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Sequential Quadratic Programming Algorithms for Optimization

by

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SEQUENTIAL QUADRATIC PROGRAMMING ALGORITHMS FOR OPTIMIZATION

Francisco Javier Prieto, Ph.D.
Stanford University, 1989

The problem considered in this dissertation is that of finding local minimizers for a function subject to general nonlinear inequality constraints, when first and perhaps second derivatives are available. The methods studied belong to the class of sequential quadratic programming (SQP) algorithms. In particular, the methods are based on the SQP algorithm embodied in the code NPSOL, which was developed at the Systems Optimization Laboratory, Stanford University.

The goal of the dissertation is to develop SQP algorithms that allow some flexibility in their design. Specifically, we are interested in introducing modifications that enable the algorithms to solve large-scale problems efficiently. The following issues are considered in detail:

- *The use of approximate solutions for the QP subproblem.* Instead of trying to obtain the search direction as a *minimizer* for the QP, the solution process is terminated after a limited number of iterations. Suitable termination criteria are defined that ensure convergence for an algorithm that uses a quasi-Newton approximation for the full Hessian. Theorems concerning the rate of convergence are also given.

- *The use of approximations for the reduced Hessian in the construction of the QP subproblems.* For many problems the reduced Hessian is considerably smaller than the full Hessian. Consequently, there are considerable practical benefits to be gained by only requiring an approximation to the reduced Hessian. Theorems are proved concerning the convergence and rate of convergence for an algorithm that uses a quasi-Newton approximation for the reduced Hessian when early termination of the QP subproblem is enforced.

- *The use of exact second derivatives.* The use of second derivatives, while having significant practical advantages, introduces new difficulties; for example, the QP subproblems may be non-convex, and even a minimizer for the subproblem is no longer guaranteed to yield a suitable search direction. It is shown how to construct suitable search directions from approximate solutions to the QP subproblem. Also, theorems are proved for the convergence and rate of convergence of these algorithms.

Finally, some numerical results, obtained from a modification of the code NPSOL, are presented.

A mis padres

Preface

"The whole of science is nothing more than a refinement of everyday thinking."

— *Albert Einstein*

The last forty years have seen the introduction of numerous methods for the solution of general nonlinear programs, and an expansion on their use as satisfactory mathematical models for problems in many different fields of human activity. Examples of this use can be found in areas as diverse as general equilibrium models in economic theory, structural optimization in mechanical engineering, microeconomic models of the firm in business administration, or optimal power flow in electrical engineering, attesting both to the universality with which the structure of the mathematical model can be recognized in Nature, and also to the existence of efficient methods to obtain accurate and satisfactory answers to the problems considered.

Despite the fact that the widespread use of these models would not have been possible without the existence of efficient solution algorithms, the opinion is frequently expressed among researchers in the field that no general-purpose algorithm available at this time combines all the desirable features, and in particular, that the algorithms available are limited regarding either the size or the difficulty of the problems they can solve.

The search for more reliable and faster algorithms constitutes the basic motivation for the work presented in this dissertation. It would have been presumptuous to have set as a goal the search for answers to all the unanswered questions left in this field; it has been our objective simply to explore some aspects promising improvements for algorithms oriented towards the solution of large-scale problems, on the understanding that it is in this area where a more substantial amount of work seems left to be done. In any event, it is our hope that the exploration of these topics, independent of the setting in which they have been studied, may help to shed some light on issues of general interest in the field.

The work presented in this dissertation would not have been possible without the financial assistance provided by the Bank of Spain, and the earlier results, generous support and assistance of the SOL algorithms group at Stanford University. Special mention is deserving of my advisor, Prof. Walter Murray, who not only suggested the main ideas explored in this dissertation and guided the course of the work to its present state, but also found the time for many enlightening conversations on the most diverse topics. Profs. Philip Gill and Michael Saunders were always willing to answer my many questions, and provided comments and suggestions from which this work has benefited greatly; the example of their behavior (and that of my advisor) has been one of my most important lessons during this period. Although I had little opportunity to benefit from her presence, Dr. Margaret Wright will be fondly remembered for her energy and dedication.

I am indebted to Prof. George B. Dantzig for his generous invitation to visit this department during the summer of 1983; this work is one of its consequences. It has been a privilege to have him in my dissertation committee.

I would like to express my gratitude to the students working with the SOL group, Samuel Eldersveld, Anders Forsgren, Aeneas Marxen and Dulce Ponceleón, for providing a very pleasant and stimulating atmosphere. Special thanks must be given to Anders Forsgren for his invaluable comments and suggestions. I am also deeply grateful to Dr. Ulf Ringertz for his many intelligent remarks, and for having provided the code for the structural optimization test problems.

Finally, I would like to thank the faculty members, staff and students at the Department of Operations Research, who helped in many different ways to make this a productive and enjoyable experience.

F.J. Prieto
Stanford, 1989

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Chapter 1

Introduction

In this chapter we introduce the subject of the report, and give some motivation for the research undertaken. In addition, a brief summary of previous work in this area is presented.

1.1. The problem and algorithms

This report is concerned with issues in the field of nonlinear programming, which in its most general form is that of finding extreme points (minimizers or maximizers) for a univariate function, subject to certain conditions on the acceptable values for the variables.

For the purpose of this work, the problem is assumed to take a more restricted form. The effort is limited to the determination of local extreme points, and the conditions on the values of the variables are assumed to be given by a system of nonlinear inequalities. The nonlinear program considered takes the following form:

$$\boxed{\begin{array}{ll} \underset{x\in\Re^n}{\text{minimize}} & F(x) \\ \text{s.t.} & c(x) \geq 0, \end{array}} \qquad \text{NLP}$$

where $F : \Re^n \rightarrow \Re$ and $c : \Re^n \rightarrow \Re^m$.

The most reliable algorithms for solving this problem make use of the derivatives of the functions defining the problem, when they exist. In this spirit, the algorithms to be studied try to exploit the structure of the problem by constructing local approximations from the derivative information available. This requires additional conditions on the form of the problem; the basic assumption is the twice continuous differentiability of the functions F and c. In addition, some other assumptions of a more technical nature are required; these assumptions will be specified later.

SQP algorithms

It is not known in general how to compute a solution of the nonlinear program NLP in a finite number of iterations (obvious exceptions being the cases of linear and quadratic programming), and so the algorithms developed for its solution are sequential in nature, that is, an infinite sequence of points $\{x_k\}_{k=0}^{\infty}$ is generated, such that the limit points of convergent subsequences are solutions for the problem.

Among sequential algorithms a particular class, that of sequential quadratic programming (SQP) algorithms, seems to be regarded as the best choice for the solution of small, dense problems (see Stoer [Sto85] or Gill *et al.* [GMSW88], for example). The algorithms considered belong to this family of SQP algorithms, and the concern of our research is to extend the class of problems for which these algorithms may be an efficient choice.

The next paragraphs are devoted to commenting upon some of the features of SQP algorithms, and their relevance to this work. We start by describing the most general form that such an algorithm may take.

- The algorithm generates a sequence of points $\{x_k\}$ converging to a solution.
- At each point, x_k, a linearly constrained quadratic program (QP) approximating locally the NLP problem is generated, and a direction p_k is obtained from it.
- The next point is defined to be either $x_k + p_k$ or the result of a linesearch from x_k along p_k, in such a way that the value of a certain merit function is decreased.

We are not concerned with the study of a general class of algorithms, like the one described above, but rather with the definition and study of specific algorithms within this class. Although the particular forms of these algorithms are presented in the following chapters, we point out here that their most significant characteristics are the use of a linesearch to determine the next point in the sequence, and the construction of quadratic subproblems of the form

$$\boxed{\begin{array}{ll} \underset{p\in\Re^n}{\text{minimize}} & \nabla F(x_k)^T p + \tfrac{1}{2} p^T H_k p \\ \text{s.t.} & c(x_k) + \nabla c(x_k) p \geq 0 \end{array}} \qquad \text{QP}$$

for some matrix H_k, whose properties are described as part of the definition of the different algorithms considered.

Goal of the report

Expanding upon previous remarks, this report is specially concerned with modifications to the way that QP approximations are constructed and solved. The modifications considered are oriented towards defining more flexible SQP algorithms in order to make them more suitable for the solution of large-scale problems. Specifically, we wish to relax the usual assumption that the search direction is obtained as a minimizer of the QP subproblem, and also to allow the use of exact second derivatives, or to require only an approximation to the reduced Hessian. Finally, it may be possible to take advantage of the increased flexibility to improve the performance of SQP methods even on small dense problems.

Incomplete QP solution

Throughout, we develop algorithms that obtain the search direction for a quadratic subproblem in a limited number of iterations, which often in practice is significantly smaller than the number required for the computation of a minimizer for the QP subproblem; the search direction obtained in this form will be referred to as an incomplete QP solution. In general, the algorithm moves from a starting point satisfying certain mild conditions to the first stationary point, and the search direction is constructed from the information known at that point.

The QP subproblems generated in the algorithms developed so far have been normally obtained by using quasi-Newton approximations to the full or the reduced Hessian; we shall also consider the option of using the exact Hessian in the definition of H_k.

Quasi-Newton approximations generate matrices that are positive definite, and at the same time allow the condition numbers of the approximating matrices to be controlled. In this way, a convex subproblem is obtained, and if it is feasible, its solution exists and is unique. In contrast, the use of exact Hessians leads to non-convex subproblems; moreover, H_k may now be singular. On the other hand, it will be seen that the use of the exact Hessian leads to stronger convergence results and an improved rate of convergence.

Convergence assumptions

The convergence of the algorithms in this family normally requires additional conditions on the form of the problem. An aim that underlies all the work presented in this report is to try to develop algorithms whose convergence proofs make use of a reasonably weak set of assumptions. The ones that can be most frequently found in the literature are:

- existence and continuity of second derivatives for the objective and constraint functions;
- full-rank Jacobians at solutions of the problem;
- bounded (above and below) eigenvalues for the approximations to the Hessian of the Lagrangian function;
- strict complementarity at solutions of the problem;
- existence of a feasible point for each subproblem;
- compactness of the feasible region, or of the region where the iterates lie.

The search direction

Together with these "regularity" assumptions on the form of the problem, it is necessary to specify the form of the direction of movement obtained from the QP subproblem, and that of the multiplier estimates. In the literature, the usual choices have been:

- the direction of movement is obtained as the exact solution of the QP subproblem, constructed as a convex program;
- the multiplier estimates to be used are either the QP multipliers at the last minimizer obtained, or the least-squares multipliers at the current point.

Details about these choices are given in the next section.

Defining a solution

In the previous paragraphs several references have been made to solutions of the NLP problem. The following remarks try to clarify what is understood by a solution.

Local solutions can be characterized in terms of what are known as the Karush-Kuhn-Tucker (KKT) conditions (see for example Fiacco and McCormick [FMC68] or Gill *et al.* [GMW81]), given in terms of the first and second derivatives of the Lagrangian function for the problem. The conditions come in different forms, and in particular there are sets of necessary conditions, and sets of sufficient conditions, but there is no practical necessary *and* sufficient characterization of this form for the general case. Given that the previous algorithms obtain points that satisfy the necessary conditions on the first and second derivatives, it is not possible to guarantee that the points obtained correspond to solutions of the problem, unless additional assumptions are satisfied.

Also, given that no convexity assumption is made on the functions defining the problem, no a priori relationship can be established between local solutions and global solutions; this implies that the algorithms to be presented will not normally be able to determine whether the solutions obtained are global solutions.

The following terms will be used to define what solution points the algorithms are able to find.

- *Stationary point.* A feasible point x such that

  $$\nabla F(x) = \nabla c(x)^T \lambda^*, \qquad \lambda_i^* c_i(x) = 0 \quad i = 1, \dots, m$$

  for some multiplier vector $\lambda^* \in \Re^m$.

- *First-order KKT point.* A stationary point x such that $\lambda^* \geq 0$.

- *Second-order KKT point.* A first-order KKT point x such that, if A denotes the rows of the Jacobian $\nabla c(x)$ corresponding to the constraints having positive multipliers at x,

  $$\forall\, v \in \mathcal{N}(A) \qquad v^T \nabla_{xx} L(x, \lambda^*) v \geq 0,$$

  where the Lagrangian function L is defined as

  $$L(x, \lambda) \equiv F(x) - \lambda^T c(x),$$

  and $\nabla_{xx} L(x, \lambda)$ denotes the Hessian of the Lagrangian function, when the (partial) derivatives are taken only with respect to the variable x.

In the case when analytical second derivatives are unknown or directions of negative curvature are not computed, the algorithms to be presented only guarantee that a solution is a first-order KKT point. When exact Hessians are known and directions of negative curvature are determined and used, the solution obtained by the algorithm will be a second-order KKT point.

1.2. Historical background

This section presents a brief history of the evolution of SQP algorithms. Surveys for this area can be found in [GMW81], [Po83] or [GMSW88], for example.

The origins

The earliest reference found to methods of this family is Wilson's doctoral dissertation [Wil63]. His algorithm, formulated for the special case of convex problems, solved an inequality constrained quadratic subproblem in each iteration, formulated using the exact Hessian of the Lagrangian function, and obtained the next iterate as $x_k + p_k$ (no linesearch was performed).

In general, a method of this form will not be globally convergent unless some precautions are taken in accepting the next step. Murray [Mu69] suggested a similar algorithm, but now a linesearch was performed on the ℓ_2 merit function, to guarantee global convergence. Also, quasi-Newton approximations to the Hessian of the Lagrangian function could be used in the generation of the subproblem, relaxing the requirement of convexity for the problem.

SQP algorithms became popular through the work of Biggs [Big72], Han [Han76] and Powell [Po78] (in the literature SQP methods are sometimes referred to as Wilson-Han-Powell algorithms). Biggs proposed an algorithm similar to the one in [Mu69], with the difference that the quadratic subproblem had only equality constraints, and a term for the multiplier estimate had been added to the constraints.

The algorithm proposed by Han solved an inequality constrained QP subproblem, where the Hessian was given by a quasi-Newton approximation to the Hessian of the Lagrangian function, although it required the assumption that the Hessian was positive definite on the whole space. Also, the "exact" (or ℓ_1) penalty function

$$P(x,\rho) \equiv F(x) + \rho \textstyle\sum_i \max\Big(0, -c_i(x)\Big)$$

was used as a merit function within the linesearch.

Powell proposed a method similar to the one in [Han76], but he was able to show that the algorithm converged superlinearly even when the Hessian of the Lagrangian function was indefinite at the solution.

In the next paragraphs we focus on the evolution of the different elements of an SQP algorithm: the merit function, second-order information, the multiplier estimate, etc.

The merit function

In all nonlinearly constrained optimization algorithms the choice of the merit function is of great importance, not only because of its role in enforcing global convergence, but also in order to ensure a satisfactory performance of the algorithm.

The ℓ_1 (exact penalty) merit function has become a very popular choice after being proposed by Han [Han76] and Powell [Po78] for SQP algorithms. Its advantage is that for large enough values of the penalty parameter, minimizers for the NLP problem are unconstrained minimizers for the exact penalty function. On the other hand, the function is not smooth, and in particular it is not differentiable at the solution of the problem.

Another option is the use of the augmented Lagrangian

$$L_A(x, \lambda, \rho) \equiv F(x) - \lambda^T c(x) + \tfrac{1}{2}\rho c(x)^T c(x)$$

as the merit function. It must be noted that this function includes an additional set of variables, the Lagrange multiplier estimates λ. In order to compute the correct value of the original variables x, it is necessary to obtain the correct value for the multiplier estimate. In fact, this merit function has the property that, if the optimal multiplier vector is used, there exists a finite value of the parameter ρ such that the solution of the problem is an unconstrained minimizer of the merit function.

A property of this merit function is that it is smooth. In extensive tests, the performance of algorithms using this merit function has been superior to that of methods using the exact penalty function. On the other hand, any algorithm that makes use of this merit function needs to take special care of the way the multipliers are estimated; a bad estimate may inhibit convergence or degrade the performance of the method. The theoretical analysis of these algorithms is also more complex because the additional variables λ need to be taken into account. The use of this merit function in an SQP framework was first suggested by Wright [Wri76] and Schittkowski [Sch81].

The search direction

An important element of the algorithms presented in this report is the use of an incomplete solution of the QP subproblem as the search direction for the merit function.

In the large-scale case, the number of QP steps required to obtain a minimizer for the QP subproblems, particularly in the early iterations, may be very high. Regardless of the inefficiency this may introduce, practical implementations must impose a strict upper limit on the number of QP steps. There is therefore a definite interest in defining an incomplete solution whose computation requires a strictly limited number of steps.

Although there have been proposals in the literature to terminate the solution process for the QP subproblems early, the great majority of SQP algorithms, including those mentioned earlier in this section, define the search direction from a minimizer for the QP subproblem.

An approach solving QP subproblems inexactly is described in Dembo and Tulowitzki [DT85], where for a generic SQP algorithm an early termination rule is given in terms of the norm of the reduced gradient for the subproblem. This rule gives a search direction p_k satisfying the condition

$$\|p_k - p_k^*\| = o(\|p_k\|),$$

where p_k^* denotes the minimizer for the kth QP subproblem.

We follow a different approach, presenting an early termination rule that is constructive in nature, and that has a guaranteed bound on the effort necessary to satisfy it.

The multiplier estimate

An important aspect in the efficient implementation of methods using merit functions based on the Lagrangian function is how to select the approximation to the Lagrange multipliers λ in each iteration.

Most SQP algorithms (for example, [Han76] or [Po78]) define λ as π, the QP multiplier obtained at the solution of the previous subproblem: $\lambda_{k+1} \equiv \pi_k$, where

$$\begin{aligned} \nabla F(x_k) + H_k p_k &= \nabla c(x_k)^T \pi_k, \\ \pi_k^T\big(\nabla c(x_k) p_k + c(x_k)\big) &= 0, \\ \pi_k &\geq 0. \end{aligned}$$

Unfortunately, in this case the change in the Lagrangian function is no longer monotonic whenever the multiplier estimate is updated.

An alternative is to use the least-squares multiplier estimate λ_L,

$$\lambda_L(x_k) = \left(\nabla c(x_k)\nabla c(x_k)^T\right)^{-1}\nabla c(x_k)\nabla F(x_k)$$

and to treat it as a function of x, rather than as an additional variable, simplifying the theoretical analysis of the algorithm. This idea appears to have been first introduced by Fletcher [Fle70], where it was used to construct an augmented Lagrangian merit function in order to solve an equality-constrained problem. For problem NLP with only equality constraints, Powell and Yuan [PY86] have considered the use of an augmented Lagrangian merit function that estimates the multipliers by λ_L, and they have shown several global and local convergence properties for this function.

Another option, compatible with the use of the QP multipliers from the previous iteration, is to treat the multiplier estimate as an additional set of variables in the linesearch. This idea was suggested by Tapia [Tap77] for equality constrained optimization, and Schittkowski [Sch81] introduced it in an SQP framework. A proof that the sequence $\{x_k\}$ converges to a first-order KKT point and the multiplier estimates converge to λ^* is given in Gill *et al.* [GMSW86b].

Trust-region methods

An alternative to the use of a linesearch on a merit function to ensure global convergence is the trust-region approach, where the size of the step is limited by imposing a constraint on the norm of the solution for the QP subproblem.

In this framework, Fletcher [Fle85] proposed an algorithm that solved a quadratic subproblem minimizing the Lagrangian function for the QP subproblem, subject to a bound on the $\|\cdot\|_\infty$ norm of the solution.

Another application of this idea is given by Celis, Dennis and Tapia [CDT85] for the case when only equality constraints are present. Their algorithm is related to the conventional trust-region approach in unconstrained optimization, in the sense that they impose a bound on the value of the $\|\cdot\|_2$ norm of the solution. Also, the linearized constraints are replaced by a second bound on the norm of their violation.

The algorithms we consider make use of a linesearch, and trust-region constraints are not specifically included in the QP subproblems.

Second derivative information

Several alternatives have been considered in the literature for the construction of the matrix H_k containing the second-order information for the quadratic subproblem.

It was mentioned earlier that in the first SQP algorithm proposed, H_k was taken to be the Hessian of the Lagrangian function at the current iterate. When the NLP problem is convex, there are no special difficulties in solving the subproblem.

If the convexity assumption is not satisfied, as is often the case in practice, the subproblem can become much more difficult to solve. To avoid this risk, and to extend the algorithm to cases where analytic derivatives may not be available, the most frequent choice of H_k has been the use of a positive definite quasi-Newton approximation to the full Hessian of the Lagrangian function. In this way, a convex subproblem is still obtained, and the subproblems can be solved efficiently. A detailed discussion of quasi-Newton updates can be found, for example, in Dennis and Moré [DM77] and Dennis and Schnabel [DS83]. Also, a description of different approaches to the implementation of this idea in an SQP framework is presented in Gurwitz [Gur87].

A difficulty with this scheme is that the Hessian of the Lagrangian function is rarely positive definite on the whole space (even at a solution). It is likely therefore that the use of quasi-Newton updates such as the BFGS method, will lead to indefinite approximations. Several alternatives have been proposed to compensate for this problem. Powell [Po78] presented a modification of BFGS for which positive definiteness was preserved and two-step superlinear convergence was achieved. Another possibility is to approximate the Hessian of the augmented Lagrangian function, where the penalty parameter has been selected large enough so that the Hessian can be kept positive definite; see Biggs [Big72], Tapia [Tap77] and Han [Han77].

Following the development of efficient QP solvers for indefinite problems, some updating methods have recently been proposed for which only the positive definiteness of $Z_k^T H_k Z_k$ is preserved, where Z_k denotes a basis for the null space of the Jacobian of the active constraints at x_k. The motivation for these approaches is that at the solution $Z^T \nabla_{xx} L(x, \lambda) Z$ will normally be positive definite. For this type of update, see for example Fenyes [Fen87].

Another alternative along a similar line is to try to approximate *only* the reduced Hessian $Z_k^T H_k Z_k$. This scheme has the advantage of requiring the storage of a matrix that in many cases is significantly smaller than the full Hessian. Reduced Hessian updating methods have been proposed among others by Murray and Wright [MW78], Coleman and Conn [CC84], Nocedal and Overton [NO85] and Gilbert [Gil87]. A study of the convergence properties of these methods for the case when only equality constraints are present is given in Byrd and Nocedal [BN88].

1.3. Contents of subsequent chapters

Chapter 2 describes the form of the general algorithm, whose variants will be studied in Chapters 4, 5 and 6. The conditions on the search direction and the multiplier estimate are presented, the assumptions used for the convergence proofs are introduced, and several results bearing on the reasonableness of the previous conditions are presented and proved.

Chapter 3 presents all results that are common to the convergence proofs for the different algorithms. Given that the algorithms studied are defined to share many elements (the merit function, the determination of the search direction, termination conditions for the linesearch, etc.), it has been considered convenient to group in this chapter the results common to all convergence proofs.

Chapter 4 studies the convergence properties of an algorithm that uses a quasi-Newton approximation to the full Hessian, and a search direction constructed from information available at a stationary point of the QP subproblem. It is shown that such an algorithm is globally convergent (that is, it converges to a solution from any initial point), and that it converges superlinearly under mild assumptions.

Chapter 5 considers the variant of the algorithm when a quasi-Newton approximation to the reduced Hessian is used, again only utilizing information at a stationary point of the QP subproblem. This algorithm is also shown to be globally convergent, but it converges two-step superlinearly to the solution.

Chapter 6 presents and studies an algorithm that uses exact second derivatives in the construction of the QP subproblem. Again, the search direction is obtained from the information at a stationary point of the quadratic subproblem. It is shown that the algorithm is globally convergent, and that it converges quadratically to the solution, under mild assumptions.

Chapter 7 presents numerical results obtained from the implementation of the algorithm introduced in Chapter 4. Finally, some remarks are included concerning the properties of all the previous algorithms.

Chapter 2

The Algorithm

Chapters 4, 5 and 6 present and study the convergence properties of three variants of an SQP algorithm. These methods differ in the way the second-order information for the QP subproblem (the matrix H_k defined in the previous chapter) is generated, but they share several common features: the merit function is the same, the search direction is generated according to similar principles and the linesearch procedure is analogous for the three methods.

This chapter describes a framework algorithm, composed of the common features mentioned earlier. Consequently, the following chapters only need to specify details that differentiate the method presented from the others.

In addition, we enumerate the general assumptions that are needed in the convergence proofs for the different methods. Again, it is left to the corresponding chapters to complete the list with any additional assumptions required for each individual method presented. Finally, as the framework algorithm specifies conditions on the way the search direction is to be computed, and on the acceptable forms that the Lagrange multiplier estimates may take, this chapter ends with a justification for the reasonableness of these conditions.

2.1. Background

The basis for the algorithms presented in this report is the algorithm NPSQP, as implemented in the code NPSOL [GMSW86a] developed at the Systems Optimization Laboratory, Stanford University. For a theoretical discussion of some properties of this algorithm, [GMSW86b] should be consulted; in fact, this reference has been the main source of information for the work described in the following chapters.

Since its inception, NPSOL has been shown to be a very efficient code for the solution of small general nonlinear problems. It provides a good starting point to propose and analyze modifications to SQP algorithms to make them suitable for the solution of large nonlinear problems.

One characteristic of NPSQP that poses difficulties in the solution of large problems is the need to compute the minimizer for the quadratic subproblem. The number of iterations required to solve the QP subproblem will in general grow with the size of the problem. This increase in QP iterations raises two issues: in the first place, it is questionable that in order to preserve overall efficiency, the effort required to compute a minimizer for the QP subproblem can be compensated by a sufficiently small *number* of subproblems to be solved. Also, any practical QP algorithm has to impose a limit on the maximum number of QP iterations allowed, and so there will exist cases in which the exact solution is not obtained; the question then is how does this affect the convergence properties of the algorithm. Both issues can be addressed if we are able to obtain a satisfactory termination criterion for a QP algorithm that is guaranteed to be achieved in a "moderate" number of iterations. In this sense, a "satisfactory" criterion will be one that is efficient in the sense that the number of nonlinear iterations is not adversely affected.

If the solution process is terminated early, the search direction for the outer iteration (the step on the original variables) is defined as the "total" step taken in the QP subproblem up to that point. The characteristics of the point at which the termination takes place clearly depend on the specific strategy used to solve the QP subproblem. NPSQP, and the algorithms described later on, use an active-set strategy to obtain the solution starting from a feasible point; this strategy dictates the kind of termination conditions that can be imposed. As mentioned earlier, the conditions imposed should have the following properties: they should limit the number of QP iterations needed to obtain the search direction to a reasonably small value, and the conditions should be easy to implement.

Terminating the QP algorithm prior to obtaining a solution impacts the SQP algorithm in a number of critical ways. Not only the search direction obtained is now of "lower quality" than before, but also the QP multipliers available will in general not be positive, and it is necessary to give some rules on what constitutes an acceptable multiplier estimate when forming the search direction in the multiplier space. The consequences of terminating the

QP solution early are therefore far reaching.

Another potential difficulty when large problems are considered is the use of a quasi-Newton approximation to the full Hessian of the Lagrangian function, as it may become too large to store in dense format, unless some scheme to generate sparse quasi-Newton approximations is used.

One possible alternative, used for example in the code MINOS, as described in [MS82], is to work with an approximation to the reduced Hessian. For many large-scale problems the size of the reduced Hessian is relatively small, and an approximation to it may therefore be stored in dense format.

Another alternative is to use exact second derivatives. In this case the sparsity of the second derivatives should alleviate the problem of storing and handling the QP Hessian, and even for the small-scale case, improvements in the rate of convergence and total computational work can be expected.

Unfortunately, this latter approach presents some drawbacks. In the first place, subproblems may no longer be convex, and an indefinite QP solver must be used. Also, a unique minimizer for the subproblem may not exist, and it is necessary to give conditions under which a specific minimizer will be an acceptable search direction. On this regard, it should be noted that while the definition of a satisfactory termination criterion for the quasi-Newton algorithms is only one aspect in the improvement of their efficiency, for the Newton-type algorithm the termination criterion is directly related to its convergence properties. Finally, given that the convergence proofs rely heavily on the similarity of the convergence properties for the sequences $\{x_k - x^*\}$ and $\{p_k\}$, if the reduced Hessian is close to singularity it is possible that no minimizer will be acceptable, and alternative termination criteria need to be specified.

The preceding topics are our main themes. The definition of the search direction will be introduced in this chapter, after the general form of the algorithm, to be completed in following chapters, has been specified. The approximation to the second-derivative information used by each algorithm will be indicated in the corresponding chapters. The next sections try to provide the framework for all subsequent results.

2.2. General form of the algorithm

This section introduces the prototype algorithm. Following the remarks made in the previous section, this algorithm is directly based on NPSQP. The prototype algorithm obtains the search direction from an incomplete solution for a QP subproblem of the form indicated in the previous chapter. The iterates are determined by performing a linesearch on the following merit function:

$$\boxed{L_A(x,\lambda,s,\rho) = F(x) - \lambda^T\big(c(x)-s\big) + \tfrac{1}{2}\rho\big(c(x)-s\big)^T\big(c(x)-s\big)} \tag{2.2.1}$$

where $s \geq 0$ are slack variables, and the scalar ρ is known as the penalty parameter. The linesearch is performed in the space of the variables x, λ and s, and the corresponding search directions are denoted by p, ξ and q.

The symbols $\phi(\alpha,\rho)$, or sometimes just $\phi(\alpha)$, are used to denote

$$\phi(\alpha,\rho) \equiv L_A(x+\alpha p, \lambda+\alpha\xi, s+\alpha q, \rho),$$

that is, the merit function as a function of the steplength. The derivative of ϕ with respect to α is denoted by ϕ'.

The following conventions will be used in the rest of the report,

$$g_k \equiv \nabla F(x_k), \qquad A_k \equiv \nabla c(x_k), \qquad c_k \equiv c(x_k),$$

although the last two symbols, A_k and c_k, will also be used with the same meaning but restricted to the set of active constraints at the given point. The term *active constraint* will be used to designate a constraint that is satisfied exactly at the current point ($c_i(x) = 0$ in the nonlinear problem, or $a_i^Tp = -c_i$ in the quadratic subproblem), and the set of all constraints active at a given point will be referred to as the *active set* at the point.

The objective function for the QP subproblem will be denoted by $\psi_k(p)$,

$$\psi_k(p) \equiv \nabla F(x_k)^T p + \tfrac{1}{2}p^T H_k p.$$

Sometimes, ψ will denote the function of one variable $\psi_k(\alpha) \equiv \psi_k(p+\alpha d)$. Finally, symbols of the form β_{abc} indicate fixed scalars related to properties of the problem, or the implementation of the algorithm, where "*abc*" identifies the specific scalar represented.

The framework algorithm

The algorithm described below will be common to the methods studied in the following chapters, in the sense that the latter will be defined as specific algorithms that lie within this framework algorithm. The framework algorithm proceeds through the following steps:

(i) Start from a point x_0 and an estimate for the Lagrange multipliers λ_0. Let H_0 be an approximation to the Hessian of the Lagrangian function at x_0, satisfying certain properties, and let $\rho_0 \geq 0$ be the initial value for the penalty parameter.

(ii) At each point x_k, form the QP subproblem

$$\begin{array}{ll} \underset{p \in \Re^n}{\text{minimize}} & g_k^T p + \tfrac{1}{2} p^T H_k p \\ \text{subject to} & A_k p \geq -c_k, \end{array}$$

where H_k denotes an approximation to the Hessian of the Lagrangian function at x_k; and obtain an incomplete solution p_k satisfying certain conditions to be specified later. Compute a vector of multipliers μ_k satisfying a second set of conditions to be specified. If $p_k = 0$, set $\lambda_k = \mu_k$ and terminate. Otherwise, define $\xi_k = \mu_k - \lambda_k$.

(iii) Compute s_k from

$$s_{k_i} = \begin{cases} \max(0, c_{k_i}) & \text{if } \rho_{k-1} = 0, \\ \max\left(0, c_{k_i} - \dfrac{\lambda_{k_i}}{\rho_{k-1}}\right) & \text{otherwise.} \end{cases}$$

Find ρ_k such that $\phi'(0)$ (or $\phi''(0)$ if a curvilinear search is used) is bounded away from zero by some fixed multiple of $\|p_k\|^2$.

Compute q_k from

$$q_k = A_k p_k + c_k - s_k. \tag{2.2.2}$$

(iv) Compute the steplength α_k as follows. If p_k is used as a direction of descent, the termination conditions for the linesearch are as follows:

If

$$\phi(1) - \phi(0) \leq \sigma \phi'(0) \tag{2.2.3}$$

set $\alpha_k = 1$. Otherwise, find an $\alpha_k \in (0, 1)$ such that

$$\phi(\alpha_k) - \phi(0) \leq \sigma \alpha_k \phi'(0) \tag{2.2.4a}$$

$$\phi'(\alpha_k) \geq \eta \phi'(0), \tag{2.2.4b}$$

where $0 < \sigma \leq \eta < \frac{1}{2}$.

If H_k is indefinite, a curvilinear search may have to be used. The definition of ϕ will be slightly modified, and the new termination conditions are given in Chapter 6.

(v) Form H_{k+1}.

(vi) Update x_k and λ_k using

$$\begin{pmatrix} x_{k+1} \\ \lambda_{k+1} \\ \bar{s}_k \end{pmatrix} = \begin{pmatrix} x_k \\ \lambda_k \\ s_k \end{pmatrix} + \alpha_k \begin{pmatrix} p_k \\ \xi_k \\ q_k \end{pmatrix}$$

and repeat the previous steps until convergence is reached.

This description of the algorithm still leaves many details to be specified. The termination criteria for the incomplete solution of the QP subproblem and the conditions on the multiplier approximation μ_k are discussed below. The specification of the form of the approximation to the Hessian of the Lagrangian function, H_k, is left to the corresponding chapters. Finally, for the case when indefinite Hessian matrices are used in the QP subproblem, the form of the modified search is given in Chapter 6.

The solution of the QP subproblem

As indicated in step (ii) of the algorithm, in each iteration the search direction is computed as the incomplete solution for the local quadratic programming approximation to the problem, by moving to a stationary point of the QP subproblem and using the information available at that point in the way indicated below. The subscript k corresponding to the iteration number will be dropped in what follows.

(i) An initial feasible point p_0 for the QP subproblem is obtained.

When an incomplete solution for the QP subproblem is used to define the search direction, the choice of p_0 becomes critical. If H_k is positive definite and the minimizer for the QP is used to determine the search direction, then, given the uniqueness of p_k, the choice of p_0 is irrelevant. If we determine the search direction from a stationary point that is not a minimizer, the sequence of stationary points that we compute depends directly on the value of p_0. We wish to define the initial point in such a manner that, at least in the positive definite case, all stationary points are satisfactory points at which to terminate the solution process. The condition that we need to impose on p_0 is one that limits the size of its norm, and in particular $\|p_0\|$ will be required to be small whenever the points x_k are close to x^*.

We start by defining vectors $\bar{s}$ and r having components

$$\bar{s}_i \equiv \max(0, c_i - \mu_i),$$
$$r_i \equiv \begin{cases} c_i - s_i & \text{if } |c_i - s_i| < |c_i - \bar{s}_i|, \\ c_i - \bar{s}_i & \text{otherwise;} \end{cases}$$

where μ denotes a multiplier estimate such that the following property holds:

$$\|x_k - \hat{x}\| \to 0 \Rightarrow \|c_k - \bar{s}_k\| \to 0$$

when $\hat{x}$ is a stationary point for the NLP problem. From this definition, r has the following property:

$$\|r\| \leq \|c - s\|. \tag{2.2.5}$$

The initial point p_0 should then satisfy:

- If $\tilde{c}$ denotes the components of c corresponding to the active constraints at p_0; for some constant $\beta_{pc} > 0$,

$$\|p_0\| \leq \beta_{pc}\|\tilde{c}\|. \tag{2.2.6}$$

- For some constant $\beta_{pcs} > 0$,

$$\|p_0\| \leq \beta_{pcs}\|r\|. \tag{2.2.7}$$

It is shown later that these conditions are easily satisfied, given a reasonable rule for the selection of the initial QP active set. A stronger condition, but perhaps of a more intuitive nature, would be to select $\|p_0\| \leq \beta_{cm}\|c^-\|$, where c^- denotes the vector of negative components of c (the norm of the infeasibilities at the current point). In this case, we would be requiring $\|p_0\|$ to be small whenever we are close to a feasible point (and not necessarily just close to a stationary point). Its disadvantage is that near a solution this rule could prevent the algorithm from having some desirable properties (such as having one QP iteration per major iteration, for example).

(ii) A sequence of Newton steps is taken until a stationary point for the QP subproblem, $\hat{p}$, is found.

(iii) If the stationary point is a second-order KKT point, the search direction is defined as $p \equiv \hat{p}$.

(iv) If the stationary point is not a second-order KKT point, either the QP multiplier vector has some components that are negative, or the reduced Hessian (assuming that exact second derivatives are used) has negative eigenvalues. In this case, an additional step, $\hat{p} + \alpha d$, may need to be taken, where α and d should satisfy the conditions indicated below.

If the multiplier vector has negative elements, the conditions on the step are:

C1. d is feasible with respect to the active constraints, $Ad \geq 0$, and its norm is bounded above and below, that is, for some constants $\beta_{und} > \beta_{lnd} > 0$ it holds that $\beta_{und} \geq \|d\| \geq \beta_{lnd}$. It is assumed that $\beta_{lnd} \leq 1$, in order to simplify the arguments in the following chapters.

C2. The rate of descent along d is sufficiently large. If $\psi(\zeta) \equiv \psi(\hat{p}+\zeta d)$, it is required that

$$\psi'(0) = (H\hat{p} + g)^T d \leq -\beta_{dsc} \max_i \mu_i^- \tag{2.2.8}$$

for some constant $\beta_{dsc} > 0$.

C3. The steplength α is defined as the step to the minimizer of the quadratic function $\psi(\zeta)$, given by $-\psi'(0)/(d^T H d)$, if ψ is convex and this step is feasible. Let α_c denote the step to the nearest inactive constraint, and define

$$\alpha_m \equiv \begin{cases} -\dfrac{\psi'(0)}{d^T H d} & \text{if } d^T H d > 0, \\ \alpha_M & \text{otherwise.} \end{cases} \tag{2.2.9}$$

Then

$$\alpha \equiv \min(\alpha_c, \alpha_m, \alpha_M), \tag{2.2.10}$$

where $\alpha_M > 0$ is a specified bound on the largest acceptable step.

If the multiplier vector is non-negative and the reduced Hessian is indefinite, the conditions are:

C4. A direction of negative curvature d for the reduced Hessian is computed satisfying

$$\|d\| = 1, \quad d^T H d \leq \beta_L \lambda_{\min}, \quad Ad = 0, \quad g^T d \leq 0,$$

where $\lambda_{\min}$ indicates the smallest eigenvalue for the reduced Hessian, and A denotes the Jacobian corresponding to the active set at $\hat{p}$.

(A weaker condition that is sufficient for the convergence of these algorithms is that for any sequence $\{d_k\}$,

$$\frac{d_k^T H_k d_k}{d_k^T d_k} \to 0 \Rightarrow \lambda_{\min_k} \to 0$$

holds.)

