Title
Primal-dual methods for nonlinear optimization

Author
Robinson, Daniel P.

Publication Date
2007

Peer reviewed|Thesis/dissertation

UNIVERSITY OF CALIFORNIA, SAN DIEGO

Primal-Dual Methods for Nonlinear Optimization

A dissertation submitted in partial satisfaction of the
requirements for the degree
Doctor of Philosophy

in

Mathematics

by

Daniel P. Robinson

Committee in charge:

Professor Philip E. Gill, Chair
Professor Randolph E. Bank
Professor Thomas Bewley
Professor Li-Tien Cheng
Professor Robert L. Parker

2007

The dissertation of Daniel P. Robinson is approved, and it is acceptable in quality and form for publication on microfilm:

Chair

University of California, San Diego

2007

To My Family–

Despite the separation of thousands of miles over the past six years, your constant love and support made this possible.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

ACKNOWLEDGEMENTS

This thesis would not have been possible without the help of many people. In particular, I would like to thank:

My family – You have endured this long process, always being there for me. You will never know how much your love and support has meant to me.

My advisor Philip Gill – Your patience and confidence in me were instrumental to my success. Thank you for the graduate research assistantship working for Northrop Grumman, for sending me to conferences, and for financially supporting me during my last year. Without this support I may not have been able to complete my thesis. For this and so much more I am eternally grateful.

Diane Nguyen – It is not possible to express my appreciation for all the little things that you have done to support me. Also thank you for making me smile when I started taking life too seriously.

My good friend Samantha Bergman – I can not thank you enough for your moral support during my first two years of graduate school. Your friendship and encouragement helped me move forward during a crucial period of my life.

My computer expert Ryan Szypowski – Thank you for being my "Rosetta Stone" for computers and for numerous insightful conversations about my research.

My roommate Jeremy Greene – I could not have asked for a more respectful and considerate roommate. Notwithstanding, you deserve acknowledgment for being exposed nightly to my unpredictable hours of research.

My committee members: Randolph Bank, Thomas Bewley, Li-Tien Cheng, and Robert Parker – Thank you for being on my committee and for your willingness to write letters of reference.

Michael Friedlander – Thank you for your help with Chapter 5. Your extensive knowledge and experience with LCL methods were invaluable.

Finally, I would like to thank everyone, too numerous to mention, that I met and shared experiences with along the way. You have all been a part of my education and I thank you.

VITA

2001	B. S., *summa cum laude*, James Madison University
2003	M. A., University of California, San Diego
2007	Ph. D., University of California, San Diego

ABSTRACT OF THE DISSERTATION

Primal-Dual Methods for Nonlinear Optimization

by

Daniel P. Robinson
Doctor of Philosophy in Mathematics

University of California San Diego, 2007

Professor Philip E. Gill, Chair

Nonlinearly constrained optimization problems may be solved by minimizing a sequence of simpler subproblems based on the properties of a so-called *merit function* that balances the (usually) conflicting aims of reducing the objective function and satisfying the constraints. Sometimes this merit function is minimized directly as an unconstrained function, in which case convergence is achieved by adjusting the relative weighting of the objective and constraints between subproblems. Alternatively, some model of the merit function is minimized subject to simple bounds and/or linearizations of the constraints. In this case, the merit function drives the algorithm by assessing the "quality" of points generated by the subproblem.

A new primal-dual augmented Lagrangian merit function is proposed that may be minimized with respect to both the primal *and* dual variables. A benefit of this approach is that each subproblem may be regularized by imposing explicit bounds on the dual variables. Two primal-dual variants of classical primal methods are given: a primal-dual bound constrained Lagrangian (pdBCL) method and a primal-dual ℓ_1 linearly constrained Lagrangian (pdℓ_1-LCL) method.

