bar{x} \in \mathcal{B}(x^*, \bar{\delta})$ and

$$\|H(x)\| = \|H(x) - H(\bar{x})\| \leq L\|x - \bar{x}\| = L\text{dist}[x, X^*]. \tag{3.5}$$

The continuity of ∇H implies that for some positive $\tilde{\delta} < \bar{\delta}$ we have that

$$\|\nabla H(x) - T(x^k)\| \leq \frac{1}{2\bar{\omega}L}, \tag{3.6}$$

whenever $x, x^k \in \mathcal{B}(x^*, \tilde{\delta})$. Thus, in this ball, (3.4), (3.5) and (3.6) lead to

$$\text{dist}[x, X^*] \leq 2\bar{\omega}\|T(x^k)H(x)\|. \tag{3.7}$$

Using Taylor's formula,

$$\|H(x^k + tv^k) - H(x^k) - t\nabla H(x^k)^\top v^k\| = o(t),$$

with $\lim_{t\to 0} o(t)/t = 0$. Then, in view of (3.3) and (3.7), there exist $\bar{k} > 0$ and $\bar{t} > 0$, so that for all $k > \bar{k}$ and $0 < t < \bar{t}$ we have that

$$\begin{aligned}\frac{1}{2\bar{\omega}}\text{dist}[x^k + tv^k, X^*] &\leq \|T(x^k)H(x^k + tv^k)\| \\ &= \|T(x^k)H(x^k + tv^k) - T(x^k)H(x^k) - tT(x^k)\nabla H(x^k)^\top v^k\| \\ &\leq \|T(x^k)\|\|H(x^k + tv^k) - H(x^k) - t\nabla H(x^k)^\top v^k\| \\ &= \sigma_1(x^*)o(t).\end{aligned}$$

On the other hand, taking (3.5) into account, we conclude that

$$\begin{aligned}\|\nabla H(x^k)^\top v^k\| &\leq \frac{o(t)}{t} + \frac{\|H(x^k + tv^k) - H(x^k)\|}{t} \\ &\leq \frac{o(t)}{t} + \frac{L}{t}\text{dist}[x^k + tv^k, X^*] \\ &\leq (1 + 2\bar{\omega}\sigma_1(x^*)L)\,\frac{o(t)}{t}.\end{aligned}$$

Taking the limit when $t \to 0^+$ we get

$$\nabla H(x^k)^\top v^k = 0,$$

which contradicts (3.2). □

3.3 Some related results

In this section we present some results related to Theorem 3.1 and discuss examples that illustrate the relevance of each hypothesis we assumed. Our first example shows that under calmness, the rank of the Jacobian must be locally constant only on the solution set, but not at other points.

Example 3.1. Consider the function $H : \mathbb{R}^2 \to \mathbb{R}^2$ defined by

$$H(x_1, x_2) = \begin{bmatrix} x_2 \\ x_2^2 \exp(x_1^2) \end{bmatrix}.$$

Thus, the Jacobian is given by

$$\nabla H(x_1, x_2)^\top = \begin{bmatrix} 0 & 1 \\ 2x_1 x_2^2 \exp(x_1^2) & 2x_2 \exp(x_1^2) \end{bmatrix}.$$

Define the sequence $\{x^k\} \not\subset X^*$ so that $x^k := (1, 1/k)$ with $k > 0$ and consider the solution $x^* := (1, 0)$. Obviously, $x^k \to x^*$ as $k \to \infty$ and $\text{rank}\left(\nabla H(x^k)\right) = 2 \neq 1 = \text{rank}\left(\nabla H(x^*)\right)$ for all $k > 0$. Nevertheless, one can easily check that $H(x) = 0$ is calm at x^*.

One may also ask if the converse of Theorem 3.1 is true, i.e., if constant rank on the solution set implies calmness. The simple example next shows that the answer to this question is negative.

Example 3.2. Let $H : \mathbb{R}^3 \to \mathbb{R}^2$ be defined by

$$H(x_1, x_2, x_3) = \begin{bmatrix} x_1 + x_2 \\ x_3^2 \end{bmatrix}.$$

The rank of the Jacobian on the solution set is always 1, but it is clear that the second component violates the error bound in Definition 3.1 around any solution.

In the convergence analysis of the Levenberg-Marquardt methods in [24] and [77] it was assumed, without loss of generality, that the Jacobian of H at x^* had at least one positive singular value. This assumption is rigorously supported by the following result.

Proposition 3.1. *Assume that Problem (3.1) is calm at $x^* \in X^*$ and that $\nabla H(x^*) = 0$. Then, there exists $\delta_1 > 0$ so that $H(x) = 0$ for all $x \in \mathcal{B}(x^*, \delta_1)$.*

Proof. Lemma 2.6 together with the assumption on $J_H(x^*)$ imply that there exists $\bar{\delta}$ such that

$$\begin{aligned}\bar{\omega}\,\mathrm{dist}[x, X^*] &\leq \|\nabla H(x)H(x)\| \\ &= \|(\nabla H(x) - \nabla H(x^*))H(x)\| \\ &\leq \|\nabla H(x) - \nabla H(x^*)\|\|H(x)\| \end{aligned} \tag{3.8}$$

for all $x \in \mathcal{B}(x^*, \bar{\delta})$. For a given x in this ball, take now $x' \in X^*$ such that $\|x - x'\| = \mathrm{dist}[x, X^*]$, and let L be the Lipschitz constant of H. It follows from (3.8) and the fact that x' belongs to X^* that

$$\begin{aligned}\bar{\omega}\,\mathrm{dist}[x, X^*] \leq \|\nabla H(x) - \nabla H(x^*)\|\|H(x)\| = \|\nabla H(x) - \nabla H(x^*)\|\|H(x) - H(x')\| \leq \\ L\|\nabla H(x) - \nabla H(x^*)\|\|x - x'\| = L\|\nabla H(x) - \nabla H(x^*)\|\mathrm{dist}[x, X^*]\end{aligned} \tag{3.9}$$

for all $x \in \mathcal{B}(x^*, \delta^\diamond)$, where $\delta^\diamond \leq \bar{\delta}$ is sufficiently small. By continuity of ∇H, there exists $\delta_1 \leq \delta^\diamond$ such that

$$\|\nabla H(x) - \nabla H(x^*)\| \leq \frac{\bar{\omega}}{2L}, \tag{3.10}$$

for all $x \in \mathcal{B}(x^*, \delta_1)$. Combining (3.9) and (3.10) we get $(\bar{\omega}/2)\mathrm{dist}[x, X^*] \leq 0$ for all $x \in \mathcal{B}(x^*, \delta_1)$, and hence the whole ball is contained in X^*. □

The next example suggests that complementarity type equations tend not to be calm at points that do not satisfy strict complementarity.

Example 3.3. Consider $H : \mathbb{R}^2 \to \mathbb{R}$ so that

$$H(x_1, x_2) := x_1 x_2.$$

The solution set correspondent to Problem (3.1) is $X^* = \{x \in \mathbb{R}^2 | x_1 = 0 \text{ or } x_2 = 0\}$ and the Jacobian is given by

$$\nabla H(x_1, x_2)^\top = \begin{bmatrix} x_2 & x_1 \end{bmatrix}.$$

Note that the rank of the Jacobian is 0 at $x^* := (0, 0)$ but it is equal to 1 at any other solution. Since the function is not identically zero in any neighborhood of x^*, Corollary 3.1 implies that Problem (3.1) cannot be calm at x^*. Nevertheless, note that in this example the systems $\nabla H(x)H(x) = 0$ and $H(x) = 0$ are equivalent around x^*. This means that the equivalence between these two systems of equations does not imply calmness.

We now show that calm problems are not that far away from full rank problems. This is formally described by the next Theorem, where we will rewrite Problem (3.1) as an equivalent full rank system of equations, also calm.

Theorem 3.2. *Assume that Problem (3.1) is calm at x^*. Then, there exists a continuously differentiable mapping $\bar{H} : \mathbb{R}^n \to \mathbb{R}^r$, with $r := \operatorname{rank}(\nabla H(x^*))$, so that the problem*

$$\bar{H}(x) = 0$$

is calm at x^* and locally equivalent to $H(x) = 0$. Moreover, there exists $\delta_2 > 0$ so that $\operatorname{rank}\left(\nabla \bar{H}(x)\right) = r$, for all $x \in \mathcal{B}(x^*, \delta_2)$.

Proof. Lemma 2.6 implies that for all $x \in \mathcal{B}(x^*, \bar{\delta})$ we have that

$$\begin{aligned} \operatorname{dist}[x, X^*] &\leq \bar{\omega}\|\nabla H(x)H(x)\| \\ &\leq \bar{\omega}\|\left(\nabla H(x) - \nabla H(x^*)\right)H(x)\| + \bar{\omega}\|\nabla H(x^*)H(x)\| \\ &\leq \bar{\omega}\|\nabla H(x) - \nabla H(x^*)\|\|H(x)\| + \bar{\omega}\|\nabla H(x^*)H(x)\|. \end{aligned} \tag{3.11}$$

Then, using the local Lipschitz continuity of H and the continuity of ∇H, we have

$$\|\nabla H(x) - \nabla H(x^*)\|\|H(x)\| \leq \frac{2}{\bar{\omega}}\operatorname{dist}[x, X^*],$$

in $\mathcal{B}(x^*, \hat{\delta})$, for $\hat{\delta} > 0$ sufficiently small, with the same argument used for obtaining the inequalities (3.9) and (3.10) in the proof of Proposition 3.1. This inequality combined with (3.11) implies that

$$\operatorname{dist}[x, X^*] \leq 2\bar{\omega}\|\nabla H(x^*)H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \hat{\delta})$. On the other hand, defining

$$\bar{H}(x) := \left(\sigma_1(x^*)\left(U_*^\top H(x)\right)_1, ..., \sigma_r(x^*)\left(U_*^\top H(x)\right)_r\right),$$

with $\sigma_1(x^*), ..., \sigma_r(x^*)$ and U_* as in Theorem 3.1, we get

$$\|\nabla H(x^*)H(x)\| = \|V_*\Sigma_*^\top U_*^\top H(x)\| = \|\bar{H}(x)\|.$$

Obviously, $\bar{H} : \mathbb{R}^n \to \mathbb{R}^r$ is continuously differentiable and $\operatorname{rank}\left(\nabla \bar{H}(x)\right) \leq r$ for all x. Furthermore, $\bar{H}(x) = 0$ is calm at x^* and equivalent to $H(x) = 0$ in a neighborhood of x^*.

In order to complete the proof we just need to show that $\operatorname{rank}(\nabla \bar{H}(x^*)) = r$, since the rank cannot diminish locally. It can be easily checked that it suffices to prove that

$$\operatorname{Kernel}\left(\nabla \bar{H}(x^*)^\top\right) \subset \operatorname{Kernel}\left(\nabla H(x^*)^\top\right). \tag{3.12}$$

So, let us prove this inclusion. We know that there exist $\delta_3 > 0$ and $\hat{\omega}$ so that

$$\operatorname{dist}[x, X^*] \leq \hat{\omega}\|\bar{H}(x)\|,$$

for all $x \in \mathcal{B}(x^*, \delta_3)$. Take $u \in \text{Kernel}\left(\nabla \bar{H}(x^*)\right)$ with $\|u\| = 1$. Then, for every $t > 0$ sufficiently small we have that

$$\begin{aligned} o(t) &= \|\bar{H}(x^* + tu) - \bar{H}(x^*) - t\nabla \bar{H}^\top u\| \\ &= \|\bar{H}(x^* + tu)\| \\ &\geq \frac{1}{\hat{\omega}} \text{dist}[x^* + tu, X^*] \\ &\geq \frac{1}{L\hat{\omega}} \|H(x^* + tu)\|, \end{aligned} \tag{3.13}$$

where the last inequality follows from the local Lipschitz continuity of H, with $L > 0$ as in Theorem 3.1. On the other hand, from Taylor's formula we know that

$$\lim_{t \to 0} \frac{1}{t} \|H(x^* + tu) - H(x^*) - t\nabla H(x^*)^\top u\| = 0.$$

This, together with (3.13), leads to

$$\nabla H(x^*)^\top u = 0,$$

which implies the inclusion (3.12). Therefore, there exists $\delta_2 > 0$ so that the rank of $\nabla \bar{H}(x)$ is r, for all $x \in \mathcal{B}(x^*, \delta_2)$. □

The next corollary characterizes the geometry of the solution set of a calm problem.

Corollary 3.1. *Assume that Problem (3.1) is calm at x^*. Then, X^* is locally, a differentiable manifold of codimension $r := rank(\nabla H(x^*))$.*

Proof. Given a continuously differentiable system $H(x) = 0$, such that the rank of $\nabla H(x)$ is constant on a neighborhood of a zero $\tilde{x}$ of H, it is well known that the set of solutions $\{x \in \mathbb{R}^n | H(x) = 0\}$ is locally a differentiable manifold (see, e.g., Proposition 12 in [72], p. 65). In view of Theorem 3.2 we conclude that this result applies to the set of zeroes of $\bar{H}$. The statement follows then from the local equivalence of $H(x) = 0$ and $\bar{H}(x) = 0$ at x^*, also proved in Theorem 3.2. □

Due to this corollary one can easily see that sets like $X^* := \{x \in \mathbb{R}^3 | x_2 = 0 \text{ or } x_1^2 + (x_2 - 1)^2 + x_3^2 = 1\}$ (the union of a sphere and a hyperplane with nonempty intersection) cannot represent the solution set of a calm problem, though it is the solution set of the differentiable system $H(x) = 0$ with

$$H(x_1, x_2, x_3) := x_2\left(x_1^2 + (x_2 - 1)^2 + x_3^2 - 1\right).$$

Another direct but interesting consequence of Corollary 3.1 is given next.

Corollary 3.2. *Assume that Problem (3.1) is calm at x^*. Then, there cannot exist a sequence of isolated solutions converging to x^*.*

Proof. Such a solution set cannot be a differentiable manifold. □

The example we will present now was given by Professor Alexey Izmailov and we use it to show how delicate Corollary 3.2 is.

Example 3.4. Let $H : \mathbb{R}^2 \to \mathbb{R}^2$ be given by

$$H(x_1, x_2) := \begin{cases} \left(x_2, x_2 - x_1^2 \sin(\frac{1}{x_1})\right), & \text{if } x_1 \neq 0; \\ (x_2, x_2), & \text{if } x_1 = 0. \end{cases}$$

In this example we have exactly one non-isolated solution, namely $x^* := (0,0)$, and x^* is the limit of the isolated solutions

$$x^k := \left(\frac{1}{2k\pi}, 0\right),$$

with k integer and $|k| \to \infty$. One can also observe that Problem (3.1) is calm at x^* and that

$$\nabla H(x^k) = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix},$$

for all $k > 0$. Nevertheless, the Jacobian of H at x^* is given by

$$\nabla H(x^*) = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}.$$

This change of rank does not contradict Corollary 3.2, since the Jacobian of H is not continuous at x^*. In this case, modifying a little bit the example in order to have continuity of the Jacobian and calmness is an impossible task. In fact, these two properties conflict with each other in the following sense. If one replaces x_1^2 by something smoother, like x_1^β, with $\beta > 2$, one gets continuity of the Jacobian but loses calmness.

Before closing the section we discuss one last example.

Example 3.5. Consider $H : \mathbb{R}^3 \to \mathbb{R}^2$ so that

$$H(x_1, x_2, x_3) := \begin{bmatrix} x_1^2 + x_2^2 - 1 \\ x_1^2 + x_3^2 - 1 \end{bmatrix},$$

The solution set X^* associated to (3.1) is the intersection of two perpendicular cylinders. The Jacobian of H is given by

$$\nabla H(x_1, x_2, x_3)^\top = \begin{bmatrix} 2x_1 & 2x_2 & 0 \\ 2x_1 & 0 & 2x_3 \end{bmatrix}.$$

The rank of the Jacobian is 2 at any solution except at $x := (1,0,0)$ and $x := (-1,0,0)$, where it is 1. Therefore, Problem (3.1) is not calm at these two solutions. But what makes this example illustrative is the fact that the equivalence of $\nabla H(x)H(x) = 0$ and $H(x) = 0$ is destroyed at $(1,0,0)$ and $(-1,0,0)$. Indeed, the solution set of $\nabla H(x)H(x) = 0$ is a surface while the solution set of $H(x) = 0$ is the union of two perpendicular ellipses that intersect each other at $(1,0,0)$ and $(-1,0,0)$.