C5. Let α_c be the step to the nearest constraint. The step α is defined as

$$\alpha \equiv \min(\alpha_c, \alpha_M).$$

Finally, for both cases we impose the following condition:

C6. It is a desirable property to avoid having search directions with very small norms, unless the corresponding point is close to a solution. The following condition is sufficient to ensure this property. Define

$$p \equiv \begin{cases} \hat{p} + \alpha d & \text{if } \|\hat{p}\| < \beta_{slp}\|\hat{p} + \alpha d\|, \\ \hat{p} & \text{otherwise,} \end{cases} \qquad (2.2.11)$$

for some constant $\beta_{slp} > 0$. In what follows it will be required that $\beta_{slp} \geq 1$.

It should be noted that in the case when H_k is obtained from the exact second derivatives, the previous rules are not sufficient for the determination of the search direction; the complete set of rules will be presented in Chapter 6.

The multiplier estimates

Step (ii) of the algorithm requires not only a search direction p_k, but also an estimate μ_k for the Lagrange multipliers at the current point. The QP solution is terminated at a stationary point, so a natural choice would be to use the QP multipliers as the estimate, but in general these may not be the best possible choice, as they may be negative, or the active set associated with the search direction may not in some cases be the same as the one for which the multiplier was obtained. The following set of conditions on μ_k is sufficient to ensure that the algorithms have the desired convergence properties.

C7. The estimates are uniformly bounded in norm.

C8.

$$\|\mu_k - \lambda^*\| = O(\|p_k\|),$$

where λ^* denotes the multiplier vector associated with the solution point closest to x_k.

C9. The complementarity condition $\mu_k^T(A_k p_k + c_k) = 0$ is satisfied at all iterations.

2.3. Assumptions and bounds

The algorithm will be applied to a problem satisfying the following general assumptions:

A1. x_k lies in a closed, bounded region $\Omega \subset \Re^n$, for all k.

A2. F, c_i and their first and second derivatives are continuous and uniformly bounded in norm on Ω.

A3. The Jacobian corresponding to the active constraints at any limit point of the sequence generated by the algorithm has full rank.

A4. The quadratic subproblems are always feasible; furthermore, there exists a subset of linearly independent constraints corresponding to the violated constraints for the NLP problem, such that its condition number is bounded and its least-norm solution is feasible.

A5. Strict complementarity holds at all stationary points for the nonlinear program in Ω.

A6. The reduced Hessian is non-singular at all solution points for the problem.

The bounds

From the previous assumptions, several quantities are uniformly bounded in the algorithm. We introduce the notation that will be used throughout the following chapters for some of these bounds. The first three bounds follow from assumption **A2**; the fourth follows from **A3**.

β_{nmA} is a bound for the norm of the Jacobian: $\|A_k\| \leq \beta_{nmA}$.

β_{nmc} is a bound for the norm of the constraint vector: $\|c_k\| \leq \beta_{nmc}$.

β_{nmg} is a bound for the norm of the gradient: $\|g_k\| \le \beta_{nmg}$.

β_{nmu} is an upper bound for the norm of the multipliers corresponding to a minimizer for the QP subproblem: $\|\tilde{\mu}_k\| \le \beta_{nmu}$.

2.4. Auxiliary results

This section presents a certain number of basic results, either justifying the conditions introduced before, or establishing properties to be used in the following chapters.

Initial points for the QP subproblem

It is of interest to show that the condition on step (i) for the solution of the QP subproblem can be satisfied. In fact, the role of assumption **A4** is to guarantee that this condition can be achieved. Condition (2.2.6) is satisfied if the Jacobians for the initial active sets have bounded condition numbers. Condition (2.2.7) requires some additional justification.

From **A4** it follows that there exist feasible points for the QP subproblem satisfying the condition

$$\|p_0\| \le \beta_{cm}\|c^-\|,$$

for some positive constant β_{cm}.

Consider now the following relationship, which will be often used in the next chapters. For any vector v defined as $v_i = \min(c_i, w_i)$, where w is any other vector, it holds that $\|c^-\| \le \|v\|$, since

$$\begin{array}{llllll} \text{if} & c_i^- = 0 & \text{then} & & & c_i^- \le |v_i|, \\ \text{if} & c_i^- > 0 & \text{then} & \text{if} \quad v_i = c_i & \text{then} & c_i^- = |v_i|, \\ & & & \text{if} \quad v_i = w_i & \text{then} & c_i^- \le |w_i| = |v_i|. \end{array}$$

This implies

$$\|c^-\| \le \|c - s\|, \qquad \|c^-\| \le \|c - \bar{s}\|$$

and

$$\|c^-\| \le \|r\| \le \|c - s\|. \tag{2.4.1}$$

Multiplier estimates

The next results explore some implications of the conditions on the multipliers given in the previous sections, and also present some examples of estimates satisfying these conditions.

A consequence of condition **C7** and the form in which multipliers are updated is the boundedness of the multipliers in the algorithm. This result is Lemma 4.2 in [GMSW86b].

Lemma 2.4.1. *For all $k \geq 1$,*

$$\|\lambda_k\| \leq \max_{0 \leq j \leq k-1} \|\mu_j\|,$$

and hence $\|\lambda_k\|$ is bounded for all k.

Proof. By definition,

$$\begin{aligned} \lambda_0 &= \mu_0 \\ \lambda_{k+1} &= \lambda_k + \alpha_k(\mu_k - \lambda_k), \quad k \geq 1. \end{aligned} \tag{2.4.2}$$

The proof is by induction. The result holds for $\lambda_0 = \mu_0$ because of the boundedness of the multiplier estimate (condition **C7**). Assume that the lemma holds for λ_k. From the definition of λ_{k+1} and norm inequalities, we have

$$\|\lambda_{k+1}\| \leq \alpha_k \|\mu_k\| + (1 - \alpha_k)\|\lambda_k\|.$$

Since $0 < \alpha \leq 1$, the inductive hypothesis gives

$$\|\lambda_{k+1}\| \leq \max_{0 \leq j \leq k} \|\mu_j\|,$$

as required. ▮

Conditions **C7**–**C9** are sufficiently general to be satisfied by most reasonable estimates, as the next lemmas show. Nonetheless, some attention must be paid to the satisfaction of condition **C7**, concerning the boundedness of the estimate, although that boundedness is guaranteed asymptotically by assumption **A3**. In general, any reasonable scheme to limit the norm of the multiplier estimate will not affect condition **C8**.

An issue that needs to be mentioned regarding condition **C8** is the necessity to identify the correct active set when x_k is close enough to x^*. (Since the problem may have several solution points, we use x^* in this context to denote the solution closest to x_k.) The next results assume that this is the case, but the formal proof for this property is given in Chapters 4, 5 and 6, where it will be shown that, independently of **C8**, if $\|x_k - x^*\|$ is small enough the correct active set must have been identified. Note that if $\|x_k - x^*\|$ is bounded away from zero, **C8** will be satisfied automatically by any multiplier estimate.

The following candidates for the estimate will be shown to satisfy **C8–C9**, assuming that the correct active set has been identified.

(i) The QP multipliers at stationary points found by the algorithm.

(ii) The least-squares multipliers at x_k.

(iii) The least-squares multipliers at $x_k + p_k$.

For the following results, let $\{x_k\}$ denote a convergent sequence such that $x_k \to x^*$, a stationary point for problem NLP with multiplier vector λ^*. Also, we assume that $\|H_k\|$ is bounded, and that

$$\|p_k\| = O(\|x_k - x^*\|).$$

In Chapters 4, 5 and 6 it will be shown that this last result holds for the points obtained by the algorithms considered there.

Lemma 2.4.2. *Let $\tilde{\mu}_k$ denote the QP multipliers at a stationary point p_k of the QP subproblem at x_k, having the same set of active constraints as x^*. If $\|p_k\| = O(\|x_k - x^*\|)$, then*

$$\|\tilde{\mu}_k - \lambda^*\| = O(\|x_k - x^*\|).$$

Proof. From the definition of $\tilde{\mu}_k$,

$$A_k^T \tilde{\mu}_k = H_k p_k + g_k,$$

and from the corresponding Taylor series expansion,

$$A_k^T \tilde{\mu}_k = A^{*T} \tilde{\mu}_k - \textstyle\sum_i \tilde{\mu}_{k_i} \nabla^2 c_i(x_k)(x^* - x_k) + O(\|x_k - x^*\|^2).$$

From the definition of λ^* and the previous equation,

$$A^{*T}(\tilde{\mu}_k - \lambda^*) = g_k - g^* + H_k p_k + \textstyle\sum_i \tilde{\mu}_{k_i} \nabla^2 c_i(x_k)(x^* - x_k) + O(\|x_k - x^*\|^2),$$

and again using a Taylor series expansion for g_k,

$$A^{*T}(\tilde{\mu}_k - \lambda^*) = \tilde{W}_k(x_k - x^*) + H_k p_k + O(\|x_k - x^*\|^2)$$

where $\tilde{W}_k$ denotes the Hessian of the Lagrangian function at x_k, defined using $\tilde{\mu}_k$ as the Lagrange multiplier estimate.

From assumptions **A2** and **A3** and the boundedness of H_k the desired result follows. ∎

The following lemma presents the corresponding results for the least-squares multiplier estimates, μ_k.

Lemma 2.4.3. *The least-squares multipliers at x_k satisfy*

$$\|\mu_k - \lambda^*\| = O(\|x_k - x^*\|)$$

and assuming $\|x_k + p_k - x^*\| = o(\|x_k - x^*\|)$, the least-squares multipliers at $x_k + p_k$ satisfy

$$\|\mu_k - \lambda^*\| = o(\|x_k - x^*\|).$$

Proof. From $A_k A_k^T \mu_k = A_k g_k$, $A^{*T}\lambda^* = g^*$ and $A_k = A^* + O(\|x_k - x^*\|)$ it follows that

$$A^* A^{*T}(\mu_k - \lambda^*) = A^*(g_k - g^*) + O(\|x_k - x^*\|) = O(\|x_k - x^*\|),$$

and from the non-singularity of $A^* A^{*T}$ we get

$$\mu_k - \lambda^* = O(\|x_k - x^*\|).$$

For the second case, under the same assumptions as before, if we denote by A_k', g_k' the corresponding values obtained at $x_k + p_k$, using $A_k' = A^* + O(\|x_k + p_k - x^*\|)$ we have

$$A^* A^{*T}(\mu_k' - \lambda^*) = A^*(g_k' - g^*) + O(\|x_k + p_k - x^*\|) = O(\|x_k + p_k - x^*\|),$$

and from the assumptions,

$$\mu_k' - \lambda^* = O(\|x_k + p_k - x^*\|) = o(\|x_k - x^*\|),$$

completing the proof. ∎

Chapter 3

General Results

The previous chapter has introduced a framework algorithm to be used in the definition of the three methods analyzed in the following chapters. The study of these algorithms centers on the determination of their convergence properties, that is, the proof that they are globally convergent, and the characterization of their asymptotic rates of convergence.

Given the many common features of the different algorithms, the arguments used to show these results naturally follow the same general pattern and present a considerable number of similar steps. This chapter introduces the general structure shared by the proofs developed in the following chapters, and proves those results that apply to all algorithms, because they are independent of the way H_k is defined, the specific details in the determination of the search direction, etc. In this way, the actual convergence proofs given in the next three chapters only need to establish those results that depend on the specific details characterizing each one of the algorithms, and will make use of the general results in this chapter for those aspects that they have in common.

The lemmas presented in the following sections leave many unjustified steps in the argument of the proofs, corresponding to those results that are particular to each algorithm. These steps are stated as properties, denoted by **Px**, where "x" is a digit, and they are assumed to hold for subsequent lemmas. The convergence proofs in Chapters 4, 5 and 6 prove that these properties hold for the different algorithms. For ease of reference, at the end of the chapter we include a list of all the properties introduced.

3.1. Convergence properties

This section motivates the common structure shared by the convergence proofs in the following chapters, by presenting the questions these proofs will address. It is important to remember that the results presented in this chapter do not try to answer the questions posed below; they only introduce a number of basic results, to be used in Chapters 4, 5 and 6 to answer these questions.

All of our algorithms generate an infinite sequence $\{x_k\}_{k=0}^{\infty}$ whose limit point is a solution for the problem. In order to establish global convergence (i.e., independently of the initial point selected, the algorithm finds a solution for the problem), we want to show that the limit point of the sequence has certain desired properties. Notice that under assumption **A1**, the sequence will always have convergent subsequences. Furthermore, from assumptions **A3** and **A6** it is possible to show that the limit point is in fact unique. Proving global convergence is then equivalent to proving that the limit point is a solution point. In what follows, we denote the limit point by x^*, so that we have $x_k \to x^*$. The proofs in Chapters 4, 5 and 6 will start by examining the properties of x^*.

In subsequent chapters we will also determine the rate of convergence of the sequence $\{\|x_k - x^*\|\}$. Specifically, we will provide answers to the following questions:

- What is the value of
$$\lim_{k\to\infty} \frac{\|x_{k+m} - x^*\|}{\|x_k - x^*\|^n}$$
when both $n = 1$ and $m = 1$?

- If the previous answer is zero, is there a value of n with $m = 1$ for which the answer is finite and strictly positive?

- If the answer to the first question is not zero, is there a value of m with $n = 1$ for which the answer is zero?

To characterize the different answers to the previous questions, we say that

(i) the algorithm converges *superlinearly* (or *one-step superlinearly*) if
$$\lim_{k\to\infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} = 0;$$

(ii) the algorithm converges *two-step superlinearly* if

$$\lim_{k\to\infty} \frac{\|x_{k+2} - x^*\|}{\|x_k - x^*\|} = 0;$$

(iii) finally, the algorithm converges *quadratically* if

$$0 < \lim_{k\to\infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^2} < \infty.$$

A further question of interest is how the penalty parameter ρ_k behaves as $k \to \infty$. A desirable property for ρ_k is that it remain bounded throughout the algorithm, and in this chapter we introduce some conditions that guarantee this property.

3.2. Structure of the proofs

In this section we present and motivate the steps that we will take to obtain the answers to the previous questions. These steps also attempt to justify the results proved in this chapter, so that they can more easily be put into the framework of the convergence proofs presented in Chapters 4, 5 and 6. Some of the results will be shown to hold in Chapters 4, 5 and 6, while some others are proved in this chapter; we try to indicate for each one of the statements where the corresponding proof can be found.

(i) A first observation is that the sequence $\{x_k - x^*\}$ is not easy to study, given that part of the information is available at iteration k, but another part, x^*, is not known until the end of the process. It will be seen that the sequence of search directions $\{p_k\}$ can be studied in its place, and this sequence mimics the behavior of $\{x_k - x^*\}$. This is done here by proving that

$$\|x_k - x^*\| = O(\|p_k\|),$$
$$\|p_k\| = O(\|x_k - x^*\|).$$

(ii) A first step in establishing these relationships is to show that the correct active set at the solution is identified after a finite number of iterations. To be more precise, for the different algorithms, and in the corresponding chapters, we prove that if $\|p_k\|$ is small enough, then the correct active set must have been identified.

(iii) The convergence of the sequence $\{p_k\}$ is proved using the boundedness of the merit function. In other words, the merit function decreases in each iteration, and the decrease is related to the value of $\|p_k\|^2$. As the merit function is bounded below, from assumptions **A1** and **A2** and Lemma 2.4.1, this implies that $\|p_k\| \to 0$, and from the previous remarks global convergence follows. This fundamental result is given in the corresponding chapters for each of the different algorithms.

(iv) To establish the bound on the decrease in the value of the merit function, it is necessary to start by showing that the search direction is an acceptable descent direction for the merit function. Again, and to be more precise, what we prove in Chapters 4, 5 and 6 is that for positive constants β_1 and β_2,

$$g_k^T p_k + \tfrac{1}{2} p_k^T H_k p_k \leq -\beta_1 \|p_k\|^2 + \beta_2 \|r_k\|.$$

(v) The descent available for the merit function in any iteration is dependent on the value chosen for ρ. This property is used to select a suitable value for the penalty parameter in each iteration. This is different from the strategy used in many algorithms, in which ρ is selected so that the Hessian of the augmented Lagrangian is positive definite at the solution. All of our algorithms define ρ so that the directional derivative at the beginning of the linesearch is sufficiently negative, that is, ϕ'_k satisfies a condition of the form

$$\phi'_k(0) \leq -\beta_H \|p_k\|^2,$$

but at the same time ρ is not large enough to prevent convergence. The particular form in which the penalty parameter is defined depends on the algorithm considered, and so it is left to the corresponding chapters.

(vi) The last requirement to ensure global convergence is to prove that the steplength is uniformly bounded away from zero. The reason for this condition is that the descent in the merit function is really bounded by $\|\alpha_k p_k\|^2$, and so in this chapter we establish that what goes to zero is the norm of the search direction, and not the steplength.

(vii) As a consequence of the global convergence of the algorithms and the conditions imposed on the estimates μ_k, the Lagrange multiplier estimates λ_k also converge to the correct value.

(viii) Concerning the rate of convergence, the significant remark is that in general the questions raised earlier have known answers for the sequence $\{x_k + p_k - x^*\}$. The proofs given in the following chapters have two parts; in one we show that eventually a unit steplength is always accepted, and so the previous sequence is the relevant one for this question, and in the other we establish the corresponding results for this sequence.

(ix) A final issue is the study of conditions under which the penalty parameter remains bounded throughout the algorithm. Using the previous results, we introduce at the end of the chapter some conditions that imply this property.

The next sections present results that are common to the proofs for all three methods, along the lines indicated above.

3.3. Properties of the search direction

The first group of results explores the relationship of stationary points for the QP subproblems and stationary points for problem NLP. The significance of this relationship is due to the fact that the search direction is obtained from information available at a stationary point of the QP subproblem. The results shown below are similar in spirit to those in Robinson [Rob74]. They will be used in subsequent chapters to show that the value of $\|p_k\|$ is "small" if and only if we are close to a solution point, with corresponding implications regarding the identification of the correct active set.

Lemma 3.3.1. *For any $x \in \Omega$, let p be a stationary point for the QP subproblem at x. Then*

$$\forall \epsilon > 0 \quad \exists\, \delta > 0 \quad \exists\, \hat{x} \quad \ni \quad \|p\| \le \delta \Rightarrow \|x - \hat{x}\| \le \epsilon,$$

where $\hat{x}$ is a stationary point for the nonlinear program NLP, with the same set of active constraints as p, or $\hat{x}$ is a feasible point where the Jacobian of the active constraints is singular.

Proof. Assume that the result does not hold; then there exist sequences $\{p_k\}_{k=1}^{\infty}$, and $\{x_k\}_{k=1}^{\infty}$, such that p_k is a stationary point for the QP subproblem at x_k satisfying $\|p_k\| \to 0$, and $\|x_k - \hat{x}\| > \epsilon$ for some $\epsilon > 0$ and all $\hat{x}$ with the previous properties.

A convergent subsequence can be extracted from $\{x_k\}$, using the compactness of Ω. Select now a sub-subsequence having fixed active set, a subset of the active set at the limit point $\tilde{x}$.

If we take limits in

$$A_k p_k + c_k \geq 0$$

and apply assumption **A2**, it immediately follows that $\tilde{x}$ must be feasible.

If the set of active constraints is non-singular at $\hat{x}$, from

$$H_k p_k + g_k = A_k^T \mu_k$$

there will exist a subsequence along which $\{\mu_k\}$ converges, $\mu_k \to \tilde{\mu}$. Taking limits along this subsequence,

$$\tilde{g} = \tilde{A}^T \tilde{\mu}.$$

This result implies that $\tilde{x}$ is a stationary point for the nonlinear problem, contradicting the assumption.

To show that the set of active constraints should be the same for p and $\hat{x}$, in the case when the Jacobian at $\hat{x}$ is non-singular, assume that sequences as described above exist, but that the set of active constraints at each p_k is not the same as the set of active constraints at $\hat{x}$. As $\|p_k\| \to 0$, the set of active constraints at each p_k must be a subset of the active constraints at $\hat{x}$; but if it is a proper subset, then there must exist an index i, active at $\hat{x}$, such that $\mu_{k_i} = 0$ for large enough k, and this will imply $\tilde{\mu}_i = 0$, violating the strict complementarity assumption. ∎

The assumptions on the form of the problem guarantee that large enough steps can be taken from stationary points in the QP subproblems when the points considered are not close to solutions for the problem. The algorithm makes use of this property to move away from stationary points for NLP. The next result establishes the existence of some of the necessary bounds.

Lemma 3.3.2. *There exist positive values β_{spc}, β_{spm}, β_{spn}, such that for all stationary points $\hat{x}$,*

$$\min_{i:\hat{c}_i>0} \hat{c}_i > \beta_{spc};$$

for those stationary points having some negative multiplier element,

$$\max_i \hat{\mu}_i^- > \beta_{spm};$$

and for those stationary points that have a non-negative multiplier vector, but are not second-order KKT points,

$$\max_i \hat{\lambda}_i^- > \beta_{spn},$$

where $\hat{\lambda}_i$ denotes the ith eigenvalue for the reduced Hessian at $\hat{x}$.

Proof. Assume that there exists a sequence $\{\hat{x}_k\}$ of stationary points for problem NLP in Ω such that

$$\min_{i:\hat{c}_{k_i}>0} \hat{c}_{k_i} \to 0.$$

From the compactness of Ω, a convergent subsequence can be extracted having fixed active set, and such that the minimum is always achieved for the same constraint (or set of constraints). Let $\hat{x}^*$ denote the limit point, which will also be a stationary point for the problem (or will have a singular Jacobian for the active constraints, except we exclude this case by invoking assumption **A3**). At x^* assumption **A5** will be violated, as the corresponding constraints are active but have zero multipliers.

If the sequence is such that

$$\max_i \hat{\mu}_{k_i}^- \to 0$$

using the same construction, assumption **A5** will again be violated at $\hat{x}^*$, since at least one of the multipliers corresponding to an active constraint will be zero.

Finally, if

$$\max_i \hat{\lambda}_{k_i}^- \to 0$$

for a sequence of first-order KKT points, the limit point will be a second-order KKT point but assumption **A6** will be violated, as the reduced Hessian will be singular. ∎

Using the previous lemmas, in Chapters 4, 5 and 6 we establish the following property for the different algorithms:

P1. There exists a value $\epsilon' > 0$ such that if $\|p_k\| \leq \epsilon'$, then the correct active set at a solution of problem NLP has been identified, and p_k is a minimizer for the QP subproblem.

In what follows, we assume that this property holds.

3.4. Equivalence of sequences

For a given sequence $\{x_k\}$, the next results establish the equivalence between the sequences $\{x_k - x^*\}$ and $\{p_k\}$, allowing us to continue the study of the convergence properties for the algorithms on the sequence of search directions.

Lemma 3.4.1. *If x^* denotes the solution point closest to x_k, then there exists a constant M_p, independent of k, such that*

$$\|x_k - x^*\| \le M_p \|p_k\|. \tag{3.4.1}$$

Proof. The proof is in essence the one for Lemma 4.1 in [GMSW86b], and takes the following form. Let c denote the vector of constraints active at x^*, let A be the Jacobian of the active constraints, and Z an orthogonal basis for the null space of A. Define

$$h(x) \equiv \begin{pmatrix} c(x) \\ Z(x)^T g(x) \end{pmatrix}.$$

Expanding $h_i(x)$ about x^*, and noting that $h(x^*) = 0$, we obtain

$$h_i(x) = H_i(\theta_i)(x - x^*),$$

for $H_i(\theta_i) \equiv \nabla h_i(x^* + \theta_i(x - x^*))$, where $0 < \theta_i \le 1$ (see Goodman [Go85], for a discussion of the definition of H_i). Define S_θ as the matrix whose rows are given by $H_i(\theta_i)$. Then

$$\begin{pmatrix} c(x) \\ Z(x)^T g(x) \end{pmatrix} = S_\theta (x - x^*). \tag{3.4.2}$$

Assume that $\|p_k\| \le \epsilon'$ for suitably small ϵ', so that property **P1** applies and the smallest singular value of the reduced Hessian of the Lagrangian function is bounded below. From assumption **A5**, S_θ is nonsingular, with smallest singular value uniformly bounded below (see, e.g., Robinson [Rob74]). Because of assumption **A1**, the relation (3.4.1) is immediate if $\|p_k\| \ge \epsilon'$, and we henceforth consider only iterations k such that $\|p_k\| < \epsilon'$.

Taking $x = x_k$ in (3.4.2), and using the nonsingularity of S_θ and norm inequalities, we obtain

$$\|x_k - x^*\| \le \beta(\|c_k\| + \|Z_k^T g_k\|) \tag{3.4.3}$$

for some bounded β. We now seek an upper bound on the right-hand side of this equation. Since the solution for the QP subproblem identifies the correct active set, p_k satisfies the equations

$$\hat{A}_k p_k = -c_k \quad \text{and} \quad Z_k^T H_k p_k = -Z_k^T g_k.$$

From these equations, assumption **A3** and the positive definiteness of the reduced Hessian, it follows that there must exist a constant $\tilde{\beta} > 0$ such that

$$\tilde{\beta}(\|c_k\| + \|Z_k^T g_k\|) \leq \|p_k\|. \tag{3.4.4}$$

Since β and $\tilde{\beta}$ are independent of k, combining (3.4.3) and (3.4.4) gives the desired result.
∎

The converse statement is proved in the next lemma. This result is not strictly necessary for the convergence proof, but it is included for completeness, and because it simplifies certain arguments. It also requires certain additional assumptions, whose validity will be established in the following chapters. In particular, if Z_k denotes a basis for the null space of the Jacobian at x_k corresponding to the constraints active at x^* (defined in the same way as before), then the sequence $\{Z_k^T H_k Z_k\}$ must be bounded, and any limit point, say $Z^{*T} H^* Z^*$, must be positive definite.

Lemma 3.4.2. *Let x^* denote the solution point closest to x_k. If any limit of the sequence $\{Z_k^T H_k Z_k\}$ is positive definite, then there exists a constant M_x, independent of k, such that*

$$\|p_k\| \leq M_x \|x_k - x^*\|.$$

Proof. We start by showing that whenever $\|x_k - x^*\| \to 0$, we must also have $\|p_k\| \to 0$.

Assume that that is not the case. Then there exists a sequence $\{p_k\}$ obtained from QP subproblems at points $\{x_k\}$ satisfying $x_k \to x^*$, and such that $\|p_k\| > \epsilon$ for all k and some $\epsilon > 0$.

Also, there must exist a first QP step d_k along the way to p_k, satisfying $\|d_k\| \geq \bar{\epsilon}$, where $\bar{\epsilon} > 0$ and all previous steps converge to zero. Define

$$\delta_k = \bar{\epsilon} \frac{d_k}{\|d_k\|}$$

so that δ_k is a feasible QP step. Extract a subsequence along which both $Z_k^T H_k Z_k$ and δ_k have a limit. Then, if $\bar{p}_k$ denotes the step taken in the QP subproblem immediately before obtaining d_k,

$$(H_k \bar{p}_k + g_k)^T d_k < 0,$$

and taking limits we obtain

$$g^{*T}\delta^* \leq 0 \Rightarrow \lambda^{*T}A^*\delta^* \leq 0,$$

but from strict complementarity and feasibility it must hold that $\delta^*_Y = 0$. Again, taking limits in

$$\psi_k(\bar{p}_k) - \psi_k(\bar{p}_k + d_k) > 0$$

we must have

$$d_Z^{*T}Z^{*T}H^*Z^*d_Z^* \leq 0,$$

contradicting the assumption that $Z^{*T}H^*Z^*$ is positive definite, so $p^* = 0$.

This result implies that there exists a $\bar{\delta} > 0$ such that for all $\delta \leq \bar{\delta}$,

$$\|x_k - x^*\| < \delta \Rightarrow \|p_k\| < \epsilon',$$

where ϵ' is the value in property **P1**, p_k is obtained as the solution of the QP subproblem and the correct active set has been identified.

If $\|x_k - x^*\| \geq \bar{\delta}$, the result follows trivially. Assume that $\|x_k - x^*\| < \bar{\delta}$. Then, as in the proof for Lemma 3.4.1, from (3.4.2) and the boundedness of S_θ we get

$$\|x_k - x^*\| \geq \beta'(\|c_k\| + \|Z_k^T g_k\|). \tag{3.4.5}$$

Also, from the nonsingularity of $\hat{A}^*$ and $Z_k^T H_k Z_k$ for large k, for small enough $\|x_k - x^*\|$ we have, given that p_k is obtained as a minimizer of the QP subproblem,

$$\tilde{\beta}'(\|c_k\| + \|Z_k^T g_k\|) \geq \|p_k\|. \tag{3.4.6}$$

Combining (3.4.5) and (3.4.6) gives the desired result. ▮

The previous lemmas justify replacing the study of the sequence of distances to the solution set by the sequence of search directions. A result that is closely associated to the last two lemmas, and that completes the justification for the study of the sequence $\{p_k\}$, is given by the following property that, as in the previous case, will be assumed to hold for the rest of the chapter, and is proved in the following chapters.

P2. $\|p_k\| = 0$ if and only if x_k is a solution for problem NLP.

It should be remembered from the remarks in Chapter 1 that the meaning of a solution for problem NLP depends on the algorithm used, but in any case it is either a first-order or a second-order KKT point.

It was mentioned before that under assumption **A6** the sequence generated by the algorithm has a unique limit point. The next lemma proves this result.

Lemma 3.4.3. *If $\|p_k\| \to 0$ and x_{k+1} is obtained as $x_{k+1} = x_k + \alpha_k p_k$, $0 < \alpha_k \le 1$, then the sequence $\{x_k\}$ has a limit x^*, a solution point for the problem.*

Proof. From assumption **A1** and Lemma 3.4.1, it holds that any limit point for the sequence is a solution point. If there exists a unique limit point for the sequence, the proof is complete. Assume then that there exists more than one limit point.

From

$$\|x_{k+1} - x_k\| = \alpha_k \|p_k\| \to 0$$

it follows that the limit points cannot be isolated. To prove this, assume that we do have isolated solutions, and in particular that there exists a limit point x^* and a positive value ϵ such that for any other limit point $\bar{x}$ we have $\|x^* - \bar{x}\| > \epsilon$.

Let $\{x_{k_i}\}$ denote a subsequence converging to x^*, and such that $\{x_{k_i+1}\}$ is convergent, but its limit point $\bar{x}$ is different from x^*. Select i large enough to have

$$\|x_{k_i} - x^*\| \le \frac{\epsilon}{4}, \qquad \|x_{k_i+1} - \bar{x}\| \le \frac{\epsilon}{4}, \qquad \|x_{k_i} - x_{k_i+1}\| \le \frac{\epsilon}{4}.$$

We can then write

$$\|x_{k_i} - x_{k_i+1}\| \ge \|x^* - \bar{x}\| - \|x_{k_i} - x^*\| - \|x_{k_i+1} - \bar{x}\| \Rightarrow \|x^* - \bar{x}\| \le \frac{3\epsilon}{4}$$

but this contradicts the previous assumption.

If limit points are not isolated, select one of them, x^*, and construct a sequence of limit points $\{\bar{x}_k\}$ converging to x^*. From the previous remarks, as all limit points must be solution points,

$$F(\bar{x}_k) = L(\bar{x}_k) = L(x^*) = F(x^*).$$

Notice that all solution points must have the same active set, from strict complementarity and nonsingularity of the Jacobian at all limit points, implying that the terms $\lambda^T c$ are zero in all cases.

Define

$$d_k = \frac{\bar{x}_k - x^*}{\|\bar{x}_k - x^*\|}$$

and select a convergent subsequence having limit point d^*. From the Taylor series expansion for the active constraints,

$$c(\bar{x}_k) = 0 = c(x^*) + A^* d_k \|\bar{x}_k - x^*\| + O(\|\bar{x}_k - x^*\|^2),$$

which implies that for any active constraint i,

$$0 = \bar{a}_{i_k}^T d_k + O(\|\bar{x}_k - x^*\|) \Rightarrow a_i^{*T} d^* = 0,$$

and d^* must be in the null space of the active constraints at x^*.

For the Lagrangian function we can write

$$\nabla L(\bar{x}_k) = \nabla L(x^*) + \nabla^2 L(x^*)(\bar{x}_k - x^*) + o(\|\bar{x}_k - x^*\|).$$

Using the property that all points considered are solutions for the problem, and so their Lagrangian functions have zero gradients,

$$0 = \nabla^2 L(x^*) d_k + o(1) \Rightarrow \nabla^2 L(x^*) d^* = 0,$$

but this contradicts assumption **A6**, and the sequence must have a unique limit point. ∎

Descent properties

As a consequence of Lemma 3.4.1, to prove that the algorithm is globally convergent it is enough to show that $p_k \to 0$. This result follows from the boundedness of the merit function, and the fact that the merit function decreases by an amount bounded away from zero by a multiple of $\|p_k\|^2$ in each iteration. The first step along this line of reasoning will be to establish that p_k satisfies certain descent properties. These properties can be considered to be related to the well known condition for global convergence in unconstrained optimization, that the angle between the gradient and the search direction must be bounded away from orthogonality. The explicit form of the condition to be used is given (and assumed to hold) in the next paragraph.

P3. There exist constants $\beta_1 > 0$, $\beta_2 \geq 0$ such that the incomplete solution for the QP subproblem, p_k, satisfies

$$g_k^T p_k + \tfrac{1}{2} p_k^T H_k p_k \leq -\beta_1 \|p_k\|^2 + \beta_2 \|r_k\|.$$

3.5. The penalty parameter

The penalty parameter in the algorithm is modified so that at each iteration it is possible to decrease the value of the merit function by a sufficiently large amount. Chapters 4, 5 and 6 include proofs for the following property, and specific definitions for the value of the penalty parameter ensuring that the desired decrease can be achieved.

P4. There exists a value $\hat{\rho}_k$ such that for some positive constant β_H, independent of the iteration,

$$\phi_k'(0,\rho) \leq -\beta_H \|p_k\|^2$$

for all $\rho \geq \hat{\rho}_k$.

We will also assume that the sequence $\{\hat{\rho}_k\}$ is nondecreasing.

In the case when the reduced Hessian is indefinite, a slightly different condition, also proved in Chapter 6, is used; in the modified condition $\phi_k'(0,\rho)$ is replaced by $\phi_k''(0,\rho)$. The alterations that this change introduces in the results to follow will not be discussed here; they are studied in detail in Chapter 6.

Whenever ρ is mentioned in the results that follow, what is meant is not the actual value of the penalty parameter, but rather the value of the bound $\hat{\rho}$ from condition **P4**. All the results still hold if this value is replaced by a bounded multiple, $\rho \leq K\hat{\rho}$, for some $K \geq 1$. Also, we need to impose a condition on how often the value of the penalty parameter will be updated. It will be assumed that there exists a positive constant $\bar{\beta}_H > \beta_H$ such that no update is performed whenever $\phi_k'(0,\rho) \leq -\bar{\beta}_H \|p_k\|^2$.

3.6. Boundedness of the steplength

The rest of the global convergence proof consists in showing that the steplength is bounded away from zero, and so the potential decrease implied by the bound in **P4** and (2.2.3) is actually attained.

A first result, whose proof depends on the form of $\hat{\rho}_k$ and β_H introduced in the following chapters, where it will be justified, gives a first bound for the rate at which the penalty parameter is allowed to increase in the algorithm. Tighter bounds will be introduced in subsequent lemmas.

P5. For any iteration k_l in which the value of ρ is modified,

$$\rho_{k_l} \|p_{k_l}\|^2 \leq N$$

and

$$\rho_{k_l} \|c_{k_l} - s_{k_l}\| \leq N$$

for some constant N.

The notation k_l is used in all that follows to indicate iterations at which the value of the penalty parameter needs to be modified.

We now introduce an expression for $\phi'(0)$ that will be used extensively in the proofs of results related to the behavior of the merit function. To derive it, consider first the gradient of L_A with respect to x, λ and s,

$$\nabla L_A(x,\lambda,s) \equiv \begin{pmatrix} g(x) - A(x)^T\lambda + \rho A(x)^T\big(c(x) - s\big) \\ -\big(c(x) - s\big) \\ \lambda - \rho\big(c(x) - s\big) \end{pmatrix}. \tag{3.6.1}$$

It follows that $\phi'(0)$ is given by

$$\begin{aligned} \phi'(0) &= p^T g - p^T A^T \lambda + \rho\, p^T A^T (c - s) - (c - s)^T \xi + \lambda^T q - \rho q^T (c - s) \\ &= p^T g + (2\lambda - \mu)^T (c - s) - \rho \|c - s\|^2 \end{aligned} \tag{3.6.2}$$

where g, A, and c are evaluated at x.

The following results, analogous to those in [GMSW86b], complete the proof for the boundedness of the steplength. These results start by proving the boundedness of certain quantities, related to the penalty parameter, that appear in the termination conditions for the linesearch; these results provide refined bounds for the rate at which the penalty parameter may increase with respect to the ones given in property **P5**, once this property is assumed to hold. In all these results it must be remembered that there exist two cases regarding the behavior of the penalty parameter ρ. It may remain bounded throughout the algorithm, in which case the results follow trivially, or it may need to be increased in an infinite number of iterations. This last case is the one addressed by the next lemmas.

Lemma 3.6.1. *For all iterations k_l at which the penalty parameter has to be modified,*

$$c_{k_l}^T \tilde{\mu}_{k_l} < K\|p_{k_l}\|^2 + (2\lambda_{k_l} - \mu_{k_l})^T (c_{k_l} - s_{k_l}),$$

where $\tilde{\mu}_{k_l}$ denotes the QP multipliers at p_{k_l}, and K is a positive constant.

Proof. In the proof we drop the subscript k_l. If $\|p\| \geq \epsilon'$, the result follows from the assumptions and the boundedness of the multiplier estimate. Otherwise, from **P1** the search direction must have been obtained as a solution for the QP subproblem, implying that

$$g^T p + p^T H p = -c^T \tilde{\mu}. \tag{3.6.3}$$

Also, if ρ^- denotes the value of the parameter before being modified,

$$\phi'(\rho^-) > -\bar{\beta}_H \|p\|^2, \tag{3.6.4}$$

and from the definition of ϕ',

$$c^T\tilde{\mu} < -p^THp + \bar{\beta}_H\|p\|^2 + (c-s)^T(2\lambda - \mu) - \rho^-(c-s)^T(c-s).$$

From the non-negativity of $\rho^-(c-s)^T(c-s)$ and the boundedness of H the desired result follows. ∎

Lemma 3.6.2. *There exists a constant M such that for all l,*

$$\rho_{k_l}\Big(\phi_{k_l}(\rho_{k_l}) - \phi_{k_{l+1}}(\rho_{k_l})\Big) < M. \tag{3.6.5}$$

Proof. To simplify notation in this proof, we shall use the subscripts 0 and K to denote quantities associated with iterations k_l and k_{l+1} respectively. Thus, the penalty parameter is increased at x_0 and x_K in order to satisfy condition **P4**, and remains fixed at ρ_0 for iterations $1, \ldots, K-1$.