1

Introduction

1.1 Overview

A constrained optimization problem involves a set of independent variables and constraints that define acceptable values of the variables. The solution of this problem is a set of allowed values of the variables for which some objective function assumes its maximum or minimum value. Minimization will only be considered since maximizing a function $f(x)$ is equivalent to minimizing $-f(x)$. Constrained optimization problems may be categorized according to properties of the objective and constraint functions. If the objective and constraint functions are linear, then the optimization problem is called a linear program (LP). If the objective function is quadratic and the constraint function is linear, then the problem is called a quadratic program (QP). The most general problem (and perhaps the most difficult to solve) is the nonlinearly constrained problem, which is given by

$$\begin{array}{ll} \underset{x \in \mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c_\ell \le c(x) \le c_u, \\ & x_\ell \le x \le x_u, \end{array}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is the objective function, $c : \mathbb{R}^n \to \mathbb{R}^m$ is the vector of constraint functions, c_ℓ and c_u are vectors in $\mathbb{R}^m$ such that $c_\ell \le c_u$, and x_ℓ and x_u are vectors in $\mathbb{R}^n$ such that $x_\ell \leq x_u$. By introducing the vector s of slack variables, the problem (1.1) may be written in the equivalent form:

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n,\, s\in\mathbb{R}^m}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) - s = 0, \\ & x_\ell \leq x \leq x_u, \quad c_\ell \leq s \leq c_u. \end{array}$$

Therefore, there is no loss of generality in assuming that the optimization problem has the form

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = 0, \\ & x_\ell \leq x \leq x_u. \end{array}$$

To simplify the exposition, the bounds on the x-variables are often assumed to take the form $x \geq 0$. This simplified problem is given by

GNPs

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = 0, \\ & x \geq 0. \end{array} \tag{1.1}$$

The analysis of problems in this format easily carries over to the more general setting with $x_\ell \leq x \leq x_u$.

Optimization problems may be categorized further by the degree of smoothness of the objective and constraint functions. This thesis considers algorithms for solving general nonlinear optimization problems for which the objective and constraint functions are assumed to be twice continuously differentiable.

Although the primary focus will be on problem GNPs, it is convenient to begin with a simpler problem with all equality constraints. This problem is given by

NEP

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = 0. \end{array} \tag{1.2}$$

One of the most well-known methods for solving problem NEP (1.2) is based on the properties of the quadratic penalty function:

$$\mathcal{P}(x;\rho) = f(x) + \frac{\rho}{2}\|c(x)\|^2, \tag{1.3}$$

where ρ is a positive scalar known as the penalty parameter. Any approach for solving problem (1.2) must provide a way of dealing with the (usually conflicting) aims of decreasing the objective function and deceasing the constraint violation. The penalty function (1.3) combines the objective function and constraint function into one function that may be minimized using unconstrained optimization methods. A basic penalty function method computes a sequence of minimizers $x(\rho_k)$ for problem (1.3) for an increasing sequence of penalty parameters $\{\rho_k\}$. The idea is that $x(\rho_k)$ converges to a solution of problem (1.2) as $\{\rho_k\} \to \infty$.

Applying the penalty function to a certain "shifted" problem gives rise to the popular augmented Lagrangian function. This function is given by

$$\mathcal{L}_{\mathcal{A}}(x;y_e,\rho) = f(x) - c(x)^T y_e + \frac{\rho}{2}\|c(x)\|^2, \tag{1.4}$$

where y_e is an estimate of the Lagrange multiplier vector. The augmented Lagrangian function was proposed independently by Hestenes [18] and Powell [24], partly as a way to overcome the ill-conditioning in the Newton equations associated with minimizing the penalty function (1.3). The use of the Lagrange multiplier estimate allows convergence to solutions of problem NEP *without* the need to drive the penalty parameter to infinity.