3.4 Our theorem and iterative algorithms for solving systems of nonlinear equations

Although Theorem 3.1 seems to be just a result of Analysis, and refers specifically to the geometry of solution sets of calm problems, it echoes in practical algorithms for solving Problem (3.1). Apparently, our results suggest that one should not be that preoccupied with the magnitude of the regularization parameter in exact unconstrained Levenberg-Marquardt methods. In order to explain this better let us recall the description of a Levenberg-Marquardt iteration.

Interpret $s \in \mathbb{R}^n$ as the current iterate. Then, the Levenberg-Marquardt method demands solution of the following subproblem:

$$\min_{d \in \mathbb{R}^n} \|H(s) + \nabla H(s)^\top d\|^2 + \alpha(s)\|d\|^2, \tag{3.14}$$

where $\alpha(s) > 0$ is a regularization parameter. If we set this parameter equal to 0 and consider the minimum norm solution of (3.14), we recover the classical Gauss-Newton method. We will see in the next chapter that for calm problems, the local convergence rate of Gauss-Newton methods is superlinear (or quadratic) if the rank of the Jacobian is constant in a whole neighborhood of a solution. In other words, under constant rank, the Levenberg-Marquardt regularization is not needed. Of course one can easily construct functions where the Levenberg-Marquardt parameter has to be precisely chosen in order to maintain fast local convergence. In Example 3.1, for instance, quadratic convergence of the Levenberg-Marquardt method is only achieved if $\alpha(s)$ is chosen so that it remains proportional to $\|H(s)\|^\beta$, with $\beta \in [1, 3]$ (see Chapter 4). Nevertheless, in view of Lemma 3.2, such problems are kind of artificial. In fact, the numerical results in [29] have shown that the Levenberg-Marquardt parameter could be chosen with significant freedom without changing the accuracy of the method. The constant rank on the solution set of calm problems might also be the reason for the efficiency of the conjugate gradient method in solving the Levenberg-Marquardt subproblems, stated in the same reference.

Chapter 4

Projected Levenberg-Marquardt and Gauss-Newton methods under the calmness condition

In this chapter we address the problem of solving nonlinear equations subject to convex constraints under the local error bound condition. For solving the system of equations, we consider basically local versions of projected Gauss-Newton and Levenberg-Marquardt type methods. The Levenberg-Marquardt method is a regularized Gauss-Newton method that under the local error bound that characterizes the calmness condition achieves a quadratic rate of convergence, if its regularization parameter is suitably chosen. We will present sufficient conditions so that the regularization is not needed in order to achieve quadratic convergence. Roughly speaking, if the singular values of the Jacobian of the function that defines the system of equations remain of the order of the norm of the function along the iterates, the Levenberg-Marquardt regularization parameter can be set equal to zero, i.e., the Gauss-Newton converges quadratically. Additionally, we propose a theoretical algorithm that removes small singular values that may destroy quadratic convergence. The relation between the order of the singular values and quadratic convergence of projected Levenberg-Marquardt methods is given and illustrated by examples.

4.1 Introduction

Let us consider the following system of nonlinear equations subject to constraints

$$H(x) = 0, \quad x \in \Omega, \tag{4.1}$$

where $H : \mathbb{R}^n \to \mathbb{R}^m$ is differentiable with a locally Lipschitz Jacobian and $\Omega \subseteq \mathbb{R}^n$ is closed, convex and nonempty. We denote by X^* the set of solutions of (4.1) and suppose it is nonempty.

Projected Levenberg-Marquardt methods for solving systems of nonlinear equations were introduced in [46] (see Chapter 2). The subproblems of these methods consist of calculating an unconstrained Levenberg-Marquardt step and projecting the resulting point onto the feasible set Ω. The local error bound considered in such methods is precisely the local error bound used in [76], for the unconstrained case. In [29] it was proved that the projected Levenberg-Marquardt method can be seen as an inexact unconstrained one. In this chapter we focus on the influence of the Levenberg-Marquardt regularization parameter on the rate of convergence of the method. We show how the parameter should be chosen in order to get quadratic convergence.

The chapter is organized as follows. In the first section we have some preliminary results and assumptions taken from the background material. We then formally recall the Gauss-Newton method, and in Section 4.3.3 we prove its quadratic convergence assuming that no positive singular value of the Jacobian of $\nabla H(x)$ converge to zero faster than $\|H(x)\|$ along the iterates. In Section 4.4 we simply reformulate the Gauss-Newton method considering a rule that removes singular values that may destroy local quadratic convergence. In Section 4.6 we present a theorem that relates the order of singular values and the value of the Levenberg-Marquardt parameter required for getting quadratic convergence.

4.2 Preliminaries

Next, we formally introduce the basic assumptions needed in the convergence analysis of the algorithms we are going to present.

Assumption 4.1. *$H : \mathbb{R}^n \to \mathbb{R}^m$ is differentiable with a locally Lipschitz continuous Jacobian.*

Assumption 4.2. *$\Omega \subseteq \mathbb{R}^n$ is closed, convex and nonempty and $X^* := \{x \in \Omega | H(x) = 0\}$ is nonempty.*

Notice that Assumption 4.1 implies that X^* is closed. From now on let $x^* \in X^*$ be a fixed solution of Problem 4.1.

Assumption 4.3. *There exist $\omega > 0$ and $\delta_1 \in (0, 1]$ so that*

$$\omega\, dist[x, X^*] \leq \|H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \delta_1)$.

Despite the fact that Problem 4.1 has convex constraints, we consider an error bound that does not involve the feasible set Ω. In the next chapter, the error bound we will deal with is significantly weaker than Assumption 4.3, in the sense that it will be asked to hold in a neighborhood of x^* intersected with Ω. Next, we recall Lemma 2.1 in Chapter 2.

Lemma 2.1. *There exist $L > 0$ and $\delta_2 > 0$ such that for all $x, y \in \mathcal{B}(x^*, \delta_2)$ the following inequalities hold:*

$$\|H(y) - H(x) - \nabla H(x)^\top (y - x)\| \le L\|y - x\|^2, \tag{4.2}$$

$$\|H(y) - H(x)\| \le L\|y - x\|, \tag{4.3}$$

$$\|\nabla H(y) - \nabla H(x)\| \le L\|y - x\|, \tag{4.4}$$

$$\|\nabla H(x)\| \le L. \tag{4.5}$$

4.3 Sufficient conditions for quadratic convergence of the Gauss-Newton method

Algorithm 2.1, presented in Chapter 2, reduces to the projected Gauss-Newton algorithm we are going to present next, when setting $\alpha(s) := 0$. Consider the function $\varphi_{GN}(x, s) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}_+$ defined by

$$\varphi_{GN}(x, s) := \frac{1}{2}\|H(s) + \nabla H(s)^\top (x - s)\|^2. \tag{4.6}$$

4.3.1 Algorithm

Algorithm 4.1. Projected Gauss-Newton method
Step 0. Choose $x^0 \in \Omega$
Step 1. If $H(x^k) = 0$ stop, else set $s := x^k$.
Step 2. Compute the solution $x_{GN}(s)$ of the optimization problem

$$\min_{x \in \mathbb{R}^n} \varphi_{GN}(x, s), \tag{4.7}$$

which lies closest to s with φ_{GN} defined as in (4.6).
Step 3. Set $x^{k+1} := P_\Omega(x_{GN}(s))$.
Step 4. Set $k := k + 1$ and go to Step 1.

We know that for each $s \in \mathbb{R}^n$ the quadratic function $\varphi_{GN}(\cdot, s)$ is convex and has at least one minimizer. Let $X^{GN}(s)$ denote the solution set of the subproblem (4.7). We also know that $X^{GN}(s)$ is nonempty, closed and convex. Thus, the problem

$$\min_{x \in X^{GN}(s)} \|x - s\|^2 \tag{4.8}$$

has a unique solution which is precisely $x_{GN}(s)$. This, together with the fact that Ω is nonempty, implies the following proposition.

Proposition 4.1. *Algorithm 4.1 is well defined.*

Let us now consider $\varphi_\alpha(x,s) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}_+$ defined as

$$\varphi_\alpha(x,s) := \frac{1}{2}\|H(s) + \nabla H(s)^\top (x-s)\|^2 + \alpha\|x-s\|^2, \tag{4.9}$$

with $\alpha > 0$. It is easy to see that $\varphi(\cdot, s)$ is strongly convex and thus has exactly one minimizer, which we will denote by $x_\alpha(s)$. If one replaces (4.7) by

$$\min_{x\in\mathbb{R}^n} \varphi_\alpha(x,s) \tag{4.10}$$

in Algorithm 4.1, the resulting method is a projected Levenberg-Marquardt method. Along the next sections we will use the following notation:

$$d_{GN}(s) := x_{GN}(s) - s, \tag{4.11}$$

$$d_\alpha(s) := x_\alpha(s) - s. \tag{4.12}$$

Lemma 4.1. *For all $s \in \mathbb{R}^n$ it holds that*

(a) *if $\alpha_1 > \alpha_2 > 0$ then $\|d_{\alpha_1}(s)\| \le \|d_{\alpha_2}(s)\|$. In particular, $\|d_\alpha(s)\| \le \|d_{GN}(s)\|$ for all $\alpha > 0$;*

(b) $\lim_{\alpha\to 0^+} x_\alpha(s) = x_{GN}(s)$.

Proof. See Lemma 2.5 in Chapter 2. □

4.3.2 An assumption on the magnitude of the singular values

From now on we will suppose that $\nabla H(x^*) \neq 0$, because otherwise we know from Proposition 3.1 that H is identically zero in a neighborhood of x^*. Obviously this case is not interesting since any reasonable algorithm should then converge locally in one only step. So, we are assuming in particular that $\nabla H(x^*)$ has at least one positive singular value. Due to the continuity of the Jacobian, this remains true in a neighborhood of x^*. Therefore, there exists $\delta_3 > 0$ so that for all $s \in \mathcal{B}(x^*, \delta_3)$ we can write

$$\nabla H(s)^\top = U_s \Sigma_s V_s^\top, \tag{4.13}$$

where $U_s \in \mathbb{R}^{m\times m}$ and $V_s \in \mathbb{R}^{n\times n}$ are orthogonal and Σ_s is the m by n diagonal matrix $\mathrm{diag}(\sigma_1(s), \sigma_2(s), ..., \sigma_{r_s}(s), 0, ..., 0)$ with singular values $\sigma_1(s) \ge \sigma_2(s) \ge ... \ge \sigma_{r_s}(s) > 0$. Let $\sigma(s)$ denote the smallest positive singular value $\sigma_{r_s}(s)$, where $r_s \ge 1$ indicates the rank of $\nabla H(s)^\top$.

Assumption 4.4. *There exist $\bar{L} > 0$ and $\delta_3 > 0$ so that*

$$\sigma(s) \ge \bar{L}\|H(s)\|$$

for all $s \in \mathcal{B}(x^*, \delta_3)$.

Lemma 4.2. *If the rank of the Jacobian of H is constant in a neighborhood of x^*, then Assumption 4.4 is satisfied.*

Proof. The proof is elementary, since all positive singular values remain bounded away from zero. □

4.3.3 Convergence analysis of the Gauss-Newton method

Define now

$$\delta := \min\{\delta_i | i = 1, 2, 3\}, \tag{4.14}$$

with $\delta_1, \delta_2, \delta_3$ as in Assumptions 4.3, 4.4 and Lemma 2.1. The next lemma characterizes the Gauss-Newton and the Levenberg-Marquardt steps in terms of the singular value decomposition of the Jacobian of H.

Lemma 4.3. *For any $s \in \mathbb{R}^n$ it holds that $\|d_\alpha(s)\| = \|v_\alpha(s)\|$, where $v_\alpha(s) \in \mathbb{R}^{r_s}$ is defined by*

$$v_\alpha(s)_i := -\frac{\left(U_s^\top H(s)\right)_i}{\sigma(s)_i + \frac{\alpha}{\sigma(s)_i}},$$

for $i = 1, ..., r_s$ and $\alpha \geq 0$, with $U_s, \sigma(s)_i$ as in (4.13) and $d_\alpha(s)$ as in (4.12).

Proof. Taking into account the notation $d := x - s$, $u := V_s^\top d$ and the fact that V_s and U_s are orthogonal matrices, we get

$$\begin{aligned}
2\varphi_\alpha(x,s) &= \|H(s)\|^2 + 2H(s)^\top U_s \Sigma_s V_s^\top d + d^\top V_s \Sigma_s^\top U_s^\top U_s \Sigma_s V_s^\top d + \alpha\|d\|^2 \\
&= \|H(s)\|^2 + 2\left(U_s^\top H(s)\right)^\top \Sigma_s u + u^\top \Sigma_s^\top \Sigma_s u + \alpha u^\top u \\
&= \|H(s)\|^2 + 2\sum_{i=1}^{r_s} \left(U_s^\top H(s)\right)_i u_i \sigma(s)_i + \sum_{i=1}^{r_s} u_i^2((\sigma(s)_i)^2 + \alpha) + \sum_{i=r_s+1}^{n} \alpha u_i^2.
\end{aligned}$$

Let us now consider the unconstrained optimization problem

$$\min_{u \in \mathbb{R}^n} \|H(s)\|^2 + 2\sum_{i=1}^{r_s} \left(U_s^\top H(s)\right)_i u_i \sigma(s)_i + \sum_{i=1}^{r_s} u_i^2((\sigma(s)_i)^2 + \alpha) + \sum_{i=r_s+1}^{n} \alpha u_i^2, \tag{4.15}$$

with $u \in \mathbb{R}^n$. We claim that for $\alpha \geq 0$, the vector

$$u_\alpha(s) := (\underbrace{v_\alpha(s)}_{r_s}, \underbrace{0, ..., 0}_{n-r_s}) \in \mathbb{R}^n$$

is the solution of (4.15). In order to establish the claim, note that, due to the convexity of problem (4.15) and the definition of $v_\alpha(s)$, one just needs to observe that

$$\frac{\partial\left(2\left(U_s^\top H(s)\right)_i u(s)_i \sigma(s)_i + (u(s)_i)^2((\sigma(s)_i)^2 + \alpha)\right)}{\partial u_i} = 0, \text{ for } i = 1, ..., r_s,$$

and if $\alpha > 0$,

$$\frac{\partial\left(\alpha(u_\alpha(s)_i)^2\right)}{\partial u_i} = 0, \text{ for } i = r_s + 1, ..., n.$$

It is obvious that when $\alpha = 0$ the components associated to the indices $i = r_s+1, ..., n$ of the solution of minimal norm must be zero. Hence, for $\alpha \geq 0$ we have $d_\alpha(s) = V_s u_\alpha(s)$ and $\|d_\alpha(s)\| = \|u_\alpha(s)\| = \|v_\alpha(s)\|$. □

Lemma 4.4. *Suppose that Assumptions 4.1 - 4.4 hold. Then, there exist* $C_1 > 0$ *and* $C_2 > 0$ *such that the following inequalities hold for all* $s \in \mathcal{B}(x^*, \delta/2)$*:*

(a) $\|d_{GN}(s)\| \leq C_1 \, dist\,[s, X^*]$;

(b) $\|H(s) + \nabla H(s)^\top d_{GN}(s)\| \leq C_2 \, dist[s, X^*]^2$.

Proof. For proving (a), we will compare the size of $d_{GN}(s)$ to the size of $d_\alpha(s)$ with $\alpha := \|H(s)\|^2$. If $s \in X^*$ we have $d_{GN}(s) = 0$ and then (a) holds trivially. If $s \notin X^*$ we have that, in view of Lemma 2.7, there exists a constant $\bar{C}_1 > 0$ so that

$$\|d_\alpha(s)\| \leq \bar{C}_1 \text{dist}[x^k, X^*] \tag{4.16}$$

for all $s \in \mathcal{B}(x^*, \delta/2)$. We will now use the characterization given in Lemma 4.3, which gives the vectors $v_{GN}(s), v_\alpha(s) \in \mathbb{R}^{r_s}$ associated to $d_{GN}(s)$ and $d_\alpha(s)$, respectively. We consider two cases.

(i) Suppose $\left(U_s^\top H(s)\right)_i = 0$ for some $i = 1, ..., r_k$. In this case $v_{GN}(s)_i = v_\alpha(s)_i = 0$.