From the definition of ϕ,

$$\rho_0\phi = \rho_0 F - \rho_0\lambda^T(c-s) + \tfrac{1}{2}\rho_0^2(c-s)^T(c-s). \tag{3.6.6}$$

Also, property **P5** implies

$$\rho_0\|c_0 - s_0\| < M \quad \text{and} \quad \rho_K\|c_K - s_K\| < M.$$

Since $\|\lambda\|$ is bounded (Lemma 2.4.1), the only term in (3.6.6) that might become unbounded is $\rho_0 F$. The desired relation (3.6.5) then follows if an upper bound exists for $\rho_0(F_0 - F_K)$.

Consider iterations for which $\|p_0\| < \epsilon'$, so that property **P1** applies (for all other iterations ρ is bounded, and the result holds from assumption **A2**). In this case, p_0 is obtained as a solution for the QP subproblem. Let $\tilde{\mu}_0$ denote the QP multipliers corresponding to p_0.

Expanding F_K about x_0, we have

$$F_K - F_0 = (x_K - x_0)^T g_0 + O(\|x_0 - x_K\|^2). \tag{3.6.7}$$

Similarly, if we expand c_K about x_0, we obtain

$$c_K = c_0 + A_0(x_K - x_0) + O(\|x_0 - x_K\|^2). \tag{3.6.8}$$

From Lemma 3.4.1,

$$\|x_0 - x^*\| \le M_p\|p_0\| \quad \text{and} \quad \|x_K - x^*\| \le M_p\|p_K\|,$$

and substituting the expression $g_0 = A_0^T\tilde{\mu}_0 - H_0p_0$ and (3.6.8) in (3.6.7), we obtain

$$F_0 - F_K = (c_0 - c_K)^T\tilde{\mu}_0 + O\Big(\max(\|p_0\|^2, \|p_K\|^2)\Big).$$

We thus seek to bound

$$\rho_0(F_0 - F_K) = \rho_0 c_0^T\tilde{\mu}_0 - \rho_0 c_K^T\tilde{\mu}_0 + \rho_0 O\Big(\max(\|p_0\|^2, \|p_K\|^2)\Big). \tag{3.6.9}$$

To derive a bound for the first term on the right-hand side of (3.6.9), Lemma 3.6.1 can be used to write

$$\rho_0 c_0^T\tilde{\mu}_0 < \rho_0 K\|p_0\|^2 + \rho_0(c_0 - s_0)^T(2\lambda_0 - \mu_0). \tag{3.6.10}$$

Because $\rho_0\|c_0 - s_0\|$, $\rho_0\|p_0\|^2$, $\|\lambda_0\|$ and $\|\mu_0\|$ are bounded, from (3.6.10) we conclude that

$$\rho_0 c_0^T\tilde{\mu}_0 < M. \tag{3.6.11}$$

Consider now the second term on the right-hand side of (3.6.9). If c_K^- denotes the negative parts for all components of c_K, from $\tilde{\mu}_0 \ge 0$ we must have

$$-\rho_0 c_K^T\tilde{\mu}_0 \le \rho_0 c_K^{-T}\tilde{\mu}_0 \tag{3.6.12}$$

and from (2.4.1) we have

$$\|c_K^-\| \le \|c_K - s_K\|.$$

Using property **P5** and the relation $\rho_0 < \rho_K$, we conclude that

$$-\rho_0 c_K^T\tilde{\mu}_0 < M. \tag{3.6.13}$$

Finally, consider the third term on the right-hand side of (3.6.9). It follows from property **P5** and the relation $\rho_0 < \rho_K$ that

$$\rho_0\|p_0\|^2 < N \quad \text{and} \quad \rho_0\|p_K\|^2 < N,$$

and hence

$$\rho_0 O\Big(\max(\|p_0\|^2, \|p_K\|^2)\Big) < M. \tag{3.6.14}$$

Combining (3.6.11), (3.6.13) and (3.6.14), we obtain the bound

$$\rho_0(F_0 - F_K) < 3M,$$

which implies the desired result. ∎

Lemma 3.6.3. *There exists a constant M such that, for all l,*

$$\rho_{k_l} \sum_{k=k_l}^{k_{l+1}-1} \|\alpha_k p_k\|^2 < M. \tag{3.6.15}$$

Proof. As in the previous lemma, we use the subscripts 0 and K to denote quantities associated with iterations k_l and k_{l+1} respectively. For $0 \le k \le K-1$, property (2.2.4a) imposed by the choice of α_k, and the fact that the penalty parameter is not increased, imply that

$$\phi_k - \phi_{k+1} \ge -\sigma\alpha_k\phi'_k. \tag{3.6.16}$$

We can use the identity

$$\phi_0 - \phi_K = \sum_{k=0}^{K-1}(\phi_k - \phi_{k+1}), \tag{3.6.17}$$

together with equations (3.6.17), (3.6.16) and property **P4** to obtain

$$\tfrac{1}{2}\sigma\beta_H \sum_{k=0}^{K-1} \alpha_k\|p_k\|^2 \le \phi_0 - \phi_K.$$

Rearranging this expression and using the property that $0 < \alpha_k \le 1$, we obtain

$$\tfrac{1}{2}\sigma\beta_H \sum_{k=0}^{K-1} \|\alpha_k p_k\|^2 \le \phi_0 - \phi_K. \tag{3.6.18}$$

The result follows by multiplying (3.6.18) by ρ_0 and using Lemma 3.6.2. ∎

Lemma 3.6.4. *There exists a constant M such that, for all k,*

$$\rho_k\|c_k - s_k\| \le M. \tag{3.6.19}$$

Proof. Using the notation of the two previous lemmas, observe that (3.6.19) is immediate from property **P5** for $k = 0$ and $k = K$.

To verify a bound for $k = 1, \dots, K-1$ (iterations at which the penalty parameter is not increased), we first consider x_1. Let unbarred and barred quantities denote evaluation at x_0 and x_1 respectively.

If $\bar{c}_i \ge \bar{\lambda}_i/\rho_0$, then

$$\rho_0|\bar{c}_i - \bar{s}_i| = |\bar{\lambda}_i|$$

and the bound follows from Lemma 2.4.1.

If $\bar{c}_i < \bar{\lambda}_i/\rho_0$, then $\bar{s}_i = 0$. If in addition $\bar{c}_i \geq 0$, then

$$\rho_0|\bar{c}_i - \bar{s}_i| = \rho_0\bar{c}_i < \bar{\lambda}_i$$

and the same result applies.

Therefore, assume that $\bar{c}_i < 0$, $\bar{c}_i < \bar{\lambda}_i/\rho_0$, and expand the ith constraint function around x_0:

$$\bar{c}_i = c_i + \alpha_0 a_i^T p + O(\|\alpha_0 p_0\|^2). \tag{3.6.20}$$

Rewriting the previous expression, we obtain:

$$\bar{c}_i = \bar{c}_i - \bar{s}_i = (1-\alpha_0)c_i + \alpha_0(a_i^T p + c_i) + O(\|\alpha_0 p_0\|^2). \tag{3.6.21}$$

Adding and subtracting $(1-\alpha_0)s_i$ on the right-hand side of (3.6.21) gives

$$\bar{c}_i - \bar{s}_i = (1-\alpha_0)(c_i - s_i) + (1-\alpha_0)s_i + \alpha_0(a_i^T p + c_i) + O(\|\alpha_0 p_0\|^2). \tag{3.6.22}$$

The properties of α_0, s_i and $a_i^T p + c_i$ imply that

$$(1-\alpha_0)s_i + \alpha_0(s_i + q_i) \geq 0,$$

and when $\bar{c}_i < \min(0, \bar{\lambda}_i/\rho_0)$, (3.6.22) gives the following inequality:

$$\rho_0|\bar{c}_i - \bar{s}_i| \leq \rho_0(1-\alpha_0)|c_i - s_i| + \rho_0 O(\|\alpha_0 p_0\|^2). \tag{3.6.23}$$

There are two cases to consider in analyzing (3.6.23). First, when $c_i \geq 0$, or $c_i \geq \lambda_i/\rho_0$, the term $\rho|c_i - s_i|$ is bounded above, using the same arguments as before. The second term on the right-hand side of (3.6.23) is bounded above, using Lemma 3.6.3. Thus, the desired bound

$$\rho_0|\bar{c}_i - \bar{s}_i| < M$$

follows if $c_i \geq \min(0, \lambda_i/\rho_0)$. Extending this reasoning to the sequence $k = 1, \ldots, K-1$, we see that the quantity $\rho_0|c_i(x_k) - s_i(x_k)|$ is bounded whenever $c_i(x_k) \geq \min(0, \lambda_{k_i}/\rho_0)$, or $c_i(x_{k-1}) \geq \min(0, \lambda_{(k-1)_i}/\rho_0)$.

Consequently, the only remaining case involves components of c that are negative and have $s_i = 0$ at two or more consecutive iterations. Let $\tilde{c}$ denote the subvector of such components of c. Using the componentwise inequality (3.6.23) and the fact that $0 < \alpha \leq 1$, we have

$$\rho_0\|\tilde{c}(x_1) - \tilde{s}(x_1)\| \leq \rho_0\|\tilde{c}(x_0) - \tilde{s}(x_0)\| + \rho_0 O(\|\alpha_0 p_0\|^2).$$

If we proceed over the relevant sequence of iterations, the following inequality must hold for $k = 1, \ldots, K-1$:

$$\rho_0\|\tilde{c}(x_k) - \tilde{s}(x_k)\| \le \rho_0\|\tilde{c}(x_0) - \tilde{s}(x_0)\| + \rho_0 O\Big(\sum_{j=0}^{k-1}\|\alpha_j p_j\|^2\Big). \tag{3.6.24}$$

The result then follows by applying property **P5** and Lemma 3.6.3 to (3.6.24). ∎

The next two lemmas establish the existence of a linesearch step bounded away from zero, independent of k and the size of ρ, for which a sufficient-decrease condition is satisfied.

Lemma 3.6.5. *For* $0 \le \theta \le \alpha_k$,

$$\phi_k''(\theta) \le -\phi_k'(0) + N\|p_k\|^2,$$

where N *is a constant independent of* k.

Proof. We again drop the subscript k. From (3.6.1),

$$\nabla^2 L_A = \begin{pmatrix} \nabla^2 F - \sum_i\big(\lambda_i + \rho(c_i - s_i)\big)\nabla^2 c_i + \rho A^T A & -A^T & -\rho A^T \\ -A & 0 & I \\ -\rho A & I & \rho I \end{pmatrix}$$

so that

$$\begin{aligned}\phi''(\theta) &= p^T W(\theta) p - \textstyle\sum_i \rho\big(c_i(\theta) - s_i(\theta)\big)p^T\nabla^2 c_i(\theta)p \\ &\quad + \rho\big(A(\theta)p - q\big)^T\big(A(\theta)p - q\big) - 2\xi^T\big(A(\theta)p - q\big),\end{aligned} \tag{3.6.25}$$

where

$$W(\theta) = \nabla^2 F(\theta) - \textstyle\sum_i(\lambda_i + \theta\xi_i)\nabla^2 c_i(\theta).$$

We now derive bounds on the first two terms on the right-hand side of (3.6.25). The first term is bounded in magnitude by a constant multiple of $\|p\|^2$ because of assumption **A2** and the boundedness of $\|\lambda\|$ (from Lemma 2.4.1). For the second term, we expand c_i in a Taylor series about x:

$$c_i(x + \theta p) = c_i(x) + \theta a_i(x)^T p + \tfrac{1}{2}\theta^2 p^T\nabla^2 c_i(x + \theta_i p)p,$$

where $0 < \theta_i < \theta$. Since $s_i(\theta) = s_i + \theta q_i$, using (2.2.2) and multiplying by ρ, we have

$$\rho\Big(c_i(x + \theta p) - (s_i + \theta q_i)\Big) = \rho(1 - \theta)\Big(c_i(x) - s_i\Big) + \rho\tfrac{1}{2}\theta^2 p^T\nabla^2 c_i(x + \theta_i p)p.$$

We know from Lemma 3.6.4 that $\rho|c_i(x) - s_i|$ is bounded, and Lemma 3.6.3 implies that $\rho\|\alpha p\|^2$ is bounded. Therefore,

$$\rho\left|\Big(c_i(\theta) - s_i(\theta)\Big)\right| \le J_i, \tag{3.6.26}$$

where J_i is a constant independent of the iteration. Using (3.6.26), we obtain the overall bound

$$\sum_i \left|\rho\Big(c_i(\theta) - s_i(\theta)\Big)p^T\nabla^2 c_i(\theta)p\right| \le J\|p\|^2, \tag{3.6.27}$$

where J is a constant independent of the iteration.

Now we examine the third term on the right-hand side of (3.6.25). Using Taylor series, we have

$$a_i(x + \theta p)^T p = a_i^T p + \theta p^T\nabla^2 c_i(\bar{\theta}_i)p, \tag{3.6.28}$$

where $0 < \bar{\theta}_i < \theta$. Using (2.2.2) and Lemmas 3.6.3 and 3.6.4, we obtain

$$\rho\Big(A(\theta)p - q\Big)^T\Big(A(\theta)p - q\Big) \le \rho(c - s)^T(c - s) + L\|p\|^2, \tag{3.6.29}$$

where L is a constant independent of the iteration.

From (3.6.28) and the boundedness of $\|\xi\|$ (Lemma 2.4.1), the final term on the right-hand side of (3.6.25) can be written as

$$-2\xi^T\Big(A(\theta)p - q\Big) \le 2\xi^T(c - s) + M\|p\|^2, \tag{3.6.30}$$

where M is a constant independent of the iteration.

We now observe that

$$\begin{aligned}\rho(c - s)^T(c - s) + 2\xi^T(c - s) &= -\phi'(0) + p^T g + \mu^T(c - s)\\ &= -\phi'(0) + p^T(g - A^T\mu) - \mu^T s,\end{aligned}$$

and using Taylor expansions we obtain

$$p^T(g - A^T\mu) = p^T(g^* - A^{*T}\mu) + O(\|p\|^2) = p^T A^{*T}(\lambda^* - \mu) + O(\|p\|^2).$$

Condition **C8** on the multipliers implies that there exists a constant $\tilde{M} > 0$ such that

$$p^T(g - A^T\mu) \le \tilde{M}\|p\|^2.$$

From $\mu_k \to \lambda^*$, strict complementarity at the solution, and the fact that the correct active set is identified for $\|p\|$ small enough (property **P1**), we eventually have $\mu \ge 0$ and $\mu^T s \ge 0$.

From (3.6.29), (3.6.30) and the last results, we have

$$\rho\left(A(\theta)p - q\right)^T\left(A(\theta)p - q\right) - 2\xi^T\left(A(\theta)p - q\right) \le -\phi'(0) + M'\|p\|^2. \tag{3.6.31}$$

Combining (3.6.27), (3.6.29) and (3.6.31) gives the required result. ∎

Lemma 3.6.6. *The linesearch of the algorithm defines a step length $\alpha \in (0,1]$ such that*

$$\phi(\alpha) - \phi(0) \le \sigma\alpha\phi'(0) \tag{3.6.32}$$

and $\alpha \ge \bar{\alpha}$, where $0 < \sigma < 1$ and $\bar{\alpha} > 0$ is bounded away from zero and independent of the iteration.

Proof. If condition (2.2.3) is satisfied at a given iteration, then $\alpha = 1$ and (3.6.32) holds with α trivially bounded away from zero.

Assume that (2.2.3) does not hold (i.e., α is computed by safeguarded cubic interpolation). The existence of a step length α that satisfies conditions (2.2.4) is guaranteed from standard analysis (see, for example, Moré and Sorensen [MS84]). We need to show that α is uniformly bounded away from zero. There are two cases to consider.

From the assumption that (2.2.3) does not hold, $\phi(1) - \phi(0) > \sigma\phi'(0)$. Since $\phi'(0) < 0$, there must exist at least one positive zero of the function

$$\psi(\alpha) = \phi(\alpha) - \phi(0) - \sigma\alpha\phi'(0).$$

Let α^* denote the smallest such zero. Since ψ vanishes at zero and α^*, and $\psi'(0) < 0$, the mean-value theorem implies the existence of a point $\hat{\alpha}$ ($0 < \hat{\alpha} < \alpha^*$) such that $\psi'(\hat{\alpha}) = 0$, i.e., for which

$$\phi'(\hat{\alpha}) = \sigma\phi'(0).$$

Because $\sigma \le \eta$, it follows that

$$\phi'(\hat{\alpha}) - \eta\phi'(0) = (\sigma - \eta)\phi'(0) \ge 0.$$

Therefore, since the function $\phi'(\alpha) - \eta\phi'(0)$ is negative at $\alpha = 0$ and non-negative at $\hat{\alpha}$, the mean-value theorem again implies the existence of a smallest value $\bar{\alpha}$ ($0 < \bar{\alpha} \le \hat{\alpha}$) such that

$$\phi'(\bar{\alpha}) = \eta\phi'(0). \tag{3.6.33}$$

The point $\bar{\alpha}$ is the required lower bound on the step length because (3.6.33) implies that (2.2.4b) will not be satisfied for any $\alpha \in [0, \bar{\alpha})$.

Expanding ϕ' in a Taylor series gives

$$\phi'(\bar{\alpha}) = \phi'(0) + \bar{\alpha}\phi''(\theta),$$

where $0 < \theta < \bar{\alpha}$. Therefore, using (3.6.33) and noting that $\eta < 1$ and $\phi'(0) < 0$, we obtain

$$\bar{\alpha} = \frac{\phi'(\bar{\alpha}) - \phi'(0)}{\phi''(\theta)} = (1 - \eta)\frac{|\phi'(0)|}{\phi''(\theta)}. \tag{3.6.34}$$

(Since $\bar{\alpha} > 0$, θ must be such that $\phi''(\theta) > 0$). We seek a lower bound on $\bar{\alpha}$, and hence an upper bound on the denominator of (3.6.34). We know from Lemma 3.6.5 that for some positive constant N

$$\phi''(\theta) \leq -\phi'(0) + N\|p\|^2 = |\phi'(0)| + N\|p\|^2$$

implying

$$\bar{\alpha} \geq \frac{(1 - \eta)|\phi'(0)|}{|\phi'(0)| + N\|p\|^2}.$$

Dividing by $|\phi'(0)|$ gives

$$\bar{\alpha} \geq \frac{(1 - \eta)}{1 + \dfrac{N\|p\|^2}{|\phi'(0)|}}. \tag{3.6.35}$$

From property **P1** it follows that

$$|\phi'(0)| \geq \tfrac{1}{2}\beta_H\|p\|^2,$$

and thus, the denominator of (3.6.35) may be bounded above as follows:

$$1 + \frac{N\|p\|^2}{|\phi'(0)|} \leq 1 + \frac{N\|p\|^2}{\frac{1}{2}\beta_H\|p\|^2} = 1 + \frac{2N}{\beta_H}.$$

A uniform lower bound on $\bar{\alpha}$ is accordingly given by

$$\bar{\alpha} \geq \frac{\beta_H(1 - \eta)}{\beta_H + 2N}, \tag{3.6.36}$$

satisfying the condition. ∎

From these results global convergence follows, as given by the following property, to be proved in the corresponding chapters,

P6. For the sequence generated by the algorithm,

$$\lim_{k \to \infty} \|x_k - x^*\| = 0,$$

where x^* is a solution point for the problem.

3.7. Convergence of Lagrange multiplier estimates

Once the global convergence of the algorithm has been established, the next step is to show that the multiplier estimate λ_k also converges to the desired value. The result presented below, given as Theorem 4.2 in [GMSW86b], implies that the convergence of the multiplier estimates is a consequence of the global convergence of the algorithm, and the facts that the multiplier estimates are bounded in norm, and the steplength is bounded away from zero.

Lemma 3.7.1. *Assume that* **P6** *holds, and let λ^* denote the multiplier vector at x^*. Assume also that there exists a positive value $\bar{\alpha}$ such that the steplength at any iteration is bounded away from zero: $\alpha_k \geq \bar{\alpha} > 0$. Then*

$$\lim_{k\to\infty} \|\lambda_k - \lambda^*\| = 0.$$

Proof. From (2.4.2),

$$\lambda_{k+1} = \sum_{j=0}^{k} \gamma_{jk}\mu_j, \tag{3.7.1}$$

where

$$\gamma_{kk} = \alpha'_k, \qquad \gamma_{jk} = \alpha'_j \prod_{r=j+1}^{k} (1-\alpha'_r), \quad j < k, \tag{3.7.2}$$

with $\alpha'_0 = 1$ and $\alpha'_j = \alpha_j$, $j \geq 1$. (This convention is used because of the special initial condition that $\lambda_0 = \mu_0$.) From the boundedness of α and (3.7.2), we observe that

$$0 < \bar{\alpha} \leq \alpha'_j \leq 1 \quad \text{for all } j, \tag{3.7.3a}$$

$$\sum_{j=0}^{k} \gamma_{jk} = 1, \tag{3.7.3b}$$

$$\gamma_{jk} \leq (1-\bar{\alpha})^{k-j}, \quad j < k. \tag{3.7.3c}$$

From condition **C8** on the multipliers we must have

$$\mu_k = \lambda^* + M_k d_k t_k \tag{3.7.4}$$

with $|M_k| \leq M$, $d_k = \|x_k - x^*\|$ and $\|t_k\| = 1$. From property **P6**, K_1 can be chosen so that, for $k \geq K_1$,

$$|M_k d_k| \leq \tfrac{1}{2}\epsilon. \tag{3.7.5}$$

We can also define an iteration index K_2 with the following property:

$$(1-\bar{\alpha})^k \le \frac{\epsilon}{2(k+1)(1+\beta_{nmu}+\|\lambda^*\|)} \tag{3.7.6}$$

for $k \ge K_2 + 1$, where β_{nmu} is an upper bound on $\|\mu_k\|$ for all k. Let $K = \max(K_1, K_2)$. Then, from (3.7.1) and (3.7.4), we have for $k \ge 2K$,

$$\lambda_{k+1} = \sum_{j=0}^{K} \gamma_{jk}\mu_j + \sum_{j=K+1}^{k} \gamma_{jk}(\lambda^* + M_j d_j t_j).$$

Hence it follows from (3.7.3b) that

$$\lambda_{k+1} - \lambda^* = \sum_{j=0}^{K} \gamma_{jk}(\mu_j - \lambda^*) + \sum_{i=K+1}^{k} \gamma_{jk} M_j d_j t_j.$$

From the bounds on $\|\mu_j\|$ and $\|t_j\|$ we then obtain

$$\|\lambda_{k+1} - \lambda^*\| \le (\beta_{nmu} + \|\lambda^*\|)\sum_{j=0}^{K} \gamma_{jk} + \sum_{j=K+1}^{k} \gamma_{jk}|M_j d_j|. \tag{3.7.7}$$

Since $k \ge 2K$, it follows from (3.7.3a) and (3.7.3c) that

$$\sum_{j=0}^{K} \gamma_{jk} \le \sum_{j=0}^{K}(1-\bar{\alpha})^{k-j} \le \sum_{j=0}^{K}(1-\bar{\alpha})^{2K-j} \le (K+1)(1-\bar{\alpha})^K.$$

Using (3.7.6), we thus obtain the following bound for the first term on the right-hand side of (3.7.7):

$$(\beta_{nmu} + \|\lambda^*\|)\sum_{j=0}^{K} \gamma_{jk} \le \tfrac{1}{2}\epsilon. \tag{3.7.8}$$

To bound the second term in (3.7.7), we use (3.7.3b) and (3.7.5):

$$\sum_{j=K+1}^{k} \gamma_{jk}|M_j d_j| \le \tfrac{1}{2}\epsilon \sum_{j=K+1}^{k} \gamma_{jk} \le \tfrac{1}{2}\epsilon. \tag{3.7.9}$$

Combining (3.7.7)–(3.7.9), we obtain the following result: given any $\epsilon > 0$, we can find K such that

$$\|\lambda_k - \lambda^*\| \le \epsilon \quad \text{for} \quad k \ge 2K+1,$$

which implies the convergence result. ∎

3.8. Unit steplength

As mentioned before, the determination of the rate of convergence for the algorithm proceeds in two steps. One is to show that a unit steplength is always accepted for all k large enough; the basic results used for this proof are introduced in this section, although the result will be proved in the corresponding chapters. The other step is to determine the convergence rate of the sequence $\{x_k + p_k - x^*\}$. This will be done in Chapters 4, 5 and 6.

The following lemmas determine the limiting behavior of certain subsequences related to the penalty parameter ρ. Again, for the case in which the penalty parameter remains bounded the results follow immediately, so their interest lies in the case when ρ is assumed to be unbounded.

The first result is an extension of property **P5**, and its meaning is again to obtain a better bound for the rate at which the penalty parameter may increase, once we know that the algorithm is globally convergent. As before, its proof is left to the corresponding chapters.

P7. For iterations k_l in which the penalty parameter is increased, assuming an infinite sequence of such iterations exists,

$$\lim_{l\to\infty} \rho_{k_l} \|p_{k_l}\|^2 = 0$$

and

$$\lim_{l\to\infty} \rho_{k_l} \|c_{k_l} - s_{k_l}\| = 0.$$

Other results, extensions of those given in the previous sections, and providing refinements on the rate of increase for ρ_k, are presented in the next lemmas.

Lemma 3.8.1. *If there exists an infinite subsequence* $\{k_l\}$, *then*

$$\lim_{l\to\infty} \rho_{k_l} \Big(\phi_{k_l}(\rho_{k_l}) - \phi_{k_{l+1}}(\rho_{k_l})\Big) = 0.$$

Proof. We use the same notation as in the proof of Lemma 3.6.2. From the boundedness of $\|\lambda\|$ (Lemma 2.4.1), and the fact that $\rho_0 < \rho_K$, we have

$$\rho_0 |\lambda_0^T (c_0 - s_0)| \le 2\|\lambda_0\|\, \rho_0 \|c_0 - s_0\| \to 0,$$
$$\rho_0 |\lambda_K^T (c_K - s_K)| \le 2\|\lambda_K\|\, \rho_K \|c_K - s_K\| \to 0,$$

and from property **P7** we have

$$\rho_0(\phi_0 - \phi_K) - \rho_0(F_0 - F_K) \to 0. \tag{3.8.1}$$

Using (3.6.10),

$$\rho_0 K\|p_0\|^2 + \rho_0(c_0 - s_0)^T(2\lambda_0 - \tilde{\mu}_0) > \rho_0 c_0^T\tilde{\mu}_0 \geq \rho_0(c_0 - s_0)^T\tilde{\mu}_0. \tag{3.8.2}$$

Using again property **P7**, from (3.8.2) and assumption **A3**, implying the boundedness of $\|\tilde{\mu}_0\|$, we get

$$\rho_0 c_0^T\tilde{\mu}_0 \to 0. \tag{3.8.3}$$

From (2.4.1) and (3.6.12) (keeping the same notation),

$$-\rho_0 c_K^T\tilde{\mu}_0 \leq \rho_0 \bar{c}_K^T\tilde{\mu}_0 \leq \rho_0\|\tilde{\mu}_0\|\|c_K - s_K\| \to 0. \tag{3.8.4}$$

For the last term in (3.6.9), we can again use property **P7** to obtain

$$\rho_0 O\Big(\max(\|p_0\|^2, \|p_K\|^2)\Big) \to 0. \tag{3.8.5}$$

From (3.8.1), (3.8.3), (3.8.4) and (3.8.5) we obtain

$$\rho_0(\phi_0 - \phi_K) \to 0,$$

giving the desired result. ∎

Lemma 3.8.2. *For general iterations k,*

$$\lim_{k\to\infty} \rho_k\|p_k\|^2 = 0.$$

Proof. If ρ is bounded, the result follows from property **P6** and Lemma 3.4.2. If ρ is increased in an infinite subsequence of iterations, then from (3.6.18) and Lemma 3.6.6,

$$\rho_0 \sum_{k=0}^{K-1} \|p_k\|^2 \leq \frac{2}{\bar{\alpha}\sigma\beta_H}\,\rho_0(\phi_0 - \phi_K)$$

and the result follows from Lemma 3.8.1. ∎

Lemma 3.8.3. *For general iterations k,*

$$\lim_{k\to\infty} \rho_k\|c_k - s_k\| = 0.$$

Proof. If ρ is bounded the result follows from $c^* \geq 0$, $\lambda^* \geq 0$, $\lambda^{*T}c^* = 0$, property **P6**, Lemma 3.7.1 and

$$c_i - s_i = \min(c_i, \frac{\lambda_i}{\rho}).$$

If ρ is increased in an infinite subsequence of iterations, consider two cases:

(i) If i is such that $c_i^* > 0$, then $\lambda_i^* = 0$ and as

$$\rho|c_i - s_i| = |\min(\rho c_i, \lambda_i)|,$$

from the convergence of the multiplier estimates, eventually $\rho|c_i - s_i| = |\lambda_i| \to 0$.

(ii) For those i such that $c_i^* = 0$, implying $\lambda_i^* > 0$, consider iteration indices large enough so that the correct active set is identified, implying $a_i^T p + c_i = 0$. Then, from the Taylor series expansion for c (3.6.20) and Lemma 3.6.6 (using the same notation as in Lemma 3.6.4),

$$\bar{c}_i = c_i + \alpha_0 a_i^T p + O(\|\alpha_0 p_0\|^2) = (1 - \alpha_0)c_i + O(\|p_0\|^2).$$

Recurring this relationship for the kth step between $k = 0$ and $k = K$ we get

$$\rho_k c_{k_i} = \rho_0 c_{k_i} = \rho_0 \prod_{j=0}^{k-1}(1 - \alpha_j)c_{0_i} + \rho_0 O\Big(\sum_{j=0}^{k-1} \|p_j\|^2\Big),$$

but as $0 < \alpha_j \leq 1$ we obtain

$$\rho_k|c_{k_i}| \leq \rho_0|c_{0_i}| + \rho_0 O\Big(\sum_{j=0}^{k-1} \|p_j\|^2\Big). \qquad (3.8.6)$$

From property **P7** we must have that $\rho_0|c_{0_i}| \to 0$, and using (3.8.6) and Lemma 3.8.2,

$$\rho_k|c_{k_i}| \to 0.$$

This completes the proof. ∎

Another relationship that will be needed in the following chapters is proved in the next lemma.

Lemma 3.8.4. *For large enough k,*

$$\mu_k^T s_k = 0.$$

Proof. Assume k large enough so that the correct active set has been identified.

(i) If i is such that $c_i^* > 0$, from condition **C9** on the multipliers, $\mu_{k_i} = 0$.

(ii) If i is such that $c_i^* = 0$, then, from strict complementarity, $\lambda_i^* > 0$. Also, from Lemma 3.8.3, $\rho_k(c_{k_i} - s_{k_i}) = \min(\rho_k c_{k_i}, \lambda_{k_i}) \to 0$, so for large enough k, Lemma 3.7.1 will imply $\rho_k c_{k_i} \le \lambda_{k_i}$, and

$$s_{k_i} = \max\Big(0, c_{k_i} - \frac{\lambda_{k_i}}{\rho_k}\Big) = 0,$$

proving the result. ∎

Using the previous lemmas, the following property will be established in Chapters 4, 5 and 6:

P8. There exists an iteration index $\bar{k}$ such that for all indices $k \ge \bar{k}$ the unit steplength is accepted: $\alpha_k = 1$.

The following chapters make use of these results to establish the rates of convergence of the corresponding algorithms.

3.9. Boundedness of the penalty parameter

The main consideration in the definition of the penalty parameter ρ is to ensure that the directional derivative (or the curvature along the linesearch) is sufficiently negative. This strategy leaves open the possibility that the value of the penalty parameter may be forced to grow without bounds to satisfy this condition as the algorithm progresses. Notice that for the convergence and rate of convergence proofs the boundedness of the penalty parameter is irrelevant; it is only from the point of view of the practical behavior of the algorithm that we may want to have ρ bounded.

This section presents conditions that suffice to guarantee that the penalty parameter remains bounded. The required conditions can be given either in terms of the properties of the multiplier estimates, or in terms of the behavior of the ratios $\|p_Y\|/\|p_Z\|$ (or both). The study of the sequence of ratios for quasi-Newton methods is not simple, and the conditions presented here are given only in terms of the properties of the multipliers.

The following lemma proves the basic result concerning the behavior of the penalty parameter. The notation $\tilde{\mu}_k$ is used for the QP multiplier at iteration k.

Lemma 3.9.1. *Consider an iteration index $\hat{k}$ such that for all iterations with $k \geq \hat{k}$ both properties* **P1** *and* **P8** *hold. If*

$$\|2\mu_{k-1} - \mu_k - \tilde{\mu}_k\| = O(\|p_k\|),$$

then there exists a finite value $\bar{\rho}$ such that

$$\phi_k'(0, \bar{\rho}) \leq -\beta_H \|p_k\|^2$$

for all $k \geq \hat{k}$.

Proof. From the definition of ϕ', (3.6.2), and the fact that p_k is obtained as a solution for the QP subproblem, we have

$$\phi'(0) = -p^T H p + (2\lambda - \mu - \tilde{\mu})^T (c - s) - \tilde{\mu}^T s - \rho\|c - s\|^2.$$

Also, from the correct identification of the active set and property **P8**,

$$c_i - s_i = \min\left(c_i, \frac{\lambda_i}{\rho}\right) = \begin{cases} c_i & \text{if } c_i^* = 0 \\ 0 & \text{otherwise.} \end{cases}$$

Using Lemma 3.8.4 we can write

$$\phi'(0) = -p^T H p + (2\lambda - \mu - \tilde{\mu})^T c - \rho\|c\|^2, \tag{3.9.1}$$

where c now denotes a vector where all the entries corresponding to the inactive constraints are zero.

From $AYp_Y = -c$ and the non-singularity of AY (assume k large enough, and use assumption **A3**), there must exist positive constants β_1 and β_2, independent of the iteration, such that

$$\|c\| \leq \beta_1 \|p_Y\| \quad \text{and} \quad \|p_Y\| \leq \beta_2 \|c\|.$$

The arithmetic mean/geometric mean inequality implies that for any y, z, $\gamma > 0$,

$$yz \leq \frac{\gamma}{2} y^2 + \frac{1}{2\gamma} z^2. \tag{3.9.2}$$

Using this result, we can write for an adequate β_3,

$$-p^T H p \leq -\tfrac{1}{2} p_Z^T Z^T H Z p_Z + \beta_3 \|p_Y\|^2.$$

Also, from property **P8** and the assumption on the form of $\|2\mu_{k-1} - \mu_k - \tilde{\mu}_k\|$,

$$(2\lambda_k - \mu_k - \tilde{\mu}_k)^T c \le \beta_4 \|p\| \|c\| \le \beta_5 \|p\| \|p_Y\| \le \tfrac{1}{4} p_Z^T Z^T H Z p_Z + \beta_6 \|p_Y\|^2.$$

Combining these results, we obtain

$$\phi'(0) \le -\tfrac{1}{4} p_Z^T Z^T H Z p_Z + \beta_7 \|p_Y\|^2 - \rho \|c\|^2 \le -\tfrac{1}{4} p_Z^T Z^T H Z p_Z - (\rho - \beta_7 \beta_2^2) \|c\|^2,$$

and if we select $\bar{\rho} \ge \beta_7 \beta_2^2$, the desired result follows. ∎

Note that if the multiplier estimate is such that

$$\|\mu_k - \lambda^*\| = O(\|x_k + p_k - x^*\|),$$

the condition in Lemma 3.9.1 is satisfied. Lemma 2.4.3 establishes this property for the least-squares multipliers at $x_k + p_k$, providing an example of a multiplier estimate whose use guarantees the boundedness of the penalty parameter.

3.10. Summary

The goal of this chapter has been to present the structure of the convergence proofs to be completed in the following chapters, and to establish those results that are common to the proofs for the different algorithms. The steps in the proofs that depend on the specific implementation of the different algorithms have been left to be shown in the corresponding chapters. These steps are collected below so that they can be more easily referenced.

The next chapters prove that the following results hold for the corresponding algorithms:

P1. There exists a value $\epsilon' > 0$ such that if $\|p_k\| \le \epsilon'$, then the correct active set at a solution of problem NLP has been identified, and p_k is a minimizer for the QP subproblem.

P2. $\|p_k\| = 0$ if and only if x_k is a solution for NLP.

P3. There exist constants $\beta_1 > 0$, $\beta_2 \ge 0$ such that the incomplete solution for the QP subproblem, p_k, satisfies

$$g_k^T p_k + \tfrac{1}{2} p_k^T H_k p_k \le -\beta_1 \|p_k\|^2 + \beta_2 \|r_k\|.$$

P4. There exists a value $\hat{\rho}_k$ such that for some positive constant β_H, independent of the iteration,

$$\phi'_k(0,\rho) \le -\beta_H \|p_k\|^2$$

for all $\rho \ge \hat{\rho}_k$.

P5. For any iteration k_l in which the value of ρ is modified,

$$\rho_{k_l} \|p_{k_l}\|^2 \le N$$

and

$$\rho_{k_l} \|c_{k_l} - s_{k_l}\| \le N$$

for some constant N.

P6. For the sequence generated by the algorithm,

$$\lim_{k \to \infty} \|x_k - x^*\| = 0,$$

where x^* is a solution point for the problem.

P7. For iterations k_l in which the penalty parameter is increased, assuming an infinite sequence of such iterations exists,

$$\lim_{l \to \infty} \rho_{k_l} \|p_{k_l}\|^2 = 0$$

and

$$\lim_{l \to \infty} \rho_{k_l} \|c_{k_l} - s_{k_l}\| = 0.$$

P8. There exists an iteration index $\bar{k}$ such that for all iteration indices $k \ge \bar{k}$ a unit steplength is accepted: $\alpha_k = 1$.

The theorems where the corresponding rates of convergence are established will also be proved in Chapters 4, 5 and 6.

Chapter 4

Positive Definite Approximations to the Hessian

4.1. Introduction

In this chapter we study the convergence properties of an SQP algorithm, defined along the lines of the framework algorithm introduced in Chapter 2, and such that H_k is constructed to be positive definite. The algorithm is very similar to the one implemented in the code NPSOL, as described in [GMSW86a], with the difference that the search direction in a given iteration is computed as an "incomplete solution" for the quadratic subproblem. An incomplete solution in this chapter will be a feasible point for the subproblem obtained according to the rules indicated in Chapter 2.

The goals for this chapter can be summarized as being

- the derivation of a global convergence proof for the algorithm, following the lines indicated in Chapter 3; and
- the identification of additional conditions that need to be imposed to attain superlinear convergence, and the proof that the algorithm achieves this rate of convergence.

The steps needed for these proofs have already been presented in Chapter 3, where those intermediate results that are independent of the definition of H_k have also been shown. To complete the proofs, this chapter need only establish those results that depend on the form of H_k, properties **P1**–**P8**.

4.2. Definition of the algorithm

The main point left to be specified in the description of the framework algorithm in Chapter 2, is the form of the approximation to the Hessian of the Lagrangian function, H_k. The condition on H_k that is assumed to hold in this chapter, and that should be added to conditions **C1–C9**, is:

C10. The matrices H_k used in the construction of the QP subproblems are positive definite and bounded, with bounded condition number.

This assumption is identical to the one made for NPSQP. In practice, such a sequence may be generated (see [GMSW86a]) by updating a quasi-Newton approximation to the Hessian of the Lagrangian function in each iteration.

From this condition, some quantities will be uniformly bounded in the algorithm. The notation introduced below is used throughout the chapter for these bounds.