The augmented Lagrangian has been used very successfully within different algorithmic frameworks. In the context of problem GNPs, the optimization code LANCELOT [7] approximately minimizes a sequence of bound constrained Lagrangian (BCL) problems. These problems take the form

$$\underset{x\in\mathbb{R}^n}{\text{minimize}}\ \ \mathcal{L}_{\mathcal{A}}(x;y_e,\rho) \quad \text{subject to} \ \ x \ge 0. \tag{1.5}$$

After each approximate minimization, the Lagrange multiplier estimate y_e may be updated, while parameters and tolerances are adjusted. In [8], Conn, Gould, and Toint show that this BCL method is globally convergent, exhibits R-linear convergence, and has a uniformly bounded penalty parameter ρ.

Linearly constrained Lagrangian (LCL) methods also make use of the augmented Lagrangian. LCL methods are based on the properties of Robinson's method [25], which sequentially minimizes the Lagrangian function $\mathcal{L}(x; y_e) = f(x) - c(x)^T y_e$, subject to the linearized constraints. Robinson proved that his algorithm exhibits R-quadratic convergence if started sufficiently close to a solution satisfying the second-order sufficient conditions. A positive penalty parameter was introduced in the method used by the software package MINOS [23] in order to improve convergence from poor starting points. In other words, MINOS uses the *augmented* Lagrangian function instead of the Lagrangian function. This modification improves the robustness of Robinson's method, but the question of convergence from arbitrary starting points is open. Further improvement was made by Friedlander and Saunders in [13]. Their stabilized LCL (sLCL) method remedies three drawbacks associated with MINOS. First, the sLCL subproblems are always feasible. Second, if the distance from the linearization point to the subproblem solution becomes large, it may be counteracted by decreasing the penalty parameter associated with the linearized constraints. Third, the sLCL method was proved to be globally convergent. These improvements to MINOS resulted from the definition of an elastic subproblem, which is known to be equivalent to an ℓ_1 penalization of the linearized constraint violation. They show that their sLCL algorithm is actually a continuum of algorithms with the BCL method as one extrema and Robinson's LCL method as the other. As a result, the sLCL algorithm inherits global convergence from the BCL method and R-quadratic convergence from Robinson's LCL method.

The augmented Lagrangian function may also be used as a *merit* function in sequential quadratic programming (SQP) methods. A merit function is a single function that is used to assess the quality of a pre-determined search direction. The search direction is typically given as the solution of a quadratic program that models the merit function. The most obvious choice for computing a search direction for the augmented Lagrangian, is to minimize the second-order Taylor approximation of $\mathcal{L}_\mathcal{A}(x; y_e, \rho)$. It can be shown that minimizing the second-order Taylor approximation of $\mathcal{L}_\mathcal{A}(x; y_e, \rho)$ is equivalent to minimizing a certain quadratic objective function subject to linear constraints. For more details see Section 15.3.1 of [9].

The SQP algorithm SNOPT [14] uses the augmented Lagrangian function as a merit function in a different way. Given a current approximation (x_k, y_k) to a solution of problem NEP (1.2), SNOPT generates a search direction by solving the following QP:

$$\begin{array}{ll} \underset{p\in\mathbb{R}^n}{\text{minimize}} & g_k^T p + \frac{1}{2} p^T H_k p \\ \text{subject to} & c_k + J_k p = 0, \end{array} \tag{1.6}$$

where g_k is the gradient of the objective function $f(x)$ evaluated at x_k, J_k is the Jacobian of $c(x)$ evaluated at x_k, and H_k is a symmetric positive-definite approximation to the Hessian of the Lagrangian function evaluated at (x_k, y_k). A search direction in both the x- *and* y-variables is then defined by using the minimizer p and the Lagrange multiplier vector from the QP subproblem (1.6). In this way, the augmented Lagrangian is considered a continuous function of both the primal *and* dual variables.

1.2 Contributions of this thesis

Chapter 3 considers a new *primal-dual* augmented Lagrangian merit function, which is a generalization of the Forsgren-Gill merit function for equality constraints (see [12]). First, it is shown that this function possesses properties considered mandatory of a merit function. The rest of the chapter examines additional properties of the merit function and shows that it is a viable and attractive option for use within an optimization method. In particular, since the new merit function is a function of both the primal and dual variables, explicit bounds may be imposed on the dual variables in the subproblem. This is expected to be helpful for highly nonlinear problems and in this way is a form of regularization of the subproblem. In addition, the use of primal and dual variables are expected to expedite optimization of the subproblem.