(ii) Now assume that $\left(U_s^\top H(s)\right)_i \neq 0$ for some $i = 1, ..., r_k$. According to our definition, this implies that $v_{GN}(s)_i \neq 0$ and $v_\alpha(s)_i \neq 0$. Then

$$\frac{v_{GN}(s)_i}{v_\alpha(s)_i} = \frac{\left(U_s^\top H(s)\right)_i}{\sigma(s)_i}\left(\frac{\sigma(s)_i + \frac{\|H(s)\|^2}{\sigma(s)_i}}{\left(U_s^\top H(s)\right)_i}\right) = 1 + \left(\frac{\|H(s)\|}{\sigma(s)_i}\right)^2.$$

These conclusions, together with Assumption 4.4, imply that for all $i = 1, ..., r_s$ we have

$$\begin{aligned}
|v_{GN}(s)_i| &= |v_\alpha(s)_i|\left(1 + \left(\frac{\|H(s)\|}{\sigma(s)_i}\right)^2\right) \\
&\leq |v_\alpha(s)_i|\left(1 + \left(\frac{\|H(s)\|}{\bar{L}\|H(s)\|}\right)^2\right) \\
&= |v_\alpha(s)_i|\left(1 + \frac{1}{\bar{L}^2}\right).
\end{aligned}$$

Thus,

$$\|d_{GN}(s)\| = \|v_{GN}(s)\| \leq \left(1 + \frac{1}{\bar{L}^2}\right)\|v_\alpha(s)\| = \left(1 + \frac{1}{\bar{L}^2}\right)\|d_\alpha(s)\|.$$

Using (4.16) we get

$$\|d_{GN}(s)\| \leq C_1 \text{dist}[s, X^*],$$

for all $s \in \mathcal{B}(x^*, \delta/2)$, with $C_1 := \bar{C}_1 \left(1 + \frac{1}{L^2}\right)$. This proves (a).

We now prove (b). Let $\bar{s} \in X^*$ be so that $\text{dist}[s, X^*] = \|s - \bar{s}\|$. Then, from the definition of $d_{GN}(s)$ and (4.2), we have

$$\begin{aligned}\|H(s) + \nabla H(s)^\top d_{GN}(s)\| &\leq \|H(s) - \underbrace{H(\bar{s})}_{=0} + \nabla H(s)^\top (s - \bar{s})\| \\ &\leq L\|s - \bar{s}\|^2 = L\text{dist}[s, X^*]^2.\end{aligned}$$

Hence, statement (b) holds with $C_2 := L$. □

This was the key lemma for deriving the convergence result given by the following theorem. We omit its proof since a more general analysis will be given in the next section.

Theorem 4.1. *If Assumptions 4.1 - 4.4 hold and $x^0 \in \Omega$ is chosen sufficiently close to x^*, Algorithm 4.1 generates a sequence $\{x^k\}$ that converges quadratically to some solution $\bar{x} \in X^*$.*

This theorem is more general than the results on Gauss-Newton methods given in [54], where full rank of the Jacobian was required. Note also that our theorem implies that if the singular values remain proportional to $\|H(s)\|$ along the iterates, then the Levenberg-Marquardt parameter can be chosen with a certain freedom in order to get local quadratic convergence. In fact, if one chooses the regularization parameter so that its order is less or equal to $\|H(s)\|$, the quadratic rate is achieved. Nevertheless, Assumption 4.4 is not satisfied in general. We will give examples in this chapter where small singular values destroy quadratic convergence of Levenberg-Marquardt methods for certain choices of their parameters.

4.4 A correction on the projected Gauss-Newton method

In this subsection we again study a Gauss-Newton type method for solving (4.1). Roughly speaking, given the iterate $s \in \mathbb{R}^n$ we consider a correction of $\nabla H(s)$ removing its singular values that are smaller than some constant times $\|H(s)\|$. To this end we choose an arbitrary but fixed constant $\tilde{L} > 0$ and define the regularized matrix

$$A(s)^\top = U_s \tilde{\Sigma}_s V_s^\top, \tag{4.17}$$

where $\tilde{\Sigma}_s$ is the $m \times n$ diagonal matrix $\text{diag}(\sigma_1(s), \sigma_2(s), ..., \sigma_{\tilde{r}_s}(s), 0, ..., 0)$ and $\tilde{r}_s$ is the largest index such that $\sigma_i(s) \geq \tilde{L}\|H(s)\|$. The error between the original matrix and the perturbed one will be denoted by $E(s)^\top = \nabla H(s) - A(s)$. For $s \in \mathbb{R}^n$ let $\tilde{x}_{GN}(s)$ denote the solution of the problem

$$\min_{x \in \mathbb{R}^n} \|H(s) - A(s)^\top (x - s)\|^2,$$

which lies closest to s. We set $\tilde{d}_{GN}(s) := \tilde{x}_{GN}(s) - s$ in order to shorten the notation in some manipulations.

4.4.1 Algorithm

Algorithm 4.2. A corrected projected Gauss-Newton method
Step 0. Choose $x^0 \in \Omega$ and set $k := 0$.
Step 1. Define $x^{k+1} := P_\Omega(\tilde{x}_{GN}(x^k))$.
Step 2. Set $k := k + 1$ and go to Step 1.

The fact that this algorithm is well defined can be proved with the argument used in the proof of Proposition 4.1.

Proposition 4.2. *Algorithm 4.2 is well defined.*

4.4.2 Convergence analysis of the corrected GN method

Proposition 4.3. $\|E(s)\| < \tilde{L}\|H(s)\|$.

Proof. Note that $E(s) = U_s(\Sigma_s - \tilde{\Sigma}_s)V_s^\top$ and

$$\Sigma_s - \tilde{\Sigma}_s = \text{diag}(0, ..., 0, \sigma^s_{\tilde{r}_s+1}, ..., \sigma^s_{r_s}, 0, ..., 0).$$

Hence, $\|E(s)\| = \sigma^s_{r_s+1}$. The statement then follows from this fact combined with the definition of $A(s)$. □

Lemma 4.5. *Assume that Assumption 4.1-4.3 hold. Then, there exist constants $C_3 > 0$, $C_4 > 0$ such that the following inequalities hold for all $s \in \mathcal{B}(x^*, \delta/2)$:*

(a) $\|\tilde{d}_{GN}(s)\| \leq C_3 \, dist\,[s, X^*]$;

(b) $\|H(s) + A(s)^\top \tilde{d}_{GN}(s)\| \leq C_4 \, dist[s, X^*]^2$.

Proof. The proof of (a) is similar to the proof of Lemma 4.4 (a). One just needs to observe that Assumption 2 is automatically satisfied with $\bar{L} = \tilde{L}$ due to the definition of $A(x^k)$. We now prove (b). Let $\bar{s}$ be a point in the solution set X^* so that $\|s - \bar{s}\| = \text{dist}[s, X^*]$. From the definitions of $\tilde{d}_{GN}(s)$ and $A(s)$, Lemma 2.1 and Proposition 4.3

we conclude that

$$\begin{aligned}\|H(s)+A(s)^\top \tilde{d}_{GN}(s)\| &\le \|H(s)-\underbrace{H(\bar{s})}_{=0}+A(s)^\top(s-\bar{s})\|\\ &\le \|H(s)-H(\bar{s})+\nabla H(s)^\top(s-\bar{s})\|+\|E(s)(s-\bar{s})\|\\ &\le L\|s-\bar{s}\|^2+\tilde{L}\|H(s)\|\|s-\bar{s}\|\\ &= L\|s-\bar{s}\|^2+\tilde{L}\|H(s)-H(\bar{s})\|\|s-\bar{s}\|\\ &\le (L+\tilde{L}L)\|s-\bar{s}\|^2\\ &= (L+\tilde{L}L)\text{dist}[s,X^*]^2.\end{aligned}$$

Thus (b) holds with $C_4 := (L+\tilde{L}L)$. □

Proposition 4.4. *Suppose that Assumptions 4.1-4.3 are satisfied. Let $\{x^k\}$ be the sequence generated by Algorithm 4.2. If $x^k, x^{k+1} \in B(x^*, \delta/2)$, then there exists $C_5 > 0$ so that*

$$dist[x^{k+1}, X^*] \le C_5\, dist[x^k, X^*]^2.$$

Proof. From the definition of $\tilde{x}_{GN}(x^k)$, the nonexpansiveness of the projection operator and the assumption that $x^k, \tilde{x}_{GN}(x^k) \in \mathcal{B}(x^*, \delta/2)$, we obtain

$$\begin{aligned}w\text{dist}[x^{k+1},X^*] &= w\ \text{dist}[P_\Omega(\tilde{x}_{GN}(x^k)),X^*]\\ &= w \inf_{x\in X^*}\|P_\Omega(\tilde{x}_{GN}(x^k))-x\|\\ &= w \inf_{x\in X^*}\|P_\Omega(\tilde{x}_{GN}(x^k))-P_\Omega(x)\| \qquad (4.18)\\ &\le w \inf_{x\in X^*}\|\tilde{x}_{GN}(x^k)-x\|\\ &= w\ \text{dist}[\tilde{x}_{GN}(x^k),X^*] \le \|H(\tilde{x}_{GN}(x^k))\|.\end{aligned}$$

The definition of $A(x^k)$, Lemma 2.1 and Proposition 4.3 imply that

$$\begin{aligned}\|H(x^k)-H(\tilde{x}_{GN}(x^k))+A(x^k)^\top\tilde{d}_{GN}(x^k)\| &\le L\|\tilde{d}_{GN}(x^k)\|^2+\|E(x^k)\|\|\tilde{d}_{GN}(x^k)\|\\ &\le L\|\tilde{d}_{GN}(x^k)\|^2+\tilde{L}\|H(x^k)\|\|\tilde{d}_{GN}(x^k)\|.\end{aligned} \qquad (4.19)$$

Inequalities (4.18) and (4.19) together with Lemma 4.5 lead to

$$\begin{aligned}w\text{dist}[x^{k+1},X^*] &\le \|H(\tilde{x}_{GN}(x^k)\|\\ &\le \|H(x^k)+A(x^k)^\top\tilde{d}_{GN}(x^k)\|+\|H(x^k)-H(\tilde{x}_{GN}(x^k))+A(x^k)^\top\tilde{d}_{GN}(x^k)\|\\ &\le C_4\text{dist}[x^k,X^*]^2+L\|\tilde{d}_{GN}(x^k)\|^2+\tilde{L}\|H(x^k)\|\|\tilde{d}_{GN}(x^k)\|\\ &\le (C_4+LC_3^2+\tilde{L}LC_3)\text{dist}[x^k,X^*]^2.\end{aligned}$$

Hence, the statement holds with $C_5 := w^{-1}(C_4+LC_3^2+\tilde{L}LC_3)$. □

Lemma 4.5 is the key result of our analysis and plays a decisive role in deriving the convergence theorems of this subsection. The technical tools used in the proofs of the following lemmas and theorems are based on the approach in [46] and are presented here for the sake of completeness.

Lemma 4.6. *Let Assumptions 4.1-4.3 be satisfied and x^k be a sequence generated by Algorithm 4.2 with starting point $x^0 \in \mathcal{B}(x^*, \varepsilon)$, where*

$$\varepsilon := \min\left\{\frac{\delta}{2(1+2C_3)}, \frac{1}{2C_5}\right\}. \tag{4.20}$$

Then, the sequence $\{dist[x^k, X^*]\}$ converges to zero quadratically.

Proof. Due to Proposition 4.4 we just need to prove that $x^k, \tilde{x}_{GN}(x^k) \in \mathcal{B}(x^*, \delta/2)$ for all k. Our proof will be by induction on k. Let us start with $k = 0$. Of course $x^0 \in \mathcal{B}(x^*, \delta/2)$, since $\varepsilon \le \delta/2$. Hence, from Lemma 4.5 it follows that

$$\begin{aligned}\|\tilde{x}_{GN}(x^0) - x^*\| &\le \|x^0 - x^*\| + \|\tilde{x}_{GN}(x^0) - x^0\| \\ &\le \varepsilon + C_3 \text{dist}[x^0, X^*] \\ &\le (1 + C_3)\varepsilon.\end{aligned}$$

Since $(1 + C_3)\varepsilon \le \delta/2$, we have $\tilde{x}_{GN}(x^0) \in \mathcal{B}(x^*, \delta/2)$.

Suppose now that $k > 0$ and that $x^\ell, \tilde{x}_{GN}(x^\ell) \in \mathcal{B}(x^*, \delta/2)$ for all $\ell = 0, 1, ..., k$. The nonexpansiveness of the projection operator implies that

$$\|x^{k+1} - x^*\| = \|P_\Omega(\tilde{x}_{GN}(x^k)) - P_\Omega(x^*)\| \le \|\tilde{x}_{GN}(x^k) - x^*\|. \tag{4.21}$$

Hence, $x^{k+1} \in \mathcal{B}(x^*, \delta/2)$. Next, we show that $\tilde{x}_{GN}(x^{k+1}) \in \mathcal{B}(x^*, \delta/2)$. Using (4.21), the induction hypothesis and Lemma 4.5 successively we obtain

$$\begin{aligned}\|\tilde{x}_{GN}(x^{k+1}) - x^*\| &= \|x^{k+1} + \tilde{d}_{GN}(x^{k+1}) - x^*\| \\ &\le \|x^{k+1} - x^*\| + \|\tilde{d}_{GN}(x^{k+1})\| \\ &\le \|\tilde{x}_{GN}(x^k) - x^*\| + \|\tilde{d}_{GN}(x^{k+1})\| \\ &\le \|x^k - x^*\| + \|\tilde{d}_{GN}(x^k)\| + \|\tilde{d}_{GN}(x^{k+1})\| \\ &\vdots \qquad \vdots \\ &\le \|x^0 - x^*\| + \sum_{\ell=0}^{k+1} \|\tilde{d}_{GN}(x^\ell)\| \\ &\le \varepsilon + C_3 \sum_{\ell=0}^{k+1} \text{dist}[x^\ell, X^*]. \end{aligned} \tag{4.22}$$

From Proposition 4.4 we have that for all $\ell = 1, ..., k$

$$\begin{aligned}
\text{dist}[x^\ell, X^*] &\leq C_5 \text{dist}[x^{\ell-1}, X^*]^2 \\
&\leq C_5 C_5^2 \text{dist}[x^{\ell-2}, X^*]^{2^2} \\
&\vdots \qquad \vdots \\
&\leq C_5 C_5^2 ... C_5^{2^\ell} \text{dist}[x^0, X^*]^{2^\ell} \\
&= C_5^{2^\ell - 1} \text{dist}[x^0, X^*]^{2^\ell} \\
&\leq C_5^{2^\ell - 1} \|x^0 - x^*\|^{2^\ell} \leq C_5^{2^\ell - 1} \varepsilon^{2^\ell} \qquad (4.23)
\end{aligned}$$

Taking into account the definition of ε, (4.22) and (4.23) we get

$$\begin{aligned}
\|x^{k+1} - x^*\| &\leq \varepsilon + C_3 \sum_{\ell=0}^{k} C_5^{2^\ell - 1} \varepsilon^{2^\ell} = \varepsilon + C_3 \varepsilon \sum_{\ell=0}^{k} C_5^{2^\ell - 1} \varepsilon^{2^\ell - 1} \\
&\leq \varepsilon + C_3 \varepsilon \sum_{\ell=0}^{k} \left(\frac{1}{2}\right)^{2^\ell - 1} \\
&\leq \varepsilon + C_3 \varepsilon \sum_{\ell=0}^{\infty} \left(\frac{1}{2}\right)^{2^\ell} = (1 + 2C_3)\varepsilon \leq \frac{\delta}{2}.
\end{aligned}$$

This completes the induction step. □

Now we deal with the behavior of the sequence $\{x^k\}$ itself. The next result states that the sequence generated by Algorithm 4.2 is convergent if we start sufficiently close to the solution set.