β_{lvH} is an upper bound for the largest eigenvalue of H: $p^T H p \le \beta_{lvH} \|p\|^2$.

β_{svH} is a positive lower bound for the smallest eigenvalue of H: $p^T H p \ge \beta_{svH} \|p\|^2$.

4.3. Global convergence results

The results in this section establish global convergence properties for the SQP algorithm under study.

The first step in the proof is to show that, from assumptions **A1–A2**, condition **C10**, and the form of step (i) in the solution of the QP subproblem, the norm of p will be uniformly bounded for any p obtained as an intermediate step during the solution of the QP subproblem.

From the condition $\|p_0\| \le \beta_{pc}\|\bar{c}\|$ and assumptions **A1–A2**, it follows that $\|p_0\| \le K$ and

$$\psi(p_0) \le \beta_{nmg} K + \tfrac{1}{2}\beta_{lvH} K^2 = \bar{K}.$$

For any p, $\psi(p) \le \bar{K}$, implying

$$\tfrac{1}{2}(p + H^{-1}g)^T H (p + H^{-1}g) - \tfrac{1}{2} g^T H^{-1} g \le \bar{K},$$

and hence

$$\|p + H^{-1}g\|^2 \le \frac{2\bar{K}\beta_{svH} + \beta_{nmg}^2}{\beta_{svH}^2},$$

giving the bound

$$\|p\| \le \beta_{nmp} = \frac{\beta_{nmg}}{\beta_{svH}} + \sqrt{\frac{2\bar{K}\beta_{svH} + \beta_{nmg}^2}{\beta_{svH}^2}}.$$

Properties of the search direction

The next result is the one presented in the previous chapter as property **P1**, that is, if the norm of the search direction in any given iteration $\|p_k\|$ is small enough, then the correct active set must have been identified.

If the norm of the stationary point where the search direction is computed, $\|\hat{p}_k\|$, is bounded away from zero, then condition **C6** on the search direction implies that $\|p_k\|$ is also bounded away from zero, and so the proof of **P1** needs only consider iterations where $\|\hat{p}_k\|$ is small.

From Lemma 3.3.1 we know that if this norm is small, we must be close to a stationary point for problem NLP, $\hat{x}$, and in that case we can use the results from Lemma 3.3.2 to bound the size of the search direction.

Before proving our first lemma, giving a bound on the descent from the stationary point, we introduce bounds for several quantities that are related to the descent that can be achieved in the QP subproblem at $\hat{x}$ when, starting from the origin, a step of the form indicated in Section 2.3 is taken.

The step to the nearest inactive constraint is bounded by

$$-\alpha a_i^T d = c_i \ge \beta_{spc} \Rightarrow \alpha \ge \beta_c^o = \frac{\beta_{spc}}{\beta_{nmA}\beta_{und}}.$$

The step described in condition **C3** is bounded by

$$\alpha \ge \beta_g^o = \min\Big(\beta_c^o, \frac{\beta_{dsc}\beta_{spm}}{\beta_{lvH}\beta_{und}^2}, \alpha_M\Big). \tag{4.3.1}$$

Also, the following bound on the function value holds:

$$\psi(\alpha) \le \tfrac{1}{2}\alpha g^T p \le -\beta_{spd} = -\tfrac{1}{2}\beta_{dsc}\beta_{spm}\beta_g^o.$$

Since we only have approximations to the second derivatives, we cannot guarantee finding a direction of negative curvature; consequently, we can only prove convergence to a first-order KKT point. Whenever the term "solution point" is used in the following paragraphs, what is meant is a first-order KKT point for problem NLP.

The following lemma uses the previous bounds to obtain a lower bound on the descent available from $\hat{p}$ at a point that is sufficiently close to a stationary point for problem NLP. It must be remarked that only properties of the approximation to the reduced Hessian, $Z^T HZ$, are used in the proof, and so the result still holds under the relaxed assumptions introduced in the next chapter.

Lemma 4.3.1. *There exists a value $\beta_{spr} > 0$ such that for any stationary point $\hat{x}$ not a solution of problem NLP, and any point x, if $\|x - \hat{x}\| < \beta_{spr}$ and p is the search direction obtained from a stationary point for the QP subproblem at x, $\hat{p}$, having the same active constraints as $\hat{x}$, then either*

$$\psi(\hat{p}) - \psi(p) > \tfrac{1}{8}\beta_{spd},$$

or at $\hat{x}$ the Jacobian for the active constraints is singular.

Proof. We consider only the case when the Jacobian of the active constraints at $\hat{x}$ has full rank.

If the lemma does not hold, there must exist a stationary point $\hat{x}$, not a solution for problem NLP, and a sequence $\{x_k\}$ converging to $\hat{x}$, such that there exists an associated sequence $\{\hat{p}_k\}$ of stationary points for the QP subproblems at the points x_k, having the same active constraints as $\hat{x}$, and such that

$$\psi_k(\hat{p}_k) - \psi_k(p_k) \leq \tfrac{1}{8}\beta_{spd}$$

for all k.

We show first that $\|p_k\| \to 0$. Let p^* denote any limit point for the sequence of QP stationary points (note that the sequence is bounded). From the assumption that the correct active set has been identified, it must hold that $p_Y^* = 0$ (since $\hat{c} = 0$ for the active constraints).

Also, from $H_k p_k + g_k = A_k^T \tilde{\mu}_k$, selecting any convergent sequence for H_k and using the non-singularity of A_k for large k, $H^* p^* = 0$, but from the positive definiteness of $Z_k^T H_k Z_k$, it must hold that $p_Z^* = 0$.

From this result it must hold that

$$a_{k_i}^T \hat{p}_k + c_{k_i} \to \hat{c}_i$$

and for large enough k (we assume that the correct active set has been identified),

$$\min_{i:a_{k_i}^T\hat{p}_k+c_{k_i}>0} a_{k_i}^T\hat{p}_k + c_{k_i} > \frac{\beta_{spc}}{2}.$$

In addition to this, if $\tilde{\mu}_k$ denotes the QP multipliers at $\hat{p}_k$, then $\tilde{\mu}_k \to \hat{\mu}$ and for large enough k, if $\|\hat{\mu}^-\| \neq 0$,

$$\max_i \tilde{\mu}_{k_i} > \frac{\beta_{spm}}{2}.$$

A bound similar to the one in the previous paragraphs can then be obtained for k large enough, as follows. The step to the nearest inactive constraint can be bounded by $\hat{\beta}_c^o = \frac{1}{2}\beta_c^o$. Define $e_{I_k} \equiv A_k d_k$ whenever $\|\hat{\mu}^-\| \neq 0$. Then

$$g_k^T d_k + \hat{p}_k^T H_k d_k = e_{I_k}^T \tilde{\mu}_k.$$

Consequently, for large enough k,

$$\psi'(0) = (g_k + H_k\hat{p}_k)^T d_k \le -\beta_{dsc}\frac{\beta_{spm}}{4}.$$

Hence a bound for the step to the minimizer is given by $\hat{\beta}_g^o = \frac{1}{4}\beta_g^o$, implying

$$\psi(\hat{p}_k) - \psi(\hat{p}_k + \alpha_k d_k) > \tfrac{1}{8}\beta_{spd},$$

contradicting the hypothesis. ∎

In the statement of Lemmas 3.3.1 and 4.3.1 the case when the Jacobian is singular has been explicitly considered. In the next results we make use of assumption **A3** to exclude this case. (The possibility of having a rank-deficient Jacobian will not be examined.)

We shall show that properties **P1** and **P2** hold for this algorithm, but first we need to introduce some notation.

δ^o denotes the value of δ associated with $\epsilon = \beta_{spr}$ in Lemma 3.3.1. If $\|\hat{p}_k\| < \delta^o$ then the condition in Lemma 4.3.1 is satisfied.

The main result for this section is presented in the next lemma, where p_k denotes the search direction obtained as an incomplete solution for the QP subproblem.

Lemma 4.3.2. *There exists a value $\epsilon' > 0$ such that if $\|p_k\| \le \epsilon'$ then p_k is a minimizer for the QP subproblem and the correct active set at a solution has been identified.*

Also, $\|p_k\| = 0$ if and only if x_k is a first-order KKT point for problem NLP.

Proof. From Lemma 4.3.1, it holds that if $\|\hat{p}_k\| \leq \delta^o$ and $\hat{p}_k$ was not obtained as the minimizer for the QP subproblem, then

$$\psi(\hat{p}_k) - \psi(p_k) > \tfrac{1}{8}\beta_{spd}$$

and from the continuity of ψ, there exists a $\delta > 0$ such that $\|\hat{p}_k - p_k\| > \delta$.

Define

$$\beta_1^o = \min(\delta^o, \frac{\delta}{2}).$$

If $\|\hat{p}_k\| \leq \beta_1^o$, then

$$\|p_k\| \geq \|\hat{p}_k - p_k\| - \|\hat{p}_k\| \geq \frac{\delta}{2} \geq \beta_1^o.$$

If $\|\hat{p}_k\| > \beta_1^o$, then from condition **C6**,

$$\|p_k\| \geq \frac{\|\hat{p}_k\|}{\beta_{slp}} > \frac{\beta_1^o}{\beta_{slp}}$$

and thus in all cases the final point obtained has norm bounded away from zero.

If p_k is obtained from the minimizer of the QP subproblem, then Lemma 3.3.1 can be used directly. Assume that a sequence of points $\{x_k\}$ exists such that $\|p_k\| \to 0$, and all p_k are obtained as the solutions of the corresponding QP subproblems, but the active sets do not correspond to the one at a solution. By extracting a subsequence having fixed active set (there are only a finite number of possible active sets) and taking limits, a solution for the original problem with that active set is obtained (from assumption **A6**, it must hold that the multiplier vectors converge to the multipliers at the limit point), contradicting the hypothesis. Hence, a lower bound for $\|p_k\|$ must also exist in this case.

For the second part of the lemma, from the previous remarks, $p_k = 0$ if and only if p_k is a solution for the QP subproblem. Furthermore,

$$\begin{aligned} p_k \equiv 0 \text{ is a solution of QP} &\Leftrightarrow g_k = A_k^T\mu_k,\ \mu_k \geq 0,\ c_k \geq 0,\ \mu_k^T c_k = 0 \\ &\Leftrightarrow x_k \text{ is a first-order KKT point for NLP,} \end{aligned} \tag{4.3.2}$$

completing the proof. ∎

Descent properties

As explained in Chapter 3, we need to impose some condition on the direction p_k to ensure that adequate descent can be obtained in each iteration. To be more precise, the bound on the directional derivative in step (iii) of the algorithm should be satisfied. This condition was presented in the previous chapter as property **P3**.

The next lemma shows that if the starting point for the QP subproblem is selected as indicated in Chapter 2, the search direction satisfies property **P3**. Remember that r_k was the quantity introduced in Chapter 2 to provide a bound for the norm of the initial point p_{k_0}, and that its most relevant property for the proofs that follow is its relationship to $c_k - s_k$, given in (2.2.5).

Lemma 4.3.3. *There exist constants $\beta_1 > 0$, $\beta_2 \geq 0$, and initial points for the QP subproblem that give values for p_k, the search direction, satisfying*

$$p_k^T g_k + \tfrac{1}{2} p_k^T H_k p_k \leq -\beta_1 \|p_k\|^2 + \beta_2 \|r_k\|. \tag{4.3.3}$$

Proof. In the proof we drop the subscript corresponding to the iteration number. Consider the following cases:

(i) p is obtained as the solution of the QP subproblem. Then, for some $\tilde{\mu} \geq 0$,

$$p^T g + p^T H p = p^T A^T \tilde{\mu} = -c^T \tilde{\mu} \leq -\tilde{\mu}^T c^- \leq \|\tilde{\mu}\| \|c^-\|$$
$$p^T g + \tfrac{1}{2} p^T H p \leq -\tfrac{1}{2} p^T H p + \beta_{nmu} \|c^-\|,$$

where $\beta_{nmu} > 0$ is a bound on the norm of the QP multipliers. Note that from condition **C10**, $p^T H p \geq \beta_{svH} \|p\|^2$.

(ii) p is obtained by moving from a stationary point $\hat{p}$. Different cases need to be considered separately.

- Assume that $\|\hat{p}\| > \delta^o$ and $\|\hat{p} - p_0\| \leq \frac{1}{2}\delta^o$. If $\|\tilde{c}\| \leq \epsilon_1 = \delta^o/(2\beta_{pc})$, then from (2.2.6),

$$\|\hat{p}\| \leq \tfrac{1}{2}\delta^o + \|p_0\| \leq \tfrac{1}{2}\delta^o + \beta_{pc}\|\tilde{c}\| \leq \delta^o,$$

but this is a contradiction, implying that under this condition $\|\tilde{c}\| \geq \epsilon_1$, in which case

$$\|p\| \leq \beta_{nmp} \leq \frac{\beta_{nmp}}{\epsilon_1} \|\tilde{c}\| = K \|\tilde{c}\|.$$

Defining $\beta_2^o = \beta_{nmg} + \beta_{lvH}\beta_{nmp}$, we have

$$p^T g + p^T H p \leq \beta_2^o \|p\| \leq \beta_2^o K \|\tilde{c}\| \leq \beta_2^o K \beta_{nmc}.$$

Using the condition on the initial point, it must hold that $\|p_0\| > \frac{1}{2}\delta^o$, and

$$p^T g + \tfrac{1}{2} p^T H p \leq -\tfrac{1}{2} p^T H p + \frac{2\beta_2^o K \beta_{nmc} \beta_{pcs}}{\delta^o} \|r\|.$$

- Assume that $\|\hat{p}-p_0\| > \frac{1}{2}\delta^o$. If ψ_i denotes the objective function for the QP subproblem after the ith *QP iteration*, $\psi_i = g^T p_i + \frac{1}{2}p_i^T H p_i$, we can write

$$\psi_{i-1} - \psi_i = -\alpha_i(g^T d_i + p_{i-1}^T H d_i) - \tfrac{1}{2}\alpha_i^2 d_i^T H d_i = d_i^T H d_i\, \alpha_i(1 - \tfrac{1}{2}\alpha_i).$$

Summing over all the iterations to the stationary point, and letting $\hat{\psi} = g^T\hat{p} + \frac{1}{2}\hat{p}^T H \hat{p}$,

$$\psi_0 - \hat{\psi} = \textstyle\sum_i d_i^T H d_i\, \alpha_i(1 - \frac{1}{2}\alpha_i) \geq \beta_{svH} \sum_i \|d_i\|^2 \alpha_i (1 - \frac{1}{2}\alpha_i),$$

but from $\|\hat{p} - p_0\| = \|\sum_i \alpha_i d_i\| > \frac{1}{2}\delta^o$, for at least one i we must have

$$\alpha_i \|d_i\| > \frac{\delta^o}{2m},$$

where m is a bound on the number of steps; using $\alpha_i \leq 1$, it must hold that

$$\psi_0 - \hat{\psi} \geq \beta_{svH}\left(\frac{\delta^o}{2m}\right)^2 \left(\frac{1}{\alpha_i} - \frac{1}{2}\right) \geq \bar{\gamma} = \tfrac{1}{2}\beta_{svH}\left(\frac{\delta^o}{2m}\right)^2. \tag{4.3.4}$$

From

$$\psi_0 = p_0^T g_0 + \tfrac{1}{2}p_0^T H p_0 \leq \beta_2^o \|p_0\| \leq \beta_{pcs}\beta_2^o \|r\| \tag{4.3.5}$$

we can derive the following bound:

$$p^T g + \tfrac{1}{2}p^T H p \leq \hat{\psi} \leq \psi_0 - \bar{\gamma} \leq -\beta_1 \|p\|^2 + \beta_{pcs}\beta_2^o \|r\|$$

for $0 < \beta_1 \leq \bar{\gamma}/\beta_{nmp}^2$.

- If $\|\hat{p}\| \leq \delta^o$, then from Lemma 4.3.1,

$$\psi_0 - \psi > \tfrac{1}{8}\beta_{spd},$$

and using (4.3.5)

$$p^T g + \tfrac{1}{2}p^T H p \leq \tfrac{1}{8}\beta_{spd} + \beta_{pcs}\beta_2^o \|r\| \leq -\beta_1 \|p\|^2 + \beta_{pcs}\beta_2^o \|r\|,$$

where $0 < \beta_1 \leq \beta_{spd}/(8\beta_{nmp}^2)$. ∎

Bounds for the penalty parameter

We now show that the penalty parameter can be selected in such a way that the initial descent available for the linesearch is sufficiently negative. This result is the equivalent to property **P4** in Chapter 3, although in this case (since H_k is required to be positive definite from condition **C10**) it seems natural to define the constant β_H in terms of $p_k^T H_k p_k$, as in the next lemma. In the spirit of the remarks made in the previous chapter, what we define is a bound for the value of the parameter; the actual value should be chosen so that it satisfies property **P4** and is bounded by a finite multiple of the value $\hat{\rho}$ given in the following lemma.

Lemma 4.3.4. *There exists a value $\hat{\rho}_k \geq 0$ such that*

$$\phi_k'(0, \rho) \leq -\tfrac{1}{2} p_k^T H_k p_k \tag{4.3.6}$$

for all $\rho \geq \hat{\rho}_k$.

Proof. Again, we drop the subscript corresponding to the iteration number. From (3.6.2), the condition to be satisfied can be written as

$$p^T g + (2\lambda - \mu)^T (c - s) - \rho (c - s)^T (c - s) \leq -\tfrac{1}{2} p^T H p.$$

A similar but stronger condition is

$$-\bar{b}^T (c - s) + \beta_2' v^T (c - s) + (2\lambda - \mu)^T (c - s) - \rho (c - s)^T (c - s) \leq 0 \tag{4.3.7}$$

for a vector $\bar{b}$ uniformly bounded in norm, a constant $\beta_2' \geq 0$, and $v_i \equiv \mathrm{sign}(c_i - s_i)$, so that $v^T (c - s) = \|c - s\|_1$. These parameters must satisfy

$$p^T g + \tfrac{1}{2} p^T H p \leq -\bar{b}^T (c - s) + \beta_2' v^T (c - s).$$

The following paragraphs introduce specific definitions for $\bar{b}$ and β_2'.

Rearrangement of (4.3.7) shows that a sufficient condition for ρ is

$$\rho (c - s)^T (c - s) \geq (2\lambda - \mu - \bar{b} + \beta_2' v)^T (c - s). \tag{4.3.8}$$

A value $\hat{\rho}$ such that (4.3.8) holds for all $\rho \geq \hat{\rho}$ is

$$\hat{\rho} = \frac{\|2\lambda - \mu - \bar{b} + \beta_2' v\|}{\|c - s\|}. \tag{4.3.9}$$

The value $\hat{\rho}$ can be taken as (4.3.9) if $\phi'(0,\rho^-) > -\frac{1}{2}p^THp$, where ρ^- denotes the value of the penalty parameter at the previous iteration; and as any value greater than or equal to ρ^- otherwise. ∎

An immediate consequence of (4.3.6) and condition **C10** is the satisfaction of property **P4**,

$$\phi_k'(0) \le -\tfrac{1}{2}\beta_H\|p_k\|^2 \tag{4.3.10}$$

for $\beta_H \le \beta_{svH}$.

The value of $\hat{\rho}$ in the previous lemma has been given in terms of two as yet undefined quantities, $\bar{b}$ and β_2'. The value for β_2' is related to the constant introduced in property **P3**, while the value of $\bar{b}$ is related to the QP multipliers at the current point. For the purpose of satisfying property **P4**, $\bar{b}$ can be taken to be zero, but as will be seen later, it plays an important role in ensuring that the penalty parameter is chosen in a way that does not inhibit superlinear convergence. The following paragraphs offer rules for the definition of these two quantities.

The conditions that $\bar{b}$ needs to satisfy to allow the algorithm to converge superlinearly are:

$$\bar{b}_k \to \lambda^*,$$

and for small enough $\|p_k\|$,

$$p_k^Tg_k + \bar{b}_k^T(c_k - s_k) \le -\tfrac{1}{2}p_k^TH_kp_k.$$

The values for $\bar{b}$ and β_2' in (4.3.9) can be selected as follows:

- Define $\bar{\mu}_k$ as the QP multipliers if p_k was obtained from the minimizer for the QP subproblem; otherwise define $\bar{\mu}_k$ as a multiplier estimate satisfying conditions **C7–C9**.

- Define

$$\bar{b} \equiv \begin{cases} \mu & \text{if } p^Tg + \mu^T(c-s) \le -p^THp, \\ \bar{\mu} & \text{otherwise.} \end{cases}$$

- Define

$$\beta_2' \equiv \max(0, \hat{\beta}_2),$$

  where

$$\hat{\beta}_2\|c - s\|_1 = p^Tg + \tfrac{1}{2}p^THp + \bar{b}^T(c - s).$$

Note that β_2' is bounded, since from Lemma 4.3.3,

$$p^Tg + \tfrac{1}{2}p^THp + \bar{b}^T(c-s) \le p^Tg + p^THp + \bar{b}^T(c-s) \le (\beta_2 + \|\bar{b}\|)\|c-s\|.$$

The strategy for the selection of the penalty parameter ρ_k is to define its value to satisfy property **P4**, while remaining small enough to be bounded by a multiple of $\hat{\rho}$. An example of a selection rule having these properties is as follows.

Let

$$\rho_k = \begin{cases} \rho_{k-1} & \text{if } \phi'(0,\rho_{k-1}) \le -\tfrac{1}{2}p_k^TH_kp_k, \\ \max(\hat{\rho}_k, 2\rho_{k-1}) & \text{otherwise} \end{cases} \tag{4.3.11}$$

where $\hat{\rho}_k$ is defined as in Lemma 4.3.4. Then, for any iteration k_l in which the parameter needs to be increased, it holds that $\rho_{k_l} \ge 2\rho_{k_{l-1}}$, and the penalty parameter goes to infinity if and only if its value is increased in an infinite number of iterations.

Proof of global convergence

In order to prove global convergence, we need to establish that property **P5** holds. The proof of global convergence relies on Lemmas 3.6.1 to 3.6.6 to show that the descent in each iteration is bounded away from zero by a large enough value, and on the boundedness of the merit function. The next lemma shows that property **P5** holds for this algorithm.

Lemma 4.3.5. *For any iteration k_l in which the value of ρ is modified,*

$$\rho_{k_l}\|p_{k_l}\|^2 \le N$$

and

$$\rho_{k_l}\|c_{k_l} - s_{k_l}\| \le N,$$

for some constant N.

Proof. All quantities in the proof refer to iteration k_l, and so this subscript is dropped.

From the boundedness of β_2', Lemma 2.4.1, the definition of $\bar{b}$, and condition **C7** on the multipliers, there must exist a fixed constant N_1 such that

$$\|2\lambda - \mu - \bar{b} + \beta_2'v\| \le N_1,$$

and from the definition of $\hat{\rho}$ and the condition that ρ has to be selected as a finite multiple of $\hat{\rho}$,

$$\rho\|c-s\| \le N_1.$$

For the second part, using Lemma 4.3.3 (we add the term $\bar{b}^T(c-s)$ using the boundedness of $\|\bar{b}\|$), we can write after some algebraic manipulation

$$\begin{aligned}\phi'(0) &= p^Tg + (2\lambda-\mu)^T(c-s) - \rho\|c-s\|^2 \\ &\leq -\tfrac{1}{2}p^THp - \beta_1\|p\|^2 + (2\lambda-\mu-\bar{b}+\beta_2 v)^T(c-s) - \rho\|c-s\|^2,\end{aligned}$$

and if we have $\phi'(0) > -\frac{1}{2}p^THp$, then

$$\beta_1\|p\|^2 \leq (2\lambda-\mu-\bar{b}+\beta_2 v)^T(c-s) \leq \|2\lambda-\mu-\bar{b}+\beta_2 v\|\,\|c-s\|.$$

We reorder terms to obtain

$$\|c-s\| \geq \beta_1 \frac{\|p\|^2}{\|2\lambda-\mu-\bar{b}+\beta_2 v\|}. \tag{4.3.12}$$

Multiplying both sides by ρ and using the same arguments as in the first part of the lemma yields

$$\rho\|p\|^2 \leq N_2,$$

completing the proof. ∎

We can now complete the proof of global convergence.

Theorem 4.3.1. *The algorithm described in this chapter has the property that*

$$\lim_{k\to\infty} \|p_k\| = 0 \tag{4.3.13}$$

Proof. If $\|p_k\| = 0$ for any finite k, the algorithm terminates and the theorem is true. Hence we assume that $\|p_k\| \neq 0$ for any k.

When there is no upper bound on the penalty parameter, the uniform lower bound on α of Lemma 3.6.6 and (3.6.15) implies that, for any $\delta > 0$, we can find an iteration index K such that

$$\|p_k\| \leq \delta \quad \text{for} \quad k \geq K,$$

which implies that $\|p_k\| \to 0$ as required.

In the bounded case, we know that there exists a value $\tilde{\rho}$ and an iteration index $\tilde{K}$ such that $\rho = \tilde{\rho}$ for all $k \geq \tilde{K}$. We consider henceforth only such values of k.

The proof is by contradiction. We assume that there exists $\epsilon > 0$ and an infinite subsequence $\{k_i\}$ such that $\|p_{k_i}\| \geq \epsilon$ for all i. Consider only indices i such that $k_i > \tilde{K}$.

Every iteration after $\tilde{K}$ must yield a strict decrease in the merit function because, using Lemma 3.6.6, (4.3.10) and the fact that the penalty parameter is not modified,

$$\phi(\alpha) - \phi(0) \leq \sigma\alpha\phi'(0) \leq -\tfrac{1}{2}\sigma\bar{\alpha}\beta_H\|p\|^2 < 0.$$

The adjustment of the slack variables s in step (ii) of the algorithm can only lead to a further reduction in the merit function, as L is quadratic in s and the minimizer with respect to s_i is given by $c_i - \lambda_i/\rho$. For iterations from the subsequence we have

$$\phi(x_{k_{i+1}}) - \phi(x_k) < \phi(x_{k_i+1}) - \phi(x_k) \leq -\tfrac{1}{2}\sigma\bar{\alpha}\beta_H\epsilon^2.$$

Therefore, since the merit function with $\rho = \tilde{\rho}$ decreases by at least a fixed quantity at every step in the subsequence, it must be unbounded below. But this is impossible, from assumptions **A1**, **A2** and Lemma 2.4.1, so (4.3.13) must hold. ∎

Corollary 4.3.1.

$$\lim_{k\to\infty} \|x_k - x^*\| = 0.$$

Proof. The result follows immediately from Theorem 4.3.1 and Lemma 3.4.1. ∎

A second corollary establishes the convergence for the multiplier estimates.

Corollary 4.3.2.

$$\lim_{k\to\infty} \|\lambda_k - \lambda^*\| = 0.$$

Proof. The convergence of the multiplier estimate is a consequence of Lemma 3.7.1, given the results in Lemma 3.6.6 and Corollary 4.3.1. ∎

4.4. Rate of convergence

Under suitable additional assumptions it is possible to show that the algorithm converges at a superlinear rate. To prove this result, we need to assume that H_k converges to an adequate approximation of $\nabla^2_{xx}L(x^*, \lambda^*)$, the Hessian of the Lagrangian function at the solution.

In the following results the symbol W, defined as $W \equiv \nabla^2_{xx}L$, will be used to denote the Hessian of the Lagrangian function.

The conditions that we impose, in addition to **C1**–**C10**, are:

C11. Following Boggs, Tolle and Wang [BTW82], we assume

$$\|Z_k^T(H_k - W_k)p_k\| = o(\|p_k\|),$$

where Z_k, a basis for the null space of A_k, is bounded in norm and its smallest singular value is bounded away from 0.

C12. $\|\mu_k - \lambda^*\| = o(\|x_k - x^*\|)$.

This is not the only set of conditions under which it is possible to prove that the algorithm converges superlinearly. The next chapter introduces and justifies an alternative set of conditions, where **C12** is replaced by the requirement that the penalty parameter must be chosen large enough near the solution.

The proof proceeds by showing first that the sequence $\{x_k + p_k - x^*\}$ converges superlinearly, and then proving that a steplength of one is eventually attained. We begin by showing that property **P7** holds for this algorithm.

Lemma 4.4.1. *If there exists an infinite subsequence of iterations $\{k_l\}$ at which the penalty parameter is increased, then*

$$\lim_{l\to\infty} \rho_{k_l}\|p_{k_l}\|^2 = 0$$

and

$$\lim_{l\to\infty} \rho_{k_l}\|c_{k_l} - s_{k_l}\| = 0.$$

Proof. We drop the subscript k_l in what follows. From definition (4.3.9) and boundedness of the ratio $\rho/\hat{\rho}$,

$$\rho\|c - s\| \le 2\|2\lambda - \mu - \bar{b} + \beta_2' v\|,$$

and from the definition of $\bar{b}$ after Lemma 4.3.4,

$$\bar{b}_{k_l} \to \lambda^*.$$

As the QP multipliers satisfy $p^Tg + p^THp = -c^T\tilde{\mu}$, and for ρ large enough p is obtained as the solution of the QP subproblem, $\bar{b}$ eventually satisfies

$$p^Tg + \bar{b}^T(c - s) \le -p^THp,$$

implying that we can take $\beta_2' = 0$ in (4.3.9).

From Corollary 4.3.2 and the previous remarks we have

$$\lim_{l\to\infty} \|2\lambda_{k_l} - \mu_{k_l} - \bar{b}_{k_l} + \beta'_{2_{k_l}} v_{k_l}\| = 0$$

and

$$\lim_{l\to\infty} \rho_{k_l} \|c_{k_l} - s_{k_l}\| = 0.$$

We can now use (4.3.12) to get

$$\lim_{l\to\infty} \rho_{k_l} \|p_{k_l}\|^2 = 0,$$

completing the proof. ∎

We want to show that condition (2.2.3) is satisfied for all k large enough. To do this, we need to be able to express $\phi'(0)$ in a way that is related to properties of the algorithm already established.

We start by defining $T_k = p_k^T(g_k - A_k^T\mu_k) + p_k^T W_k p_k$, where W is the Hessian of the Lagrangian function using λ_k as the Lagrange multiplier estimate. We show next that the satisfaction of (2.2.3) is directly related to the asymptotic properties of T_k. In what follows, the absence of an argument indicates values at x_k, and an argument of θ will indicate values at $x_k + \theta p_k$, for any fixed $\theta \in [0, 1]$.

Lemma 4.4.2. *The following relationships hold:*

$$\phi_k(\theta) - \phi_k(0) = \theta(1 - \tfrac{1}{2}\theta)\,\phi'_k(0) + \tfrac{1}{2}\theta^2 T_k + o(\|p_k\|^2)$$

and

$$\phi'_k(\theta) = (1 - \theta)\phi'_k(0) + \theta\, T_k + o(\|p_k\|^2).$$

Proof. From (2.2.1) we have

$$\phi(\theta) - \phi = F(\theta) - F - \Big(\lambda + \theta(\mu - \lambda)\Big)^T\Big(c(\theta) - s - \theta q\Big) + \lambda^T(c - s)$$
$$+ \tfrac{1}{2}\rho\Big(c(\theta) - s - \theta q\Big)^T\Big(c(\theta) - s - \theta q\Big) - \tfrac{1}{2}\rho(c - s)^T(c - s),$$

and using the corresponding Taylor expansions around x_k,

$$c_i(\theta) - s_i - \theta q_i = (1 - \theta)(c_i - s_i) + \tfrac{1}{2}\theta^2 p^T \nabla^2 c_i p + o(\|p\|^2),$$

we obtain

$$\begin{aligned}\phi(\theta)-\phi &= \theta g^Tp+\tfrac{1}{2}\theta^2p^T\nabla^2Fp-(1-\theta)\lambda^T(c-s)-\theta(1-\theta)\xi^T(c-s)\\ &- \tfrac{1}{2}\theta^2\textstyle\sum_i\lambda_i\,p^T\nabla^2c_ip-\tfrac{1}{2}\theta^3\sum_i\xi_i\,p^T\nabla^2c_ip+\lambda^T(c-s)\\ &+ \tfrac{1}{2}\rho(1-\theta)^2(c-s)^T(c-s)+\tfrac{1}{2}\rho(1-\theta)\theta^2\textstyle\sum_i(c_i-s_i)\,p^T\nabla^2c_ip\\ &+ \tfrac{1}{8}\rho\theta^4\textstyle\sum_i(p^T\nabla^2c_ip)^2-\tfrac{1}{2}\rho(c-s)^T(c-s)+o(\|p\|^2).\end{aligned}$$

From Lemmas 4.4.1, 3.8.2, 3.8.3 and 3.8.4,

$$\begin{aligned}\phi(\theta)-\phi &= \theta\phi'+\tfrac{1}{2}\theta^2\Big(p^TWp+2\xi^T(c-s)+\rho(c-s)^T(c-s)\Big)+o(\|p\|^2)\\ &= \theta(1-\tfrac{1}{2}\theta)\phi'+\tfrac{1}{2}\theta^2\Big(p^TWp+p^Tg+\mu^T(c-s)\Big)+o(\|p\|^2)\\ &= \theta(1-\tfrac{1}{2}\theta)\phi'+\tfrac{1}{2}\theta^2\Big(p^TWp+p^T(g-A^T\mu)\Big)+o(\|p\|^2).\end{aligned}$$

For the second result, from (3.6.1),

$$\begin{aligned}\phi'(\theta) = p^Tg(\theta) &- p^TA(\theta)^T\Big(\lambda+\theta(\mu-\lambda)\Big)+\rho p^TA(\theta)^T\Big(c(\theta)-s-\theta q\Big)\\ &- \xi^T\Big(c(\theta)-s-\theta q\Big)+q^T\Big(\lambda+\theta(\mu-\lambda)\Big)-\rho q^T\Big(c(\theta)-s-\theta q\Big),\end{aligned}$$

and again using the corresponding Taylor series expansions we obtain

$$\begin{aligned}\phi'(\theta) &= p^Tg+\theta p^T\nabla^2Fp-p^TA^T\lambda-\theta p^TA^T\xi-\theta\textstyle\sum_i\lambda_i\,p^T\nabla^2c_ip\\ &- \theta^2\textstyle\sum_i\xi_i\,p^T\nabla^2c_ip+\rho(1-\theta)p^TA^T(c-s)+\tfrac{1}{2}\rho\theta^2\sum_i(a_i^Tp)\,p^T\nabla^2c_ip\\ &+ \rho\theta(1-\theta)\textstyle\sum_i(c_i-s_i)\,p^T\nabla^2c_ip+\tfrac{1}{2}\rho\theta^3\sum_i(p^T\nabla^2c_ip)^2\\ &- (1-\theta)\xi^T(c-s)-\tfrac{1}{2}\theta^2\textstyle\sum_i\xi_i\,p^T\nabla^2c_ip+q^T\lambda+\theta q^T\xi\\ &- \rho(1-\theta)q^T(c-s)-\tfrac{1}{2}\rho\theta^2\textstyle\sum_iq_i\,p^T\nabla^2c_ip+o(\|p\|^2).\end{aligned}$$

From Lemmas 4.4.1, 3.8.2, 3.8.3 and 3.8.4 we finally get

$$\begin{aligned}\phi'(\theta) &= \phi'+\theta\Big(p^TWp+2\xi^T(c-s)+\rho(c-s)^T(c-s)\Big)+o(\|p\|^2)\\ &= (1-\theta)\phi'+\theta\Big(p^TWp+p^T(g-A^T\mu)\Big)+o(\|p\|^2),\end{aligned}$$

completing the results. ∎

The following results make use of the relationships introduced in this lemma only for the particular case $\theta=1$.

Condition **C11** implies the superlinear convergence of the sequence $\{x_k+p_k-x^*\}$, as the next lemma shows.

Lemma 4.4.3. *If condition* **C11** *holds, then*

$$\|x_k + p_k - x^*\| = o(\|x_k - x^*\|). \tag{4.4.1}$$

Proof. Assume k to be large enough that p_k is obtained as the solution of the QP subproblem, and the correct active set has been identified.

In what follows, all values refer to iteration k, except those corresponding to the solution. Consider first the decomposition of $x + p - x^*$ into null-space and range-space components:

$$x - x^* = Zu + Yv.$$

For the range-space component we make use of the series expansion, restricted to the active constraints at x:

$$0 = c^* = c + A(x^* - x) + o(\|x - x^*\|).$$

From $Ap = -c$ and the previous decomposition,

$$AYv = o(\|x - x^*\|),$$

and from assumption **A3**,

$$v = o(\|x - x^*\|).$$

For the null-space component, consider the corresponding Taylor series expansions around x:

$$\begin{aligned} A^{*T}\lambda^* &= g^* = g + \nabla^2 F(x^* - x) + o(\|x - x^*\|), \\ A^{*T}\lambda^* &= A^T\lambda^* + \textstyle\sum_i \lambda_i^* \nabla^2 c_i(x^* - x) + o(\|x - x^*\|). \end{aligned}$$

Combining these two results and denoting the Hessian of the Lagrangian function by W,

$$W(x - x^*) + A^T\lambda^* = g + \textstyle\sum_i (\lambda_i - \lambda_i^*)\nabla^2 c_i(x - x^*) + o(\|x - x^*\|).$$

From Corollary 4.3.2 and $Hp + g = A^T\tilde{\mu}$,

$$W(x + p - x^*) + A^T(\lambda^* - \tilde{\mu}) = (H - W)p + o(\|x - x^*\|).$$

Using the decomposition of $x + p - x^*$ into null-space and range-space components, the previous result gives

$$Z^T W Z u = Z^T(H - W)p - Z^T W Y v + o(\|x - x^*\|),$$

and from the properties of v, condition **C11** and the nonsingularity of Z^TWZ near the solution,

$$u = o(\|x - x^*\|),$$

completing the proof. ∎

The main result of this section is given in the next theorem, where it is shown that after a finite number of iterations a steplength of one is taken for all iterations thereafter, implying that the algorithm achieves superlinear convergence.