Chapter 4 examines a primal-dual bound constrained Lagrangian (pdBCL) method similar to the BCL algorithm used by the optimization package LANCELOT [7] (see Section 1.1). In the context of problem GNPs (1.1), the pdBCL subproblem takes the form

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n,\, y\in\mathbb{R}^m}{\text{minimize}} & \mathcal{M}(x,y;y_e,\mu) \\ \text{subject to} & x\geq 0, \;\; -\gamma e\leq y\leq \gamma e, \end{array} \tag{1.7}$$

where $\mathcal{M}$ is the primal-dual augmented Lagrangian function, e is a vector of ones, γ is a positive scalar, μ is a positive penalty parameter, and y_e is an estimate of the Lagrange multiplier vector. Note that explicit bounds on the dual variables are enforced in the subproblem. The theoretical development follows that of Conn, Gould, and Toint in [8]. In this way, the primal theory developed by Conn, Gould, and Toint is extended to the *primal-dual* setting.

Chapter 5 examines a primal-dual ℓ_1 linearly constrained Lagrangian (pdℓ_1-LCL) method similar to the sLCL algorithm given by Friedlander and Saunders in [13] (see Section 1.1). In the context of problem GNPs (1.1), the pdℓ_1-LCL subproblem takes the form

$$\begin{array}{ll} \underset{x,\,y,\,u,\,v}{\text{minimize}} & \mathcal{M}(x,y;y_e,\rho)+\sigma e^T(u+v) \\ \text{subject to} & \bar{c}_k(x)+u-v=0, \\ & x\geq 0,\;\; -\gamma e\leq y\leq \gamma e,\;\; u\geq 0,\;\; v\geq 0, \end{array} \tag{1.8}$$

where $\mathcal{M}$ is the primal-dual augmented Lagrangian function, e is a vector of ones, γ is a positive number, y_e is an estimate of the Lagrange multiplier vector, ρ is a penalty parameter associated with $c(x)$, $\bar{c}_k(x)$ is a linearization of the constraint function, and σ is a penalty parameter associated with $\bar{c}_k(x)$. Note that explicit bounds on the dual variables are enforced in the subproblem. The chapter follows the development given by Friedlander and Saunders. In this way, the primal theory developed by Friedlander and Saunders is extended to the *primal-dual* setting.

It is anticipated that future convergence proofs using the primal-dual augmented Lagrangian function will be possible under less stringent conditions. This thesis is the first step towards this goal.

1.3 Notation

- e_i, the ith coordinate basis vector.
- $e = (1, 1, \ldots, 1)^T$, the column vector of all ones.
- E and I, both are used to represent the identity matrix.
- $\mathrm{In}(A)$, Given a real symmetric matrix A, the inertia of A, denoted $\mathrm{In}(A)$, is the integer 3-tuple (i_+, i_-, i_0) indicating the number of positive, negative, and zero eigenvalues of the matrix A.
- $A \succeq \alpha$, Given a real symmetric matrix A, the notation $A \succeq \alpha$ means that the smallest eigenvalue of A is greater than or equal to α.
- $A \succ \alpha$, Given a real symmetric matrix A, the notation $A \succ \alpha$ means that the smallest eigenvalue of A is greater than α.
- $x \cdot y$, if x and y are vectors in $\mathbb{R}^n$, then $x \cdot y$ is defined to be the vector such that $[x \cdot y]_i = x_i\, y_i$.
- $f(x)$, the objective function evaluated at x.
- $g(x)$, the gradient of $f(x)$ evaluated at x.
- $H(x)$, the Hessian of $f(x)$ evaluated at x.