Theorem 4.2. *Let Assumptions 4.1-4.3 be satisfied and x^k be a sequence generated by Algorithm 4.2 with starting point $x^0 \in \mathcal{B}(x^*, \varepsilon)$, where ε is defined as in (4.20)). Then the sequence $\{x^k\}$ converges to a solution $\bar{x}$ of (4.1) belonging to the ball $\mathcal{B}(x^*, \delta/2)$.*

Proof. We will verify that $\{x^k\}$ is a Cauchy sequence. Indeed, for any integers k and m such that $k > m$, we obtain

$$\begin{aligned}
\|x^k - x^m\| &= \|P_\Omega(x^{k-1} + \tilde{d}_{GN}(x^{k-1}) - P_\Omega(x^m)\| \\
&\leq \|x^{k-1} + \tilde{d}_{GN}(x^{k-1}) - x^m\| \\
&\leq \|x^{k-1} - x^m\| + \|\tilde{d}_{GN}(x^{k-1})\| \\
&= \|P_\Omega(x^{k-2} + \tilde{d}_{GN}(x^{k-2})) - P_\Omega(x^m)\| + \|\tilde{d}_{GN}(x^{k-1})\| \\
&\leq \|x^{k-2} + \tilde{d}_{GN}(x^{k-2}) - x^m\| + \|\tilde{d}_{GN}(x^{k-1})\| \\
&\leq \|x^{k-2} - x^m\| + \|\tilde{d}_{GN}(x^{k-2})\| + \|\tilde{d}_{GN}(x^{k-1})\| \\
&\vdots \qquad \vdots \\
&\leq \sum_{\ell=m}^{k-\ell} \|\tilde{d}_{GN}(x^\ell)\| \leq \sum_{\ell=m}^{\infty} \|\tilde{d}_{GN}(x^\ell)\|.
\end{aligned}$$

Now, as in the proof of Lemma 4.6, due to (4.20) and (4.23), we have

$$\|\tilde{d}_{GN}(x^\ell)\| \leq C_3 \text{dist}[x^\ell, X^*] \leq C_3 C_5^{2^\ell - 1} \varepsilon^{2^\ell} \leq C_3 \varepsilon \left(\frac{1}{2}\right)^{2^\ell - 1} \leq C_3 \varepsilon \left(\frac{1}{2}\right)^\ell.$$

Consequently, we get $\|x^k - x^m\| \leq C_3 \varepsilon \sum_{\ell=m}^{\infty} \left(\frac{1}{2}\right)^\ell \to 0$ as $m \to \infty$. This means that $\{x^k\}$ is a Cauchy sequence and hence convergent to a point in X^*. □

Lemma 4.7. *Let $x^0 \in \mathcal{B}(x^*, \varepsilon)$ and $\{x^k\}$ be a sequence generated by Algorithm 4.2 and $\bar{x} \in X^*$ its limit when $k \to \infty$. Then, there exist positive constants C_6, C_7, C_8, C_9 such that*

(a) *$\text{dist}[x^k, X^*] \leq C_6 \|\tilde{d}_{GN}(x^k)\|$*

(b) $\|\tilde{d}_{GN}(x^{k+1})\| \leq C_7 \|\tilde{d}_{GN}(x^k)\|^2$

(c) $C_8 \|x^k - \bar{x}\| \leq \|\tilde{d}_{GN}(x^k)\| \leq C_9 \|x^k - \bar{x}\|$

hold for all $k \in \mathbb{N}$ sufficiently large.

Proof. First note that Lemma 4.6 implies that $\text{dist}[x^{k+1}, X^*] \leq \frac{1}{2}\text{dist}[x^k, X^*]$ for $k \in \mathbb{N}$ sufficiently large. Let $\bar{x}^{k+1} \in X^*$ be a solution that satisfies $\text{dist}[x^{k+1}, X^*] = \|\bar{x}^{k+1} - x^{k+1}\|$. From the nonexpansiveness of the projection operator we obtain

$$\begin{aligned}
\|\tilde{d}_{GN}(x^k)\| &= \|x^k + \tilde{d}_{GN}(x^k) - x^k\| \geq \|P_\Omega(x^k + \tilde{d}_{GN}(x^k)) - P_\Omega(x^k)\| \\
&= \|x^{k+1} - x^k\| \geq \|\bar{x}^{k+1} - x^k\| - \|x^{k+1} - \bar{x}^{k+1}\| \\
&\geq \text{dist}[x^k, X^*] - \text{dist}[x^{k+1}, X^*] \\
&\geq \text{dist}[x^k, X^*] - \frac{1}{2}\text{dist}[x^k, X^*] = \frac{1}{2}\text{dist}[x^k, X^*]
\end{aligned}$$

for all $k \in \mathbb{N}$ large enough. Hence, (a) holds with $C_6 := 1/2$.

Lemma 4.5, Proposition 4.4 and item (a) imply that

$$\|\tilde{d}_{GN}(x^{k+1})\| \leq C_3 \text{dist}[x^{k+1}, X^*] \leq C_3 C_5 \text{dist}[x^{k+1}, X^*]^2 \leq \frac{1}{4} C_3 C_5 \|\tilde{d}_{GN}(x^k)\|^2$$

for all $k \in \mathbb{N}$ sufficiently large. Therefore, (b) follows by setting $C_7 := \frac{1}{4} C_3 C_5$.

We now prove (c). Item (a) from Lemma 4.5 yields the right inequality with $C_9 := C_3$. Consider then the left inequality. One can show that for some sufficiently large (but fixed) index $k \in \mathbb{N}$ we have

$$\|\tilde{d}_{GN}(x^{k+j})\| \leq \left(\frac{1}{2}\right)^j \|\tilde{d}_{GN}(x^k)\| \quad \text{for all } j = 0, 1, 2, \dots.$$

Furthermore, the nonexpansiveness of the projection operator yields

$$\begin{aligned}
\|x^k - x^{k+\ell}\| &= \|P_\Omega(x^k) - P_\Omega(x^{x+\ell-1} + \tilde{d}_{GN}(x^{k+\ell-1})\| \\
&\le \|x^k - x^{k+\ell-1} - \tilde{d}_{GN}(x^{k+\ell-1})\| \\
&\le \|x^k - x^{k+\ell-1}\| + \|\tilde{d}_{GN}(x^{k+\ell-1})\| \\
&\vdots \qquad \vdots \\
&\le \sum_{j=0}^{\ell-1} \|\tilde{d}_{GN}(x^{k+j})\|.
\end{aligned}$$

Since $\bar{x} = \lim_{\ell\to\infty} x^{k+\ell}$, we therefore obtain from the continuity of the norm

$$\begin{aligned}
\|x^k - \bar{x}\| = \lim_{\ell\to\infty} \|x^k - x^{k+\ell}\| &\le \lim_{\ell\to\infty} \sum_{j=0}^{\ell-1} \|\tilde{d}_{GN}(x^{k+j})\| \\
&\le \|\tilde{d}_{GN}(x^k)\| \lim_{\ell\to\infty} \sum_{j=0}^{\ell-1} \left(\frac{1}{2}\right)^j = 2\|\tilde{d}_{GN}(x^k)\|.
\end{aligned}$$

Since this holds for an arbitrary (sufficiently large) $k \in \mathbb{N}$, we obtain (c) by setting $C_9 := 1/2$. □

We are now able to state the main result of this subsection.

Theorem 4.3. *Let Assumptions 4.1-4.3 be satisfied and $\{x^k\}$ be a sequence generated by Algorithm 4.2 with starting point $x^0 \in \mathcal{B}(x^*, \varepsilon)$, where ε is defined as in (4.20). Then, the sequence $\{x^k\}$ converges quadratically to a solution $\bar{x}$ of (4.1) belonging to the ball $\mathcal{B}(x^*, \delta/2)$.*

Proof. Theorem 4.2 says that the sequence $\{x^k\}$ converges to a solution $\bar{x} \in X^*$. From Lemmas 4.5, 4.7 and Proposition 4.4 we obtain

$$\begin{aligned}
\frac{\|x^{k+1} - \bar{x}\|}{\|x^k - \bar{x}\|^2} &\le \frac{\|\tilde{d}_{GN}(x^{k+1})\|}{C_8 C_9^2 \|\tilde{d}_{GN}(x^k)\|^2} \\
&\le \frac{C_3 C_6^2 \mathrm{dist}[x^{k+1}, X^*]}{C_8 C_9^2 \mathrm{dist}[x^k, X^*]^2} \\
&\le \frac{C_3 C_6^2 C_5}{C_8 C_9^2}.
\end{aligned}$$

Thus, the convergence to $\bar{x}$ is quadratic. □

4.5 Examples

Consider the function $H : \mathbb{R}^2 \to \mathbb{R}^2$ defined by

$$H(x_1, x_2) = \begin{bmatrix} x_2^{\rho} \\ x_2 \exp(x_1^2) \end{bmatrix}, \tag{4.24}$$

where $\rho > 0$ and let $\Omega := \mathbb{R}^2$. Then, the solution set of (4.1) is clearly given by $X^* = \{(x_1, x_2) \in \mathbb{R}^2 | x_2 = 0\}$, and obviously every solution is nonisolated. We have introduced the term $\exp(x_1^2)$ in the second component in order to generate positive singular values converging to zero without violating the local error bound condition. In fact, it is easy to see that Assumptions 4.1-4.3 are satisfied locally at any solution x^*. Next, we calculate the Jacobian of H.

$$\nabla H(x_1, x_2)^{\top} = \begin{bmatrix} 0 & \rho x_2^{\rho-1} \\ 2x_1 x_2 \exp(x_1^2) & \exp(x_1^2) \end{bmatrix}.$$

Observe that the Jacobian is locally Lipschitz continuous if, and only if, $\rho \notin (0, 2)\backslash\{1\}$. The singular values of $\nabla H(x)$ are given by

$$\sigma_1(x) = \frac{1}{2}\left(1 + \sqrt{1 + 8\rho |x_1||x_2|^{\rho} \exp(-x^2)}\right),$$
$$\sigma_2(x) = \frac{2\rho |x_1||x_2|^{\rho}}{\sigma_1(x)}.$$

This implies that

$$\operatorname{rank}(\nabla H(x)) = \begin{cases} 2, & \text{if } x_1 \neq 0 \text{ and } x_2 \neq 0; \\ 1, & \text{otherwise.} \end{cases}$$

We will discuss examples based on (4.24) considering different choices of ρ.

Example 4.1. $\rho = 1$: For this choice of ρ, for any starting point, the Gauss-Newton method converges exactly in one only step, while Levenberg-Marquardt type methods (with its regularization parameter larger than zero) generate an infinite sequence. This behavior of the Gauss-Newton method is easy to understand, since the problem has a quite linear structure. Note that in this case, Assumption 4.4 holds around any solution different from $(0, 0)$, and thus, according to Theorem 4.3, at least locally quadratic convergence was already expected. Close to $(0, 0)$, there are points so that $\sigma_2(s)$ is quite smaller than $\|H(s)\|$, but the Gauss-Newton method step is incisive enough in the direction of the solution set, so that the method does not follow a trajectory where such singular values appear.

Example 4.2. $\rho = 2$: In this case the quadratic convergence of the Gauss-Newton method is lost. Moreover, this rate is destroyed for Levenberg-Marquardt methods if we take $\alpha(s) = \|H(s)\|^{\beta}$, with $\beta > 3$. We deduced this by seeing that the limit

$$\lim_{s_2 \to 0} \frac{\operatorname{dist}[s + d_{\alpha}(s), X^*]}{(\operatorname{dist}[s, X^*])^2} = \lim_{s_2 \to 0} \frac{|s_2 + d_{\alpha}(s)|}{s_2^2},$$

explodes if $\beta > 3$ and is finite if $\beta \in [1, 3]$. In this example a Levenberg-Marquardt method follows a trajectory with $\sigma_2(s)$ proportional to $\|H(s)\|^2$ and this affects the Gauss-Newton method, which in this case, converges just linearly, no matter what starting point outside the solution set one chooses.

Example 4.3. $\rho = \frac{4}{3}$: Whit this ρ the Jacobian is not Lipschitz continuous (just Holder continuous). Using the same approach as above we can check that the Levenberg-Marquardt method converges quadratically if $\beta \in [1, 2]$ and diverges if $\beta > 2$.

Example 4.4. $\rho = \frac{11}{13}$: This example shows that the local Lipschitz continuity of the Jacobian is decisive if one expects quadratic convergence for the Levenberg-Marquardt method (as it is in the classical Newton method). The Jacobian again is just Holder continuous around a solution and the Levenberg-Marquardt method loses its quadratic convergence if $\beta \in [1, 2]$.

The following example shows that the structure of the problem may not cause only a deceleration on the convergence of a Gauss-Newton method. We conclude that even when the local error bound condition holds, a point that is arbitrary close to the solution set can be thrown away by the Gauss-Newton method. This undesirable behavior emphasizes the relevance of the regularizing technics, as in Levenberg-Marquardt methods, once again.

Example 4.5. Let $H : \mathbb{R}^2 \to \mathbb{R}^2$ be given by

$$H(x_1, x_2) = \begin{bmatrix} x_1^2 + x_2^2 - 1 \\ (x_1^2 + x_2^2 - 1)^\eta \exp(-x_1^2) \end{bmatrix},$$

and consider $\Omega := \mathbb{R}^2$. Assumptions 4.1-4.3 are satisfied locally at any solution x^* in X^*, which is the unit sphere center in $(0, 0)$. In this example we will be particularly interested in Gauss-Newton steps calculated at points $s \in \mathbb{R}^2$ so that $s_1 = s_2 = \gamma$, where $\gamma > \frac{\sqrt{2}}{2}$. For such points we have that

$$d_{GN}(s) = -\frac{1}{2\gamma} \begin{bmatrix} \eta - 1 \\ 2\gamma^2 - \eta \end{bmatrix}, \; s + d_{GN}(s) = \frac{1}{2\gamma} \begin{bmatrix} 2\gamma^2 + 1 - \eta \\ \eta \end{bmatrix}.$$

Hence,

$$\lim_{\gamma \to \frac{\sqrt{2}}{2}^+} s + d_{GN}(s) = \frac{\sqrt{2}}{2} \begin{bmatrix} 2 - \eta \\ \eta \end{bmatrix}.$$

Thus, one has that if $\eta := 1$ the structure of the problem is quite simple and guarantees the convergence of the Gauss-Newton method in one only step. Nevertheless, for $\eta = 2$ the limit above is $\bar{x} = (0, \sqrt{2}) \in \mathbb{R}^2$. This indicates that a point arbitrary close to the solution set, can be strongly repelled by a Gauss-Newton method.

4.6 The relation between quadratic convergence and the order of the singular values

In this section we study the relation between quadratic convergence of Levenberg-Marquardt type methods and the order of singular values that converge to zero. Our analysis will clarify the conclusions in the examples we have seen in the previous section. Before giving the main theorem we present a result related to Lemma 2.3 of [24], but significantly stronger than it.

Lemma 4.8. *Let Assumptions 4.1-4.3 be satisfied and assume that for all $s \in \mathcal{B}(x^*, \delta/2)$ it holds that $\sigma_{i_s}(s) \leq L_1\|H(s)\|$, for some index i_s with $1 \leq i_s \leq r_s$. Then, there exists $C_{10} > 0$ so that for all $s \in \mathcal{B}(x^*, \delta/2)$ we have*

$$|(U_s^\top H(s))_{i_s}| \leq C_{10}\, dist[s, X^*]^2,$$

for all $s \in \mathcal{B}(x^*, \delta/2)$

Proof. Set $\alpha := \|H(s)\|^2$. We know that for this choice of α there exists a constant $\bar{C} > 0$ so that

$$\|H(s) + \nabla H(s)^\top d_\alpha(s)\| \leq \bar{C}\operatorname{dist}[s, X^*]^2, \tag{4.25}$$

for all $s \in \mathcal{B}(x^*, \delta/2)$. Consider $v_\alpha(s)$ as in Lemma 4.3. Then, from the orthogonality of U_s we conclude that

$$\begin{aligned}\|H(s) + \nabla H(s)^\top d_\alpha(s)\| &= \|U_s^\top H(s) + \Sigma_s V_s^\top d_\alpha(s)\| \\ &= \|U_s^\top H(s) + \Sigma_s^\top v_\alpha(s)\|.\end{aligned}$$

Hence,

$$\left|\left(U_s^\top H(s) + \Sigma_s^\top v_\alpha(s)\right)_{i_s}\right| = \left|\left(U_s^\top H(s)\right)_{i_s}\right| \left|1 - \frac{\sigma_{i_s}(s)}{\sigma_{i_s}(s) + \frac{\|H(s)\|^2}{\sigma_{i_s}(s)}}\right|.$$

Thanks to $\sigma_{i_s}(s) \leq L_1\|H(s)\|$ we obtain that

$$\left|1 - \frac{\sigma_{i_s}(s)}{\sigma_{i_s}(s) + \frac{\|H(s)\|^2}{\sigma_{i_s}(s)}}\right| \geq \frac{1}{L_1^2 + 1}.$$

Thus, using (4.25) we get

$$\left|\left(U_s^\top H(s)\right)_{i_s}\right| \leq C_{10}\operatorname{dist}[s, X^*]^2,$$

for all $s \in \mathcal{B}(x^*, \delta/2)$, with $C_{10} := \bar{C}(L_1^2 + 1)$. □

The next theorem shows how one can choose the Levenberg-Marquardt parameter α taking into account the order of singular values without destroying quadratic convergence.