Theorem 4.4.1. *Under the previous conditions, the algorithm converges superlinearly.*

Proof. As in Powell and Yuan [PY86], observe that the continuity of second derivatives gives the following relationships:

$$\begin{aligned} F(x+p) &= F(x) + \tfrac{1}{2}\Big(g(x) + g(x+p)\Big)^T p + o(\|p\|^2) \\ c(x+p) &= c(x) + \tfrac{1}{2}\Big(A(x) + A(x+p)\Big)p + o(\|p\|^2). \end{aligned}$$

From the Taylor series expansions we have

$$\begin{aligned} F(x+p) &= F(x) + g(x)^T p + \tfrac{1}{2} p^T \nabla^2 F(x) p + o(\|p\|^2) \\ c_i(x+p) &= c_i(x) + a_i(x)^T p + \tfrac{1}{2} p^T \nabla^2 c_i(x) p + o(\|p\|^2), \end{aligned}$$

and since (4.4.1) implies $g(x+p) = g^* + o(\|p\|)$, $a_i(x+p) = a_i^* + o(\|p\|)$, we get

$$\begin{aligned} p^T \nabla^2 F p &= (g^* - g)^T p + o(\|p\|^2) \\ p^T \nabla^2 c_i p &= (a_i^* - a_i)^T p + o(\|p\|^2). \end{aligned}$$

Given that $\sum_i \lambda_i p^T \nabla^2 c_i p = \sum_i \mu_i p^T \nabla^2 c_i p + o(\|p\|^2)$, we must have

$$p^T W p = p^T (g^* - A^{*T}\mu) - p^T (g - A^T \mu) + o(\|p\|^2). \tag{4.4.2}$$

Condition **C12** implies $p^T(g^* - A^{*T}\mu) = o(\|p\|^2)$, and from (4.4.2),

$$p^T W p + p^T (g - A^T \mu) = o(\|p\|^2). \tag{4.4.3}$$

From Lemma 4.4.2 and (4.4.3),

$$\begin{aligned} \phi(1) - \phi(0) &= \tfrac{1}{2}\phi'(0) + o(\|p\|^2) \\ \phi'(1) &= o(\|p\|^2), \end{aligned}$$

but from (4.3.10) condition (2.2.3) is eventually satisfied, and we have $x_{k+1} = x_k + p_k$ for all k large enough. In this case, from (4.4.1),

$$\lim_{k\to\infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} = 0,$$

i.e. superlinear convergence, completing the proof. ∎

4.5. Summary

In this chapter we have introduced and analyzed an algorithm that is based on the framework algorithm of Chapter 2. It uses a positive definite approximation to the full Hessian of the Lagrangian function, and an incomplete solution for the QP subproblems. The study of the convergence properties of this algorithm has produced the following results:

- When the search direction and the multiplier estimate are defined satisfying conditions **C1–C9**, and the Hessian approximation H_k satisfies condition **C10**, the algorithm is *globally convergent.*

- The algorithm converges *superlinearly* if the following conditions are satisfied:

  C11. $\|Z_k^T(H_k - W_k)p_k\| = o(\|p_k\|)$, where Z_k, a basis for the null space of A_k, is bounded in norm and its smallest singular value is bounded away from 0, and

  C12. $\|\mu_k - \lambda^*\| = o(\|x_k - x^*\|)$.

In the chapter that follows, we will show superlinear convergence for this algorithm under condition **C11** and an alternative to **C12**:

C12'. When the iterates are close to the solution, the penalty parameter is chosen to be large enough.

Chapter 5

Approximations to the Reduced Hessian

5.1. Introduction

This chapter considers an algorithm similar to the one presented in Chapter 4, with the difference that conditions **C10** and **C11** are relaxed. We shall now only impose conditions on the approximation to the reduced Hessian (but not on the full Hessian approximation).

There are three main reasons to consider relaxing our requirements. From the second-order optimality conditions, only the reduced Hessian can be expected to be positive semidefinite at a solution of the problem, and so it seems unreasonable to attempt to approximate the full Hessian by a matrix that is required to be positive definite. We may wish instead to impose positive definiteness only on the approximation to the reduced Hessian. Secondly, the size of the reduced Hessian is usually smaller than that of the full Hessian, and in many cases the difference in size is significant. For large-scale problems, approximating the full Hessian is problematic, whereas approximating the reduced Hessian can be straightforward. Finally, it is not known in general how to construct matrices H_k that satisfy conditions **C10** and **C11**, but on the other hand, it is not too difficult to enforce satisfactory conditions on the asymptotic properties of the reduced Hessian approximation.

The conditions that replace **C10**–**C11** take the form:

C10'. H_k is uniformly bounded, and $\tilde{Z}_k^T H_k \tilde{Z}_k$ is positive definite with smallest singular value bounded away from zero, where $\tilde{Z}_k$ is a basis for the null space of the active constraints at the *initial* point for the QP subproblem at x_k.

C11'. $\|Z_k^T(H_k - W_k)Z_k p_{Z_k}\| = o(\|p_k\|)$, where W_k denotes the Hessian of the Lagrangian function at x_k.

The definition of the reduced Hessian requires the specification of a set of active constraints. Crucial to the issues presented in this chapter is the notion that at each iteration an initial "active set" of constraints, whose characteristics will be specified later, is selected prior to attempting to solve the QP subproblem. Condition **C10'** makes use of this assumption when imposing conditions on the reduced Hessian approximation. From iteration to iteration this active set may change, and this requires the definition of a strategy to cope with the changing size of the reduced Hessian approximation. Fortunately, this is not an issue in the limit, provided we can show convergence, since any reasonable definition of the initial active set for the QP subproblem will eventually remain unaltered for successive nonlinear iterations.

Conditions **C10'** and **C11'** apply only to the reduced Hessian approximation, and the convergence proofs presented in this chapter impose no requirements on the matrices $H_k\tilde{Y}_k$. It seems reasonable then to ask what is the role of these matrices, if any, in the algorithm considered. The answer is that $\tilde{Z}_k^T H_k \tilde{Y}_k$ is needed for the computation of the null-space component of the search direction p_{Z_k}, and $\tilde{Y}_k^T H_k \tilde{Y}_k$ is used to obtain the QP multipliers. If our main concern is to define an algorithm able to deal with large-scale problems, we may take advantage of the freedom we have in the definition of these matrices, and select them so that the computations in which they appear become as simple as possible. A common choice has been to take $\tilde{Z}_k^T H_k \tilde{Y}_k$ equal to zero and $\tilde{Y}_k^T H_k \tilde{Y}_k$ to be a well-behaved positive definite matrix, for example the identity. With these choices and condition **C10'**, it is clear that **C10** is automatically satisfied, and the proofs in Chapter 4 only need to be modified wherever they make use of **C11**, that is, for the purpose of establishing the rate of convergence of the algorithm. (In this setting **C11** can no longer be expected to be satisfied.) The modified proof using **C11'** is given at the end of the chapter.

The preceding paragraph considers only a particular set of options for the definition of H_k. A more general approach to the problem would be to define an algorithm with similar convergence properties, but requiring only condition **C10'**, instead of **C10**. This situation arises if for a program of moderate size we are approximating the whole matrix H_k, but we only require $\tilde{Z}_k^T H_k \tilde{Z}_k$ to be positive definite. Constructing H_k in this way would allow us to achieve better rates of convergence than the ones attainable when we only approximate the reduced Hessian.

One case that this approach would cover is the use of one of the recently proposed quasi-Newton updates that preserve only the positive definiteness of the reduced Hessian approximation (see for example [Fen87]).

The chapter proves global convergence for an algorithm that assumes only that **C10'** holds. Again, note that for particular definitions of H_k that satisfy condition **C10**, like the one indicated above, the global convergence proof in Chapter 4 is immediately applicable. The chapter ends with a proof for the rate of convergence of the algorithm when the approximation to the Hessian is required to satisfy the relaxed convergence condition **C11'**.

5.2. Global convergence results

We begin by introducing some notation for this chapter. Let $\tilde{Z}_k$, as above, be a basis for the null space of $\tilde{A}_k$, the Jacobian corresponding to the constraints active at the *initial* point p_{k_0}, for the QP subproblem at x_k. Let $\tilde{c}_k$ denote the value of the constraints in this set at the current point, and $\tilde{Y}_k$ a basis for the range space of $\tilde{A}_k^T$. The vectors p_Z and p_Y are used to denote the components for p in some null-space and range-space decomposition, respectively; the specific decomposition will in general be clear from the basis matrices used in the corresponding expressions. Finally, $w_c \leq 0$ is a vector such that $\tilde{A}p = -(\tilde{c} + w_c)$, and we extend it to a full m-dimensional vector by adding zero entries corresponding to the inactive constraints at the initial point.

Under condition **C10'**, $p_k^T H_k p_k$ may take negative values, in which case $\beta_{svH} < 0$. On the other hand, this cannot happen for vectors in the null space of $\tilde{A}_k$. We therefore use the following constant:

β_{szH} is a positive lower bound for the smallest eigenvalue of H_k on the subspace spanned by $\tilde{Z}_k$: $p_Z^T \tilde{Z}_k^T H_k \tilde{Z}_k p_Z \geq \beta_{szH} \|\tilde{Z}_k p_Z\|^2$.

Properties **P1** and **P2** still hold under the new conditions. They may be proved using arguments similar to the ones presented in Chapter 4, with only a minor modification introduced in Lemma 5.2.1. The main change to be made to the algorithm given in Chapter 4 is the introduction of a new bound for the directional derivative of the merit function. In Chapter 4 the bound was given as $-\frac{1}{2}p_k^T H_k p_k$, but under the relaxed assumptions on H_k this quantity may not be positive in all iterations. The new bound should preserve the property that the directional derivative is bounded away from zero by a quantity related to $\|p\|^2$. A reasonable choice is to use a linear combination of $p_Z^T \tilde{Z}^T H \tilde{Z} p_Z$ and $\|\tilde{c}\|^2$ to form the bound.

A second change is the definition of p_k, to take into account our lack of knowledge about the properties of H_k outside the null space of the "active" constraints. In Chapter 4 the search direction was obtained from the QP stationary point by taking a descent step with respect to the QP objective function. In this section the step from the stationary point is computed in terms of the value of the descent available for the linesearch, as this function in general has better properties (convexity) than the QP objective function. A more general approach is presented in a slightly different setting in Chapter 6.

Definition of the search direction

As mentioned above, we modify slightly the way the incomplete solution p_k is obtained from the QP subproblem, with respect to the conditions given in Chapter 2.

The value of p_k is now obtained by moving to the *first* stationary point for the QP subproblem found by the algorithm, $\hat{p}_k$, and from there, if the stationary point is not a minimizer for the QP subproblem, by taking a step along a descent direction. To proceed further does not seem worthwhile. Since only an approximation to a particular reduced Hessian is known, it becomes necessary to define artificially the curvature in an enlarged space, when any constraints are removed from the active set. If we have an approximation to the full Hessian, and the properties of the approximation outside the current subspace are not controlled, the search directions computed may be unacceptable unless special precautions are taken. In Chapter 6 we introduce conditions that would allow us to prevent these difficulties.

The requirement to stop at the first stationary point allows us to work with the reduced Hessian approximation for the initial active set exclusively, and so the possible lack of positive definiteness outside the corresponding subspace does not affect any of the steps taken during the solution process for the QP subproblem. In particular, conditions **C4** and **C5** will not be used in what follows.

Define v_c to be such that if $p = \hat{p} + \alpha d$, then $w_c = \alpha v_c$, where clearly $v_c \leq 0$. Assume that d is computed so that conditions **C1**, **C2** and **C6** are satisfied, and in particular the following condition holds,

$$g^T d + \hat{p}^T H d \leq \beta_{dsc} v_c^T \mu$$

for some $\beta_{dsc} > 0$. Note that condition **C1** implies that v_c must be bounded, $\|v_c\| \leq \beta_{nmv}$.

Condition **C3** is replaced by the following condition:

C3'. The step α is taken as the step to the minimizer of $\varphi(\zeta)$, where

$$\varphi(\zeta) = g^T(p+\zeta d) + \tfrac{1}{2}\Big((\hat{p}_z+\zeta d_z)^T \tilde{Z}^T H \tilde{Z}(\hat{p}_z+\zeta d_z) + \|\tilde{c}+\zeta v_c\|^2\Big).$$

To be more precise, if $\varphi'(0) \geq 0$ then let $\alpha = 0$. Otherwise, let α_c be the step to the nearest inactive constraint and define

$$\begin{aligned} \alpha_m &= -\frac{\varphi'(0)}{\varphi''} \\ \alpha &= \min(\alpha_c, \alpha_m, \alpha_M), \end{aligned}$$

where α_M is a specified bound on the largest acceptable step.

Also, from the conditions on p_0 in step (i) of the rules to compute the incomplete search direction, and from the way α and d are obtained, we can show again that $\|p\|$ is uniformly bounded for any p obtained during the solution of the QP subproblem.

If K denotes a uniform bound on the norm of the initial point obtained from (2.2.6) and assumption **A2**, $\|p_0\| \leq K$, we have

$$\varphi(p_0) \leq \beta_{nmg}K + \tfrac{1}{2}(\beta_{lzH} + \beta_{nmA}^2)K^2 = \bar{K},$$

and for any p up to $\hat{p}$, as $p_Y = p_{Y_0}$, it holds that $\varphi(p) \leq \bar{K}$, and hence

$$\tfrac{1}{2}\Big(p_Z + (\tilde{Z}^T H \tilde{Z})^{-1}\tilde{Z}^T g\Big)^T \tilde{Z}^T H \tilde{Z}\Big(p_Z + (\tilde{Z}^T H \tilde{Z})^{-1}\tilde{Z}^T g\Big) - \tfrac{1}{2} g^T \tilde{Z}(\tilde{Z}^T H \tilde{Z})^{-1}\tilde{Z}^T g \leq \bar{K}.$$

From this result, we get the bound

$$\|p_Z + (\tilde{Z}^T H \tilde{Z})^{-1}\tilde{Z}^T g\|^2 \leq \frac{2\bar{K}\beta_{szH} + \beta_{nmg}^2}{\beta_{szH}^2},$$

implying

$$\|p_Z\| \leq \tilde{K} = \frac{\beta_{nmg}}{\beta_{szH}} + \sqrt{\frac{2\bar{K}\beta_{szH} + \beta_{nmg}^2}{\beta_{szH}^2}}.$$

For the step along d, note that

$$\alpha \leq \frac{\beta_{nmg} + \beta_{szH}\tilde{K} + \beta_{nmA}K}{\beta_{szH}\beta_{lnd}^2},$$

and from $\|d\| \leq \beta_{und}$ we must have that for some β_{nmp},

$$\|p\| \leq \beta_{nmp}.$$

The argument in the proof of Lemma 4.3.2 still applies to this algorithm, except for one minor change induced by the introduction of condition **C3'**. It now becomes necessary to prove that a bound similar to the one in (4.3.1) still applies to this algorithm, at least for the case when $\|\hat{p}\|$ is small enough (otherwise, condition **C6** is sufficient to imply the result). The following lemma establishes this result, and so it indirectly proves the validity of properties **P1** and **P2** for the algorithm.

Lemma 5.2.1. *If* $\|\hat{p}\| \leq \delta^1$, *where*

$$\delta^1 = \min\Big(\delta^o, \frac{\beta_{dsc}\beta_{spm}}{8\beta_{lvH}\beta_{und} + 4\beta_{nmv}\beta_{nmA}}\Big),$$

then α *is bounded away from zero in condition* **C3'**.

Proof. From the definition of $\varphi'(0)$,

$$\begin{aligned}\varphi'(0) &= g^T d + \hat{p}_Z^T \tilde{Z}^T H \tilde{Z} d_Z + \tilde{c}^T v_c \\ &= g^T d + \hat{p}^T H d - \hat{p}^T H \tilde{Y} d_Y - \hat{p}_Y^T \tilde{Y}^T H \tilde{Z} d_Z - v_c^T \tilde{A}\hat{p} \\ &\leq v_c^T \mu + (2\beta_{lvH}\beta_{und} + \beta_{nmv}\beta_{nmA})\|\hat{p}\|.\end{aligned}$$

For $\|\hat{p}\| \leq \delta^1$,

$$\varphi'(0) \leq v_c^T \mu + \tfrac{1}{4}\beta_{dsc}\beta_{spm} \leq \tfrac{1}{2} v_c^T \mu,$$

and from condition **C2**,

$$\varphi'(0) \leq -\tfrac{1}{4}\beta_{dsc}\beta_{spm}.$$

The step to the minimizer of $\varphi(\zeta)$ is given by $\alpha = -\varphi'(0)/\varphi''$, and as

$$\varphi'' = d_Z^T \tilde{Z}^T H \tilde{Z} d_Z + \|v_c\|^2 \leq \max(\beta_{lvH}, \beta_{nmA}^2)\beta_{und}^2 = \beta''$$

we can write a bound for this step as

$$\alpha \geq \beta_m^1 = \frac{\beta_{dsc}\beta_{spm}}{4\beta''}.$$

Again, selecting $\beta_g^1 = \min(\beta_c^o, \beta_m^1)$ and using the same reasoning as in the discussion before Lemma 4.3.2, we get that the step satisfies $\alpha \geq \frac{1}{2}\beta_g^1$. ∎

From this result, properties **P1** and **P2** follow along the lines presented in Lemma 4.3.2.

Descent properties

The next result that we need to establish is that the descent condition given in property **P3** holds for this algorithm.

Lemma 5.2.2. *There exist constants $0 < \beta_1 \le \frac{1}{2}$, $\beta_2 \ge 0$, and initial points for the QP subproblem that give values for the search direction p_k satisfying*

$$p_k^T g_k + \tfrac{1}{2}(p_{Z_k}^T \tilde{Z}_k^T H_k \tilde{Z}_k p_{Z_k} + \|\tilde{c}_k + w_{c_k}\|^2) \le -\beta_1(p_{Z_k}^T \tilde{Z}_k^T H_k \tilde{Z}_k p_{Z_k} + \|\tilde{c}_k + w_{c_k}\|^2) + \beta_2\|r_k\|.$$

Proof. Since no constraints are deleted from the active set until a stationary point is reached, we must have $\hat{p}_Y = p_{Y_0}$. Consider the following cases:

(i) p is obtained as the solution of the QP subproblem. Then for some $\tilde{\mu} \ge 0$,

$$p^T g + p^T H p = p^T A^T \tilde{\mu} = -c^T \tilde{\mu} \le \|\tilde{\mu}\|\|c^-\| \le \|\tilde{\mu}\|\|r\|$$

and as $w_c = 0$ at the solution, $\|\tilde{c}\| \le \beta_{nmA}\|p_0\|$ and $p_Y = p_{Y_0}$,

$$p^T H p = p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + (p + \tilde{Z} p_Z)^T H \tilde{Y} p_{Y_0} \le p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + 2\beta_{lvH}\beta_{nmp}\beta_{pcs}\|r\|,$$

and we finally get

$$p^T g + \tfrac{1}{2}(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c}\|^2) \le -\tfrac{1}{2}(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c}\|^2) + K\|r\|,$$

where

$$K = \beta_{nmu} + 2\beta_{lvH}\beta_{nmp}\beta_{pcs} + \beta_{nmA}\beta_{pcs}.$$

(ii) p is obtained by taking a descent step on φ from a stationary point $\hat{p}$. There are a number of possibilities:

- If $\|\hat{p}\| > \delta^1$ and $\|\hat{p} - p_0\| \le \frac{1}{2}\delta^1$, we need to consider different values for $\|\tilde{c}\|$. If $\|\tilde{c}\| < \epsilon_1 = \delta^1/(2\beta_{pc})$, then

$$\|\hat{p}\| \le \tfrac{1}{2}\delta^1 + \|p_0\| \le \tfrac{1}{2}\delta^1 + \beta_{pc}\|\tilde{c}\| \le \delta^1,$$

but this is a contradiction, so we must have $\|\tilde{c}\| \ge \epsilon_1$, in which case

$$\|p\| \le \beta_{nmp} \le \frac{\beta_{nmp}}{\epsilon_1}\|\tilde{c}\| = K\|\tilde{c}\|,$$

implying that for $\beta_2^1 = \beta_{nmg} + (\beta_{lvH} + \beta_{nmA}^2)\beta_{nmp}$,

$$p^T g + (p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c}\|^2) \le \beta_2^1 \|p\| \le \beta_2^1 K \|\tilde{c}\|.$$

Finally, using $\|\tilde{c}\| \le \beta_{nmA}\|p_0\| \le \beta_{nmA}\beta_{pcs}\|r\|$,

$$p^T g + \tfrac{1}{2}(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c}\|^2) \le -\tfrac{1}{2}(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c}\|^2) + \bar{K}\|r\|$$

where $\bar{K} = 2\beta_2^1 \beta_{nmp}\beta_{nmA}\beta_{pcs}/\delta^1$.

- Let φ_k denote the function used to bound the desired descent. If $\|\hat{p} - p_0\| > \frac{1}{2}\delta^1$ then, after the kth *QP iteration*,

$$\varphi_k = g^T p_k + \tfrac{1}{2}(p_{Z_k}^T \tilde{Z}^T H \tilde{Z} p_{Z_k} + \|\tilde{c}\|^2).$$

Making use of the fact that $p_{Y_k} = p_{Y_0}$ for all k up to the stationary point, we can write

$$\varphi_{k-1} - \varphi_k = \psi_{k-1} - \psi_k + p_{Y_0}^T \tilde{Y}^T H \tilde{Z}(p_{Z_k} - p_{Z_{k-1}}),$$

where ψ_k is the QP objective function after iteration k. For all iterations between the initial point and the stationary point, it holds that

$$\varphi_0 - \hat{\varphi} = \psi_0 - \hat{\psi} + p_{Y_0}^T \tilde{Y}^T H \tilde{Z}(\hat{p}_Z - p_{Z_0}).$$

We can use (4.3.4) to write

$$|p_{Y_0}^T \tilde{Y}^T H \tilde{Z}(\hat{p}_Z - p_{Z_0})| \le 2\beta_{lvH}\beta_{nmp}\|p_0\| \le 2\beta_{lvH}\beta_{nmp}\beta_{pcs}\|r\| = K'\|r\|.$$

If we let $\bar{\gamma} = \psi_0 - \hat{\psi}$, it follows that

$$\varphi \le \hat{\varphi} \le \varphi_0 - \bar{\gamma} + K'\|r\|.$$

From one of the intermediate results in the proof of Lemma 4.3.3, we have $\bar{\gamma} \ge \frac{1}{2}\beta_{szH}(\delta^o/2m)^2$. Consequently,

$$p^T g + \tfrac{1}{2}(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c} + w_c\|^2) \le -\beta_1(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c} + w_c\|^2) + \hat{K}\|r\|,$$

where $\hat{K} = K' + \beta_2^1$ and

$$0 < \beta_1 \le \frac{\bar{\gamma}}{\beta_{lvH}\beta_{nmp}^2}.$$

- If $\|\hat{p}\| \leq \delta^1$, we know from Lemma 5.2.1 that we have descent for φ, and the minimal descent rate is bounded by

$$\hat{\varphi} - \varphi\Big(\hat{p} - \frac{\varphi'(0)}{\varphi''}\, d\Big) = \frac{\varphi'(0)^2}{2\varphi''},$$

where $-\varphi'(0)/\varphi''$ is the step to the minimizer. As the step is at least $\frac{1}{2}\beta_g^1$, by assuming the same (minimum) rate of descent as before, we get for the descent from $\hat{p}$,

$$\hat{\varphi} - \varphi \geq \tfrac{1}{2}\varphi'(0)\, \tfrac{1}{2}\beta_g^1 \geq \tfrac{1}{8}\beta_{dsc}\beta_{spm}\, \beta_g^1.$$

By selecting

$$0 < \beta_1 \leq \frac{\beta_{dsc}\beta_{spm}\beta_g^1}{8\beta_{lvH}\beta_{nmp}{}^2}$$

we can write

$$p^T g + \tfrac{1}{2}(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c} + w_c\|^2) \leq -\beta_1 (p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c} + w_c\|^2) + \tilde{K}\|r\|$$

for $\tilde{K} = \beta_{pcs}\beta_2^1$. This completes the proof. ∎

Bounds for the penalty parameter

We now determine modified bounds for the penalty parameter. We assume that the multiplier estimates are obtained according to conditions **C7–C9**, given in Chapter 2, and in addition we impose an extra condition on the choice of the initial working set made at each iteration:

C13. The initial active set must be selected so that there exists an $\epsilon'' > 0$ such that if $\|p_k\| < \epsilon''$, then the active set at p_k is the initial active set.

From the definition of the search direction, p_k, this condition implies that eventually p_k must be the solution of the QP subproblem, and it must be determined in just one QP iteration (no constraints added or deleted).

Define the auxiliary vector

$$w_g \equiv \tilde{Z}^T g - \tilde{Z}^T H p. \tag{5.2.1}$$

Property **P4** is an immediate consequence of the following lemma:

Lemma 5.2.3. *There exists a value $\hat{\rho}_k$ such that*

$$\phi_k'(0,\rho) \leq -\tfrac{1}{2}(p_{Z_k}^T \tilde{Z}_k^T H_k \tilde{Z}_k p_{Z_k} + \|\tilde{c}_k + w_{c_k}\|^2) \tag{5.2.2}$$

for all $\rho \geq \hat{\rho}_k$.

Proof. From the expression for $\phi'(0)$ given in (3.6.2), we can write, using (5.2.1),

$$\begin{aligned}\phi'(0) &= p_Z^T\tilde{Z}^Tg + p_Y^T\tilde{Y}^Tg + \mu^T(c-s) - 2\xi^T(c-s) - \rho\|c-s\|^2\\ &= -p_Z^T\tilde{Z}^TH\tilde{Z}p_Z - p_Z^T\tilde{Z}^TH\tilde{Y}p_Y + p_Z^Tw_g + p_Y^T\tilde{Y}^Tg - \mu^TA\tilde{Y}p_Y\\ &\qquad - \mu^TA\tilde{Z}p_Z - \mu^Ts - 2\xi^T(c-s) - \rho\|c-s\|^2\\ &= -p_Z^T\tilde{Z}^TH\tilde{Z}p_Z - \|\tilde{c}+w_c\|^2 + b^T(\tilde{c}+w_c) + p_Z^T(w_g - \tilde{Z}^TA^T\mu)\\ &\qquad - \mu^Ts - 2\xi^T(c-s) - \rho\|c-s\|^2,\end{aligned}$$

where $\xi \equiv \mu - \lambda$ and b is defined from

$$\begin{aligned}\theta &= \|\tilde{c}+w_c\|^2 - p_Y^T\tilde{Y}^T(H\tilde{Z}p_Z + A^T\mu - g)\\ b &= \begin{cases} 0 & \text{if } \|\tilde{c}+w_c\| = 0\\ \dfrac{\theta}{\|\tilde{c}+w_c\|^2}(\tilde{c}+w_c) & \text{otherwise.}\end{cases}\end{aligned}$$

Consequently, $b^T(\tilde{c}+w_c) = \theta$, as $\|\tilde{c}+w_c\| = 0 \Rightarrow p_Y = 0$.

If b and w_c are redefined to be full m-vectors by giving the value zero to all components corresponding to constraints not in the initial active set, we may rewrite the previous equation as

$$\begin{aligned}\phi'(0) = -p_Z^T\tilde{Z}^TH\tilde{Z}p_Z &- \|\tilde{c}+w_c\|^2 + b^Tw_c + p_Z^T(w_g - \tilde{Z}^TA^T\mu) + (b-\mu)^Ts\\ &+ (b-2\xi)^T(c-s) - \rho\|c-s\|^2.\end{aligned}$$

The condition to be satisfied can then be expressed as

$$\begin{aligned}b^Tw_c &+ p_Z^T(w_g - \tilde{Z}^TA^T\mu) + (b-\mu)^Ts + (b-2\xi)^T(c-s) - \rho\|c-s\|^2\\ &\le \tfrac{1}{2}(p_Z^T\tilde{Z}^TH\tilde{Z}p_Z + \|\tilde{c}+w_c\|^2),\end{aligned}$$

and a stronger condition on ρ is given by

$$\rho(c-s)^T(c-s) \ge (b-2\xi)^T(c-s) + b^Tw_c + p_Z^T(w_g - \tilde{Z}^TA^T\mu) + (b-\mu)^Ts. \qquad (5.2.3)$$

A value $\hat{\rho}$ such that (5.2.3) holds for all $\rho \ge \hat{\rho}$ is

$$\hat{\rho} = \frac{\|b\| + 2\|\xi\|}{\|c-s\|} + \frac{\max(0, b^Tw_c + p_Z^T(w_g - \tilde{Z}^TA^T\mu) + (b-\mu)^Ts)}{\|c-s\|^2}, \qquad (5.2.4)$$

completing the result. ∎

We now prove property **P4**. As a consequence of assumption **A3** and the definition of w_c, there exists a constant β_{pcf} such that

$$\frac{\|\tilde{Y}_k p_{Y_k}\|}{\|\tilde{c}_k + w_{c_k}\|} \leq \beta_{pcf}. \tag{5.2.5}$$

From condition **C10'** and (5.2.5), we then have

$$p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c} + w_c\|^2 \geq \beta_{szH} \|\tilde{Z} p_Z\|^2 + \beta_{pcf}^2 \|\tilde{Y} p_Y\|^2 \geq \min(\beta_{pcf}^2, \beta_{szH}) \|p\|^2. \tag{5.2.6}$$

Defining $\beta_H = \frac{1}{2} \min(\beta_{pcf}^2, \beta_{szH})$ we obtain property **P4**,

$$\phi'(0) \leq -\beta_H \|p\|^2. \tag{5.2.7}$$

Another result that is useful in the lemmas that follow is the boundedness of the auxiliary variable b. From (5.2.5), assumptions **A1–A2** and condition **C10'**, we have that

$$\|b\| \leq \|\tilde{c} + w_c\| + \frac{\|\tilde{Y} p_Y\|}{\|\tilde{c} + w_c\|} \|H \tilde{Z} p_Z + A^T \mu - g\| \leq N'. \tag{5.2.8}$$

Regarding the penalty parameter, the same approach that was presented in the previous chapter still applies in this case; that is, we define its value to satisfy property **P4** and to be small enough so that $\rho/\hat{\rho}$ is bounded. An example of a selection rule having these properties is given in the next paragraph.

Let $\varphi_k = p_{Z_k}^T \tilde{Z}_k^T H_k \tilde{Z}_k p_{Z_k} + \|\tilde{c}_k + w_{c_k}\|^2$. As in (4.3.11), we define the bound for the penalty parameter by

$$\rho_k = \begin{cases} \rho_{k-1} & \text{if } \phi'(0, \rho_{k-1}) \leq -\frac{1}{2}\varphi_k \\ \max(\hat{\rho}_k, 2\rho_{k-1}) & \text{otherwise,} \end{cases} \tag{5.2.9}$$

where $\rho_0 = 0$ and $\hat{\rho}_k$ is defined by (5.2.4).

The next result establishes property **P5**.

Lemma 5.2.4. *Assuming the bound given in (5.2.9) for the multipliers, for any iteration k_l in which the value of ρ is modified,*

$$\rho_{k_l} \|p_{k_l}\|^2 \leq N$$

and

$$\rho_{k_l} \|c_{k_l} - s_{k_l}\| \leq N,$$

for some constant N.

Proof. If the penalty parameter is increased only at a finite number of iterations, the result follows from assumption **A2**, Lemma 2.4.1 and the boundedness of $\|p_k\|$. For the rest of the proof we then assume that there exists an infinite sequence of iterations along which the penalty parameter is increased without bound.

From Lemma 5.2.2,

$$\begin{aligned}\phi'(0) &= p^T g + (2\lambda - \mu)^T(c - s) - \rho\|c - s\|^2 \\ &\leq -(\tfrac{1}{2} + \beta_1)(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c} + w_c\|^2) + (2\lambda - \mu + \beta_2 v)^T(c - s) - \rho\|c - s\|^2,\end{aligned}$$

and if $\phi'(0) > -\frac{1}{2}(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c} + w_c\|^2)$ then, from the boundedness of the multipliers and β_2, and from (5.2.6),

$$\|c - s\| > \frac{\beta_1}{\|2\lambda - \mu + \beta_2 v\|}(p_Z^T \tilde{Z}^T H \tilde{Z} p_Z + \|\tilde{c} + w_c\|^2) \geq N_1\|p\|^2. \tag{5.2.10}$$

From assumptions **A1** and **A2**, Lemma 2.4.1, (5.2.8) and definition (5.2.4),

$$\rho\|c - s\|^2 \leq N_2,$$

and from (5.2.10) it follows that

$$\rho\|p\|^4 \leq N_3. \tag{5.2.11}$$

Under the assumption that $\hat{\rho}_{k_l} \to \infty$, this result implies that $\|p_{k_l}\| \to 0$.

We now show that for a large enough value of the penalty parameter $\hat{\rho}_{k_l}$ it must hold that

$$\max\Big(0\,,\, b_{k_l}^T w_{ck_l} + p_{Zk_l}^T(w_{gk_l} - \tilde{Z}_{k_l}^T A_{k_l}^T \mu_{k_l}) + (b_{k_l} - \mu_{k_l})^T s_{k_l}\Big) = 0.$$

If $\|p_{k_l}\| \to 0$, we can show that $\|b_{k_l}\| \to 0$. From condition **C13** we must eventually have $w_{ck_l} = 0$, and so $\|\tilde{c}_{k_l} + w_{ck_l}\| \to 0$. Furthermore, from Lemma 3.4.1 and condition **C8** on the multipliers, $\|A_{k_l}^T \mu_{k_l} - g_{k_l}\| \to 0$. From (5.2.8) we can write the bound

$$\|b_{k_l}\| \leq \|\tilde{c}_{k_l} + w_{ck_l}\| + \beta_{pcf}(\|H_{k_l}\tilde{Z}_{k_l} p_{Zk_l}\| + \|A_{k_l}^T \mu_{k_l} - g_{k_l}\|),$$

and therefore we have $\|b_{k_l}\| \to 0$.

Since $\|b_{k_l}\| \to 0$, there exists an index K such that $b_{k_l} \leq \mu_{k_l}$ for all $k_l \geq K$. (We use strict complementarity at the solution.) Also, for k_l large enough it must hold that $\|p_{k_l}\| < \epsilon''$, and from condition **C13** in that iteration we must have $w_{gk_l} = 0$, $\mu_{k_l}^T A_{k_l} \tilde{Z}_{k_l} = 0$ and $w_{ck_l} = 0$. Hence,

$$b_{k_l}^T w_{ck_l} + p_{Zk_l}^T(w_{gk_l} - \tilde{Z}_{k_l}^T A_{k_l}^T \mu_{k_l}) + (b_{k_l} - \mu_{k_l})^T s_{k_l} = (b_{k_l} - \mu_{k_l})^T s_{k_l} \leq 0.$$

From this inequality and (5.2.4) it follows that for k_l large enough, $\hat{\rho}_{k_l}$ must satisfy

$$\hat{\rho}_{k_l} = \frac{\|b_{k_l}\| + 2\|\xi_{k_l}\|}{\|c_{k_l} - s_{k_l}\|}. \tag{5.2.12}$$

In this case

$$\rho_{k_l}\|c_{k_l} - s_{k_l}\| \leq N,$$

and (5.2.10) implies

$$\rho_{k_l}\|p_{k_l}\|^2 \leq N_3\rho_{k_l}\|c_{k_l} - s_{k_l}\| \leq N,$$

proving the result. ∎

Proof of global convergence

The proof of global convergence follows along the same lines as in the previous chapter.

Theorem 5.2.1. *The algorithm described in this chapter has the property that*

$$\lim_{k\to\infty} \|p_k\| = 0. \tag{5.2.13}$$

Proof. Follows from the same arguments used in the proof of Theorem 4.3.1. ∎

Corollary 5.2.1.

$$\lim_{k\to\infty} \|x_k - x^*\| = 0.$$

Proof. The result follows immediately from Theorem 5.2.1 and Lemma 3.4.1. ∎

Corollary 5.2.2.

$$\lim_{k\to\infty} \|\lambda_k - \lambda^*\| = 0.$$

Proof. The result follows from Lemma 3.7.1, given the results in Lemma 3.6.6 and Corollary 5.2.1. ∎

5.3. Rate of convergence

In this chapter we assume that our approximation to the Hessian is only accurate on the null space of the active constraints. A consequence of the use of less precise information is a degradation in the rate of convergence for the algorithm. We are now only able to show that under condition **C11'** the algorithm converges two-step superlinearly (as opposed to the one-step superlinear convergence established in Chapter 4). The proof follows the same general pattern presented in Chapter 3.

We start by establishing property **P7**.

Lemma 5.3.1. *For iterations k_l in which the penalty parameter is increased, assuming an infinite sequence of such iterations occurs in the algorithm,*

$$\lim_{l\to\infty} \rho_{k_l}\|p_{k_l}\|^2 = 0$$

and

$$\lim_{l\to\infty} \rho_{k_l}\|c_{k_l} - s_{k_l}\| = 0.$$

Proof. For large enough ρ, from definition (5.2.4) and the remarks in Lemma 5.2.4,

$$\rho\|c - s\| \le 2\|b\| + 4\|\xi\|.$$

From Corollary 5.2.2, $\|\xi_{k_l}\| \to 0$, $\|A_{k_l}^T\mu_{k_l} - g_{k_l}\| \to 0$, and using Theorem 5.2.1 and Corollary 5.2.1, from (5.2.8) and condition **C13**,

$$0 \le \|b_{k_l}\| \le \|\tilde{c}_{k_l} + w_{ck_l}\| + \frac{\|\tilde{Y}_{k_l}p_{Y k_l}\|}{\|\tilde{c}_{k_l} + w_{ck_l}\|}\|H_{k_l}\tilde{Z}_{k_l}p_{Z k_l} + A_{k_l}^T\mu_{k_l} - g_{k_l}\| \to 0,$$

giving

$$\lim_{l\to\infty} \rho_{k_l}\|c_{k_l} - s_{k_l}\| = 0.$$

But (5.2.10) implies

$$\lim_{l\to\infty} \rho_{k_l}\|p_{k_l}\|^2 = 0,$$

completing the proof. ∎

Our goal is to prove a result similar to Theorem 4.4.1 for the algorithm introduced in this chapter. As in the previous chapter, some additional conditions need to be imposed. It was mentioned at the beginning of the chapter that our interest is to study the consequences of approximating only the reduced Hessian. In this case, condition **C11** cannot be enforced, and it is replaced by

C11'. Following Powell [Po78], we assume

$$\|Z_k^T(H_k - W_k)Z_k p_{Z_k}\| = o(\|p_k\|).$$

Note that this condition, together with condition **C10'**, implies that for points close enough to the solution we must have

$$p_{Z_k}^T Z_k^T W Z_k p_{Z_k} \geq \tfrac{1}{2}\beta_{szH}\|Z_k p_{Z_k}\|^2.$$

As a consequence of the use of less restrictive conditions on H_k, condition **C12** is no longer adequate, and it also needs to be replaced. The new condition does not apply to the multiplier estimates, which now are only required to satisfy **C7**–**C9**; instead, it limits the acceptable values for the penalty parameter ρ_k.

C12'. When the iterates are close to the solution, the penalty parameter is chosen to be "large enough".

The following results will make clear what is a suitable lower bound for the penalty parameter.

If these conditions hold, using the previous results and Lemmas 3.8.2 to 4.4.3, we can show that the algorithm converges two-step superlinearly.

Theorem 5.3.1. *There exists a value $\bar{\rho}$, such that if ρ_k is selected satisfying $\rho_k \geq \bar{\rho}$, then the algorithm converges two-step superlinearly.*

Proof. We start by proving that if ρ_k is large enough, condition (2.2.3) is satisfied for all large k. In the rest of the proof we drop the subscript denoting the iteration number.

As in Byrd and Nocedal [BN88], we let

$$L(x,\lambda,s) = F(x) - \lambda^T(c(x) - s). \tag{5.3.1}$$

We can now use a Taylor series expansion to write

$$\Delta L \equiv L(x+p,\lambda,s) - L(x,\lambda,s) = g^T p - \lambda^T A p + \tfrac{1}{2}p^T W p, \tag{5.3.2}$$

where $W = \nabla_{xx}^2 L(x+\theta p,\lambda,s)$ and $0 \leq \theta \leq 1$.