- $c(x)$, the m-dimensional constraint vector evaluated at x.
- $J(x) = c'(x)$, the $m \times n$ Jacobian of $c(x)$ evaluated at x.
- $H_i(x) = \nabla^2 c_i(x)$, the Hessian of $c_i(x)$ evaluated at x.
- f_k, g_k, c_k, J_k, functions and gradients evaluated at x_k.
- $\mathcal{I}$, set of indices corresponding to inequality constraints.
- $\mathcal{A}_\mathcal{I}(x) = \{\, i \in \mathcal{I} : c_i(x) = 0 \,\}$, the index set of all active inequalities.
- $\mathcal{E}$, set of indices corresponding to equality constraints.
- $\mathcal{A}(x) = \mathcal{A}_\mathcal{I}(x) \cup \mathcal{E}$, the set of active constraints.
- $x_\mathcal{A}$, If $\mathcal{A}$ is *any* index set, then $x_\mathcal{A}$ is the sub-vector of x corresponding to the index set $\mathcal{A}$.
- $S_\mathcal{A}$, If $\mathcal{A}$ is *any* index set and S is a matrix, then $S_\mathcal{A}$ will be the sub-matrix of S consisting of the rows corresponding to the index set $\mathcal{A}$.

1.4 Terminology

Definition 1.4.1 (Feasible Set)**.** *The feasible set is denoted by $\mathcal{F}$. Consider problem* NEP*, which is given by*

$$\begin{array}{ll} \underset{x \in \mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = 0 \ . \end{array}$$

The feasible set for problem NEP *is given by $\mathcal{F} = \{\, x \in \mathbb{R}^n : c(x) = 0 \,\}$.*

Definition 1.4.2 (Constrained Local Minimizer)**.** *Let f be a function defined for all $x \in \mathbb{R}^n$. A point x^* is a constrained local minimizer of f if there is an open ball $B(x^*; \delta)$ such that*

$$f(x^*) \le f(x) \ \text{ for all } x \in B(x^*; \delta) \cap \mathcal{F}.$$

Definition 1.4.3 (Strict Constrained Local Minimizer). *Let f be a function defined for all $x \in \mathbb{R}^n$. A point x^* is a strict constrained local minimizer of f if there is an open ball $B(x^*;\delta)$ such that*

$$f(x^*) < f(x) \text{ for all } x \neq x^*,\ x \in B(x^*;\delta) \cap \mathcal{F}.$$

Definition 1.4.4 (Isolated Constrained Local Minimizer). *A constrained local minimizer x^* is* isolated *if there is an open ball $B(x^*;\delta)$ such that x^* is the only constrained local minimizer in $B(x^*;\delta)$.*

The next three definitions pertain to the following problem:

$$\text{NIP} \qquad \begin{array}{ll} \underset{x \in \mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) \geq 0. \end{array} \tag{1.9}$$

Definition 1.4.5 (Feasible Path). *A feasible path for problem* NIP (1.9) *is a differentiable, directed curve $x(\alpha)$ emanating from a feasible point x, parameterized by a scalar α such that*

$$x(0) = x \text{ and } c\big(x(\alpha)\big) \geq 0$$

for all α satisfying $0 \leq \alpha < \sigma$ for some $\sigma > 0$ and where $dx(\alpha)/d\alpha|_{\alpha=0} \neq 0$.

Definition 1.4.6 (Binding Feasible Path). *A feasible path for problem* NIP (1.9) *is called a binding feasible path with respect to $c_i(x)$ if there exists an $\hat{\alpha} > 0$ such that $c_i\big(x(\alpha)\big) = 0$ for all α satisfying $0 \leq \alpha < \hat{\alpha}$.*

Definition 1.4.7 (Non-Binding Feasible Path). *A feasible path for problem* NIP (1.9) *is called a non-binding feasible path with respect to $c_i(x)$ if there exists an $\hat{\alpha} > 0$ such that $c_i\big(x(\alpha)\big) > 0$ for all $0 < \alpha < \hat{\alpha}$.*

Analogous definitions can be given for other problem formats.