Theorem 4.4. *Let Assumptions 4.1-4.3 be satisfied and suppose there exist $L_2, L_3 > 0$ so that for every $i = 1, ..., \min\{n, m\}$, one of the following properties holds*

(a) $\sigma_i(s) \geq L_2 \|H(s)\|$*;*

(b) $\sigma_i(s) \leq L_3 \|H(s)\|^{\beta-1}$*,*

for all $s \in \mathcal{B}(x^*, \delta/2)$ with $\beta \geq 2$ fixed. Then, the Levenberg-Marquardt method is locally quadratically convergent for $\alpha := \|H(s)\|^\beta$.

Proof. If i is an index so that (a) is satisfied one can conclude, using similar arguments as in Lemma 4.4, that there exists $C_{11} > 0$ (that does not depend on i) such that

$$|v_\alpha(s)_i| \leq C_{11} \text{dist}[s, X^*],$$

for all $s \in \mathcal{B}(x^*, \delta/2)$. For any index i satisfying (b) we obtain

$$\begin{aligned}
|v_\alpha(s)_i| &= \frac{\sigma_i(s) | \left(U_s^\top H(s)\right)_i |}{\sigma_i(s)^2 + \|H(s)\|^\beta} \leq \frac{\sigma_i(s) C_{10} \text{dist}[s, X^*]^2}{\sigma_i(s)^2 + \|H(s)\|^\beta} \\
&\leq \frac{\sigma_i(s) C_{10} \text{dist}[s, X^*]^2}{\|H(s)\|^\beta} \leq \frac{C_{10} L_3 \|H(s)\|^{\beta-1} \text{dist}[s, X^*]^2}{\|H(s)\|^\beta} \\
&= \frac{C_{10} L_3 \text{dist}[s, X^*]^2}{\|H(s)\|} \leq C_{10} L_3 w \text{dist}[s, X^*].
\end{aligned}$$

Hence,

$$\|d_\alpha(s)\| \leq C_{12} \text{dist}[s, X^*] \tag{4.26}$$

for all $s \in \mathcal{B}(x^*, \delta/2)$ with $C_{12} := \min\{C_{11}, C_{10} L_3 w\}$. Thus, under conditions (a) and (b) we

$$\begin{aligned}
\|H(s) + \nabla H(s)^\top d_\alpha(s)\|^2 &\leq \|H(s) + \nabla H(s)^\top d_\alpha(s)\|^2 + \|H(s)\|^\beta \|d_\alpha(s)\|^2 \\
&\leq \|H(s) - \underbrace{H(\bar{s})}_{=0} + \nabla H(s)^\top (s - \bar{s})\|^2 + \|H(s)\|^\beta \|s - \bar{s}\|^2 \\
&\leq L \|s - \bar{s}\|^4 + L^\beta \|s - \bar{s}\|^{\beta+2} \\
&\leq \left(L + L^\beta \delta^{\beta-2}\right) \text{dist}[s, X^*]^4.
\end{aligned}$$

Hence,

$$\|H(s) + \nabla H(s)^\top d_\alpha(s)\| \leq \sqrt{L + L^\beta \delta^{\beta-2}} \text{dist}[s, X^*]^2. \tag{4.27}$$

Using (4.26) and (4.27) one can carry out the remaining convergence analysis as in Section 4.4. □

Let us explain what this theorem says. Consider the choice $\alpha := \|H(s)\|^\beta$ with $\beta := 4$. Then, if in our problem the singular values that converge to zero remain of the order of $\|H(s)\|$, or smaller than the order of $\|H(s)\|^3$, Theorem 4.4 guarantees quadratic convergence of the Levenberg-Marquardt method. If some singular values lie strictly between these orders of magnitude, then the theorem does not guarantee this rate. To clarify this more, consider Example 4.2 using $\beta := 4$. We have seen that in this case, singular values proportional to $\|H(s)\|^2$ appear along the Levenberg-Marquardt iterates, i.e., the hypothesis of Theorem 4.4 are not fulfilled. This might be the reason why the Levenberg-Marquardt method does not converge quadratically for the choice $\alpha := \|H(s)\|^4$.

Notice that, due to Theorem 4.4, if one intended to destroy the local quadratic convergence of a Levenberg-Marquardt method for $\beta := 3$, one should be able to follow iterates so that correspondent singular values were strictly between the orders of $\|H(s)\|$ and $\|H(s)\|^2$. Of course there exist trajectories of points that do this job (take $t \geq 0$ and consider Example 4.1 with $x_1 := \sqrt{t}$ and $x_2 := t$ in order to produce singular values proportional to $\|H(s)\|^{\frac{3}{2}}$ for instance). But it seems that Levenberg-Marquardt iterates tend not to follow such trajectories. At least this was true in the examples we have constructed. Thus, the question whether, in general, one has local quadratic convergence for Levenberg-Marquardt methods with a fixed $\beta \in (2, 3]$, remains an open issue.

4.7 Concluding remarks

It was already known that unconstrained Levenberg-Marquardt do not converge quadratically in general if $\alpha := \|H(s)\|^\beta$ with $\beta \in (0, 1)$. In [46] it was proved that defining $\alpha := \|H(s)\|^2$ this rate is achieved by a projected Levenberg-Marquardt type method. In [28] it was proved that these projected methods can be interpreted as inexact unconstrained ones, and that $\beta \in [1, 2]$ implies quadratic convergence of them. The reader has probably realized that the set Ω was not mentioned that much in this chapter, unless when the nonexpansiveness of the projection operator was needed. The tie between the unconstrained and the projected methods is related to the fact that the error bound assumed is precisely the same. We will see in the next chapter that projected methods may have problems when dealing with boundary points of Ω.

In this chapter we have dealt with projected Gauss-Newton and Levenberg-Marquardt methods. Sometimes a singular value decomposition was explicitly required. Of course this decomposition is computationally very expensive in actual implementations of the method. Nevertheless, our analysis clarified a couple of questions on the relation between the exponent β and quadratic convergence. We have concluded that quadratic convergence is lost in general if $\beta > 3$, but we still do not know what happens if $\beta \in (2, 3]$. What may weaken some of our conclusions is our strong result in Chapter 3, that states that singular values converging to zero are related to duplications on the system (4.1). Nevertheless, we have seen examples with duplications that may affect the efficiency of Levenberg-Marquardt algorithms, if the regularization parameter α is not chosen with $\beta \in [1, 2]$.

Chapter 5

A unified local convergence analysis of inexact constrained Levenberg-Marquardt methods

In this chapter we present the local convergence analysis given in our article [5] for an inexact version of a constrained Levenberg-Marquardt method. It is shown that the best results known for the unconstrained case also hold for the constrained Levenberg-Marquardt method. Moreover, the influence of the regularization parameter on the level of inexactness and the convergence rate is described. Our results improve and unify several existing ones on the local convergence of Levenberg-Marquardt methods.

5.1 Introduction

Let a sufficiently smooth mapping $H : \mathbb{R}^n \to \mathbb{R}^m$ and a closed convex nonempty set $\Omega \subseteq \mathbb{R}^n$ be given. As in the previous chapter, we consider the following system of nonlinear equations subject to constraints

$$H(x) = 0, \quad x \in \Omega. \tag{5.1}$$

In the present chapter we are interested in extending and unifying results on the local convergence of inexact Levenberg-Marquardt methods for smooth problems (5.1) that can have non-isolated solutions. We are now going to discuss this in more detail.

It is known that Levenberg-Marquardt methods guarantee a local quadratic (or superlinear) convergence under the error bound that characterizes the calmness condition. The level of inexactness in the subproblems of Levenberg-Marquardt methods that is possible without losing a given superlinear convergence rate was investigated in [14, 23, 29] for the unconstrained case, i.e., if $\Omega := \mathbb{R}^n$. Recall that the inexact Levenberg-Marquardt subproblems read as follows

$$\min_x \frac{1}{2}\|H(s) + \nabla H(s)^\top (x - s)\|^2 + \frac{1}{2}\alpha(s)\|x - s\|^2 + \pi(s)^\top (x - s),$$

where $s \in \mathbb{R}^n$ can be understood as the current iterate, $\alpha(s) > 0$ denotes the regularization parameter, and $\pi(s) \in \mathbb{R}^n$ is used to formally describe the inexactness that may result from approximate data, truncated solution algorithms, or numerical errors. In order to obtain a large level for the inexactness under a given convergence rate, the regularization parameter $\alpha(s)$ plays a crucial role.

In order to recall the results for inexact unconstrained Levenberg-Marquardt methods, let us assume that a quadratic convergence rate should be guaranteed. We have seen in Chapter 1 and 2 that $\alpha(s) \sim \|H(s)\|^2$ was used in [14] and that this choice enables an inexactness level of (at least) $\|\pi(s)\| \sim \|H(s)\|^4$. The inexactness level of $\|\pi(s)\| \sim \|H(s)\|^3$ was obtained in [23] if a significantly larger regularization parameter is used, namely if

$$\alpha(s) \sim \|H(s)\|. \tag{5.2}$$

Remember also that for this choice of $\alpha(s)$ the inexactness level was further improved to $\|\pi(s)\| \sim \|H(s)\|^2$ in [29]. This result motivated us when considering the constrained case. The subproblems of the constrained Levenberg-Marquardt method in [46] (see Chapter 2) read as follows

$$\min_x \frac{1}{2}\|H(s) + \nabla H(s)^\top (x - s)\|^2 + \frac{1}{2}\alpha(s)\|x - s\|^2 \qquad \text{s.t.} \quad x \in \Omega.$$

The constrained Levenberg-Marquardt method is known to converge locally with a quadratic rate if $\alpha(s) \sim \|H(s)\|^2$ is assumed, see [46] (and [77] under slightly different conditions). Nothing was known on the behavior of inexact versions of the constrained Levenberg-Marquardt method and it was not even clear whether a quadratic rate was possible if the larger value (5.2) were used for the regularization parameter $\alpha(s)$.

In this chapter, answers to these issues are given. It will turn out that the regularization parameter $\alpha(s)$ in terms of $\|H(s)\|^\beta$ with $\beta \in (0, 2]$ is responsible for the rate of convergence of the exact constrained Levenberg-Marquardt method. Moreover, inexactness does not worsen this rate if it is at most proportional to $\|H(s)\|^{\beta+1}$. It will also be shown in Section 5.5 that this level of inexactness is sharp. The results in this chapter improve or extend previous results, in particular those in [14, 23, 29, 46, 77].

In Section 5.2 problem (5.1) is reformulated as an optimization problem and its necessary optimality conditions are represented as a generalized equation. Based on this an auxiliary lemma on the upper Lipschitz-continuity for a perturbation of the generalized equation is proved. In Section 5.3 the subproblems of the inexact constrained Levenberg-Marquardt method and the resulting method are formally defined. The main local convergence analysis is presented in Section 5.4. By an example the sharpness of the inexactness level is demonstrated in Section 5.5. Some concluding remarks are presented at the end of the chapter.

5.2 An upper Lipschitz-continuity result

Throughout this chapter we adopt basically the same notation as in the previous one, and also assume that the solution set of problem (5.1) is nonempty, i.e.,

$$X^* := \{x \in \Omega \,|\, H(x) = 0\} \neq \emptyset.$$

Then, any solution of (5.1) solves the minimization problem

$$\min \frac{1}{2}\|H(x)\|^2 \quad \text{s.t. } x \in \Omega, \tag{5.3}$$

and vice versa. If H is differentiable then every solution of the minimization problem satisfies the necessary optimality condition

$$0 \in \nabla H(x)H(x) + \mathrm{N}_\Omega(x), \tag{5.4}$$

where

$$\mathrm{N}_\Omega(x) := \begin{cases} \{y \in \mathbb{R}^n \,|\, y^\top(z - x) \leq 0 \text{ for all } z \in \Omega\} & \text{if } x \in \Omega, \\ \emptyset & \text{if } x \notin \Omega \end{cases}$$

denotes the normal cone to the set Ω at x (see Chapter 2). In addition to the generalized equation (5.4) we also consider the perturbed generalized equation

$$p \in \nabla H(x)H(x) + \mathrm{N}_\Omega(x) \tag{5.5}$$

for perturbation parameters $p \in \mathbb{R}^n$. Let $X(p)$ denote the solution set of (5.5). Obviously, $X^* \subseteq X(0)$ holds.

Assumption 5.1. *The function $H : \mathbb{R}^n \to \mathbb{R}^m$ is differentiable and $\nabla H : \mathbb{R}^n \to \mathbb{R}^{n\times m}$ is locally Lipschitz continuous.*

In order to formulate the calmness condition (Assumption 5.2 below) let $x^* \in X^*$ be an arbitrary but fixed solution. Assumption 5.2 could be restricted to some neighborhood of x^* which, however, is avoided for simplicity.

Assumption 5.2. *There exist $w > 0$ and $\delta \in (0, 1]$ so that*

$$w \operatorname{dist}[x, X^*] \leq \|H(x)\|,$$

for all $x \in \mathcal{B}(x^*, \delta) \cap \Omega$.

For enabling subproblems simpler than those we use in this paper (see Section 5.3), projected Levenberg-Marquardt steps can be employed, see [46] and [55] (within a local phase). Then, however, the corresponding local convergence analysis requires that the inequality in Assumption 5.2 holds for all $x \in \mathcal{B}(x^*, \delta)$ (see Chapter 4) although the set Ω in problem (5.1) is a proper subset of $\mathbb{R}^n$. This implies that, in a neighborhood of x^*, problem (5.1) is equivalent to $H(x) = 0$. Therefore, depending on the problem, Assumption 5.2 can be significantly weaker than assuming that the inequality holds for all $x \in \mathcal{B}(x^*, \delta)$. It is shown in [29, Section 3] that such projected Levenberg-Marquardt steps can be regarded as solutions of unconstrained Levenberg-Marquardt subproblems (5.1) with an appropriate definition of the perturbation π. Due to this, the advantage from enlarging the regularization parameter, i.e., that the level of inexactness increases without destroying quadratic convergence (see the discussion in Section 5.1), applies to the projected steps in [46, 55].

The following lemma shows that the mapping $p \mapsto X(p)$ is upper Lipschitz continuous at x^* under the previous assumptions.

Lemma 5.1. *Let Assumptions 5.1 and 5.2 be satisfied. Then, there exist* $\mu > 0$ *and* $\delta_* > 0$ *so that*

$$X(p) \cap \mathcal{B}(x^*, \delta_*) \subseteq X^* + \mu \|p\| \mathcal{B}$$

for all $p \in \mathbb{R}^n$.