Rearranging terms,

$$\begin{aligned}\Delta L &= p_Y^T Y^T(g - A^T\lambda) + p_Z^T Z^T g + \tfrac{1}{2} p_Z^T Z^T W Z p_Z + (\tfrac{1}{2} Y p_Y + Z p_Z)^T W Y p_Y \\ &= p_Y^T Y^T(g - A^T\lambda) + \sigma p_Z^T Z^T g + (1-\sigma) p_Z^T Z^T (W - H) Z p_Z \\ &\quad - (1-\sigma) p_Z^T Z^T H Y p_Y + (\tfrac{1}{2} Y p_Y + Z p_Z)^T W Y p_Y - (\tfrac{1}{2} - \sigma) p_Z^T Z^T W Z p_Z.\end{aligned}$$

Assume now that k is large enough so that $\|W\| \le 2\|W^*\| = \beta^*$, where W^* indicates the Hessian of the Lagrangian function at the solution, and also that the bound $p_Z^T Z^T W Z p_Z \ge \frac{1}{2}\beta_{szH}\|Zp_Z\|^2$ holds. We may rewrite condition **C11'** in the form

$$p_{Z_k}^T Z_k^T (W_k - H_k) Z_k p_{Z_k} = \omega_k \|Z_k p_{Z_k}\| \|p_k\|,$$

where $\omega_k \to 0$. Consequently

$$\begin{aligned}\Delta L &\le p_Y^T Y^T(g - A^T\lambda) + \sigma p_Z^T Z^T g - \Big((\tfrac{1}{2} - \sigma)\tfrac{1}{2}\beta_{szH} - (1-\sigma)\omega\Big)\|Zp_Z\|^2 \\ &\quad + \tfrac{1}{2}\beta^*\|Yp_Y\|^2 + \Big((1-\sigma)(\beta_{lvH} + \omega) + \beta^*\Big)\|Zp_Z\|\|Yp_Y\|.\end{aligned}$$

For k large enough, there exist positive constants a_1, a_2 (e.g., take $a_1 = 2(1-\sigma)\beta_{lvH} + \beta^*$ and $a_2 = \frac{1}{4}(\frac{1}{2} - \sigma)\beta_{szH}$), such that

$$\Delta L \le p_Y^T Y^T(g - A^T\lambda) + \sigma p_Z^T Z^T g + \tfrac{1}{2}\beta^*\|Yp_Y\|^2 + a_1\|Zp_Z\|\|Yp_Y\| - a_2\|Zp_Z\|^2.$$

We now study the merit function (2.2.1) at $\alpha = 1$. We can write it as

$$\begin{aligned}\phi(1) &= L(x+p,\lambda,s) + \Big(L(x+p,\mu,s+q) - L(x+p,\lambda,s)\Big) + \tfrac{1}{2}\rho\|c(x+p) - s - q\|^2 \\ &= L(x,\lambda,s) + \Big(\lambda^T(c(x+p) - s) - \mu^T(c(x+p) - s - q)\Big) + \tfrac{1}{2}\rho\|c(x+p) - s - q\|^2 \\ &\quad + p_Y^T Y^T(g - A^T\lambda) + \sigma p_Z^T Z^T g + \tfrac{1}{2}\beta^*\|Yp_Y\|^2 + a_1\|Zp_Z\|\|Yp_Y\| - a_2\|Zp_Z\|^2.\end{aligned}$$

Using $c_i(x+p) - s_i - q_i = p^T\nabla^2 c_i(z_i)p$, where $z_i = x + \theta_i p$ for some $\theta_i \in [0,1]$, we have

$$\begin{aligned}\phi(1) &= \phi(0) + p_Y^T Y^T(g - A^T\lambda) + \sigma p_Z^T Z^T g + \lambda^T q - \textstyle\sum_i \xi_i p^T\nabla^2 c_i(z_i)p - \tfrac{1}{2}\rho\|c - s\|^2 \\ &\quad + \tfrac{1}{2}\rho\textstyle\sum_i\Big(p^T\nabla^2 c_i(z_i)p\Big)^2 + a_1\|Zp_Z\|\|Yp_Y\| - a_2\|Zp_Z\|^2 + \tfrac{1}{2}\beta^*\|Yp_Y\|^2 \\ &\le \phi(0) + \sigma\phi'(0) - \sigma p_Y^T Y^T g - \sigma(2\lambda - \mu)^T(c - s) + \lambda^T q + p_Y^T Y^T(g - A^T\lambda) \\ &\quad - (\tfrac{1}{2} - \sigma)\rho\|c - s\|^2 + a_1'\|Zp_Z\|\|Yp_Y\| - a_2'\|Zp_Z\|^2 + \beta^*\|Yp_Y\|^2,\end{aligned}$$

where we have made use of Lemma 3.8.2 and the facts that $\xi_k \to 0$ and the second derivatives of the constraint functions are uniformly bounded. This result holds for large enough k, and positive constants a_1', a_2' (again, take for example $a_1' = 2a_1$, $a_2' = \frac{1}{2}a_2$).

Rewriting this expression, we get

$$\phi(1)-\phi(0) \le \sigma\phi'(0) + (1-\sigma)p_Y^T Y^T(g - A^T\mu) - (1-2\sigma)\xi^T(c-s) - (1-\sigma)\mu^T q$$
$$-(\tfrac{1}{2}-\sigma)\rho\|c-s\|^2 + a_1'\|Zp_Z\|\|Yp_Y\| - a_2'\|Zp_Z\|^2 + \beta^*\|Yp_Y\|^2.$$

From Lemma 4.4.3, condition **C8** on the multipliers, and selecting k large enough so that $\mu^T q = 0$, it follows that

$$\|g - A^T\mu\| \le \bar{\beta}\|p\|$$

for some constant $\bar{\beta}$. Finally, we can select ρ large enough so that for large k,

$$-(1-2\sigma)\xi^T(c-s) - (\tfrac{1}{2}-\sigma)\rho\|c-s\|^2 \le -\tfrac{1}{2}(\tfrac{1}{2}-\sigma)\rho\|c-s\|^2;$$

for example, let ρ be larger than twice the bound given in (5.2.12). We then have

$$\phi(1)-\phi(0) \le \sigma\phi'(0) - \tfrac{1}{2}(\tfrac{1}{2}-\sigma)\rho\|c-s\|^2 + a_1''\|Zp_Z\|\|Yp_Y\| - a_2'\|Zp_Z\|^2 + a_3\|Yp_Y\|^2,$$

where $a_1'' = a_1' + \bar{\beta}$ and $a_3 = \beta^* + \bar{\beta}$.

Assume that k is large enough so that p is obtained as the solution for the QP subproblem, the correct active set has been identified and $\rho c_i < \lambda_i$ for all active constraints (this follows from Lemma 3.8.3). From (5.2.5),

$$\|Yp_Y\| \le \beta_{pcf}\|\bar{c}\| \le \beta_{pcf}\|c-s\|,$$

and

$$\phi(1)-\phi(0) \le \sigma\phi'(0) + \Big(a_3' - \tfrac{1}{2}(\tfrac{1}{2}-\sigma)\rho\Big)\|c-s\|^2 + a_1'''\|Zp_Z\|\|c-s\| - a_2'\|Zp_Z\|^2,$$

where $a_1''' = \beta_{pcf}a_1''$ and $a_3' = \beta_{pcf}a_3$.

From the arithmetic mean/geometric mean inequality,

$$a_1'''\|Zp_Z\|\|c-s\| \le \tfrac{1}{2}\Big(a_2'\|Zp_Z\|^2 + \frac{a_1'''^2}{a_2'}\|c-s\|^2\Big), \tag{5.3.3}$$

we finally obtain

$$\phi(1)-\phi(0) \le \sigma\phi'(0) - \tfrac{1}{2}a_2'\|Zp_Z\|^2 + \Big(a_3' + \frac{a_1'''^2}{2a_2'} - \tfrac{1}{2}(\tfrac{1}{2}-\sigma)\rho\Big)\|c-s\|^2. \tag{5.3.4}$$

If ρ is chosen so that

$$\rho \ge \frac{4a_3'a_2' + 2a_1'''^2}{(1-2\sigma)a_2'}$$

then the step of $\alpha = 1$ will satisfy condition (2.2.3).

Finally, applying Theorem 1 from Powell [Po78], we obtain the desired convergence result. ∎

Most of the proof for the previous theorem is devoted to showing that a unit steplength is eventually acceptable if the penalty parameter is sufficiently large. Clearly, the proof given here still holds for the algorithm presented in Chapter 4, and this gives a second set of alternative conditions for superlinear convergence, where the condition on the multiplier estimate **C12** is replaced by a condition on the penalty parameter **C12'**.

5.4. Summary

In this chapter we have studied an algorithm similar to the one presented in Chapter 4, but where the conditions on the approximation to the Hessian have been relaxed, so that now only the approximation to the reduced Hessian is required to be positive definite.

The results obtained have been:

- Under conditions **C1**–**C9** on the search direction and multiplier estimate, and condition **C10'** on the approximation to the reduced Hessian, if the approximation for the rest of the Hessian is assumed to be such that H_k is positive definite, then the algorithm is *globally convergent.*

- An alternative algorithm has also been shown to be *globally convergent,* where no assumption is made about the Hessian approximation outside the null space of the active constraints, but requiring the additional condition:

  C13. the initial active set must be selected so that there exists an $\epsilon'' > 0$ such that if $\|p_k\| < \epsilon''$, then the active set at p_k is the initial active set.

- Finally, we have proved that the algorithm is *two-step superlinearly convergent* if in addition the following conditions are satisfied:

  C11'. $\|Z_k^T(H_k - W_k)Z_k p_{z_k}\| = o(\|p_k\|)$.

  C12'. When the iterates are close to the solution, the penalty parameter is chosen to be large enough.

Note that when no conditions are required on the approximation to the Hessian on subspaces other than the null space of the active constraints, the algorithm leaves open the possibility of using an approximation scheme satisfying condition **C11** from the previous chapter (instead of condition **C11'**). This would allow the algorithm to attain a one-step superlinear rate of convergence.

Chapter 6

Exact Second Derivatives

This chapter considers a third variant of the framework algorithm presented in Chapter 2. Again, a partial solution for the QP subproblem is used as the search direction, but in this case the Hessian approximation H_k is taken to be the exact Hessian of the Lagrangian function at the last iterate, that is

$$H_k \equiv \nabla^2_{xx} L(x_k, \lambda_k) = \nabla^2 F(x_k) - \textstyle\sum_i \lambda_{k_i} \nabla^2 c_i(x_k),$$

where now H_k, and even the reduced Hessian $Z_k^T H_k Z_k$, can be indefinite.

There are numerous theoretical and practical benefits deriving from the explicit use of second derivatives. For example, it will be seen in this chapter how to define an algorithm generating a sequence that converges to a second-order KKT point. Also, in practice it has been observed that second-derivative methods usually converge in much fewer iterations than those required by first-order methods. However, the use of second derivatives presents a number of technical difficulties, all of which stem from the loss of control over the properties of H_k. In order to reap all the benefits from the availability of second derivatives, we need to redefine the way the search direction is obtained. In all other respects the basic principles introduced in Chapter 2 will still be preserved.

The next section presents the definition of the incomplete solution for the QP subproblems, to be used as the search direction in each iteration. The rest of the chapter proves global convergence for the algorithm, and shows that under mild conditions the algorithm converges quadratically.

6.1. The search direction

The definition of the search direction given in Chapter 2 needs to be modified for the algorithm presented in this chapter, to take into account the possible lack of convexity in the subproblems, implying the possible indefiniteness of H_k and rank-deficiency in the reduced Hessians.

In the case when the Hessian is indefinite, the descent directions that can be obtained from the QP subproblems may no longer provide enough descent to guarantee the convergence of the algorithm; that is, the quantities $\phi_k'(0)$ may no longer be sufficiently negative to ensure that $\phi_k - \phi_{k+1}$ satisfies the condition used in the proofs of Theorems 4.3.1 and 5.2.1. In this section we present a procedure to generate search directions that either give sufficient descent, or are directions of negative curvature (satisfying $p_k^T H_k p_k < 0$) allowing a sufficient decrease in the value of the merit function to ensure convergence.

The search direction p_k is defined by the following steps:

(i) Obtain a feasible initial point p_0 for the QP subproblem such that conditions (2.2.6) and (2.2.7) are satisfied.

(ii) Solve the QP subproblem until a stationary point $\hat{p}$ is found, or until a direction of infinite descent d is obtained. The convergence results presented in this chapter do not assume the use of any specific QP algorithm, but the following conditions must be satisfied by the method selected.

- It must be an active-set algorithm, taking feasible descent steps in each iteration. If steps having a positive directional derivative for $\alpha = 0$ are taken, the total descent must be uniformly bounded away from zero.
- It must be able to find a stationary point (or a direction of infinite descent) in a number of iterations uniformly bounded by a function of the size of the problem.
- Each QP iteration must produce a minimum descent, unless we are at a stationary point for the QP subproblem. To be more precise, let p denote any intermediate point along the solution of the QP subproblem and let d be the QP search direction at p; also let α indicate the step taken from p along d, obtained as the minimum of the steps to the unidimensional minimizer, the nearest inactive constraint and a specified upper bound, in the same spirit as in the definition of α given in condition **C3**. Finally, let g_R denote the projection of $g + Hp$ onto

the null space of the active QP constraints at p. We require that d satisfies the following condition:

$$\frac{\psi(p) - \psi(p + \alpha d)}{\|\alpha d\|} \geq \beta_{qpd} \|g_R\|, \tag{6.1.1}$$

where β_{qpd} is some positive constant.

The reason for this condition is that it prevents the algorithm from taking steps that give arbitrarily small descent unless $\|g_R\|$ is small, that is, the point p is close to being a QP stationary point.

(iii) Define $\tilde{p}$ from $\hat{p}$ or d as follows,

(a) If a direction of infinite descent d satisfying (6.1.1) is obtained at a point p along the solution of the QP subproblem, define

$$\tilde{p} \equiv p + \alpha d,$$

where $\alpha > 0$ is chosen so that $\|\tilde{p}\|$ is uniformly bounded above and below.

(b) If $\hat{p}$ is a second-order KKT point for the QP subproblem, let

$$\tilde{p} \equiv \hat{p}.$$

(c) Otherwise, select $\tilde{p}$ by computing a direction d and a steplength α satisfying conditions **C1**–**C6**.

(iv) The following condition is introduced to identify the circumstances under which near singularity in the reduced Hessian may be a problem:

C14. $\|c^-\| \leq \epsilon_1$, and

$$\frac{\psi(p_0) - \psi(\tilde{p})}{\|p_0 - \tilde{p}\|} \leq \beta_d.$$

If **C14** holds, obtain an estimate for the active set at the current point, x_k, and compute a direction $\bar{p}$ by taking a step αd from p_0 satisfying **C1**–**C6**. If no feasible step satisfying these conditions exists, let $\bar{p} \equiv p_0$.

(v) Select the search direction p as

$$p \equiv \begin{cases} \tilde{p} & \text{if } \psi(\tilde{p}) \leq \psi(\bar{p}), \textbf{ C14} \text{ does not hold, or } \bar{p} = p_0 \\ \bar{p} & \text{otherwise.} \end{cases}$$

Several remarks are in order regarding the definition of p. Condition (6.1.1) could be replaced by the alternative condition

$$(g + Hp)^T \frac{d}{\|d\|} \leq \beta_{qpd}\|g_R\|,$$

which may provide a better expression for the stated goal of linking the lack of descent associated with the direction d and the proximity to a QP stationary point; but this is achieved at the expense of limiting the choice in the selection of directions of negative curvature.

In point (iv) it is required that the correct active set at a nearby stationary point should be identified. Under condition (6.1.1), an estimate for this active set having the desired properties is given by the QP active set at the initial point for the first finite QP step (the first step that is bounded away from zero).

Finally, condition **C5** requires the computation of a direction of negative curvature. In the case when n is small this is straightforward. For the large-scale case, efficient methods are known when the reduced Hessian is not too large. Although some work has been carried out for problems of arbitrary size, see for example Conn and Gould [CG84], such methods are not very efficient. Our hope is that satisfactory methods for computing feasible directions of negative curvature for arbitrarily large problems will be developed in the near future. If a direction of negative curvature is not determined, the proofs would still hold if we characterize solution points to be first-order KKT points for the problem (instead of second-order KKT points).

Properties of the search direction

As in the previous chapters, the first result required for the convergence proof is to show that if $\|p\|$ is small enough, the correct active set must have been identified. We start by introducing the following constant, implied by the non-singularity assumption **A6**:

β_{svH} is a positive lower bound for the smallest eigenvalue of the reduced Hessian of the Lagrangian function at all second-order KKT points for the NLP problem in Ω.

The following lemma establishes property **P1** for this algorithm.

Lemma 6.1.1. *There exists an $\epsilon > 0$ such that $\|p\| \leq \epsilon$ implies that p was obtained as a second-order KKT point of the QP subproblem and the correct active set has been identified.*

Proof. The correct identification of the active set follows from strict complementarity at the solution point (see proof for Lemma 4.3.2).

Assume that the lemma does not hold, in the sense that there exists a sequence $\{x_k\}$ such that $x_k \to x^*$ and $\|p_k\| \to 0$, where p_k denotes the search direction obtained for the QP subproblem at x_k in the form described in the previous section, but p_k has not been obtained as a second-order KKT point for the QP subproblem.

If $p_k = \bar{p}_k$ and $\|\bar{p}_k\| > \epsilon_a$ for an infinite subsequence and some $\epsilon_a > 0$, then as $\bar{p}_k$ must be feasible, we must have $\|c_k^-\| \to 0$. Also, as $\psi_k(\bar{p}_k) \to 0$, we must have $\psi_k(\tilde{p}_k) \to 0$. From this and condition (6.1.1) it must follow that x^* is a stationary point for the NLP problem, given that it is feasible and in the QP subproblem we have no descent when taking a nonzero step from the origin to a stationary point.

If x^* is a second-order KKT point, eventually $\bar{p}_k = p_{k_0}$ and $p_k = \bar{p}_k$. If x^* is a stationary point but not a second-order KKT point, for $\|x_k - x^*\|$ small enough we can find a direction d_k and a steplength α_k such that $p_{k_0} + \alpha_k d_k$ is feasible, as $\|p_{k_0}\| \to 0$ and the information used is asymptotically correct. From the bound given in (4.3.1) and condition **C1**,

$$\alpha_k \geq \tfrac{1}{2}\beta_g^o, \qquad \|d_k\| \geq \beta_{lnd},$$

implying that

$$\|\bar{p}_k\| = \|p_{k_0} + \alpha_k d_k\| \geq \tfrac{1}{4}\beta_g^o \beta_{lnd}.$$

However, this contradicts our hypothesis.

Assume now that $\|\tilde{p}_k\| \to 0$. From condition **C6**, this implies $\|\hat{p}_k\| \to 0$, and from Lemma 3.3.1 we must have that x^* is a stationary point. Suppose x^* is a second-order KKT point. Then strict complementarity at x^* and the fact that $\|p_k\| \to 0$ imply that the correct active set is eventually identified. Hence, from the positive definiteness of the reduced Hessian at x^*, we must have that for large enough k, $\hat{p}_k$ is a second-order KKT point for the QP subproblem.

If x^* is a stationary point, but not a second-order KKT point, using the bounds given in Section 4.3 and assuming $\|x_k - x^*\|$ to be small enough, we can find a direction d_k and a steplength α_k such that

$$\alpha_k \geq \tfrac{1}{2}\beta_g^o, \qquad \|d_k\| \geq \beta_{lnd},$$

implying that

$$\|\tilde{p}_k\| = \|\hat{p}_k + \alpha_k d_k\| \geq \tfrac{1}{4}\beta_g^o \beta_{lnd}.$$

Again, this is a contradiction. ∎

As in previous chapters, the proof proceeds by showing that property **P3** holds for this algorithm, that is, the search direction computed according to the rules introduced in Section 6.1 satisfies a descent condition.

In order to prove **P3**, we need a preliminary result. In Chapters 4 and 5 it was possible to show that

$$\psi_k(p_{k_0}) - \psi_k(p_k) \to 0 \Rightarrow \|p_{k_0} - p_k\| \to 0,$$

using the positive definiteness of H_k, or of $Z_k^T H_k Z_k$ at least. This argument is not valid in this case, and we give an alternative proof for the result in the next lemmas.

In the following lemmas the notation $\{y_m\}_{m=1}^{\infty}$ is used to represent a subsequence from the sequence of iterates, $\{y_m\} \subseteq \{x_k\}$. The symbol c_m denotes the vector $c(y_m)$, H_m corresponds to the Hessian of the Lagrangian function at y_m, and p_m indicates the search direction obtained at y_m.

Lemma 6.1.2. *If the convergent sequence $\{y_m\}$, $y_m \to y^*$, satisfies $\|c_m^-\| \to 0$, it must hold that*

$$\psi_m(p_m) \to 0 \Rightarrow \|p_m\| \to 0,$$

where p_m denotes the search direction obtained from the process described above. Also, y^* must be a stationary point of the NLP *problem.*

Proof. Assume that the lemma does not hold, i.e., that $\psi_m(p_m) \to 0$ but $\|p_m\| \geq \delta > 0$ for all m.

Since the norm of the initial QP point goes to zero ($\|p_{m_0}\| \to 0$), condition **C14** must hold for large enough m.

To show that y^* is a stationary point, take a subsequence along which the number of QP steps is fixed (it is bounded), and all intermediate steps converge to limit points; in the limit all steps give zero descent, as $\psi_m(\tilde{p}_m) \to 0$, implying that all intermediate points, and in particular the origin, must be stationary points from condition (6.1.1).

Assume that y^* is a second-order KKT point, and that a set of limit points for intermediate steps has been obtained as indicated in the previous paragraph. For the first nonzero step from the origin d^*, it must hold that $\|d_Y^*\| > 0$, as otherwise we would have $d_Z^{*T} Z^{*T} H Z^* d_Z^* = 0$, contradicting assumption **A6**. But then $g^{*T} d^* > 0$, violating the first condition imposed on the QP solution method.

It follows that at y^* there exists either a direction of negative curvature or a negative multiplier. Since $\bar{\mu}_m \to \mu^*$ (the Jacobian of the active constraints at y^* has full rank), then from the bounds introduced in (4.3.1) and Lemma 3.3.2, it follows for m large enough that

$$\psi_m(\bar{p}_m) \le -\tfrac{1}{4}\alpha_m^2 |d_m^T H_m d_m| \le -\tfrac{1}{32}\beta_g^{o^2}\beta_L\beta_{spn}$$

when there exists a direction of negative curvature, or

$$\psi_m(\bar{p}_m) \le -\tfrac{1}{4}\alpha_m |\psi_m'(0)| \le -\tfrac{1}{16}\beta_g^o\beta_{dsc}\beta_{spm}$$

when there exists a negative multiplier.

Consequently, in either case $\psi_m(\bar{p}_m)$ is bounded away from zero, which contradicts our assumption. ∎

Lemma 6.1.3. *There exists a constant $\epsilon_c > 0$ such that for any sequence $\{y_m\}$ satisfying $\|c_m^-\| \le \epsilon_c$, we must have*

$$\psi_m(p_{m_0}) - \psi_m(p_m) \to 0 \Rightarrow \|p_{m_0} - p_m\| \to 0.$$

Proof. Assume that the result does not hold. Consider any sequence $\{\epsilon_j\}$, such that $\epsilon_j \to 0$ and $\epsilon_j \le \epsilon_1$. For each ϵ_j, we can construct a sequence $\{y_j^l\} \subseteq \{y_m\}$ such that $\|c_j^{l-}\| \le \epsilon_j$ for all l, $y_j^l \to y_j^*$ as $l \to \infty$ for all j, $\psi_j^l(p_{j0}^l) - \psi_j^l(p_j^l) \to 0$ but $\|p_{j0}^l - p_j^l\| > \delta_j$ for some $\delta_j > 0$ for all l. Finally, we can assume that $y_j^* \to y^*$.

From the previous properties, condition **C14** must hold eventually for any of the sequences. Select one element from each sequence $y_j^l \equiv \bar{y}_j$, such that for that point **C14** is satisfied and $\bar{y}_j \to y^*$. Then from the previous lemma we must have that $\bar{p}_j \to 0$ and y^* is a stationary point of the problem.

Using the same arguments as in Lemma 6.1.2, if y^* is not a second-order KKT point, then at y^* we will have either a direction of negative curvature or a negative multiplier, and since $\bar{\mu}_j \to \mu^*$ (the Jacobian at y^* has full rank from assumption **A3**), and a similar property holds for the reduced Hessian, we must have that

$$\psi_j(\bar{p}_{j0}) - \psi_j(\bar{p}_j) \ge \tfrac{1}{32}\beta_g^o \min(2\beta_{dsc}\beta_{spm}, \beta_g^o\beta_L\beta_{spn}),$$

contradicting our assumption.

If y^* is a second-order KKT point, then consider the sequence $\{y_j^*\}$. For this sequence and for j large enough, p_{j0}^* (the initial point for the QP subproblem) must be a second-order KKT point. This follows from condition (6.1.1), implying that all p_{j0}^* must be QP stationary points, and from $\|p^*_{j0}\| \to 0$, the identification of the correct active set from strict complementarity at y^* and assumption **A6**. But from arguments used in the previous lemma, the fact that we have no descent from p^*_{j0} implies that the reduced Hessian must be singular at p^*_{j0} for large enough j, and the reduced Hessian must also be singular at y^*, contradicting assumption **A6**. ∎

We can now prove property **P3** for the algorithm.

Lemma 6.1.4. *There exist constants $\beta_1 > 0$ and $\beta_2 > 0$ such that*

$$g_k^T p_k + \tfrac{1}{2} p_k^T H_k p_k \le -\beta_1 \|p_k\|^2 + \beta_2 \|r_k\|. \tag{6.1.2}$$

Proof. Define ϵ_H satisfying $\epsilon \ge \epsilon_H > 0$, where ϵ is the value from Lemma 6.1.1, and such that $\|p\| < \epsilon_H$ implies that p is a second-order KKT point, the correct active set has been identified, and the smallest eigenvalue for the reduced Hessian is greater than $\frac{1}{2}\beta_{svH}$.

Also, from Lemma 6.1.3, let $\delta > 0$ be the value such that, if $\|c^-\| \le \epsilon_c$,

$$\|p_0 - p\| > \tfrac{1}{2}\epsilon_H \Rightarrow \psi(p_0) - \psi(p) > \delta.$$

Define

$$\epsilon' = \frac{\delta}{2(\beta_{nmg} + \beta_{nmH}\beta_{nmp})},$$

having the property that $\|p_0\| \le \epsilon'$ implies $|\psi(p_0)| \le \frac{1}{2}\delta$. Select

$$\epsilon_1 = \min\left(1, \epsilon_c, \frac{\epsilon'}{\beta_{pcs}}, \frac{\epsilon_H}{2\beta_{pcs}}\right).$$

From condition (2.2.6) and assumption **A2**, there exists a constant β_{nmp} such that

$$\|p_0\| \le \beta_{pc}\|\bar{c}\| \le \beta_{nmp}.$$

One of the following conditions must hold:

- $\|r\| > \epsilon_1$. From the boundedness of $\|p_0\|$ we can write

$$\begin{aligned}\psi(p) &= g^T p + \tfrac{1}{2} p^T H p \le \psi(p_0) \le \beta_{nmp}(\beta_{nmg} + \tfrac{1}{2}\beta_{nmH}\beta_{nmp}) \\ &\le -\beta_1\|p\|^2 + \frac{\beta_{nmp}}{\epsilon_1}(\beta_1\beta_{nmp} + 2\beta_{nmg} + \beta_{nmH}\beta_{nmp})\|r\|.\end{aligned}$$

- $\|r\| \le \epsilon_1$ and $\|p\| \ge \epsilon_H$. This implies $\|p_0\| \le \beta_{pcs}\epsilon_1 \le \epsilon'$ and $|\psi(p_0)| \le \frac{1}{2}\delta$. Also, $\|p_0 - p\| > \epsilon_H - \beta_{pcs}\epsilon_1 \ge \frac{1}{2}\epsilon_H$, and

$$\psi(p_0) - \psi(p) > \delta \quad \Rightarrow \quad \psi(p) < -\tfrac{1}{2}\delta \quad \Rightarrow \quad \psi(p) < -\frac{\delta}{2\beta_{nmp}^2}\|p\|^2.$$

- $\|r\| \le \epsilon_1$ and $\|p\| < \epsilon_H$. In this case, as p is a second-order KKT point for the QP subproblem,

$$g^Tp + p^THp = -c^T\mu \le \beta_{nmu}\|c^-\| \le \beta_{nmu}\|r\|.$$

Using the notation $\Delta p \equiv p - p_0$,

$$\begin{aligned} p^THp &= p_0^THp_0 + 2\Delta p^THp_0 + \Delta p^TH\Delta p \\ &\ge -\beta_{nmH}\beta_{spc}^2\|r\|^2 - 2\beta_{nmH}\beta_{spc}\|r\|\|\Delta p\| + \tfrac{1}{2}\beta_{svH}\|\Delta p\|^2, \end{aligned}$$

and from the arithmetic mean/geometric mean inequality,

$$2\|r\|\|\Delta p\| \le \frac{4\beta_{spc}\beta_{nmH}}{\beta_{svH}}\|r\|^2 + \frac{\beta_{svH}}{4\beta_{spc}\beta_{nmH}}\|\Delta p\|^2,$$

we obtain

$$p^THp \ge \tfrac{1}{4}\beta_{svH}\|\Delta p\|^2 - \beta_{nmH}\beta_{spc}^2\Big(1 + \frac{4\beta_{nmH}}{\beta_{svH}}\Big)\|r\|^2.$$

The inequalities

$$\tfrac{1}{2}\|p\|^2 \le \tfrac{1}{2}\|\Delta p\|^2 + \tfrac{1}{2}\|p_0\|^2 + \|\Delta p\|\|p_0\| \le \|\Delta p\|^2 + \|p_0\|^2$$

imply that we can write

$$p^THp \ge \tfrac{1}{8}\beta_{svH}\|p\|^2 - \beta'\|r\|^2,$$

where

$$\beta' = \beta_{spc}^2\Big(\beta_{nmH}\Big(1 + \frac{4\beta_{nmH}}{\beta_{svH}}\Big) + \tfrac{1}{4}\beta_{svH}\Big).$$

Putting all these results together, we have

$$\psi(p) \le \beta_{nmu}\|r\| - \tfrac{1}{2}p^THp \le -\tfrac{1}{16}\beta_{svH}\|p\|^2 + (\tfrac{1}{2}\beta' + \beta_{nmu})\|r\|,$$

completing the proof. ∎

6.2. Definition of the linesearch

As a consequence of the way we have defined the matrices H_k and the incomplete solutions for the QP subproblems in this chapter, the search direction p_k may no longer be a descent direction, but rather a direction of negative curvature. The linesearch model presented in the previous chapters is not adequate for this case. We can no longer be assured that the directional derivative at the beginning of the linesearch is bounded by a multiple of $\|p_k\|^2$. The structure of the global convergence proof would then fail to hold. We need to modify the linesearch model introduced in Chapter 2, and we will do so according to the ideas introduced in McCormick [McC77], and further developed in Moré and Sorensen [MS84].

The problem considered in [MS84] is that of minimizing an unconstrained function when in each iteration a direction of descent v, or a direction of negative curvature w, or both, are available. The search is carried out along the curve $C = \{x(\alpha) : x(\alpha) = x + \alpha w + \alpha^2 v\}$, and the termination conditions when the direction of negative curvature is available are specified in terms of the curvature at the initial point. In our case we generate only one search direction p_k for the original variables x in each iteration, but the search on the merit function is made not only in the space of the original variables, but also in the space of the Lagrange multipliers and the slack variables. Whenever we make use of p_k as a direction of negative curvature, we need to define not just one search direction but both a direction of descent and a direction of negative curvature in this expanded space. If p_k can be treated as a direction of descent, we prefer to avoid the complications associated with the curvilinear search by reverting to the linesearch model introduced in Chapter 2.

The next paragraphs present the definitions of the expanded directions for the curvilinear search. To motivate them, we start by studying the form of the derivatives for the merit function along the curve C. We define the unidimensional merit function along the curve of search, ϕ^C, starting from the point y and moving along the vectors

$$y = \begin{pmatrix} x \\ \lambda \\ s \end{pmatrix}, \qquad \bar{v} = \begin{pmatrix} v \\ t_1 \\ u_1 \end{pmatrix}, \qquad \bar{w} = \begin{pmatrix} w \\ t_2 \\ u_2 \end{pmatrix}, \tag{6.2.1}$$

as

$$\phi^C(\alpha) = L(y + \alpha^2 \bar{v} + \alpha \bar{w}) = F(x_\alpha) - \phi_1^C(\alpha) + \rho \phi_2^C(\alpha),$$

where

$$\phi_1^C(\alpha) = \lambda_\alpha^T \big(c(x_\alpha) - s_\alpha\big),$$

$$\phi_2^C(\alpha) = \tfrac{1}{2}\|c(x_\alpha) - s_\alpha\|^2.$$

To simplify the expressions that appear in the analysis of the different functions related to the merit function, we introduce the notation

$$\begin{aligned} x_\alpha &\equiv x + \alpha^2 v + \alpha w, \\ \lambda_\alpha &\equiv \lambda + \alpha^2 t_1 + \alpha t_2, \\ s_\alpha &\equiv s + \alpha^2 u_1 + \alpha u_2. \end{aligned}$$

In the case when a normal linesearch is performed, the value of the merit function along the line of search will be denoted by ϕ^N. This linesearch can be viewed as a particular case of the curvilinear search, when $\bar{w} = 0$, and in fact for the definitions of the vectors t_i and u_i given in this section the form of the search directions is identical if we let $w = 0$, but it must be noted that the termination conditions are different in the two cases.

Our interest in what follows is to assign values to u_i and t_i in terms of the known quantities at the current point; the definitions for v and w will be specified later as a function of the properties of the search direction p_k. In order to identify satisfactory values for these vectors in the curvilinear search, we need to study the form of the first and second derivatives of the merit function at zero, as these are the values that will be used in the termination criteria. We start by forming the corresponding derivatives at any point. The first derivative is given by

$$\phi^{C'}(\alpha) = \nabla F(x_\alpha)^T(2\alpha v + w) - \phi_1^{C'}(\alpha) + \rho\phi_2^{C'}(\alpha),$$

where

$$\phi_1^{C'}(\alpha) = (2\alpha t_1 + t_2)^T\Big(c(x_\alpha) - s_\alpha\Big) + \lambda_\alpha^T\Big(\nabla c(x_\alpha)(2\alpha v + w) - 2\alpha u_1 - u_2\Big)$$

and

$$\phi_2^{C'}(\alpha) = \Big(c(x_\alpha) - s_\alpha\Big)^T\Big(\nabla c(x_\alpha)(2\alpha v + w) - 2\alpha u_1 - u_2\Big).$$

For the second derivative we have

$$\phi^{C''}(\alpha) = (2\alpha v + w)^T\nabla^2 F(x_\alpha)(2\alpha v + w) + 2\nabla F(x_\alpha)^T v - \phi_1^{C''}(\alpha) + \rho\phi_2^{C''}(\alpha),$$

where

$$\begin{aligned} \phi_1^{C''}(\alpha) = {} & 2(2\alpha t_1 + t_2)^T\Big(\nabla c(x_\alpha)(2\alpha v + w) - 2\alpha u_1 - u_2\Big) + 2t_1^T\Big(c(x_\alpha) - s_\alpha\Big) \\ & + \lambda_\alpha^T\Big(2\nabla c(x_\alpha)v - 2u_1\Big) + \textstyle\sum_i \lambda_{\alpha_i}(2\alpha v + w)^T\nabla^2 c_i(x_\alpha)(2\alpha v + w) \end{aligned}$$

and

$$\phi_2^{C''}(\alpha) = \|\nabla c(x_\alpha)(2\alpha v + w) - 2\alpha u_1 - u_2\|^2 + \Big(c(x_\alpha) - s_\alpha\Big)^T\Big(2\nabla c(x_\alpha)v - 2u_1\Big)$$
$$+ \textstyle\sum_i \Big(c_i(x_\alpha) - s_{\alpha_i}\Big)(2\alpha v + w)^T\nabla^2 c_i(x_\alpha)(2\alpha v + w).$$

As we mentioned earlier, we are interested in studying the values of these derivatives when $\alpha = 0$, given that the termination criteria for the linesearch make use of these values; their form will determine the definition of u_i, t_i. For the first derivative we have

$$\phi^{C'}(0) = g^T w - t_2^T(c - s) - \lambda^T(Aw - u_2) + \rho(c - s)^T(Aw - u_2),$$

and letting

$$u_2 \equiv Aw, \qquad t_2 \equiv 0, \tag{6.2.2}$$

we obtain

$$\phi^{C'}(0) = g^T w. \tag{6.2.3}$$

For the second derivative,

$$\phi^{C''}(0) = w^T\nabla^2 F w + 2g^T v - 2t_1^T(c - s) - 2t_2^T(Aw - u_2) - 2\lambda^T(Av - u_1)$$
$$+ \textstyle\sum_i \Big(\rho(c_i - s_i) - \lambda_i\Big) w^T\nabla^2 c_i w + \rho\|Aw - u_2\|^2 + 2\rho(c - s)^T(Av - u_1),$$

and after replacing the expressions for u_2 and t_2, we obtain

$$\phi^{C''}(0) = w^T\nabla^2 F w + 2g^T v - 2t_1^T(c - s) + 2\Big(\rho(c - s) - \lambda\Big)^T(Av - u_1)$$
$$+ \textstyle\sum_i \Big(\rho(c_i - s_i) - \lambda_i\Big) w^T\nabla^2 c_i w.$$

Define

$$u_1 \equiv Av + c - s + \omega, \quad t_1 \equiv \mu - \lambda, \tag{6.2.4}$$

for some vector ω to be defined later on, implying

$$\phi^{C''}(0) = w^T\nabla^2 L w + 2g^T v + 2(2\lambda - \mu)^T(c - s) - 2\rho\|c - s\|^2$$
$$+ 2\omega^T\Big(\lambda - \rho(c - s)\Big) + \textstyle\sum_i \rho(c_i - s_i) w^T\nabla^2 c_i w. \tag{6.2.5}$$

To make sure that the last terms in (6.2.5) take acceptable values, we select ω to satisfy

$$\omega_i = \begin{cases} 0 & \text{if } (c_i - s_i)w^T\nabla^2 c_i w \le 0, \quad |w^T\nabla^2 c_i w| \le |c_i - s_i|, \\ & \quad \text{or } \sum_i (c_i - s_i)w^T\nabla^2 c_i w \le \|c - s\|^2; \\ -\dfrac{\rho}{2}\dfrac{(c_i - s_i)w^T\nabla^2 c_i w}{\lambda_i - \rho(c_i - s_i)} & \text{otherwise.} \end{cases}$$

If $\lambda_i - \rho(c_i - s_i)$ is very small or zero, and the first set of conditions does not apply, this definition is unsatisfactory because ω_i is either undefined or unacceptably large. To avoid this problem, we modify the current value of ρ, attempting to attain two goals: we want the new value for ρ, say $\bar{\rho}$, to be bounded by a finite multiple of its existing value, and we want ω to be bounded by a multiple of $\|w\|^2$. We start by imposing the following condition:

$$\left|\frac{\bar{\rho}}{2}\frac{c_i - s_i}{\lambda_i - \bar{\rho}(c_i - s_i)}\right| \leq K \tag{6.2.6}$$

for some $K > 1$. Note that this bound implies that our second goal, $\|\omega\| = O(\|w\|^2)$, is attained.