The next definition concerns rates of convergence of sequences.

Definition 1.4.8 (Order Notation). *Let ϕ be a scalar, vector, or matrix function of a positive variable h, let p be fixed, and let k_u and k_l denote constants.*

1. *If there exists* $k_u > 0$ *such that* $\|\phi(h)\| \le k_u h^p$ *for all sufficiently small* h*, then we write* $\phi = O(h^p)$ *and say "*ϕ *is of order* h^p*" (or "*ϕ *is big oh of* h^p*").*

2. *If, for any* $\epsilon > 0$*,* $\|\phi(h)\|/h^p < \epsilon$ *for all sufficiently small* h*, then we write* $\phi = o(h^p)$ *and say, "*ϕ *is little oh of* h^p*".*

3. *If there exists* $k_l > 0$ *such that* $\|\phi(h)\| \ge k_l h^p$ *for all sufficiently small* h*, then we write* $\phi = \Omega(h^p)$ *and say "*ϕ *is omega of* h^p*".*

4. *If there exist* $k_l > 0$ *and* $k_u > 0$ *such that* $k_l h^p \le \|\phi(h)\| \le k_u h^p$ *for all sufficiently small* h*, then we write* $\phi = \Theta(h^p)$ *and say, "*ϕ *is theta of* h^p*".*

1.5 Useful Results

Lemma 1.5.1 (Debreu 1)**.** *Let* H *denote a symmetric* $n \times n$ *matrix, and let* J *denote an* $m \times n$ *matrix. Then* H *is positive definite on the null space of* J *(i.e.,* $p^T H p > 0$ *for all* $p \ne 0$ *such that* $Jp = 0$*) if and only if there exists a positive* $\bar{\mu}$ *such that* $H + \frac{1}{\mu} J^T J$ *is positive definite for all* μ *satisfying* $0 < \mu \le \bar{\mu}$*.*

Proof. ($\Leftarrow$) For a contrapositive proof, let there exist an $x_0 \ne 0$ such that $Jx_0 = 0$ and $x_0^T H x_0 \le 0$. Then

$$x_0^T (H + \frac{1}{\mu} J^T J) x_0 = x_0^T H x_0 + \frac{1}{\mu} x_0^T J^T J x_0 = x_0^T H x_0 \le 0 \quad \text{for all } \mu > 0.$$

This says that $H + \frac{1}{\mu} J^T J$ is not positive definite for all positive μ.
($\Rightarrow$) For another contrapositive proof, suppose that there *does not* exist a positive $\bar{\mu}$ such that $H + \frac{1}{\mu} J^T J$ is positive definite for all $0 < \mu \le \bar{\mu}$. Define any sequence $\{\mu_k\}$ such that $\{\mu_k\} \to 0$ and $\mu_k > 0$ for all k. Then define a corresponding sequence $\{x_k\}$ with the property that

$$x_k^T (H + \frac{1}{\mu_k} J^T J) x_k \le 0. \tag{1.10}$$

Without loss of generality assume that $\|x_k\|_2 = 1$. A sequence with this property may always be found since if $\{y_k\}$ is any sequence satisfying $y_k^T(H + \frac{1}{\mu}J^TJ)y_k \le 0$, then the sequence $\{z_k\}$ defined as $z_k = y_k/\|y_k\|_2$ satisfies

$$z_k^T(H + \frac{1}{\mu_k}J^TJ)z_k = \frac{1}{\|y_k\|_2^2} y_k^T(H + \frac{1}{\mu_k}J^TJ)y_k \le 0 \quad \text{and} \quad \|z_k\|_2 = 1.$$

Since $\{x_k\}$ is contained in a compact set, there exists a convergent subsequence $\{x_k\}_K$ such that $\lim_{k\in K} x_k = \bar{x}$. Since $\|x_k\|_2 = 1$ for all $k \in K$, it follows that $\|\bar{x}\|_2 = 1$, and in particular that $\bar{x} \ne 0$. Multiplying (1.10) by μ_k yields

$$x_k^T(\mu_k H + J^TJ)x_k \le 0. \tag{1.11}$$

Taking limits on $k \in K$ gives

$$\|J\bar{x}\|_2^2 = \bar{x}^TJ^TJ\bar{x} = \lim_{k\in K} x_k^T(\mu_k H + J^TJ)x_k \le 0.$$

This implies that $J\bar{x} = 0$.