Proof. Let us first fix some $\delta_* \in (0, \delta]$ and let $p \in \mathbb{R}^n$ be arbitrarily chosen. If $X(p) \cap \mathcal{B}(x^*, \delta_*)$ is empty, then nothing has to be shown. Otherwise, let x_p denote any element of $X(p) \cap \mathcal{B}(x^*, \delta_*)$. Then, there exists $y_p \in \mathrm{N}_\Omega(x_p)$ so that

$$p = \nabla H(x_p) H(x_p) + y_p. \tag{5.6}$$

Since X^* is nonempty and closed there exists $\hat{x}_p \in X^*$ such that $\|x_p - \hat{x}_p\| = \operatorname{dist}[x_p, X^*]$. This implies

$$\hat{x}_p \in \mathcal{B}(x^*, 2\delta_*). \tag{5.7}$$

Assumption 5.1 ensures (due to Taylor's formula) that there exists $C_1 > 0$ so that, for any $z \in X^* \cap \mathcal{B}(x^*, 2\delta_*)$ and any $x \in \mathcal{B}(x^*, 2\delta_*)$,

$$\|H(x) + \nabla H(x)^\top (z - x)\|^2 \leq C_1 \|z - x\|^4.$$

Therefore, by (5.7), $\hat{x}_p \in X^*$, and $x_p \in \mathcal{B}(x^*, \delta)$, we have

$$\begin{aligned} r(x_p) &:= \|H(x_p) + \nabla H(x_p)^\top (\hat{x}_p - x_p)\|^2 \\ &\leq C_1 \|\hat{x}_p - x_p\|^4 \\ &= C_1 \operatorname{dist}[x_p, X^*]^4. \end{aligned} \tag{5.8}$$

For the left hand side of (5.7) we obtain

$$\begin{aligned} r(x_p) \quad = \quad & 2(\hat{x}_p - x_p)^\top \nabla H(x_p) H(x_p) + (\hat{x}_p - x_p)^\top \nabla H(x_p) \nabla H(x_p)^\top (\hat{x}_p - x_p) \\ & + \|H(x_p)\|^2 \end{aligned}$$

and

$$2(\hat{x}_p - x_p)^\top \nabla H(x_p) H(x_p) + \|H(x_p)\|^2 \leq r(x_p).$$

Since $\hat{x}_p, x_p \in \Omega$ and $y_p \in \mathrm{N}_\Omega(x_p)$ we have $(\hat{x}_p - x_p)^\top y_p \leq 0$ and, with (5.6), get

$$p^\top(\hat{x}_p - x_p) = (\hat{x}_p - x_p)^\top \nabla H(x_p) H(x_p) + (\hat{x}_p - x_p)^\top y_p \leq \frac{1}{2}(r(x_p) - \|H(x_p)\|^2).$$

By (5.8) and Assumption 5.2, this implies

$$p^\top(\hat{x}_p - x_p) \leq \frac{1}{2}(C_1 \operatorname{dist}[x_p, X^*]^4 - w^2 \operatorname{dist}[x_p, X^*]^2).$$

Due to $x_p \in \mathcal{B}(x^*, \delta_*)$, choosing $\delta_* \in (0, \delta]$ sufficiently small leads to $C_1 \operatorname{dist}[x_p, X^*]^2 \leq \frac{1}{2}w^2$ and

$$p^\top(\hat{x}_p - x_p) \leq -\frac{1}{4}w^2 \operatorname{dist}[x_p, X^*]^2$$

follows. Thus, dividing this inequality by $\|\hat{x}_p - x_p\|$ (which is the same as $\operatorname{dist}[x_p, X^*]$) yields

$$\frac{1}{4}w^2 \operatorname{dist}[x_p, X^*] \leq \|p\|.$$

Setting $\mu := 4w^{-2}$ completes the proof. □

Lemma 5.1 implies that $X(0) \cap \mathcal{B}(x^*, \delta_*) \subseteq X^*$. This means that, although the generalized equation (5.4) is only a necessary optimality condition for the minimization problem (5.3), all vectors that satisfy this necessary condition and are not too far away from x^* also solve the minimization problem.

5.3 Subproblems and method

Given some $s \in \Omega$ the algorithm we are going to analyze the following subproblem

$$0 \in \nabla_x \psi(x, s) + \mathrm{N}_\Omega(x), \tag{5.9}$$

where $\psi : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is defined by

$$\psi(x, s) := \frac{1}{2}\|H(s) + \nabla H(s)^\top (x - s)\|^2 + \frac{1}{2}\alpha(s)\|x - s\|^2 + \pi(s)^\top (x - s)$$

and $\pi(s) \in \mathbb{R}^n$ denotes a perturbation that enables inexactness within the subproblem. The level of inexactness is described by Assumption 5.3 below. It depends on the exponent $\beta \in (0, 2]$ in the following definition of the regularization parameter.

$$\alpha(s) := \begin{cases} \|H(s)\|^\beta & \text{if } s \notin X^*, \\ 1 & \text{if } s \in X^*. \end{cases} \tag{5.10}$$

Note that the convergence theorem does not change if an appropriate less restrictive rule is used to define $\alpha(s)$ for $s \notin X^*$. For example,

$$\alpha_0 \|H(s)\|^\beta \leq \alpha(s) \leq \alpha_1 \|H(s)\|^\beta$$

for some constants $\alpha_1 \geq \alpha_0 > 0$ can be employed.

By the convexity of Ω and $\psi(\cdot, s)$, the generalized equation (5.9) is equivalent to the quadratic minimization problem

$$\min_x \psi(x, s) \quad \text{s.t.} \quad x \in \Omega. \tag{5.11}$$

Due to the fact that $\alpha(s) > 0$, the function $\psi(\cdot, s)$ is strongly convex. Since the convex set Ω is also nonempty and closed, problem (5.11) has the unique solution denoted by $x(s)$.

Assumption 5.3. *There exists $c_\pi > 0$ so that*

$$\|\pi(s)\| \leq c_\pi \|H(s)\|^{\beta+1},$$

for all $s \in \mathcal{B}(x^*, \delta)$.

The constrained Levenberg-Marquardt method we are going to deal with is given next.

Algorithm 5.1. Constrained Levenberg-Marquardt method
Step 0. Choose $x^0 \in \Omega$ and $\beta \in (0, 2]$.
Step 1. Set $s := x^k$ and compute the solution $x(s)$ of Problem (5.11) with $\alpha(s)$ as in (5.10) and set

$$x^{k+1} := x(s) \tag{5.12}$$

Step 2. Set $k := k + 1$ and go to Step 1.
End

Roughly speaking, the following lemma shows that locally the length of a Levenberg-Marquardt step is bounded by a constant times the distance of the current iterate to X^*. The lemma is related to similar results in literature, see, for example, [14, 46]. However, since these results are either proved for the unconstrained case or do not deal with inexactness, a proof will be given.

Lemma 5.2. *Let Assumptions (5.1) – (5.3) be satisfied. Then, there exists $\kappa > 0$ so that*

$$\|x(s) - s\| \leq \kappa \operatorname{dist}[s, X^*] \quad \text{for all } s \in \mathcal{B}(x^*, \delta).$$

Proof. Recall that X^* is nonempty and bounded. Thus, for any $s \in \mathbb{R}^n$, there is $\hat{s} \in X^*$ with

$$\|s - \hat{s}\| = \operatorname{dist}[s, X^*]. \tag{5.13}$$

As $x(s)$ solves the minimization problem (5.11), we have

$$\frac{1}{2}\alpha(s)\|x(s) - s\|^2 + \pi(s)^\top (x(s) - s) \leq \psi(x(s), s) \leq \psi(\hat{s}, s). \tag{5.14}$$

From Assumption 5.1 and Taylor's formula, it follows that there exists $L_0 > 0$ so that

$$\|H(s)\| = \|H(s) - H(\hat{s})\| \leq L_0 \|\hat{s} - s\| \tag{5.15}$$

and

$$\|H(s) + \nabla H(s)^\top (\hat{s} - s)\|^2 \leq L_0 \|\hat{s} - s\|^4$$

hold for all $s \in \mathcal{B}(x^*, \delta)$. With the latter inequality, (5.14) implies

$$\|x(s) - s\|^2 \leq \alpha(s)^{-1} \left(L_0 \|\hat{s} - s\|^4 + 2\|\hat{s} - s\| \|\pi(s)\| + 2\|x(s) - s\| \|\pi(s)\| \right) + \|\hat{s} - s\|^2$$

for all $s \in \mathcal{B}(x^*, \delta)$. Because $\alpha(s)^{-1}\|\pi(s)\| \leq c_\pi \|H(s)\|$ holds by (5.10) and Assumption 5.3, we obtain from (5.10), Assumption 5.2, (5.15), and (5.13) that

$$\begin{aligned} \|x(s) - s\|^2 \quad &\leq \quad \operatorname{dist}[s, X^*]^2 (\operatorname{dist}[s, X^*]^{2-\beta} L_0 w^{-\beta} + 2c_\pi L_0 + 1) \\ &\quad\quad + 2c_\pi L_0 \|x(s) - s\| \operatorname{dist}[s, X^*]. \end{aligned}$$

Since $\operatorname{dist}[s, X^*] \leq \delta$ is valid for all $s \in \mathcal{B}(x^*, \delta)$ there is $L_1 > 0$ so that

$$\|x(s) - s\|^2 - 2c_\pi L_0 \operatorname{dist}[s, X^*] \|x(s) - s\| - L_1 \operatorname{dist}[s, X^*]^2 \leq 0$$

holds for all $s \in \mathcal{B}(x^*, \delta)$. Now, it can easily be seen that the inequalities

$$h^2 - 2c_\pi L_0 \operatorname{dist}[s, X^*] h - L_1 \operatorname{dist}[s, X^*]^2 \leq 0, \quad h \geq 0$$

are satisfied both if and only if

$$0 \leq h \leq \left(c_\pi L_0 + \sqrt{c_\pi^2 L_0^2 + L_1} \right) \operatorname{dist}[s, X^*].$$

Hence, the assertion of the lemma follows for $\kappa := c_\pi L_0 + \sqrt{c_\pi^2 L_0^2 + L_1}$. □

5.4 Local convergence

The local convergence results obtained below could also be derived by means of the general iterative framework for generalized equations in [27]. For simplicity, we decided however to provide proofs that are more instructive for Levenberg-Marquardt methods. To proceed, let us first define

$$\Delta(x, s) := \nabla H(x) H(x) - \nabla_x \psi(x, s)$$

for all $s, x \in \mathbb{R}^n$. By the definition of ψ this can be rewritten as

$$\begin{aligned} \Delta(x, s) \quad &= \quad (\nabla H(x) - \nabla H(s)) H(x) + \nabla H(s)(H(x) - H(s) - \nabla H(s)^\top (x - s)) \\ &\quad\quad - \alpha(s)(x - s) - \pi(s). \end{aligned} \tag{5.16}$$

Moreover, in the remainder of the chapter

$$\tau := \min\{\beta + 1, 2\}$$

will be used to describe a convergence rate.

Lemma 5.3. *Let Assumptions 5.1 – 5.3 be satisfied. Then, there exists* $C > 0$ *so that*

$$\|\Delta(x(s), s)\| \leq C \operatorname{dist}[s, X^*]^\tau \quad \text{for all } s \in \mathcal{B}(x^*, \delta_0),$$

where $\delta_0 := (\kappa + 1)^{-1}\delta$.

Proof. Recall that, for any $s \in \mathbb{R}^n$, $\hat{s} \in X^*$ is defined by (5.13). From Assumptions 5.1 and 5.3, Lemma 5.2, and (5.16) we obtain that, for all $s, x \in \mathcal{B}(x^*, \delta)$ with $s \notin X^*$, there exists $L \geq L_0 >$ so that

$$\|H(s)\| = \|H(s) - H(\hat{s})\| \leq L \operatorname{dist}[s, X^*], \tag{5.17}$$

$$\begin{aligned} \|H(x(s))\| &= \|H(x(s)) - H(\hat{s})\| \\ &\leq L\|x(s) - \hat{s}\| \\ &\leq L(\|x(s) - s\| + \|s - \hat{s}\|) \\ &\leq L(\kappa + 1) \operatorname{dist}[s, X^*], \end{aligned} \tag{5.18}$$

and

$$\|\Delta(x, s)\| \leq L\|H(x)\|\|x - s\| + L\|x - s\|^2 + \|H(s)\|^\beta\|x - s\| + c_\pi\|H(s)\|^{\beta+1}. \tag{5.19}$$

By Lemma 5.2, we have, for all $s \in \mathcal{B}(x^*, \delta_0)$,

$$\|x(s) - x^*\| \leq \|x(s) - s\| + \|s - x^*\| \leq \kappa \operatorname{dist}[s, X^*] + \delta_0 \leq (\kappa + 1)\delta_0 = \delta. \tag{5.20}$$

Therefore, the variable x within (5.19) can be replaced by $x(s)$. This together with (5.17), (5.18), and Lemma 5.2 leads to

$$\|\Delta(x(s), s)\| \leq C \operatorname{dist}[s, X^*]^\tau \tag{5.21}$$

for all $s \in \mathcal{B}(x^*, \delta_0) \setminus X^*$, where $C := L^2\kappa(\kappa+1) + L\kappa^2 + L^\beta\kappa + c_\pi L^{\beta+1}$. Since $x(s) = s$ for $s \in X^*$, it follows by (5.16) and Assumption 5.3 that (5.21) also holds for $s \in X^*$. □

Lemma 5.4. *Let Assumptions 5.1 – 5.3 be satisfied. Then, there exist* $\hat{C} > 0$ *and* $\delta_\diamond > 0$ *so that*

$$\operatorname{dist}[x(s), X^*] \leq \hat{C} \operatorname{dist}[s, X^*]^\tau \leq \frac{1}{2} \operatorname{dist}[s, X^*] \quad \text{for all } s \in \mathcal{B}(x^*, \delta_\diamond).$$

Proof. Let $s \in \mathbb{R}^n$ be arbitrary but fixed. Then, subproblem (5.9) is equivalent to the generalized equation

$$\Delta(x, s) \in \nabla H(x)H(x) + \mathrm{N}_\Omega(x).$$

Hence, $x(s)$ is the unique solution of this equation. Therefore, $x(s)$ is also a solution of the perturbed generalized equation (5.5) with $p := \Delta(x(s), s)$, i.e., $x := x(s)$ solves

$$\Delta(x(s), s) \in \nabla H(x)H(x) + \mathrm{N}_\Omega(x).$$

This means

$$x(s) \in X(\Delta(x(s), s)).$$

In order to apply Lemma 5.1, we also need that $x(s) \in \mathcal{B}(x^*, \delta_*)$. To this end and for later use, let us define

$$\delta_\diamond := \min\left\{\delta_0, \frac{\delta_*}{\kappa+1}, (2\mu C)^{\frac{-1}{\tau-1}}\right\}.$$

Now, for $s \in \mathcal{B}(x^*, \delta_\diamond)$, similar to (5.20) we obtain from Lemma 5.2 that $\|x(s) - x^*\| \leq \delta_*$. Thus, $x(s) \in X(\Delta(x(s), s)) \cap \mathcal{B}(x^*, \delta_*)$ is valid for all $s \in \mathcal{B}(x^*, \delta_\diamond)$. Lemma 5.1, Lemma 5.3, and the definition of $\delta_\diamond$ imply

$$\operatorname{dist}[x(s), X^*] \leq \mu\|\Delta(x(s), s)\| \leq \mu C \operatorname{dist}[s, X^*]^\tau \leq \frac{1}{2} \operatorname{dist}[s, X^*]$$

for all $s \in \mathcal{B}(x^*, \delta_\diamond)$. With $\hat{C} := \mu C$ the proof is complete. □

Lemma 5.5 (Lemma 2.9 in [29]). *Let $\{w^k\} \subset \mathbb{R}^n$, $r_k \subset [0, \infty)$ be sequences, and $r \in [0, 1)$, $R > 0$ numbers so that, for $k = 0, 1, 2, \ldots$,*

$$\|w^k - w^0\| \leq r_0 \frac{R}{1-r} \tag{5.22}$$

implies

$$r_{k+1} \leq r\, r_k \quad \textit{and} \quad \|w^{k+1} - w^k\| \leq R r_k. \tag{5.23}$$

Then, $\{r^k\}$ converges to 0 and $\{w^k\}$ converges to some $\hat{w} \in \mathbb{R}^n$. If, for some $t > 1$ and $c > 0$,

$$r_{k+1} \leq c r_k^t \quad \textit{and} \quad \|\hat{w} - w^k\| \geq r_k \tag{5.24}$$

is satisfied for $k = 0, 1, 2, \ldots$ then $\{w^k\}$ converges to $\hat{w}$ with the Q-order of t.

Theorem 5.1. *Let Assumptions 5.1 – 5.3 be satisfied and let $\{x^k\}$ be a sequence generated by the Levenberg-Marquardt method defined in Algorithm 5.1. Then, there exists $\epsilon > 0$ so that $x^0 \in \mathcal{B}(x^*, \epsilon)$ implies that the sequence $\{x^k\}$ converges to some $\hat{x} \in X^*$ with the Q-order τ.*

Proof. To apply Lemma 5.5 we set $w^k := x^k$ and $r_k := \operatorname{dist}[x^k, X^*]$ for $k = 0, 1, 2, \ldots$ and

$$r := \frac{1}{2}, \quad R := \kappa, \quad c := \hat{C}, \quad t := \tau = \min\{\beta + 1, 2\}.$$

Then, assuming (5.22) provides

$$\|x^k - x^*\| \leq \|x^k - x^0\| + \|x^0 - x^*\| \leq 2\kappa \operatorname{dist}[x^0, X^*] + \|x^0 - x^*\|.$$

Setting $\epsilon := (2\kappa + 1)^{-1}\delta_\diamond$ we have

$$\|x^k - x^*\| \leq (2\kappa + 1)\|x^0 - x^*\| \leq (2\kappa + 1)\epsilon \leq \delta_\diamond \leq \delta.$$

Thus, Lemmas 5.4 and 5.2 can be applied for $s := x^k$. This leads to

$$\operatorname{dist}[x^{k+1}, X^*] \leq \frac{1}{2} \operatorname{dist}[x^k, X^*] \quad \text{and} \quad \|x^{k+1} - x^k\| \leq \kappa \operatorname{dist}[x^k, X^*],$$

i.e., (5.23) is valid. Therefore, by Lemma 5.5, the sequence $\{\operatorname{dist}[x^k, X^*]\}$ converges to 0 and $\{x^k\}$ converges to some $\hat{x} \in X^*$.