We now show that our first goal can also be achieved. If the previous condition is not satisfied for the current value of ρ, then we must have

$$\left|\frac{\lambda_i}{\rho(c_i - s_i)} - 1\right| < \frac{1}{2K}, \tag{6.2.7}$$

and for that to hold it must also be true that $\lambda_i(c_i - s_i) > 0$, so we can write

$$\frac{\lambda_i}{c_i - s_i}\frac{2K}{2K+1} < \rho < \frac{\lambda_i}{c_i - s_i}\frac{2K}{2K-1}; \tag{6.2.8}$$

but if ρ is in this interval, then

$$\frac{2K+1}{2K-1}\rho \geq \frac{\lambda_i}{c_i - s_i}\frac{2K}{2K-1}, \tag{6.2.9}$$

and in general there exists a value

$$\bar{\rho} \in \left[\rho, \left(\frac{2K+1}{2K-1}\right)^m \rho\right] \tag{6.2.10}$$

for which the desired bound on ω holds.

With this definition,

$$-2\rho\|c - s\|^2 + 2\omega^T\big(\lambda - \rho(c - s)\big) + \textstyle\sum_i \rho(c_i - s_i) w^T \nabla^2 c_i w \leq -\rho\|c - s\|^2.$$

Negative curvature and descent

We now present the rules to decide how to select the linesearch model used in each iteration, and if the curvilinear search is to be used, how to define the values for v and w. Once the search direction p has been computed, let

a) $v = 0,\ w = p$ if $p^T H p < 2g^T p \le 0$,
b) $v = (1+\gamma)p,\ w = -\gamma p$ if $p^T H p < 0,\ g^T p > 0$ and $-p^T H p \ge k g^T p$,
c) use a normal linesearch otherwise,

where k is a constant satisfying $0 < k \le 1$, and γ is defined from

$$k = 2\left(\frac{2\gamma+1}{2\gamma^2-1}\right).$$

The convergence proofs make use of several properties that follow from the definitions of v and w. If we define

$$f_p \equiv \begin{cases} 2g^T v + w^T H w & \text{for cases a) and b)}, \\ 2g^T p & \text{for case c)}, \end{cases}$$

then for the different cases,

a) $f_p = p^T H p \le g^T p + \frac{1}{2} p^T H p$,
b) $f_p = 2(\gamma+1) g^T p + \gamma^2 p^T H p \le g^T p - (\gamma^2 - \frac{1}{2}) p^T H p + \gamma^2 p^T H p = g^T p + \frac{1}{2} p^T H p$,
c) $f_p = 2g^T p \le g^T p + \frac{1}{2} p^T H p$ if $g^T p \le p^T H p$,
$f_p = 2g^T p \le 2g^T p + p^T H p$ if $0 \le p^T H p < 2g^T p$,
$f_p = 2g^T p \le 2g^T p + \frac{2}{2-k}(k g^T p + p^T H p) = \frac{2}{2-k}(2g^T p + p^T H p)$ otherwise.

From (6.1.2) and these results,

$$f_p \le \min\Big(-\beta_1\|p\|^2 + \beta_2\|r\|, \frac{4}{2-k}(-\beta_1\|p\|^2 + \beta_2\|r\|)\Big) \le -\beta_1\|p\|^2 + 4\beta_2\|r\|. \tag{6.2.11}$$

A second useful inequality is

$$f_p \le 2g^T p, \tag{6.2.12}$$

following from one of the alternative cases

a) $f_p = p^T H p < 2g^T p$,
b) $f_p = 2(\gamma+1) g^T p + \gamma^2 p^T H p \le (2(\gamma+1) - k\gamma^2) g^T p = \frac{1}{2}(2-k) g^T p \le 2g^T p$,
c) $f_p = 2g^T p$.

Another interesting property of the previous definition is given in the next lemma.

Lemma 6.2.1. *There exists an $\epsilon_d > 0$ such that if $\|p_k\| < \epsilon_d$, then a normal linesearch is used.*

Proof. Assume that the lemma does not hold. Then there exists a sequence $\{x_k\}$, and an associated sequence of search directions $\{p_k\}$, such that $p_k \to 0$ and p_k satisfies the conditions for cases a) or b). Without loss of generality, assume that the sequence $\{x_k\}$ is convergent, and let the limit point be x^*, a second-order KKT point for problem NLP, from Lemma 6.1.1.

Define a new sequence of vectors $\{\nu_k\}$ from

$$\nu_k = \frac{p_k}{\|p_k\|},$$

and select a convergent subsequence where either case a) or case b) holds for all k. (The index k will also be used to denote the elements in the subsequence.) Let ν^* be the limit point for the subsequence.

From the conditions for cases a) and b),

$$|p_k^T H_k p_k| \geq k|g_k^T p_k| \Rightarrow |p_k^T H_k \nu_k| \geq k|g_k^T \nu_k|,$$

and in the limit $g^{*T}\nu^* = 0$. But this implies $\lambda^{*T}A^*\nu^* = 0$, and from strict complementarity $\nu^* \in \mathcal{N}(\hat{A}^*)$. We also have

$$\forall k \quad p_k^T H_k p_k < 0 \Rightarrow \nu^{*T}H^*\nu^* \leq 0,$$

but this contradicts the fact that we must have a strong minimizer, from assumption **A6**, proving the result. ∎

This result allows us to define the following constant. From Lemmas 6.1.1 and 3.4.1, assumption **A6** and Lemma 6.2.1,

ϵ_s is a positive constant such that $\|p_k\| \leq \epsilon_s$ implies that p_k has been obtained as a second-order KKT point, the correct active set has been identified, the smallest eigenvalue of the reduced Hessian is at least $\frac{1}{2}\beta_{svH}$, and a normal linesearch is used.

Finally, note that for cases a) and b), $\phi^{C'}(0) \leq 0$.

Linesearch termination

When we use the curvilinear search, it may no longer be possible to satisfy the termination conditions given for the normal linesearch in Chapter 2, (2.2.3) and (2.2.4); consequently, they need to be replaced. Satisfactory termination criteria of a similar type to those given in Chapter 2 are now presented. A check is made whether the condition

$$\phi^C(1) \leq \phi^C(0) + \tfrac{1}{2}\sigma\phi^{C''}(0) \tag{6.2.13}$$

is satisfied by the step $\alpha = 1$. If not, then a value $\alpha \in (0,1)$ satisfying

$$\phi^c(\alpha) \le \phi^c(0) + \sigma\frac{\alpha^2}{2}\phi^{c''}(0) \tag{6.2.14a}$$

$$\phi^{c'}(\alpha) \ge \eta\Big(\phi^{c'}(0) + \alpha\phi^{c''}(0)\Big) \tag{6.2.14b}$$

for $1 > \eta > \sigma > 0$ and $\frac{1}{2} > \sigma$, is computed as the step length. The existence of a value α satisfying (6.2.14) will be shown in Lemma 6.3.6.

From the definitions of v and w, when case b) applies the form of the step in the original variables is given by $\alpha((1+\gamma)\alpha - \gamma)p$. A consequence of this expression is that for a value

$$\alpha = \frac{\gamma}{1+\gamma}$$

we get no change in the x variables. Though this step has no effect on the convergence proofs (since we are still making finite changes in the other variables), such a step may be considered unsatisfactory from a practical point of view. We present an alternative linesearch criterion for this case.

Let

$$\hat{\alpha} = \frac{\gamma}{2(1+\gamma)}.$$

If (6.2.13) holds, then let $\alpha = 1$; otherwise, check condition (6.2.14a) for $\alpha = \hat{\alpha}$:

$$\phi^c(\hat{\alpha}) \le \phi^c(0) + \sigma\frac{\hat{\alpha}^2}{2}\phi^{c''}(0). \tag{6.2.15}$$

If this condition is not satisfied either, compute a value $\alpha \in (0, \hat{\alpha})$ satisfying (6.2.14).

6.3. Definition and properties of the penalty parameter

To guarantee convergence of the algorithm, each step must satisfy a sufficient descent condition. This implies the need to select the penalty parameter in such a way that the initial derivatives of the merit function (the quantities bounding the descent achieved in the linesearch) take acceptable values, and in particular, property **P4** (suitably extended) holds for the algorithm, both when the normal linesearch and when the curvilinear search are used. The next paragraphs indicate a way in which this can be done for both cases, and the rest of the section presents the properties associated with this definition.

Definition of the penalty parameter

When trying to show that property **P4** holds for this algorithm, we face an immediate complication. There is no longer any quantity readily available that provides a good measure for the bound $\beta_H\|p_k\|^2$ on the initial derivatives for the linesearch. For example, the values used in Chapters 4 and 5, p^THp and $p_Z^T\bar{Z}^TH\bar{Z}p_Z + \|\bar{c} + w_c\|^2$ respectively, may not even be positive. Consequently, we introduce in this section a definition of ρ_k based on the value of the penalty parameter that makes the corresponding derivatives zero, with the addition of adequate safeguards.

Let

$$\Upsilon \equiv \begin{cases} 2w^T(\lambda - \rho(c-s)) + \sum_i \rho(c_i - s_i)w^T\nabla^2 c_i w & \text{for the curvilinear search,} \\ 0 & \text{for the normal linesearch;} \end{cases}$$

and

$$f_\rho \equiv f_p + 2(2\lambda - \mu)^T(c - s).$$

From (6.2.11),

$$f_\rho \le -\beta_1\|p\|^2 + \beta_2'\|c - s\|,$$

where we can assume that $\beta_2' \ge \beta_1$.

Define ρ_1' from

$$\rho_1' \equiv \begin{cases} \dfrac{2f_\rho}{\|c-s\|^2} & \text{if } \Upsilon > 0, \\ \dfrac{f_\rho}{\|c-s\|^2} & \text{otherwise.} \end{cases}$$

Let ρ^- denote the value of the penalty parameter at the previous iteration. If $\rho^- = 0$ and $\rho_1' \le 0$, replace f_ρ in the previous definition by $f_\rho + \beta_h\|p\|^2$, where $\beta_h > 0$ is some specified parameter, and recompute the value for ρ_1 accordingly.

Let

$$\theta = \|\bar{c}\|^2 + (\mu - \hat{\mu})^T c - (p + Zp_Z)^T HYp_Y,$$

$$b_i = \begin{cases} 0 & \text{if } \|\bar{c}\| = 0 \text{ or the constraint is not active,} \\ -\dfrac{\theta}{\|\bar{c}\|^2}c_i & \text{otherwise,} \end{cases}$$

where $\hat{\mu}$ denotes the QP multipliers at the solution of the QP subproblem, if available, or the multiplier estimate otherwise.

From the non-singularity of the Jacobian at any limit point of the sequence $\{x_k\}$ (assumption **A3**), there exists a constant $\beta_{svA} > 0$ such that

$$AYp_Y \geq \beta_{svA}\|Yp_Y\| \Rightarrow \frac{\|Yp_Y\|}{\|\bar{c}\|} \leq \frac{1}{\beta_{svA}} = N.$$

It follows that b satisfies

$$\|b\| \leq \|\bar{c}\| + \|\mu - \hat{\mu}\| + N\|H(p + Zp_Z)\|.$$

This implies the boundedness of $\|b\|$ and also from Lemma 3.4.1 and condition **C8**,

$$\|p_k\| \to 0 \Rightarrow \|b_k\| \to 0.$$

Define ρ_2 from

$$\rho_2 \equiv \begin{cases} \dfrac{\|2\xi + b\|}{2\|c - s\|} & \text{if } \frac{1}{2}\phi^{C''}(0,\rho^-) > -p_Z^T Z^T H Z p_Z - \|\bar{c}\|^2 \\ & \quad \text{or } \phi^{N'}(0,\rho^-) > -p_Z^T Z^T H Z p_Z - \|\bar{c}\|^2, \\ 0 & \text{otherwise.} \end{cases}$$

To define a bound for the penalty parameter, we introduce a positive constant β_{th}, and let

$$\bar{\rho} \equiv \begin{cases} \max(\rho_1, \rho_2) & \text{if } \|p\| < \beta_{th} \text{ and } \|c - s\| > \|p\|^2, \\ \max(\rho_1, 0) & \text{otherwise.} \end{cases}$$

Also, let

$$\rho_m \equiv \begin{cases} \rho_{\min} & \text{if } \rho^- = 0, \\ 2\rho^- & \text{otherwise.} \end{cases}$$

Finally, the bound $\hat{\rho}$ is given by

$$\hat{\rho} \equiv \begin{cases} 2\bar{\rho} & \text{if } 2\bar{\rho} > \rho_m, \\ \rho_m & \text{if } \rho_m \geq 2\bar{\rho} > \rho^-, \\ \rho^- & \text{if } \rho^- \geq 2\bar{\rho}. \end{cases}$$

From this definition it immediately follows that $\hat{\rho} \geq 2\bar{\rho}$, and if $\hat{\rho} > 0$ then $\hat{\rho} \geq \rho_{\min}$.

Properties of the penalty parameter

From the previous definition we can show that property **P4** holds for the algorithm.

Lemma 6.3.1. *For $\hat{\rho}_k \geq 0$ defined as above, there exists a constant $\beta_H > 0$ such that either*

$$\begin{aligned} \phi_k^{C''}(0,\rho) &\leq -\beta_H \|p_k\|^2, \quad \text{or} \\ \phi_k^{N'}(0,\rho) &\leq -\beta_H \|p_k\|^2, \end{aligned} \tag{6.3.1}$$

for all $\rho \geq \hat{\rho}_k$.

Proof. Define a value ϵ' such that $\min(\beta_{th}, \epsilon_s) \geq \epsilon' > 0$, and whenever $\|p_k\| \leq \epsilon'$ we have $(\mu_k + b_k)^T s_k \geq 0$. Consider the following cases:

- If $\|c - s\| \leq \dfrac{\beta_1}{2\beta_2'}\|p\|^2$, then

$$\begin{aligned} \phi^{C''}(0,\hat{\rho}) &= f_\rho + \Upsilon - 2\hat{\rho}\|c - s\|^2 \leq f_\rho \leq -\tfrac{1}{2}\beta_1\|p\|^2, \\ \phi^{N'}(0,\hat{\rho}) &= \tfrac{1}{2}f_\rho - \hat{\rho}\|c - s\|^2 \leq \tfrac{1}{2}f_\rho \leq -\tfrac{1}{4}\beta_1\|p\|^2. \end{aligned}$$

- If $\|c - s\| > \dfrac{\beta_1}{2\beta_2'}\|p\|^2$ and $\|p\| > \epsilon'$, then if $\hat{\rho} > 0$, from $\hat{\rho} \geq \rho_1$,

$$f_\rho + \Upsilon - 2\hat{\rho}\|c - s\|^2 \leq -\tfrac{1}{2}\hat{\rho}\|c - s\|,$$

  implying

$$\begin{aligned} \phi^{C''}(0,\hat{\rho}) &\leq -\tfrac{1}{2}\rho_{\min}\|c - s\|^2 \leq -\tfrac{1}{2}\rho_{\min}\Big(\frac{\epsilon'\beta_1}{2\beta_2'}\Big)^2\|p\|^2, \\ \phi^{N'}(0,\hat{\rho}) &\leq -\tfrac{1}{2}\rho_{\min}\|c - s\|^2 \leq -\tfrac{1}{2}\rho_{\min}\Big(\frac{\epsilon'\beta_1}{2\beta_2'}\Big)^2\|p\|^2. \end{aligned}$$

  If $\hat{\rho} = 0$,

$$\begin{aligned} \phi^{C''}(0,\hat{\rho}) &\leq -\beta_h\|p\|^2, \\ \phi^{N'}(0,\hat{\rho}) &\leq -\tfrac{1}{2}\beta_h\|p\|^2. \end{aligned}$$

- If $\|c - s\| > \dfrac{\beta_1}{2\beta_2'}\|p\|^2$ and $\|p\| \leq \epsilon'$, from $\|p\| \leq \epsilon_s$ we must have used the normal linesearch, and from the definition of $\hat{\rho}$ it must hold that $\hat{\rho} \geq \max(\rho^-, \rho_2)$.

$$\begin{aligned} \phi^{N'}(0,\hat{\rho}) &= -p^T H p - \bar{\mu}^T c + (2\lambda - \mu)^T(c - s) - \hat{\rho}\|c - s\|^2 \\ &= -p_z^T Z^T H Z p_z - \|\bar{c}\|^2 - (2\xi + b)^T(c - s) - (\mu + b)^T s - \hat{\rho}\|c - s\|^2 \\ &\leq -2p_z^T Z^T H Z p_z - 2\|\bar{c}\|^2 \\ &\leq -\beta_q\|p\|^2, \end{aligned} \tag{6.3.2}$$

implying that property **P4** holds. ∎

Following the procedure outlined in Chapter 3 for the global convergence proof, the next step is to establish bounds for the rate of growth of the penalty parameter. The next lemma shows that property **P5** holds for this algorithm.

Lemma 6.3.2. *For any iteration k_l in which the value of ρ is modified,*

$$\rho_{k_l}\|p_{k_l}\|^2 \le N$$

and

$$\rho_{k_l}\|c_{k_l} - s_{k_l}\| \le N,$$

for some constant N.

Proof. We show first that for some positive constant K, whenever the value of ρ has to be modified,

$$\|c - s\| \ge K\|p\|^2. \tag{6.3.3}$$

Considering the cases introduced in the last lemma, whenever

$$\|c - s\| \ge \frac{\beta_1}{2\beta_2'}\|p\|^2$$

the result holds immediately. If this is not the case, assuming that $\beta_2' > \beta_1 + \beta_h$ it follows that $\bar{\rho} = \max(\rho_1, 0)$ and from

$$f_\rho \le -\beta_1\|p\|^2 + \beta_2'\|c - s\| < -\beta_2'\|c - s\| < 0,$$

we must have $\rho_1 \le 0$ and $\hat{\rho}$ is not modified.

Also,

$$\rho_2\|c - s\| = \|2\xi + b\| \le N_1,$$

and

$$\rho_1\|c - s\|^2 \le f_\rho + \beta_h\|p\|^2 \le (\beta_h - \beta_1)\|p\|^2 + \beta_2'\|c - s\| \le \left(\beta_2' + \frac{\beta_h - \beta_1}{K}\right)\|c - s\|,$$

implying

$$\rho_1\|c - s\| \le N_2$$

and

$$\hat{\rho}\|c - s\| \le N,$$

but from $\|c - s\| \geq K\|p\|^2$ it follows that

$$\hat{\rho}\|p\|^2 \leq N,$$

completing the desired result. ∎

The proof now proceeds along the same lines as those given in Chapter 3. If the normal linesearch is used, for the corresponding iterations the results given in Lemmas 3.6.1 to 3.6.6 hold as given in Chapter 3. If the curvilinear search is used, it is necessary to modify the proofs for some of these results, as follows.

Lemma 6.3.3. *At any iteration where ρ has to be modified,*

$$c^T\tilde{\mu} < N_1\|p\|^2 + N_2\|c - s\|,$$

where $\tilde{\mu}$ denotes the QP multipliers, and N_1 and N_2 are positive constants.

Proof. If $\|p\| \geq \epsilon_s$, the result follows from assumptions **A2** and **A3**. If $\|p\| < \epsilon_s$, then p has been obtained as the solution for the QP subproblem, and it satisfies

$$g^Tp + p^THp = -c^T\tilde{\mu}.$$

Furthermore, a normal linesearch has been performed.

Let ρ^- denote the value of the parameter before being modified; if $\bar{\rho} = \rho_1$, then

$$\phi^{N'}(0, \rho^-) > \phi^{N'}(0, \hat{\rho}) \geq -\tfrac{1}{2}f_\rho \geq \tfrac{1}{2}\beta_1\|p\|^2 - \tfrac{1}{2}\beta_2'\|c - s\|, \tag{6.3.4}$$

and if $\bar{\rho} = \rho_2$,

$$\phi^{N'}(0, \rho^-) > -p_Z^TZ^THZp_Z - \|\bar{c}\|^2 \geq -\beta_{lh}\|p\|^2. \tag{6.3.5}$$

From

$$\phi^{N'}(0, \rho^-) = p^Tg + (2\lambda - \mu)^T(c - s) - \rho^-\|c - s\|^2$$

and the previous equations,

$$\begin{aligned} c^T\tilde{\mu} &= -p^THp - \phi^{N'}(0, \rho^-) + (2\lambda - \mu)^T(c - s) - \rho^-\|c - s\|^2 \\ &< \beta_{lh}\|p\|^2 + (\beta_2' + \|2\lambda - \mu\|)\|c - s\| - \rho^-\|c - s\|^2. \end{aligned}$$

From the nonnegativity of $\rho^-\|c - s\|^2$ and the boundedness of the Lagrange multiplier estimate the desired result follows. ∎

The proof of Lemma 3.6.2 does not require any modification for this case. The proof of Lemma 3.6.3 needs to be slightly modified, as follows.

Lemma 6.3.4. *There exists a bounded constant M such that, for all l,*

$$\rho_{k_l} \sum_{k=k_l}^{k_{l+1}-1} \|\alpha_k p_k\|^2 < M. \tag{6.3.6}$$

Proof. In the case when a normal linesearch is used, the proof follows along the same lines as the proof for Lemma 3.6.3. For the case when a curvilinear search is used, consider the following argument.

The subscripts 0 and K denote quantities associated with iterations k_l and k_{l+1} respectively. Consider the identity

$$\phi_0^C - \phi_K^C = \sum_{k=0}^{K-1} (\phi_k^C - \phi_{k+1}^C), \tag{6.3.7}$$

and observe that the termination criterion for the linesearch (6.2.14) and the fact that the penalty parameter is not increased, imply that for $0 \le k \le K-1$,

$$\phi_k^C - \phi_{k+1}^C \ge -\sigma\alpha_k^2 \phi_k^{C''}, \tag{6.3.8}$$

where $0 < \sigma < 1$. Since α_k, σ and β_H are positive, combining (6.3.7), (6.3.8) and the result of Lemma 6.3.1 gives

$$\tfrac{1}{2}\sigma\beta_H \sum_{k=0}^{K-1} \alpha_k^2 \|p_k\|^2 \le \phi_0^C - \phi_K^C.$$

Rearranging terms we obtain

$$\tfrac{1}{2}\sigma\beta_H \sum_{k=0}^{K-1} \|\alpha_k p_k\|^2 \le \phi_0^C - \phi_K^C. \tag{6.3.9}$$

The result then follows by multiplying (6.3.9) by ρ_0 and using Lemma 3.6.2. ∎

Lemma 3.6.4 does not require any modification.

Lemma 3.6.5 applies directly to the case when a normal linesearch is performed. The corresponding version of this result for the case when we use a curvilinear search is given in the following lemma.

Lemma 6.3.5. *For $0 \le \theta < \alpha_k$,*

$$\phi_k^{C'''}(\theta) \le -6\alpha_k \phi_k^{C''}(0) - 12\alpha_k \phi_k^{C'}(0) + N\|p_k\|^2,$$

where N is a constant independent of k.

Proof. The third derivative of ϕ^C is given by

$$\begin{aligned}\phi^{C'''}(\alpha) &= 6v^T\nabla^2F(x_\alpha)(2\alpha v+w)+\textstyle\sum_i(2\alpha v_i+w_i)(2\alpha v+w)^T\nabla_i^3F(x_\alpha)(2\alpha v+w)\\ &\quad -\phi_1^{C'''}(\alpha)+\rho\phi_2^{C'''}(\alpha),\end{aligned}$$

where

$$\begin{aligned}\phi_1^{C'''}(\alpha) &= 6t_1^T\Big(\nabla c(x_\alpha)(2\alpha v+w)-2\alpha u_1-u_2\Big)+6(2\alpha t_1+t_2)^T\Big(\nabla c(x_\alpha)v-2u_1\Big)\\ &+3\textstyle\sum_i(2\alpha t_{1_i}+t_{2_i})(2\alpha v+w)^T\nabla^2c_i(x_\alpha)(2\alpha v+w)+6\sum_i\lambda_{\alpha_i}v^T\nabla^2c_i(x_\alpha)(2\alpha v+w)\\ &+\textstyle\sum_i\lambda_{\alpha_i}\sum_k(2\alpha v_k+w_k)(2\alpha v+w)^T\nabla_k^3c_i(x_\alpha)(2\alpha v+w)\end{aligned}$$

and

$$\begin{aligned}\phi_2^{C'''}(\alpha) &= 6\Big(\nabla c(x_\alpha)(2\alpha v+w)-2\alpha u_1-u_2\Big)^T\Big(2\nabla c(x_\alpha)v-2u_1\Big)\\ &\quad+3\textstyle\sum_i\Big(\nabla c_i(x_\alpha)(2\alpha v+w)-2\alpha u_{1_i}-u_{2_i}\Big)(2\alpha v+w)^T\nabla^2c_i(x_\alpha)(2\alpha v+w)\\ &\quad+\textstyle\sum_i\Big(c_i(x_\alpha)-s_{\alpha_i}\Big)\sum_k(2\alpha v_k+w_k)(2\alpha v+w)^T\nabla_k^3c_i(x_\alpha)(2\alpha v+w)\\ &\quad+6\textstyle\sum_i\Big(c_i(x_\alpha)-s_{\alpha_i}\Big)v^T\nabla^2c_i(x_\alpha)(2\alpha v+w).\end{aligned}$$

To compute a bound for the third derivative, the following Taylor expansions are useful:

$$\begin{aligned}\nabla c_i(x_\alpha)(2\alpha v+w)-2\alpha u_{1_i}-u_{2_i} &= -2\alpha\Big(c_i-s_i+\omega_i-w^T\nabla^2c_iw-(2\alpha v+w)^T\nabla^2c_i(z_i)(2\alpha v+w)\Big),\\ c_i(x_\alpha)-s_{\alpha_i} &= (1-\alpha^2)(c_i-s_i)-\alpha^2\Big(\omega_1+\tfrac{1}{2}w^T\nabla^2c_iw-\tfrac{1}{2}(2\alpha v+w)^T\nabla^2c_i(z_i')(2\alpha v+w)\Big).\end{aligned}$$

From these results, the definitions of v and w and Lemmas 6.3.4 and 3.6.4, it follows that

$$\begin{aligned}\phi^{C'''}(\alpha) &= 24\alpha t_1^T(c-s)+12\alpha\rho\|c-s\|^2+O(\|p\|^2)\\ &= 24\alpha t_1^T(c-s)+6\alpha w^T\nabla^2Fw+12\alpha g^Tv+12\alpha(\lambda-t_1)^T(c-s)-6\alpha\phi^{C''}(0)+O(\|p\|^2)\\ &= 12\alpha\mu^T(c-s)+12\alpha g^Tv-6\alpha\phi^{C''}(0)+O(\|p\|^2).\end{aligned}$$

We must now consider two cases. If $v\neq 0$ we can write

$$\phi^{C'''}(\alpha)=12\alpha v^T(g-A^T\mu)-6\alpha\phi^{C''}(0)-12\alpha\mu^Ts+O(\|p\|^2), \tag{6.3.10}$$

and if $w\neq 0$ but $v=0$ then

$$\phi^{C'''}(\alpha)=12\alpha w^T(g-A^T\mu)-6\alpha\phi^{C''}(0)-12\alpha\phi^{C'}(0)-12\alpha\mu^Ts+O(\|p\|^2). \tag{6.3.11}$$

From condition **C8** on the multipliers, implying that for large enough k, $\mu^T s \geq 0$, the final result follows:

$$\phi^{C'''}(\alpha) \leq -6\alpha\phi^{C''}(0) - 12\alpha\phi^{C'}(0) + N\|p\|^2 \tag{6.3.12}$$

for some positive constant N. ∎

It is now possible to prove that the steplength α_k is also bounded away from zero in the case when a curvilinear search is performed. For the normal linesearch, the equivalent result is given in Lemma 3.6.6.

Lemma 6.3.6. *If a curvilinear search is performed, the steplength α_k $(0 < \alpha_k \leq 1)$ satisfies*

$$\phi_k^C(\alpha_k) - \phi_k^C(0) \leq \sigma\frac{\alpha_k^2}{2}\phi_k^{C''}(0)$$

and $\alpha_k \geq \bar{\alpha}$, where $0 < \sigma < 1$, and $\bar{\alpha} > 0$ is independent of the iteration.

Proof. We show that a step satisfying the conditions for the curvilinear search termination criteria exists and is uniformly bounded away from zero. To take into account the variant in the termination conditions introduced for case b), let $\tilde{\alpha}$ denote a given initial value, to be selected as either 1 or $\hat{\alpha}$.

Assume that condition (6.2.14a) is not satisfied for $\alpha = \tilde{\alpha}$; that is,

$$\phi^C(\tilde{\alpha}) > \phi^C(0) + \sigma\frac{\tilde{\alpha}^2}{2}\phi^{C''}(0).$$

Define

$$\psi_\sigma(\alpha) = \phi^C(\alpha) - \phi^C(0) - \sigma\frac{\alpha^2}{2}\phi^{C''}(0),$$

so that

$$\begin{aligned}\psi'_\sigma(\alpha) &= \phi^{C'}(\alpha) - \sigma\alpha\phi^{C''}(0),\\ \psi''_\sigma(\alpha) &= \phi^{C''}(\alpha) - \sigma\phi^{C''}(0).\end{aligned}$$

For $\alpha = 0$,

$$\begin{aligned}\psi_\sigma(0) &= 0,\\ \psi'_\sigma(0) &= \phi^{C'}(0) \leq 0,\\ \psi''_\sigma(0) &= (1-\sigma)\phi^{C''}(0) < 0.\end{aligned}$$

Define also

$$\psi_\eta(\alpha) = \phi^C(\alpha) - \phi^C(0) - \eta\alpha\phi^{C'}(0) - \eta\frac{\alpha^2}{2}\phi^{C''}(0).$$

From $\psi_\sigma(\tilde{\alpha}) > 0$, there must exist a value $\alpha_1 \in (0, \tilde{\alpha})$ for which $\psi_\eta'(\alpha_1) \geq 0$. Otherwise, if $\psi_\eta'(\alpha) < 0$ for all $\alpha \in [0, \tilde{\alpha})$, integrating on this interval we have

$$\phi^C(\tilde{\alpha}) < \phi^C(0) + \eta\tilde{\alpha}\phi^{C'}(0) + \eta\frac{\tilde{\alpha}^2}{2}\phi^{C''}(0), \tag{6.3.13}$$

implying

$$\psi_\sigma(\tilde{\alpha}) < \eta\tilde{\alpha}\phi^{C'}(0) + \frac{\eta-\sigma}{2}\tilde{\alpha}^2\phi^{C''}(0) < 0. \tag{6.3.14}$$

Let α_1 be the smallest such point, implying that $\psi_\eta'(\alpha) < 0$ for all $\alpha \in [0, \alpha_1)$. If we integrate again between 0 and α_1,

$$\phi^C(\alpha_1) < \phi^C(0) + \eta\alpha_1\phi^{C'}(0) + \eta\frac{\alpha_1^2}{2}\phi^{C''}(0), \tag{6.3.15}$$

and

$$\psi_\sigma(\alpha_1) < \eta\alpha_1\phi^{C'}(0) + (\eta-\sigma)\frac{\alpha_1^2}{2}\phi^{C''}(0) < 0, \tag{6.3.16}$$

so α_1 satisfies the termination conditions.

For α_1 we have

$$\phi^{C'}(\alpha_1) - \eta\phi^{C'}(0) - \eta\alpha_1\phi^{C''}(0) = 0, \tag{6.3.17}$$

and using a series expansion for $\phi^{C'}$

$$\phi^{C'}(\alpha_1) = \phi^{C'}(0) + \alpha_1\phi^{C''}(0) + \frac{\alpha_1^2}{2}\phi^{C'''}(\theta), \tag{6.3.18}$$

where $\theta \in (0, \alpha_1]$.

The previous equations imply

$$(1-\eta)\phi^{C'}(0) + \alpha_1(1-\eta)\phi^{C''}(0) + \frac{\alpha_1^2}{2}\phi^{C'''}(\theta) = 0, \tag{6.3.19}$$

and as we know that a positive root exists, we must have $\phi^{C'''}(\theta) > 0$. The root is given by

$$\alpha_1 = -(1-\eta)\frac{\phi^{C''}(0)}{\phi^{C'''}(\theta)} + \sqrt{(1-\eta)^2\left(\frac{\phi^{C''}(0)}{\phi^{C'''}(\theta)}\right)^2 - 2(1-\eta)\frac{\phi^{C'}(0)}{\phi^{C'''}(\theta)}}, \tag{6.3.20}$$

and the following bound holds:

$$\alpha_1 \geq \max\left(-2(1-\eta)\frac{\phi^{C''}(0)}{\phi^{C'''}(\theta)}, \sqrt{-2(1-\eta)\frac{\phi^{C'}(0)}{\phi^{C'''}(\theta)}}\right). \tag{6.3.21}$$

From property **P4**, $\phi^{C''}(0) \le -\beta_H \|p\|^2$ and

$$\phi^{C'''}(\theta) \le -18 \min\Big(\phi^{C''}(0), \phi^{C'}(0)\Big) + N\|p\|^2$$

for some $N > 0$, giving

$$\alpha_1 \ge \max\left(\frac{2(1-\eta)\beta_H}{18\beta_H + N}, \sqrt{\frac{2(1-\eta)\beta_H}{18\beta_H + N}} \right), \tag{6.3.22}$$

completing the proof. ∎

We can now present the global convergence theorem for this algorithm.

Theorem 6.3.1. *The algorithm described in this chapter has the property that*

$$\lim_{k\to\infty} \|p_k\| = 0. \tag{6.3.23}$$

Proof. The proof is similar to the one for Theorem 4.3.1. We include it here for completeness.

If $\|p_k\| = 0$ for any finite k, the algorithm terminates and the theorem is true. Hence we assume that $\|p_k\| \ne 0$ for any k.

When there is no upper bound on the penalty parameter, the uniform lower bound on α from Lemmas 3.6.6 and 6.3.6, and the bounds on the growth of the penalty parameter given by Lemmas 3.6.3 and 6.3.4, imply that for any $\delta > 0$ we can find an iteration index K such that

$$\|p_k\| \le \delta \quad \text{for} \quad k \ge K,$$

which implies that $\|p_k\| \to 0$, as required.

In the bounded case, we know that there exists a value $\tilde{\rho}$ and an iteration index $\tilde{K}$ such that $\rho = \tilde{\rho}$ for all $k \ge \tilde{K}$. We consider henceforth only such values of k.

The proof is by contradiction. We assume that there exists $\epsilon > 0$ and an infinite subsequence $\{k_i\}$ such that $\|p_{k_i}\| \ge \epsilon$ for all i. Consider only indices i such that $k_i > \tilde{K}$. Every iteration after $\tilde{K}$ must yield a strict decrease in the merit function because, using Lemmas 3.6.6, 6.3.1 and 6.3.6, and the fact that the penalty parameter is not modified,

$$\phi(\alpha) - \phi(0) \le -\tfrac{1}{2}\sigma\bar{\alpha}^2\beta_H\|p\|^2 < 0.$$

The adjustment of the slack variables s in step (ii) of the algorithm can only lead to a further reduction in the merit function, as L is quadratic in s and the minimizer with respect to s_i is given by $c_i - \lambda_i/\rho$. For iterations from the subsequence we have

$$\phi(x_{k_{i+1}}) - \phi(x_k) < \phi(x_{k_i+1}) - \phi(x_k) \le -\tfrac{1}{2}\sigma\bar{\alpha}^2\beta_H\epsilon^2.$$

Therefore, since the merit function with $\rho = \tilde{\rho}$ decreases by at least a fixed quantity at every step in the subsequence, it must be unbounded below. But this is impossible, from assumptions **A1**, **A2** and Lemma 2.4.1. Therefore, (6.3.23) must hold. ∎

Corollary 6.3.1.

$$\lim_{k\to\infty} \|x_k - x^*\| = 0.$$

Proof. The result follows immediately from Theorem 6.3.1 and Lemma 3.4.1. ∎

Corollary 6.3.2.

$$\lim_{k\to\infty} \|\lambda_k - \lambda^*\| = 0.$$

Proof. The result follows from Lemma 3.7.1, given the results in Lemma 3.6.6 and Corollary 6.3.1. ∎

6.4. Rate of convergence

After global convergence has been established, the next step is to prove that under certain conditions the algorithm has a quadratic rate of convergence. Note that in this section we can always assume that Lemma 6.2.1 applies, as we are only interested in the limiting behavior of the algorithm. Consequently, we need only consider the case when a normal linesearch is used.

Again, it is necessary to start by presenting some results on the growth rate of the penalty parameter. The next lemma establishes property **P7** for the algorithm.

Lemma 6.4.1. *If there exists an infinite subsequence $\{k_l\}$ of iterations in which the penalty parameter is modified,*

$$\lim_{l\to\infty} \rho_{k_l} \|p_{k_l}\|^2 = 0,$$

and

$$\lim_{l\to\infty} \rho_{k_l} \|c_{k_l} - s_{k_l}\| = 0.$$

Proof. We drop the subscript k_l in what follows. From the definition of $\hat{\rho}$,

$$\rho_2 \|c - s\| = \|2\xi + b\|,$$

and from the fact that $\|b_k\| \to 0$ as $\|p_k\| \to 0$, it must hold that

$$\lim_{l\to\infty} \|2\xi_{k_l} + b_{k_l}\| = 0.$$

Assume that $\|p\| \le \epsilon_s$. From (6.3.2),

$$\phi^{N'}(0,\rho_2) \le -\beta_q\|p\|^2 < 0,$$

and from

$$\phi^{N'}(0,\tfrac{1}{2}\rho_1) = 0$$

it must hold that $\rho_1 \le 2\rho_2$, implying that

$$\lim_{l\to\infty} \rho_{k_l}\|c_{k_l} - s_{k_l}\| = 0.$$

We can now use (6.3.3) to get

$$\lim_{l\to\infty} \rho_{k_l}\|p_{k_l}\|^2 = 0,$$

completing the proof. ∎

The proofs for Lemmas 3.8.1, 3.8.2 and 3.8.3 hold for this algorithm.

Conditions for quadratic convergence

The last requirement for the proof of quadratic convergence is to establish that a unit step is always taken for points close enough to the solution (property **P8**). The condition needed to prove this result, and to ensure that the sequence $\{x_k - x^*\}$ converges quadratically, is a slightly modified version of condition **C12** on the multipliers:

C12". The multiplier estimate satisfies

$$\|\mu_k - \lambda^*\| = O(\|x_k + p_k - x^*\|).$$

Lemma 6.4.2. *If condition* **C12"** *is satisfied, there exists an iteration index $\bar{k}$ such that for all indices $k \ge \bar{k}$ a unit steplength is accepted: $\alpha_k = 1$.*

Proof. Assume that $\|p\|$ is small enough so that a normal linesearch has been performed. Given that condition **C11** in Chapter 4 is trivially satisfied for this algorithm (remember that $H_k \equiv W_k$), from Lemma 4.4.3 we have that

$$\|x_k + p_k - x^*\| = o(\|x_k - x^*\|);$$

using this result in condition **C12"** we obtain

$$\|\mu_k - \lambda^*\| = o(\|x_k - x^*\|).$$

Hence condition **C12** is also satisfied. We can now use the same argument presented in the proof of Theorem 4.4.1 to conclude that the desired result holds for this algorithm. ∎

The proof of quadratic convergence is given in the following theorem.