Next, equation (1.10) implies

$$\mu_k x_k^T H x_k + x_k^T J^T J x_k = \mu_k x_k^T H x_k + \|Jx_k\|_2^2 \le 0.$$

Since $\|Jx_k\|_2 \ge 0$, it must follow that

$$\mu_k x_k^T H x_k \le 0 \;\text{ for all } k,$$

and since $\mu_k > 0$ it then follows that

$$x_k^T H x_k \le 0 \;\text{ for all } k.$$

Finally, taking limits on $k \in K$ yields

$$\bar{x}^T H \bar{x} = \lim_{k\in K} x_k^T H x_k \le 0.$$

Thus, it has been shown that $\bar{x}$ satisfies the following properties:

$$\text{(i) } \bar{x} \ne 0, \qquad \text{(ii) } J\bar{x} = 0, \qquad \text{(iii) } \bar{x}^T H \bar{x} \le 0.$$

This completes the proof. □

The following theorem is a reformulation of Debreu's Lemma in terms of the null space matrix Z. The proof is different and has the advantage of implicitly defining a value for $\bar{\mu}$.

Lemma 1.5.2 (Debreu 2)**.** *Let H denote a symmetric $n \times n$ matrix, and let J denote an $m \times n$ matrix with null space spanned by the columns of Z. If Z^THZ is positive definite, then there exists a finite $\bar{\mu}$ such that $H + \frac{1}{\mu}J^TJ$ is positive definite for all $0 < \mu < \bar{\mu}$.*

Proof. Let r denote the rank of J, so that $r \leq \min\{m, n\}$. The *singular-value decomposition* of J can be written as

$$J = U \begin{pmatrix} S_r & 0 \\ 0 & 0 \end{pmatrix} V^T,$$

where U and V are orthogonal, and S_r is an $r \times r$ diagonal matrix with positive diagonal entries. Suppose that U and V are partitioned conformally with S_r so that $U = \begin{pmatrix} U_r & U_{m-r} \end{pmatrix}$ and $V = \begin{pmatrix} V_r & V_{n-r} \end{pmatrix}$. It follows that

$$J = U_r S_r V_r^T.$$

The $n \times n$ matrix Q such that $Q = \begin{pmatrix} V_{n-r} & V_r S_r^{-1} \end{pmatrix}$ is nonsingular, and it can be verified by direct multiplication that

$$JQ = \begin{pmatrix} 0 & U_r \end{pmatrix}.$$

Define $Z = V_{n-r}$ and $Y = V_r S_r^{-1}$. Then $Q = \begin{pmatrix} Z & Y \end{pmatrix}$, with the $n - r$ columns of Z forming a basis for the null-space of J. Since Q is nonsingular, $H + \frac{1}{\mu}J^TJ$ must have the same inertia as $Q^T(H + \frac{1}{\mu}J^TJ)Q$ from Sylvester's Law of Inertia. Pre- and post-multiplying $H + \frac{1}{\mu}J^TJ$ by Q^T and Q gives

$$Q^T(H + \frac{1}{\mu}J^TJ)Q = Q^THQ + \frac{1}{\mu}Q^TJ^TJQ = \begin{pmatrix} Z^THZ & Z^THY \\ Y^THZ & Y^THY + \frac{1}{\mu}I \end{pmatrix}.$$