Thanks to Lemma 5.4 and since $\|\hat{x} - x^k\| \geq \operatorname{dist}[x^k, X^*]$ is obviously valid for $k = 0, 1, 2, \ldots$, we see that (5.24) is satisfied. Thus, Lemma 5.5 guarantees that $\{x^k\}$ converges to $\hat{x}$ with the Q-order τ. □

5.5 Sharpness of the level of inexactness

In this section we show that, in general, the level of inexactness given by Assumption 5.3 cannot be increased without reducing the convergence rate $\tau = \min\{\beta+1, 2\}$ of the Levenberg-Marquardt method (5.12). To this end let us consider the simple example, where $\Omega := \mathbb{R}^2$ and $H : \mathbb{R}^2 \to \mathbb{R}$ is given by

$$H(x) := \|x\|^2 - 1. \tag{5.25}$$

Obviously, the solution set X^* of $H(x) = 0$ is the unit sphere and Assumptions 5.1 is valid. Moreover, since

$$\operatorname{dist}[x, X^*] \leq (\|x\| + 1) \operatorname{dist}[x, X^*] = (\|x\| + 1)|\|x\| - 1| = |\|x\|^2 - 1| = |H(x)|,$$

Assumption 5.2 is satisfied for $w = 1$ and any $\delta > 0$ regardless which solution $x^* \in X^*$ is taken. For later use let, for some $\rho \in (0, \frac{1}{4}]$,

$$S(\rho) := \{x \in \mathbb{R}^2 \setminus X^* \mid \operatorname{dist}[x, X^*] \leq \rho\}$$

denote a set surrounding the solution set X^*. Then, according to (5.10), the regularization parameter is

$$\alpha(s) = |H(s)|^\beta \tag{5.26}$$

for any $s \in S(\rho)$ with some $\beta \in (0, 2]$. Let us assume that, for some $\eta \in (0, 1)$, the perturbation vector is given by

$$\pi(s) := -\sigma(s)s + \pi(s)_\perp \in \mathbb{R}^2 \tag{5.27}$$

with

$$\sigma(s) := |H(s)|^{\beta+\eta}, \quad \|\pi(s)_\perp\| = |H(s)|^{\beta+\eta}, \quad \text{and} \quad s^\top \pi(s)_\perp = 0. \tag{5.28}$$

Then, $\|\pi(s)\| \leq \sqrt{5}|H(s)|^{\beta+\eta}$ is valid for all $s \in \mathcal{B}(0, 2)$. Note that for $\eta \geq 1$ Assumption 5.3 would be satisfied for any $x^* \in X^*$ and the level of inexactness is not increased in comparison with Theorem 5.1. Therefore, only $\eta \in (0, 1)$ need to be considered.

Now, in order to estimate the influence of the inexactness on the convergence rate of the Levenberg-Marquardt method, we analyze the ratio

$$\frac{\operatorname{dist}[x(s), X^*]}{\operatorname{dist}[s, X^*]^\nu} \tag{5.29}$$

for $\|s\| \to 1$ and $\nu > 1$. By the definition of H in (5.25) we know that

$$\operatorname{dist}[x(s), X^*] = |\|x(s)\| - 1| = \frac{|\|x(s)\|^2 - 1|}{\|x(s)\| + 1}. \tag{5.30}$$

Recall that, due to $\Omega = \mathbb{R}^2$, the solution $x(s)$ of the subproblem (5.11) is the unique solution of the linear system

$$(\nabla H(s) \nabla H(s)^T + \alpha(s) I)(x - s) = -\nabla H(s) H(s) - \pi(s).$$

For our example (5.25), we obtain

$$(4ss^\top + \alpha(s) I)(x(s) - s) = -2(\|s\|^2 - 1)s - \pi(s). \tag{5.31}$$

Then, with (5.31), (5.27), and (5.28), a simple calculation shows that, for any $s \in S(\rho)$,

$$x(s) = \frac{2\|s\|^2 + 2 + \alpha(s) + \sigma(s)}{4\|s\|^2 + \alpha(s)} s - \frac{1}{\alpha(s)} \pi(s)_\perp$$

and, by (5.26) and (5.28),

$$\|x(s)\|^2 = \left(\frac{2\|s\|^2 + 2 + \alpha(s) + \sigma(s)}{4\|s\|^2 + \alpha(s)} \right)^2 \|s\|^2 + |H(s)|^{2\eta}$$

are valid. This implies that $\|x(s)\| + 1$ is bounded above on $S(\frac{1}{4})$. Moreover, taking into account (5.30), Assumption 5.2, and (5.28) as well as $\beta \in (0, 2]$ and $\eta \in (0, 1)$, we obtain after a longer calculation that there exist $c_1, c_2 > 0$ and $\hat{\rho} \in (0, \frac{1}{4}]$ so that

$$\operatorname{dist}[x(s), X^*] \geq c_1 \operatorname{dist}[s, X^*]^{\beta + \eta} + c_2 \operatorname{dist}[s, X^*]^{2\eta}$$

holds for all $s \in S(\hat{\rho})$. Hence, if

$$\nu > \nu(\beta, \eta) := \min\{\beta + \eta, 2\eta\},$$

the ratio (5.29) tends to ∞ for $\|s\| \to 1$, i.e., in the above example the Levenberg-Marquardt method cannot converge to a solution with an order of ν. Since

$$\nu(\beta, \eta) = \min\{\eta + \beta, 2\eta\} < \min\{1 + \beta, 2\} = \tau,$$

the convergence rate τ in Theorem 5.1 cannot be guaranteed if the level of inexactness is larger than required in Assumption 5.3.

5.6 Final remarks

Before we derived this unified convergence approach we got motivated by a result for $\beta = 1$. We had shown, using a certain induction technique, that this choice of β leaded to a Q-order convergence of $2 - \epsilon$ of the Levenberg-Marquardt method, with $\epsilon > 0$ arbitrary small. Nevertheless, we were not able to substitute $2 - \epsilon$ by 2 using our approach. Fortunately, we found the key for our analysis, namely, the upper Lipschitz continuity property of the map $p \to X(p)$. Indeed, let the regularization parameter $\alpha(s)$ be given by (5.10), i.e., $\alpha(s) = \|H(s)\|^{\beta}$. For $\beta = 1$, Theorem 5.1 tells us that the local convergence rate of the constrained Levenberg-Marquardt method (5.12) is $\tau = 2$, where an inexactness level of $\|H(s)\|^2$ is enabled. For the unconstrained case ($\Omega = \mathbb{R}^n$) a corresponding result has been shown recently in [29]. However, for the constrained Levenberg-Marquardt methods in [46, 77], $\beta = 2$ is required to achieve a quadratic rate. With our results, the local behavior of an inexact constrained Levenberg-Marquardt method is analyzed for the first time. A sharp maximal level of inexactness depending on $\beta \in (0, 2]$ is derived. In particular, this shows that $\beta = 1$ should be used to allow a maximal inexactness without reducing the quadratic rate. Numerical results in [29] underline this in the unconstrained case. If $\beta = 2$ is considered the level of inexactness given in [14] for the unconstrained case could be improved from $\|H(s)\|^4$ to $\|H(s)\|^3$ and also holds if constraints are present. According to Theorem 5.1, $\beta \in (0, 1)$ implies a convergence rate less than 2. Nevertheless, this choice of β may be useful to allow larger perturbations.

We now show by a very simple example that the constrained method may have a significant advantage over the projected Levenberg-Marquardt method. Consider $H : \mathbb{R}^2 \to \mathbb{R}$ defined by

$$H(x_1, x_2) = x_2,$$

and $\Omega = \{(x_1, x_2) \in \mathbb{R}^2 | x_2 \geq -x_1\}$. Let a starting point $x^0 \in \Omega$ so that $x_1^0 < 0$ be given. Then, any projected Levenberg-Marquardt (for any choice of $\alpha(s)$) generates a sequence that converges at most linearly to the the solution $x^* := (0, 0) \in \Omega$. Now the pure constrained Levenberg-Marquardt method (with $\pi \equiv 0$) achieves quadratic convergence if $\alpha(s)$ is taken so that the exponent β lies in the interval $[1, 2]$ (the Gauss-Newton converges in one only step). The reason why the constrained method performs much better in terms of the rate of convergence, lies on the fact that the local error bound required for the projected method (see Chapter 4) is not satisfied at $x^* := (0, 0)$, while Assumption 5.2 holds trivially. Note that in our example H is linear. This means that projected methods might have deficiencies when dealing with solutions that are boundary points of Ω.

We would like to explain more in detail the notion of the inexactness used in the subproblems. It will be proved next that points sufficiently close to the solution of the exact Levenberg-Marquardt subproblem are solutions of inexact subproblems.

Lemma 5.6. *Let $s \in \Omega$ and $x(s)$ be the unique minimizer of $\psi_0(\cdot, s)$ subject to Ω, where ψ_0 is the function ψ with $\pi(s) \equiv 0$. Then, for each $y \in \Omega$ so that $\|y - x(s)\| \leq$*

$\|s - x(s)\|^{\beta+1}$ *we have that* y *is the unique minimizer of* $\psi_{\pi_y}(\cdot, s)$ *in* Ω*, where*

$$\psi_{\pi_y}(x, s) := \psi_0(x, s) + \pi_y(s)^\top (x - s),$$

with

$$\pi_y(s) := (\nabla H(s) \nabla H(s)^\top + \alpha(s) I)(x(s) - y).$$

Moreover, π_y *satisfies Assumption 5.3.*

Proof. Elementary. □

It may be interesting, from the theoretical point of view, to see what happens with a constrained Gauss-Newton method under the hypothesis that the positive singular values of the Jacobian do not converge faster to zero than the norm of H along the iterates. We think that the extension of the results from Chapter 4 to the constrained case might be natural. Nevertheless, we do not have the proofs yet. This can be a subject for future work.

Another topic we could explore in the future, is the impact of the error bound condition given in Assumption 5.2 on the the solution set of (5.1). One can easily see that Theorem 3.1, that implies constant rank of the Jacobian matrix on the solution set, no longer holds under the assumptions in this chapter. Take for instance $H : \mathbb{R}^2 \to \mathbb{R}$ with $H(x_1, x_2) = x_1 x_2$, and $\Omega := \{x \in \mathbb{R}^2 | x_1 \geq 0 \text{ and } x_2 = 0\}$. Clearly, Assumption 5.2 is satisfied and the rank of the Jacobian matrix changes on the solution set X^*. Nevertheless, this might happen because $\Omega \subset X^*$. Maybe without this inclusion, one can expect certain extensions of the results given in Chapter 3.

Chapter 6

Primal-dual relations between the central path and the Levenberg-Marquardt trajectory, with an application to quadratic programming

In this chapter we consider the problem of minimizing a convex function subject to a compact polyhedron defined by linear equality constraints and nonnegative variables. We scale the problem around the analytic center of the polyhedron and define associated Levenberg-Marquardt and a central path trajectories and show that they have relations that go beyond primal properties. In fact, these relations provide primal-dual feasible points for initializations in path following methods. From a practical point of view, this is particularly relevant in convex quadratic programming, where calculating such primal-dual points based on the Levenberg-Marquardt trajectory requires just the resolution of linear systems of equations. Our results therefore overcome the common deficiency of infeasibility in the initialization of some trust region subproblems. Similar results were previously known only for linear programming.

6.1 Introduction

Consider the convex problem

$$\begin{array}{ll} \text{minimize} & f_0(w) \\ \text{subject to} & A_0 w = b \\ & w \geq 0 \end{array} \tag{6.1}$$

where $f_0 : \mathbb{R}^n \to \mathbb{R}$ is a convex continuously differentiable function, $A_0 \in \mathbb{R}^{m\times n}$ and $b \in \mathbb{R}^m$. We will assume the polyhedron $\Omega_0 := \{w \in \mathbb{R}^n | Aw = b, w \geq 0\}$ to have an analytic center which we will denote by w_{AN}.

Problem (6.1) appears in many contexts in optimization, specially if f_0 is in addition quadratic. In this case, several kinds of trust region subproblems can be rewritten in the format of (6.1) as we have already seen in Chapter 2. Methods with quadratic subproblems belong to the family of sequential quadratic programming algorithms (SQP), a powerful tool in optimization. Among the numerous articles and also books that address the subject, we cite [3, 7, 9, 11, 13, 55]. In the last decade, a subfamily of SQP methods known as inexact restoration methods were developed. The first work in this direction is due to Martínez and Pilotta [57]. Their methods treat optimality and feasibility separately. Inexact restoration subproblems, the work by Ferris et al. [25] and the paper by Gonzaga [33], were the main motivation of our study, which aimed to provide primal-dual feasible points in quadratic programming that could be easily computed. Nevertheless, the results we will present encompass general convex problems with the form (6.1).

For the sake of simplicity we will consider a scaled version of (6.1).

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & Ax = b \\ & x \geq 0 \end{array} \tag{6.2}$$

where $A := A_0 W_{AN}$, with $W_{AN} := \text{diag}(w_{AN})$, where w_{AN} is the analytic center of the polyhedron Ω_0 defined above, $f : \mathbb{R}^n \to \mathbb{R}$, with $f(x) := f_0(W_{AN}x)$, and $\Omega := \{x \in \mathbb{R}^n | Ax = b, x \geq 0\}$.

Note that, since W_{AN} is a positive definite matrix, Problem (6.2) inherits the convexity of Problem (6.1). Moreover, they are in an obvious correspondence due to the change of variables $w = W_{AN}x$.

The applicability of (6.2), when f is quadratic, is not restricted to sequential quadratic programming or trust region methods in general. In the symmetric case, monotone linear complementarity problems can be regarded as quadratic programs. In order to conclude this, one only needs to rewrite conveniently the Karush-Kuhn-Tucker conditions associated to (6.2), which are given by

$$P_{\mathcal{K}(A)}\left(\nabla f(x) - s\right) = 0 \tag{6.3}$$

$$Ax = b \tag{6.4}$$

$$x \geq 0 \tag{6.5}$$

$$s \geq 0 \tag{6.6}$$

$$x \cdot s = 0. \tag{6.7}$$

where P is the Euclidean projection operator, $x \cdot s := (x_1 s_1, ..., x_n s_n) \in \mathbb{R}^n$ is the Hadamard product and $\mathcal{K}(A)$ is a short notation for Kernel(A). Due to convexity, these conditions are necessary and sufficient for optimality of (6.2) for any convex function f. Recall that (6.3) is called Lagrange condition, (6.4) and (6.5) indicate primal feasibility, (6.6) dual feasibility and (6.7) is the complementarity condition. We say that $(x, s) \in \mathbb{R}^n \times \mathbb{R}^n$ is a feasible pair, or a feasible primal dual point associated to (6.2), if it satisfies (6.3)-(6.6). We recall from Chapter 2 that interior feasible points are feasible points so that $x, s > 0$ and its set is denoted by Γ°. Remember also that the central path associated to (6.2) is based on the logarithmic barrier and consists of the interior feasible points $(x, s) \in \Gamma^\circ$ with the property

$$x \cdot s = \mu e,$$

for some $\mu > 0$, where $e := (1, ...1) \in \mathbb{R}^n$.

In this chapter we will define a primal-dual Levenberg-Marquardt trajectory associated to (6.2), starting from the analytic center of Ω. We will prove that its primal part is tangent to the central path, while its dual part provide primal dual interior feasible points. This is done in Sections 6.2 and 6.3. An application in quadratic programming is given in Section 6.4 followed by some concluding remarks.