Theorem 6.4.1. *The algorithm presented in this chapter converges quadratically.*

Proof. It is enough to show that $\|x + p - x^*\| = O(\|x - x^*\|^2)$, as the previous lemma showed that a unit step is always taken for large k. Assume k to be large enough so that p_k is obtained as the solution of the QP subproblem, and the correct active set has been identified.

We drop the iteration index k in all that follows. Consider first the decomposition of $x + p - x^*$ into null-space and range-space components:

$$x - x^* = Zu + Yv.$$

For the range-space component, consider the series expansion restricted to the active constraints at the point:

$$0 = c^* = c + A(x^* - x) + O(\|x - x^*\|^2).$$

From $Ap = -c$ and the previous decomposition,

$$A(x + p - x^*) = O(\|x - x^*\|^2).$$

For the null-space component, consider the corresponding Taylor series expansions around x:

$$\begin{aligned} A^{*T}\lambda^* &= g^* = g + \nabla^2 F(x^* - x) + O(\|x - x^*\|^2), \\ A^{*T}\lambda^* &= A^T\lambda^* + \textstyle\sum_i \lambda_i^* \nabla^2 c_i(x^* - x) + O(\|x - x^*\|^2). \end{aligned}$$

Combining these two results,

$$H(x - x^*) + A^T\lambda^* = g + \textstyle\sum_i (\lambda_i - \lambda_i^*)\nabla^2 c_i(x - x^*) + O(\|x - x^*\|^2),$$

and from $Hp + g = A^T\tilde{\mu}$,

$$H(x + p - x^*) + A^T(\lambda^* - \tilde{\mu}) = \textstyle\sum_i(\lambda_i - \lambda_i^*)\nabla^2 c_i(x - x^*) + O(\|x - x^*\|^2).$$

Now using condition **C12"** on the multiplier estimate,

$$\mu_k - \lambda^* = O(\|x_k + p_k - x^*\|),$$

and assuming that $\|p\|$ is small enough so that a step of one is taken in all iterations and therefore $\lambda_k = \mu_{k-1}$, the previous equation reduces to

$$H(x + p - x^*) + A^T(\lambda^* - \tilde{\mu}) = O(\|x - x^*\|^2).$$

Putting these results together,

$$\begin{pmatrix} H & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} x + p - x^* \\ \lambda^* - \tilde{\mu} \end{pmatrix} = O(\|x - x^*\|^2),$$

and using the non-singularity of the reduced Hessian and the Jacobian of the active constraints at the solution,

$$\begin{pmatrix} x + p - x^* \\ \lambda^* - \tilde{\mu} \end{pmatrix} = O(\|x - x^*\|^2),$$

implying

$$\lim_{k\to\infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^2} = K < \infty,$$

completing the proof. ∎

6.5. Summary

In this chapter we have introduced and analyzed a third algorithm based on the framework algorithm of Chapter 2. Its distinctive feature is the use of exact Hessian matrices of the objective and constraint functions. As before, the search direction is obtained from an incomplete solution for the QP subproblem. Some conditions on the incomplete solution have been presented that allow some convergence properties of the algorithm to be established. The results are:

- When the search direction satisfies the conditions introduced in Section 6.1, the multiplier estimate satisfies conditions **C7–C9**, and the Hessian for the QP subproblem, H_k, is the exact Hessian of the Lagrangian function, then the algorithm is *globally convergent*.

- If the multiplier estimates μ_k satisfy the following condition:

  C12". $\|\mu_k - \lambda^*\| = O(\|x_k + p_k - x^*\|)$.

  Then the algorithm *converges quadratically.*

Chapter 7

Numerical Results

In this chapter we present numerical results obtained from an implementation of the algorithm described and analyzed in Chapter 4. The implementation has been written as a modification of NPSOL, with the only difference being the use of an incomplete solution for the QP subproblem as the search direction, and the consequences of this change on the rest of the algorithm. The details of the modification are given in the following section.

The purpose of the testing reported in this chapter is to demonstrate that the efficiency and robustness of the modified algorithm are comparable to those of NPSOL. Naturally, we can only test the hypothesis on the domain of problems NPSOL is designed to solve, namely problems having a moderate number of variables and constraints, although on these problems the opportunities for improvement are limited, as we discuss in later sections. What this implementation really tests is whether the introduction of flexibility in the determination of the search direction has a significant cost.

7.1. Implementation

In this section we describe the implementation used for the early-termination rules introduced in Chapter 2. The rest of the algorithm is identical to NPSOL, and a detailed description of other implementation issues can be found in Gill *et al.* [GMSW86a].

From the kth QP subproblem, the search direction p_k is computed according to the following steps. (The subscript k corresponding to the iteration number is dropped from now on.)

- An initial feasible point p_0 is obtained following the same procedure as NPSOL. Conditions (2.2.6) and (2.2.7) have *not* been implemented, as the feasibility phase in NPSOL seems to give results that are adequate with respect to these conditions.

- The solution process continues until the *first* stationary point $\hat{p}$ is reached, and the corresponding QP multipliers $\tilde{\mu}$ are computed. In all that follows we work with a multiplier vector μ that is weighted by the norms of the corresponding constraints,

$$\mu_i \equiv \tilde{\mu}_i \|a_i\|.$$

- Let ϵ_M denote machine precision. If

$$\forall i \quad \mu_i \geq -\sqrt{\epsilon_M}, \tag{7.1.1}$$

then $\hat{p}$ is taken as the search direction.

- If (7.1.1) does not hold, we can take a step away from a subset of the active constraints while decreasing the value of the QP objective function. To identify the set of active constraints to be deleted, define

$$\mu_{\min} \equiv \min_i \mu_i,$$

and introduce a vector e_I as

$$e_{I_i} \equiv \begin{cases} \|a_i\| & \text{if } \mu_i \leq \beta_{mb}\mu_{\min}, \\ 0 & \text{otherwise.} \end{cases}$$

For the results presented in the following sections, $\beta_{mb} = 10^{-3}$.

- There is also a limit on the maximum number of constraints to be deleted. If the previous condition is satisfied by more than a specified number of active constraints, β_{ml}, only the β_{ml} ones having the smallest multipliers are deleted. For the results given, $\beta_{ml} = 50$. For most problems this limit has no effect, since the total number of constraints is less than 50.

- The direction away from the selected constraints is obtained as the least-norm solution of the system

$$Ad = e_I;$$

that is, we define

$$d_Y = (AY)^{-1}e_I, \qquad d_Z = 0,$$

to obtain

$$d = Yd_Y.$$

- If α_c denotes the step to the nearest inactive constraint, and α_m is defined as in (2.2.9):

$$\alpha_m = -\frac{(g + H\hat{p})^T d}{d^T H d},$$

we define α as in condition **C3**:

$$\alpha = \min(\alpha_c, \alpha_m, \alpha_M),$$

where α_M is 10^{10} for this case.

- We obtain the search direction p from (2.2.11):

$$p \equiv \begin{cases} \hat{p} + \alpha d & \text{if } \|\hat{p}\| < \beta_{slp}\|\hat{p} + \alpha d\|, \\ \hat{p} & \text{otherwise,} \end{cases}$$

where $\beta_{slp} = 100$; with this value the step αd is accepted in nearly all cases.

- Finally, the multiplier estimate used in the linesearch is taken to be the QP multiplier if $p = \hat{p}$. Otherwise, it is taken to be the least-squares estimate λ_L obtained from

$$AA^T\lambda_L = Ag.$$

7.2. Test problems

The two algorithms, NPSOL and its variant using an incomplete solution for the QP subproblem as the search direction, have been compared by solving a collection of 114 problems from the literature. Some features of these test problems are given in Table 1, along with the "optimal" function values obtained in the actual runs.

The problems have been obtained from the following sources:

- Problem 1 is the example problem distributed with NPSOL; its description can be found in [GMSW86a]. Problems 3 and 4 are slight reformulations of the same problem, where the bounds $-1 \leq x_3 \leq 1$ have been replaced by the constraint $x_3^2 \leq 1$. Problem 4 uses the same starting point as Problem 1. Problem 3 uses the starting point

$$(\tfrac{1}{3}, \tfrac{2}{3}, \tfrac{11}{10}, \tfrac{2}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{2}{3}, -\tfrac{1}{3}, -\tfrac{1}{3}).$$

- Descriptions for problems 6 and 12–15 can be found in [MS82]. The version of problem 6 considered is the one corresponding to a value $T = 10$. Problems 12 and 13 start from point (d) for Wright No. 4 as indicated in the reference, while problems 14 and 15 start from points (a) and (b) for Wright No. 9, respectively.
- A description of the SQUARE ROOT problems (17–20) and of EXP6 (9) can be found in Fraley [Fra88].
- Problems 21–30 were obtained from Boggs and Tolle [BT84].
- All problems having names starting with "HS" are from Hock and Schittkowski [HS81].
- Problems 85–95 can be found in Dembo [Dem76].

All the above problems have been used in the past to test NPSOL. It should be noted that the problems in this group are small; the average number of variables is 10, and the average number of constraints is 6. Nevertheless, many of these problems are considered hard to solve. Moreover, for some of these problems the assumptions made in Chapter 2 to establish the convergence results fail to hold; for example, in some cases the Jacobian at the solution is singular, or no feasible points exist for some QP subproblems.

In addition to the previous set, the algorithms have been tested on another group of problems:

- The structural optimization problems 99–114 are described in Ringertz [Rin88]. The letters "I" and "E" in the problem name indicate if the formulation used included explicitly the displacement variables ("E") or eliminated them in advance. Also, the following number (10, 25, 36 or 63) denotes the number of bars in the truss considered. Finally, whenever a number is included at the end of the name (006, 040 or 060), the initial point has been modified to be $x_j = 6, 40$ or 60 respectively.

These problems have been introduced because of the atypical behavior of quasi-Newton SQP algorithms on them. For this group, the ratio of QP to nonlinear iterations is large when compared to the size of the problem; on the first test set (problems 1–98) the average ratio for NPSOL is 2 QP iterations per nonlinear iteration, while on problems 99–114 the average ratio is 30.

The normal behavior of NPSOL on the first set of test problems is to require a relatively large number of QP iterations in the first few nonlinear iterations. Typically, the number of QP iterations declines exponentially until near the solution, when only one iteration is required. As a result, significant savings achieved by incomplete solution of QP subproblems in the early iterations are masked by a large number of subproblems requiring only a few QP iterations. As an example, for problem 98 the largest number of QP iterations needed in any nonlinear iteration is reduced from 57 for NPSOL to 15 for the algorithm using early termination. This effect is much less clear when we look at total numbers of QP iterations (244 for NPSOL vs. 170 for early termination).

The STRUC problems depart from this "standard" behavior, in the sense that the number of QP iterations declines much more gradually. (Although only one QP iteration is required in the end, most nonlinear iterations require more.) This offers the possibility of observing the reductions that can be achieved by using the early-termination criterion, with limited distortion from the asymptotic behavior of NPSOL.

Finally, the problems in this second group are larger than the ones presented above; the average number of variables is now 55, and the average number of constraints is 100. For all the reasons mentioned, this set of problems provides a better environment in which to test the ability of the proposed early-termination criterion to reduce the total number of QP iterations.

Computing environment

Version 4.02 of NPSOL was used in the comparisons, and all parameters used in the code were given their default values (see [GMSW86a]). No attempt has been made to improve the results by selecting a different set of parameters, as the main goal of the comparison is to determine the reliability of the changes introduced in NPSOL.

The runs were performed as batch jobs on a DEC VAXstation II with 5 megabytes of main memory. The operating system was VAX/VMS version 4.5, and the compiler used was VAX FORTRAN version 4.6 with default options.

TABLE 1

Problem Set Description

No.	Problem name	Variables	Linear constraints	Nonlinear constraints	Optimal objective
1	NPSOL SAMPLE PROBLEM	9	4	14	−.1349963e+01
2	SINGULAR	2	0	2	.0000000e+00
3	HEXAGON	9	4	15	−.1349963e+01
4	HEXAGON (ALT. START)	9	4	15	−.1349963e+01
5	LC7	7	7	0	.9295973e+06
6	ALAN MANNE'S PROBLEM	30	10	10	−.2670099e+01
7	ROSEN-SUZUKI	4	0	3	−.4400000e+02
8	QP PROBLEM	7	7	0	−.1847785e+07
9	EXP6	6	0	0	.1866481e−19
10	STEINKE2	6	0	4	.4000131e−03
11	NORWAY	7	6	0	−.2402344e+02
12	MHW4	5	0	3	.2787187e+02
13	MHW9	5	0	3	−.3618808e+02
14	MHW9 INEQUALITY 1	5	0	3	−.2104078e+03
15	MHW9 INEQUALITY 2	5	0	3	−.6043539e+04
16	WOPLANT	12	3	5	.1555716e+02
17	SQUARE ROOT 1	9	0	9	.2500000e+04
18	SQUARE ROOT 2	9	0	9	.2999795e+01
19	SQUARE ROOT 3	9	0	9	.2000000e+01
20	SQUARE ROOT 4	4	0	4	.2500000e+04
21	BT1	2	0	1	−.1000000e+01
22	BT2	3	0	1	.3256820e−01
23	BT3	5	3	0	.4093023e+01
24	BT4	3	1	1	−.4551055e−03
25	BT5–HS63	3	1	1	.9577426e+03
26	BT6–HS77	5	0	2	.2415051e+00
27	BT7	5	0	3	.3065000e+03
28	BT8	5	0	2	.1000000e+01
29	BT9–HS39	4	0	2	−.1000000e+01
30	BT10	2	0	2	−.1000000e+01
31	BT11–HS79	5	0	3	.9171343e−01
32	BT12	5	0	3	.6188119e+01
33	BT13	5	0	1	.0000000e+00
34	POWELL TRIANGLES	7	0	5	.2331371e+02
35	POWELL BADLY SCALED	2	0	1	.1305195e−23
36	POWELL WRIGGLE	2	0	2	−.1911618e−15
37	POWELL-MARATOS	2	0	1	−.1000000e+01
38	HS72	4	0	2	.7266794e+03
39	HS73 (CATTLE FEED)	4	2	1	.2989438e+02
40	HS107	9	0	6	.5055012e+04
41	MUKAI-POLAK	6	0	2	.5000000e+01
42	INFEASIBLE SUBPROBLEM	2	1	1	—
43	HS26	3	0	1	.1969433e−20
44	HS32	3	1	1	.1000000e+01
45	HS46	5	0	2	.1936782e−22
46	HS51	5	3	0	.3851860e−32
47	HS52	5	3	0	.5326648e+01
48	HS53	5	3	0	.4093023e+01
49	PENALTY1 A	50	1	0	.4313635e−01
50	PENALTY1 B	50	1	0	.4313635e−01
51	PENALTY1 C	50	1	0	.4313635e−01
52	HS13	2	0	1	.1002181e+01
53	HS64	3	0	1	.6299842e+04
54	HS65	3	0	1	.9535289e+00
55	HS70	4	0	1	.7498464e−02
56	HS71	4	0	2	.1701402e+02
57	HS74	4	2	3	.5126498e+04

TABLE 1 (CONT.)

Problem Set Description

No.	Problem name	Variables	Linear constraints	Nonlinear constraints	Optimal objective
58	HS75	4	2	3	.5174413e+04
59	HS78	5	0	3	−.2919700e+01
60	HS80	5	0	3	.5394985e−01
61	HS81	5	0	3	.5394985e−01
62	HS84	5	0	3	−.5329025e+07
63	HS85	5	0	38	−.1905155e+01
64	HS86 (COLVILLE 1)	5	10	0	−.3234868e+02
65	HS87 (COLVILLE 6)	6	0	4	.8927598e+04
66	HS93	6	0	2	.1350760e+03
67	HS95	6	0	4	.1561953e−01
68	HS96	6	0	4	.1561953e−01
69	HS97	6	0	4	.3135809e+01
70	HS98	6	0	4	.3135809e+01
71	HS99	7	0	2	−.8290102e+09
72	HS100	7	0	4	.6806301e+03
73	HS104	8	0	5	.3951163e+01
74	HS105	8	1	0	.1138418e+04
75	HS108 (HEXAGON)	9	0	13	−.8660254e+00
76	HS109	9	1	8	.5362069e+04
77	HS110	10	0	0	−.4577847e+02
78	HS111	10	0	3	−.4773239e+02
79	HS112 (CHEMICAL EQ.)	10	3	0	−.4776109e+02
80	HS113	10	3	5	.2430621e+02
81	HS114	10	5	6	−.1768807e+04
82	HS117 (COLVILLE 2)	15	0	5	.3234868e+02
83	HS118 (LC PROBLEM)	15	17	0	.6648204e+03
84	HS119 (COLVILLE 7)	16	8	0	.2448997e+03
85	DEMBO 1B	12	0	3	.3168222e+01
86	DEMBO 2–HS83	5	0	6	.1012243e+05
87	DEMBO 3	7	4	10	.1227226e+04
88	DEMBO 4A	8	0	4	.3951163e+01
89	DEMBO 4C	9	0	5	.3952139e+01
90	DEMBO 5–HS106	8	3	3	.7049248e+04
91	DEMBO 6–HS116	13	3	10	.9758751e+02
92	DEMBO 7	16	8	11	.1747870e+03
93	DEMBO 8A	7	0	4	.1809765e+04
94	DEMBO 8B	7	0	4	.9118806e+03
95	DEMBO 8C	7	0	4	.5436680e+03
96	OPF	67	0	60	.9927005e+00
97	GBD EQUILIBRIUM MODEL	44	38	6	.4510281e−16
98	WEAPON ASSIGNMENT	100	12	0	−.1735019e+04
99	STRUCI10KON	10	0	11	.4156398e+04
100	STRUCE10KON	18	10	8	.4156398e+04
101	STRUCI10VAN	10	0	12	.5076669e+04
102	STRUCE10VAN	18	10	8	.5076669e+04
103	STRUCI25006	8	0	74	.5451627e+03
104	STRUCE25006	44	50	36	.5451627e+03
105	STRUCI25DAT	8	0	74	.5451627e+03
106	STRUCE25DAT	44	50	36	.5451627e+03
107	STRUCI36DAT	21	0	76	.3389915e+05
108	STRUCE36DAT	75	72	54	.3389915e+05
109	STRUCI63040	63	0	128	.6117064e+04
110	STRUCE63040	147	126	84	.6117064e+04
111	STRUCI63060	63	0	128	.6117064e+04
112	STRUCE63060	147	126	84	.6117064e+04
113	STRUCI63DAT	63	0	128	.6117064e+04
114	STRUCE63DAT	147	126	84	.6117064e+04

7.3. Results

The results obtained from running both algorithms on the test set described in the previous section are presented in Table 4.

The parameters chosen to characterize the relative performance of both algorithms have been: the number of outer (nonlinear) iterations for each problem; the number of calls to the routine computing the values of the objective function, the constraint functions and their derivatives (function evaluations); the total number of inner (QP) iterations for the problem (including the number of iterations necessary to compute a feasible point); and the running (CPU) time needed to solve the problem. The results corresponding to both algorithms are given as a single entry in the tables, in the form

NPSOL result/Early-termination result.

Given that many of the problems are not convex, the algorithms may converge to different solutions. A few such events are indicated in Table 4. Another possible outcome is failure—that is, the algorithm terminates without finding a solution, because the iteration limit has been exceeded, because no significant progress can be made at the current point with respect to the merit function, or because the objective or constraint functions need to be evaluated at a point for which they are not defined in the code. Such failures are indicated by "—".

To summarize the results from the test set we now give statistics for the whole set of problems. We start by presenting in the following table the number of failures for both algorithms. These values illustrate the reliability of the early-termination algorithm: it is able to solve 98% of the number of problems solved by NPSOL, and 92% of all the problems attempted.

TABLE 2
Problems Successfully Solved

NPSOL	Early termination
107	105

Table 3 presents a summary of the results for the four quantities monitored in Table 4.

The values have been computed as the geometric means for the ratios of the values for NPSOL and for the early-termination algorithm; that is, entries larger than one indicate that the corresponding value for NPSOL is larger than the value for the early-termination code (excluding those problems where one of the algorithms failed). Separate entries have been provided for problems 1–98 (the smaller problems), and for problems 99–114 (the structural optimization problems).

TABLE 3
Average Behavior: NPSOL vs. Early Termination

	Problems		
	All	1–98	99–114
Nonlinear iterations	.988	.979	1.044
Function evaluations	.994	.999	.963
QP iterations	1.190	1.112	1.884
CPU time	1.043	1.022	1.200

We now comment briefly on the implications of these results.

- The early-termination rule seems to behave very well regarding the numbers of nonlinear iterations and function evaluations; even if we are now using a search direction of "worse quality" than in NPSOL, the numbers are very close for both algorithms.

- The number of QP iterations is reduced by 20% for the complete set. When judging this figure we must take into account that the problems are small, implying that the number of QP iterations required per nonlinear iteration is also small. (In fact, the average value for the test set is 5.6 QP iterations per nonlinear iteration.) The opportunity for improvement is correspondingly limited. Moreover, both codes use the active set at the solution of the previous QP subproblem as a prediction for the correct active set in the current subproblem, resulting in a small number of QP iterations close to the solution. Finally, the early-termination rule still requires a feasible point, and the feasibility phase is the same as in NPSOL. When this phase accounts for most of the total number of iterations, as with the STRUC problems, the possibility of improvement is further diminished.

Nonetheless, it should be noted that for problems 99–114 the improvement obtained is significantly greater than 20%, as the mean ratio is now 1.88; in fact, when we look only at the larger problems, the relative performance of the early-termination algorithm improves markedly. This offers the promise that for even larger problems the results obtained may be substantially better than the values shown above.

- The CPU time required by the early-termination algorithm is lower than the time for NPSOL, but by a factor that is much smaller than for the number of QP iterations. This is due not only to the fact that function evaluations can be expensive when compared to the effort to solve each QP subproblem, but also to some details in the implementation that have been chosen to affect the number of QP iterations, even at the expense of running time. For example, the multiplier estimate used for the linesearch (the least-squares multiplier) is expensive to compute when many constraints are deleted in the last step, as the factorization for the Jacobian of the active constraints must be updated. There are still options to be explored that might improve the running times for the modified algorithm.

Finally, Figures 1 and 2 show plots of the results included in Table 4, in an attempt to make these results more easily understandable. The vertical axes give the base 2 logarithms of the ratios between the corresponding values for NPSOL and the early-termination (ET) algorithm. A value of 1 would correspond to a case in which NPSOL requires twice the number of nonlinear iterations, or function evaluations, etc. needed by the early termination algorithm.

TABLE 4

Numerical Results

No.	Problem name	Nonlinear iterations	Function evaluations	QP iterations	CPU time (s)
1	NPSOL SAMPLE PROBLEM	12/13	16/18	45/34	3.69/3.61
2	SINGULAR	15/15	16/16	4/4	1.03/1.05
3	HEXAGON	15/16	21/23	32/29	4.41/4.41
4	HEXAGON (ALT. START)	11/11	16/14	35/26	3.56/3.26
5	LC7	7/9	9/11	13/16	.76/.95
6	ALAN MANNE'S PROBLEM	17/17	18/18	40/37	21.13/21.92
7	ROSEN-SUZUKI	8/8	11/11	9/9	.81/.81
8	QP PROBLEM	8/10	9/11	23/15	1.10/1.04
9	EXP6	33/53	35/57	38/57	1.96/3.08
10	STEINKE2	—*/5	—/6	—/14	—/.87
11	NORWAY	4/6†	5/7	34/13	1.23/.65
12	MHW4	10/10	18/15	14/12	1.31/1.25
13	MHW9	30/19†	56/28	42/24	3.71/2.31
14	MHW9 INEQUALITY 1	28/23	38/28	59/40	3.41/2.73
15	MHW9 INEQUALITY 2	41/14†	58/27	80/24	4.83/1.77
16	WOPLANT	25/29	29/33	44/35	6.85/7.17
17	SQUARE ROOT 1	—*/—*	—/—	—/—	—/—
18	SQUARE ROOT 2	23/23	36/36	0/0	5.01/5.32
19	SQUARE ROOT 3	6/6	9/9	7/7	.95/.94
20	SQUARE ROOT 4	—*/—*	—/—	—/—	—/—
21	BT1	11/11	19/19	11/11	.81/.83
22	BT2	9/9	14/14	9/9	.71/.70
23	BT3	2/2	5/5	2/2	.19/.19
24	BT4	12/12	18/18	13/13	.92/.92
25	BT5–HS63	6/6	9/9	8/8	.58/.58
26	BT6–HS77	15/15	21/21	16/16	1.52/1.54
27	BT7	31/31	56/56	32/32	3.36/3.43
28	BT8	17/17	19/19	17/17	1.25/1.44
29	BT9–HS39	13/13	16/16	14/14	.95/1.19
30	BT10	8/8	11/11	0/0	.48/.52
31	BT11–HS79	9/9	12/12	10/10	1.05/1.06
32	BT12	27/27	57/57	28/28	3.04/3.04
33	BT13	32/32	44/44	34/34	2.61/2.62
34	POWELL TRIANGLES	23/15	37/16	36/23	3.27/2.28
35	POWELL BADLY SCALED	12/12	15/15	13/13	.85/.85
36	POWELL WRIGGLE	34/32	69/55	60/40	2.77/2.39
37	POWELL-MARATOS	6/6	7/7	6/6	.44/.44
38	HS72	7/7	8/8	8/8	.69/.67
39	HS73 (CATTLE FEED)	4/4	5/5	4/4	.38/.36
40	HS107	11/11	18/18	27/18	2.77/2.56
41	MUKAI-POLAK	10/10	16/16	13/13	1.08/1.11
42	INFEASIBLE SUBPROBLEM	—*/—*	—/—	—/—	—/—
43	HS26	47/47	64/64	48/48	3.39/3.41
44	HS32	2/4	3/5	3/5	.25/.38
45	HS46	55/55	58/58	56/56	5.26/4.98
46	HS51	2/2	5/5	2/2	.18/.14
47	HS52	2/2	5/5	2/2	.19/.16
48	HS53	2/2	5/5	2/2	.19/.16
49	PENALTY1 A	16/16	18/19	77/41	20.01/16.49
50	PENALTY1 B	6/7	14/19	67/32	14.77/11.77
51	PENALTY1 C	29/15	85/40	152/65	24.35/11.65
52	HS13	22/19	23/20	13/10	1.29/1.22
53	HS64	29/43	39/62	47/60	2.34/3.33
54	HS65	8/9	10/11	16/16	.70/.78
55	HS70	36/—*	39/—	39/—	3.33/—
56	HS71	5/7	6/9	9/9	.53/.67
57	HS74	10/26	15/48	14/28	1.17/2.68

* Failed to solve the problem.

† Converged to a different minimizer.

TABLE 4 (CONT.)

Numerical results

No.	Problem name	Nonlinear iterations	Function evaluations	QP iterations	CPU time (s)
58	HS75	6/8	10/11	7/9	.72/.90
59	HS78	10/10	14/14	11/11	1.15/1.15
60	HS80	8/8	10/10	8/8	.92/.92
61	HS81	14/14	20/20	15/15	1.57/1.60
62	HS84	—*/4	—/5	—/9	—/.51
63	HS85	17/14	18/15	33/20	4.00/3.12
64	HS86 (COLVILLE 1)	6/7	8/8	11/11	.62/.64
65	HS87 (COLVILLE 6)	11/8	18/9	18/14	1.63/1.23
66	HS93	12/12	15/15	14/14	1.36/1.38
67	HS95	1/1	2/2	1/1	.15/.15
68	HS96	1/1	2/2	1/1	.17/.15
69	HS97	3/3	6/6	3/3	.40/.41
70	HS98	3/3	6/6	8/8	.43/.44
71	HS99	23/—*	44/—	74/—	3.99/—
72	HS100	14/14	29/29	18/18	2.07/2.02
73	HS104	18/18	20/20	23/23	3.36/3.37
74	HS105	43/—*	61/—	97/—	27.14/—
75	HS108 (HEXAGON)	24/32	45/49	57/87	6.78/9.36
76	HS109	11/10	13/11	25/29	3.23/3.26
77	HS110	6/6	9/9	24/15	.78/.69
78	HS111	41/49	64/75	44/52	8.08/9.05
79	HS112 (CHEMICAL EQ.)	19/—*	39/—	54/—	2.78/—
80	HS113	14/16	19/23	38/36	3.12/3.41
81	HS114	18/16	19/24	36/33	3.81/3.60
82	HS117 (COLVILLE 2)	17/18	21/27	96/39	6.75/5.34
83	HS118 (LC PROBLEM)	4/4	6/6	20/20	1.35/1.40
84	HS119 (COLVILLE 7)	12/17	16/19	41/47	4.25/5.60
85	DEMBO 1B	281/—*	437/—	296/—	75.46/—
86	DEMBO 2–HS83	4/4	6/6	4/4	.54/.54
87	DEMBO 3	9/8	11/9	37/20	2.01/1.78
88	DEMBO 4A	19/19	23/23	24/24	3.53/3.31
89	DEMBO 4C	13/13	15/15	20/23	3.10/3.20
90	DEMBO 5–HS106	17/18	21/24	30/31	2.90/3.04
91	DEMBO 6–HS116	36/43	96/69	144/248	21.84/29.65
92	DEMBO 7	19/12	24/15	126/68	15.54/9.82
93	DEMBO 8A	33/42	85/118	105/99	7.52/9.17
94	DEMBO 8B	29/29	69/71	88/73	6.51/6.45
95	DEMBO 8C	25/27	60/68	89/65	6.19/6.06
96	OPF	18/17	19/18	53/51	468.12/456.10
97	GBD EQUILIBRIUM MOD.	5/6	6/7	37/26	6.22/6.10
98	WEAPON ASSIGNMENT	96/73	98/76	244/170	120.78/114.93
99	STRUCI10KON	18/17	34/30	65/42	13.67/11.73
100	STRUCE10KON	26/29	49/67	87/84	17.68/20.75
101	STRUCI10VAN	23/19	41/34	54/51	16.30/13.85
102	STRUCE10VAN	—*/24	—/48	—/91	—/19.44
103	STRUCI25006	42/37	68/62	147/85	92.44/80.99
104	STRUCE25006	20/28	32/36	178/95	357.83/260.79
105	STRUCI25DAT	11/12	19/21	24/22	24.75/27.11
106	STRUCE25DAT	52/21	106/37	687/65	647.13/191.44
107	STRUCI36DAT	23/20	38/34	59/46	120.79/108.02
108	STRUCE36DAT	29/30	53/62	87/90	971.16/1021.87
109	STRUCI63040	117/112	211/202	6116/3091	8182.13/7159.03
110	STRUCE63040	375/—*	794/—	3545/—	77286.64/—
111	STRUCI63060	—*/98	—/244	—/3899	—/8281.02
112	STRUCE63060	63/115	150/316	6675/3407	25090.15/33228.42
113	STRUCI63DAT	246/136	354/412	9043/2060	12591.61/11424.54
114	STRUCE63DAT	52/72	86/145	8049/2858	41793.84/22740.66

* Failed to solve the problem.

† Converged to a different minimizer.

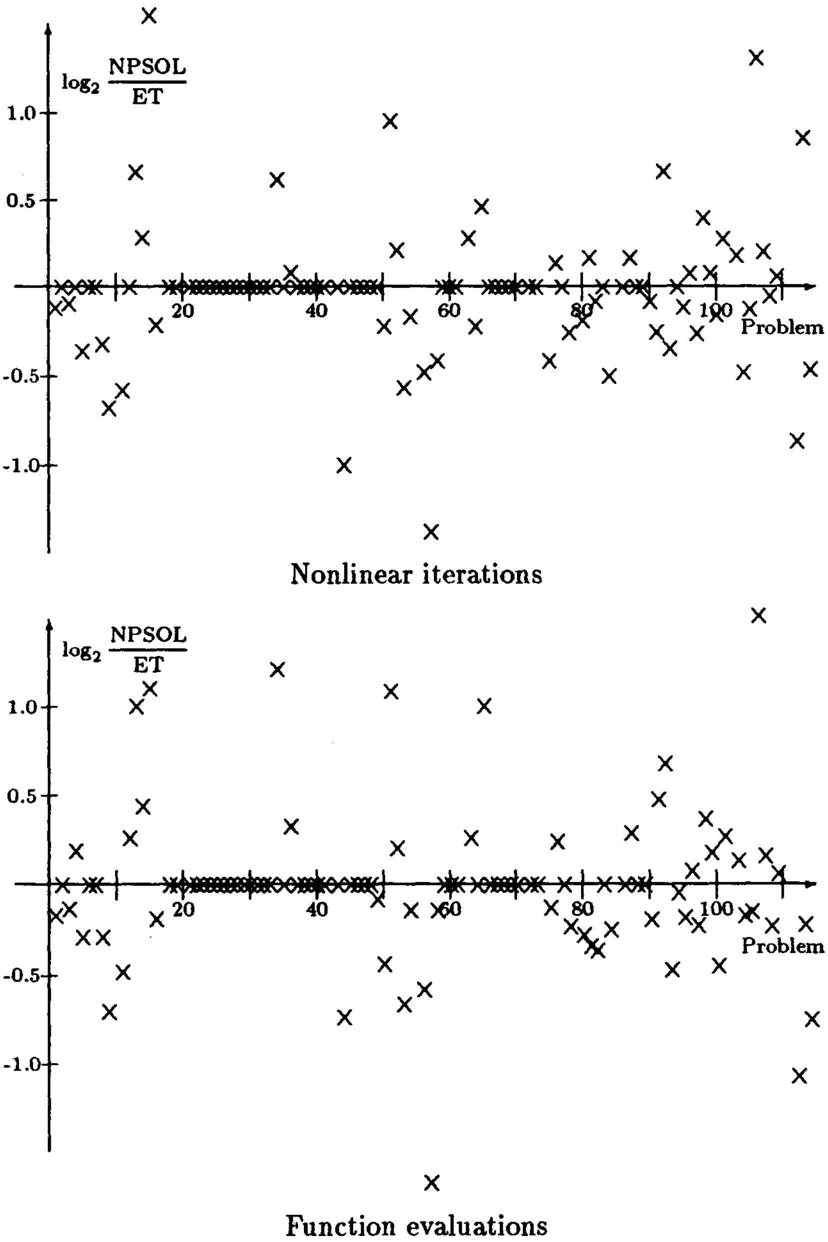

Figure 1. Nonlinear iterations and function evaluations: NPSOL vs. Early termination

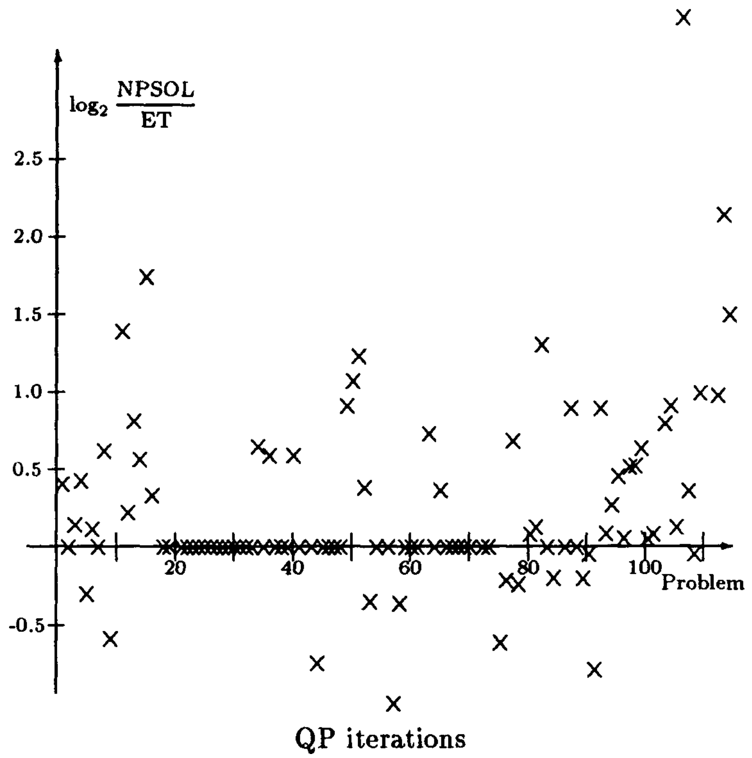

Figure 2. QP iterations: NPSOL vs. Early termination

From Figures 1 and 2 it can be noticed that the results obtained present a significant lack of correlation from one problem to the next; the comments offered earlier in this section apply when the average behaviors are considered, rather than for each individual problem. In Figure 1, the values for the numbers of nonlinear iterations and function evaluations are clearly clustered around zero, with relatively small deviations from the average. In contrast to these results, the predominance of positive values for the number of QP iterations can be easily appreciated in Figure 2, especially for those (larger) problems beyond problem 92.

7.4. Further work

We conclude the report with some comments on those areas where further improvement in the algorithm is desirable.

- Two of the assumptions introduced in Chapter 2 were the nonsingularity of the Jacobian for the active constraints at the solution, and the existence of a feasible region for all QP subproblems. Many of the failures in the solution of the test problems can be attributed to the corresponding subproblems lacking one of these properties (or being close to violating them). NPSOL includes rules to deal with these difficulties but they are not guaranteed to be able to cope with all possible situations, particularly in the case of infeasible subproblems. A third related issue that appeared several times in the solution of the problem set, was the need for a disproportionate effort to obtain feasible points for the QP subproblems. In some of the problems the work to obtain a feasible point was far greater than the remaining work needed to compute a satisfactory search direction. For example, in problem number 114, 80% of the quite considerable solution time was spent in the feasibility phase by both algorithms.

  These last two issues are closely related. It can be expected that a procedure to terminate the feasibility phase early may not only yield further reductions in the total number of QP iterations needed to solve the problems, but at the same time may provide a way to deal with infeasible QP subproblems.

- Another open area, also related to the assumptions made in Chapter 2, is the theoretical study of the relaxation of the strict complementarity requirement. Some recent work on this topic by Burke [Bur89] indicates that it might still be possible to identify a satisfactory active set at the solution in a finite number of iterations. Several other associated issues are also open: for example, determination of the best strategy to compute a Lagrange multiplier estimate when the Jacobian is becoming progressively more ill-conditioned, and study of the theoretical rate of convergence achievable by the algorithm when strict complementarity does not hold.

- Finally, a more general issue is identification of the best strategy for the solution of the QP subproblems in the large-scale case. This report focused on active-set methods, but recently there has been great interest in the use of interior-point methods, in which the inequality constraints are rewritten in the form of equality constraints and simple bounds, and a barrier function formulation is used to move the simple bounds into the objective function. These methods may become a promising alternative for use within our framework (to solve the QP subproblems), as they seem able to avoid the exponential complexity associated with determination of the correct active set.

Exploration of these alternatives offers a great number of possibilities for further research in the quest for a satisfactory method to solve large-scale nonlinear programs.

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