6.2 Preliminaries

Remember that the logarithmic barrier $p_{\log} : \mathbb{R}^n_{++} \to \mathbb{R}$ is given by

$$p_{\log}(x) := -\sum_{i=1}^{n} \log(x_i),$$

and that, by definition, x_{AN} is precisely the unique solution of the optimization problem

$$\begin{array}{ll} \text{minimize} & p_{\log}(x) \\ \text{subject to} & Ax = b \ . \\ & x > 0 \end{array} \tag{6.8}$$

Lemma 6.1. *We have that $x_{AN} := e \in \mathbb{R}^n$ is the analytic center of Ω, $\nabla p_{log}(e) = e$ and $\nabla^2 p_{log}(e) = I$.*

Proof. The fact that $x_{AN} = e$ follows directly from our change of variables together with the fact that the logarithm of a product is the sum of the logarithms. The remaining claims are also elementary. □

Let us now consider the Levenberg-Marquardt regularization function $p_{LM} : \mathbb{R}^n \to \mathbb{R}$ with

$$p_{LM}(x) := \frac{1}{2}\|x\|^2.$$

Then, as we have seen in Chapter 2, the Levenberg-Marquardt trajectory is based on the following optimization problem

$$\begin{array}{ll} \text{minimize} & f(x) + \alpha p_{LM}(x) \\ \text{subject to} & Ax = b \end{array} , \tag{6.9}$$

where $\alpha > 0$. For each $\alpha > 0$, the system above has the unique solution that we will denote by $x_{LM}(\alpha)$. The parametrization $\alpha \mapsto x_{LM}(\alpha)$, with $\alpha > 0$, will also be called as the primal Levenberg-Marquardt trajectory.

Lemma 6.2. *The unique minimizer of p_{LM} subject to $Ax = b$ is e. Moreover, $\nabla p_{LM}(e) = e$ and $\nabla^2 p_{LM}(e) = I$.*

Proof. From the definition of p_{LM} it follows directly that $\nabla p_{LM}(e) = e$ and $\nabla^2 p_{LM}(e) = I$. From Lemma 6.1 we know that the projection of e onto $\mathcal{K}(A)$ is zero. Therefore, taking $\nabla p_{LM}(e) = e$ into account, we have that e minimizes p_{LM} subject to $Ax = b$. □

Hence, e is not only the minimizer of the two penalization functions introduced above. Indeed, the first and the second derivatives of the logarithmic barrier and the Levenberg-Marquardt regularization coincide at e.

Now, we get into a subsection where we prove an auxiliary lemma that will be important to state primal relations between the central path and the Levenberg-Marquardt trajectory.

6.2.1 An auxiliary result

For each $\alpha > 0$ consider the problem

$$\begin{array}{ll} \text{minimize} & f(x) + \alpha p(x) \\ \text{subject to} & Ax = b, \end{array} \tag{6.10}$$

where $p : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is a strongly convex function.

Lemma 6.3. *Let $\bar{x}$ be the minimizer of p subject to $Ax = b$ and suppose that p is two times continuously differentiable with a locally Lipschitz Hessian $\nabla^2 p(\cdot)$ in a neighborhood of $\bar{x}$. Assume also that $\nabla^2 p(\bar{x}) = I$. Then, considering that $x(\alpha)$ denotes the solution of the optimization problem (6.10), with $\alpha > 0$, it follows that:*

(a) *The trajectory $\{x(\alpha) \in \mathbb{R}^n | \alpha > 0\}$ is well defined and $\lim_{\alpha\to\infty} x(\alpha) = \bar{x}$;*

(b) *$x(\alpha)$ minimizes f in the convex trust region $\{x \in \mathbb{R}^n | p(x) \leq p(x(\alpha)), Ax = b\}$ and $\alpha > 0 \mapsto p(x(\alpha))$ is a nonincreasing function;*

(c) $\lim_{\alpha\to\infty} \alpha\,(x(\alpha) - \bar{x}) = -P_{\mathcal{K}(A)}(\nabla f(\bar{x}))$.

Proof. For any $\alpha > 0$, the function $f + \alpha p$ is strongly convex. Hence, (6.10) has the unique solution $x(\alpha)$. In particular, $\{x(\alpha) \in \mathbb{R}^n | \alpha > 0\}$ is well defined. From the definition of $x(\alpha)$ and $\bar{x}$ we have, for all $\alpha \geq 1$, that

$$\begin{aligned} f(x(\alpha)) + p(x(\alpha)) - p(\bar{x}) &\leq f(x(\alpha)) + \alpha\,(p(x(\alpha)) - p(\bar{x})) \\ &\leq f(\bar{x}) + \alpha\,(p(\bar{x}) - p(\bar{x})) = f(\bar{x}). \end{aligned}$$

This inequality, together with the compactness of the level sets of $f + p$, implies that $\{x(\alpha) \in \mathbb{R}^n | \alpha \geq 1\}$ is bounded. Consequently, $\{f(x(\alpha))\}_{\alpha \geq 1}$ must be bounded. Therefore, the second inequality leads to

$$\lim_{\alpha \to \infty} \alpha(p(x(\alpha)) - p(\bar{x})) < \infty.$$

Hence,

$$\lim_{\alpha \to \infty} p(x(\alpha)) - p(\bar{x}) = 0.$$

Then, the strong convexity of p guaranties that

$$\lim_{\alpha \to \infty} x(\alpha) = \bar{x},$$

proving (a).

The Karush-Kuhn-Tucker conditions of (6.10), necessary and sufficient due to convexity, read as follows

$$P_{\mathcal{K}(A)} \left(\nabla f(x(\alpha)) + \alpha \nabla p(x(\alpha)) \right) = 0; \tag{6.11}$$

$$A \left(x(\alpha) \right) = b. \tag{6.12}$$

From (6.11) and (6.12) we conclude that $x(\alpha)$ minimizes f in the convex set $\{x \in \mathbb{R}^n | p(x) \leq p(x(\alpha)), Ax = b\}$. Moreover, the Lagrange multiplier correspondent to the inequality constraint is α. Now take $0 < \alpha_2 < \alpha_1$. Then,

$$f\left(x(\alpha_2)\right) + \alpha_2 p\left(x(\alpha_2)\right) \leq f\left(x(\alpha_1)\right) + \alpha_2 p\left(x(\alpha_1)\right)$$

$$f\left(x(\alpha_1)\right) + \alpha_1 p\left(x(\alpha_1)\right) \leq f\left(x(\alpha_2)\right) + \alpha_1 p\left(x(\alpha_2)\right).$$

Adding these inequalities we get $p\left(x(\alpha_1)\right) \leq p\left(x(\alpha_2)\right)$, proving (b).

Note that if for some $\bar{\alpha} > 0$ we have $x(\bar{\alpha}) = \bar{x}$, the strong convexity of p and (b) guarantee that $x(\alpha) = \bar{x}$ for every $\alpha > \bar{\alpha}$. In this case, (6.11) implies (c). Therefore, let us assume from now on that $x(\alpha) \neq \bar{x}$ for all α sufficiently large. From Taylor's formula we have that

$$p(x) - p(\bar{x}) - \nabla p(\bar{x})^\top (x - \bar{x}) - \frac{1}{2}(x - \bar{x})^\top \nabla^2 p(\bar{x})(x - \bar{x}) = o(\|x - \bar{x}\|^2), \tag{6.13}$$

with

$$\lim_{x \to \bar{x}} \frac{o(\|x - \bar{x}\|^2)}{\|x - \bar{x}\|^2} = 0.$$

Moreover, from the local Lipschitz continuity of $\nabla^2 p$ around $\bar{x}$, we know that there exist $L > 0$ and $\delta > 0$, so that for all $x \in \mathcal{B}(\bar{x}, \delta)$ it holds that

$$\|v(x)\| \leq L \|x - \bar{x}\|^2, \tag{6.14}$$

where

$$v(x) := \nabla p(x) - \nabla p(\bar{x}) - \underbrace{\nabla^2 p(\bar{x})}_{I}(x - \bar{x}).$$

Since $\bar{x}$ is the minimizer of p subject to $Ax = b$, we conclude that $\nabla p(\bar{x})$ is orthogonal to $\mathcal{K}(A)$. Then, taking also (6.13) and $\nabla^2 p(\bar{x}) = I$ into account, we get

$$p(x(\alpha)) - p(\bar{x}) = \|x(\alpha) - \bar{x}\|^2 \left(\frac{1}{2} + \frac{o(\|x(\alpha) - \bar{x}\|^2)}{\|x(\alpha) - \bar{x}\|^2} \right), \tag{6.15}$$

for all α sufficiently large. Due to (6.12) and the feasibility of $\bar{x}$, it follows that $x(\alpha) - \bar{x} \in \mathcal{K}(A)$, for all $\alpha > 0$. Then, using the linearity of $P_{\mathcal{K}(A)}$ and (6.11) we obtain

$$\begin{aligned} 0 &= P_{\mathcal{K}(A)} \left(\nabla f(x(\alpha)) + \alpha \nabla p(x(\alpha)) \right) \\ &= P_{\mathcal{K}(A)} \left(\nabla f(x(\alpha)) + \alpha \nabla p(\bar{x}) + \alpha (x(\alpha) - \bar{x}) + \alpha v(x(\alpha)) \right) \\ &= P_{\mathcal{K}(A)}(\nabla f(x(\alpha))) + \alpha P_{\mathcal{K}(A)}(\nabla p(\bar{x})) + \alpha P_{\mathcal{K}(A)}(x_\alpha - \bar{x}) + P_{\mathcal{N}(A)}(\alpha v(x(\alpha))) \\ &= P_{\mathcal{K}(A)}(\nabla f(x(\alpha))) + \alpha (x(\alpha) - \bar{x}) + P_{\mathcal{K}(A)}(\alpha v(x(\alpha))). \end{aligned} \tag{6.16}$$

In order to finish the proof we will show that $\lim_{\alpha \to \infty} \alpha v(x(\alpha)) = 0$. Note that the definition of $x(\alpha)$ implies that

$$0 \leq \alpha (p(x(\alpha)) - p(\bar{x})) \leq f(x(\alpha)) - f(\bar{x}).$$

Using (a) we get

$$\lim_{\alpha \to \infty} \alpha (p(x(\alpha)) - p(\bar{x})) = 0. \tag{6.17}$$

Now, multiplying (6.15) by α and taking limits we obtain

$$\lim_{\alpha \to \infty} \alpha \|x(\alpha) - \bar{x}\|^2 = 0. \tag{6.18}$$

On the other hand, for all $\alpha > 0$ sufficiently large, (6.14) leads to

$$\alpha \|v(x(\alpha))\| = \frac{\|v(x(\alpha))\|}{\|x(\alpha) - \bar{x}\|^2} \alpha \|x(\alpha) - \bar{x}\|^2 \leq L\alpha \|x(\alpha) - \bar{x}\|^2.$$

Therefore, $\lim_{\alpha \to \infty} \alpha v(x(\alpha)) = 0$. This fact, combined with (6.16), implies (c). □

6.3 Primal dual relations between the Levenberg-Marquardt and the central path trajectories

Before arriving to the main result of this chapter let us define our dual Levenberg-Marquardt trajectory.

For each $\alpha > 0$ set $s_{LM}(\alpha) := \alpha(2x_{AN} - x_{LM}(\alpha))$.

Theorem 6.1. *It holds that:*

(a) $P_{\mathcal{K}(A)}\left(\nabla f(x_{LM}(\alpha)) - s_{LM}(\alpha)\right) = 0$ *for all* $\alpha > 0$*;*

(b) $\sigma(x_{LM}(\alpha)), s_{LM}(\alpha), \alpha) \leq \|x_{LM}(\alpha) - x_{AN}\|^2$*, with* σ *as in* (2.22)*;*

(c) *the Levenberg-Marquardt trajectory and the central path associated to* (6.2) *are tangent at* x_{AN}*;*

(d) *for all* $\alpha > 0$ *sufficiently large,* $(x_{LM}(\alpha), s_{LM}(\alpha)) \in \mathbb{R}^n \times \mathbb{R}^n$ *is an interior feasible primal-dual point associated to* (6.2)*;*

(e) $\lim_{\alpha\to 0^+} s_{LM}(\alpha) = 0$ *and* $\lim_{\alpha\to\infty} \frac{s_{LM}(\alpha)}{\alpha} = x_{AN}$.

Proof. From the linearity of $P_{\mathcal{K}(A)}$ and the definition of $x_{LM}(\alpha)$ and $s_{LM}(\alpha)$, we conclude that

$$\begin{aligned} P_{\mathcal{K}(A)}\left(\nabla f(x_{LM}(\alpha)) - s_{LM}(\alpha)\right) &= P_{\mathcal{K}(A)}\left(\nabla f(x_{LM}(\alpha)) + \alpha x_{LM}(\alpha) - 2\alpha x_{AN}\right) \\ &= P_{\mathcal{K}(A)}\left(\nabla f(x_{LM}(\alpha)) + \alpha x_{LM}(\alpha)\right) - 2\alpha P_{\mathcal{K}(A)}\left(x_{AN}\right) \\ &= 0 - 2\alpha P_{\mathcal{K}(A)}(e) = 0. \end{aligned}$$

This proves (a). Let us now prove (b).

Invoking the definition of the measure σ given in (2.22) and remembering that $x_{AN} = e$, we conclude that

$$\begin{aligned} \sigma(x_{LM}(\alpha), s_{LM}(\alpha), \alpha) :&= \left\| \frac{x_{LM}(\alpha)\cdot s_{LM}(\alpha)}{\alpha} - e \right\| \\ &= \|x_{LM}(\alpha)\cdot(2x_{AN} - x_{LM}(\alpha)) - e\| \\ &= \|(x_{AN} + (x_{LM}(\alpha) - x_{AN}))\cdot(x_{AN} - \\ &\quad (x_{LM} - x_{AN})(\alpha)) - e\| \\ &= \|(x_{LM}(\alpha) - x_{AN}(\alpha))\cdot(x_{LM}(\alpha) - x_{AN}(\alpha))\| \\ &\leq \|x_{LM}(\alpha) - x_{AN}\|^2. \end{aligned}$$

Item (c) is a direct consequence of item (c) in Lemma 6.3 together with Lemmas 6.1 and 6.2.

Due to item (a), and the fact that $Ax_{LM}(\alpha) = 0$, we only need to check the positivity of $x_{LM}(\alpha)$ and $s_{LM}(\alpha)$ in order to prove (d). But this follows for sufficiently large $\alpha > 0$, since $x_{AN} > 0$ and $\lim_{\alpha\to\infty} x_{LM}(\alpha) = x_{AN}$. This limit also makes item (e) elementary. □

6.4 An application to convex quadratic programming

Our theorem is specially interesting when f is quadratic, because in this case one can calculate points on the Levenberg-Marquardt trajectory by solving linear systems of equations. So, assume in this section that $f : \mathbb{R}^n \to \mathbb{R}$ is a convex quadratic function defined as in the following

$$f(x) := x^\top Q x + c^\top x,$$

where $c \in \mathbb{R}^n$ and $Q \in \mathbb{R}^{n\times n}$ is positive semidefinite. Then, the Karush-Kuhn-Tucker conditions of Problem 6.9, that defines the Levenberg-Marquardt trajectory, read as follows

$$\begin{bmatrix} Q+\alpha I & A^\top \\ A & 0 \end{bmatrix} \begin{bmatrix} x \\ \lambda \end{bmatrix} = \begin{bmatrix} -c \\ 0 \end{bmatrix}. \tag{6.19}$$

For each $\alpha > 0$ this system is always solvable and has a unique solution in x, which is precisely $x_{LM}(\alpha)$. One gets uniqueness in λ if, and only if, A is full rank. We now arrive at a practical algorithm for calculating feasible interior primal-dual points in quadratic programming.

Algorithm 6.1. Primal-Dual feasible points
Step 0. Choose $\alpha_0 > 0$ and $\rho > 1$.
Step 1. Calculate the solution $x_{LM}(\alpha)$ of the system (6.19) with $\alpha := \alpha_k$.
Step 2. If $x_{LM}(\alpha_k) > 0$ and $s_{LM}(\alpha) >$ stop, else set $\alpha := \rho\alpha_k$.
Step 4. Set $k := k + 1$ and go to Step 1.

Due to Theorem 6.1 this algorithm is well defined and produces interior primal-dual feasible points $(x_{LM}(\alpha), s_{LM}(\alpha))$ in quadratic programming for sufficiently large values of α.

6.5 Concluding remarks

Theorem 6.1 says that the pairs $(x_{LM}(\alpha), s_{LM}(\alpha))$ are close to the primal-dual central path associated to Problem 6.2. This is a nice property since getting points on the central path is almost as difficult as solving the main problem. This result is established for convex problems with constraints described by linear equalities and nonnegative variables in a way that the feasible set has an analytic center. We have seen in Chapter 2 how one can rewrite certain quadratic programs in order to get the constraints in the format of Ω having e as its analytic center. This means that Algorithm 6.1 can be useful in path following algorithms for a large class of quadratic programs.

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