Note that this matrix is of the form

$$\begin{pmatrix} H_{11} & H_{21}^T \\ H_{21} & H_{22} + \frac{1}{\mu} I \end{pmatrix}, \tag{1.12}$$

where $H_{11} = Z^T HZ$, $H_{21} = Y^T HZ$ and $H_{22} = Y^T HY$. Since $Z^T HZ$ is positive definite by assumption, H_{11} is positive definite and (1.12) can be written as

$$\begin{pmatrix} I & 0 \\ H_{2,1} H_{11}^{-1} & I \end{pmatrix} \begin{pmatrix} H_{11} & 0 \\ 0 & H_{22} - H_{21} H_{11}^{-1} H_{21}^T + \frac{1}{\mu} I \end{pmatrix} \begin{pmatrix} I & H_{11}^{-1} H_{21}^T \\ 0 & I \end{pmatrix}.$$

Sylvester's Law of Inertia then implies that the inertia of $H + \frac{1}{\mu} J^T J$ is the same as the inertia of $\operatorname{diag}(H_{11}, H_{22} - H_{21} H_{11}^{-1} H_{21}^T + \frac{1}{\mu} I)$. This matrix is positive definite for all $0 < \mu < \bar{\mu}$, where $\bar{\mu} = 1/\max\{-\lambda_{\min}, 0\}$, with $\lambda_{\min}$ the smallest eigenvalue of $H_{22} - H_{21} H_{11}^{-1} H_{21}^T$. □

Theorem 1.5.1. *Given an $n \times n$ symmetric matrix H and an $m \times n$ matrix J, let r denote the rank of J and let Z be a matrix whose columns form a basis for the null space of J. If K is defined as*

$$K = \begin{pmatrix} H & J^T \\ J & 0 \end{pmatrix}$$

then

$$\operatorname{In}(K) = \operatorname{In}(Z^T HZ) + (r, r, m - r).\ \square$$

The following corollary is immediate.

Corollary 1.5.1. *Given an $n \times n$ symmetric matrix H and an $m \times n$ matrix J of rank m, let Z be a matrix whose columns form a basis for the null space of J. If K is defined as*

$$K = \begin{pmatrix} H & J^T \\ J & 0 \end{pmatrix} \tag{1.13}$$

then

$$\operatorname{In}(K) = \operatorname{In}(Z^T HZ) + (m, m, 0).$$

Proof. Let $r = m$ in Theorem 1.5.1. □

Note: If $Z^T H Z$ is nonsingular and J has full row rank, then the matrix given by (1.13) is nonsingular.

Lemma 1.5.3. *Define the matrix*

$$K = \begin{pmatrix} H & J^T \\ J & -\mu I \end{pmatrix}. \tag{1.14}$$

Then

$$\text{In}(K) = \text{In}(H + \frac{1}{\mu} J^T J) + (0, m, 0).$$

Proof. Define the nonsingular matrix S as

$$S = \begin{pmatrix} I & 0 \\ \frac{1}{\mu} J & I \end{pmatrix}. \tag{1.15}$$

Sylvester's Law of Inertia implies

$$\begin{aligned} \text{In}(K) &= \text{In}(S^T K S) \\ &= \text{In} \begin{pmatrix} H + \frac{1}{\mu} J^T J & 0 \\ 0 & -\mu I \end{pmatrix} \\ &= \text{In}(H + \frac{1}{\mu} J^T J) + (0, m, 0). \end{aligned}$$

□

The following result concerns the *exact* ℓ_1 penalty function given by

$$P_1(x, \rho) = f(x) + \rho \sum_{i=1}^{m} |c_i(x)| = f(x) + \rho \|c(x)\|_1.$$

Lemma 1.5.4. *If x^* is an unconstrained local minimizer of $P_1(x, \rho)$, then x^* is a solution of the constrained problem*

$$\begin{aligned} \underset{x,u,v}{\text{minimize}} \quad & f(x) + \rho e^T (u + v) \\ \text{subject to} \quad & c(x) - u + v = 0, \\ & u \geq 0, \ v \geq 0, \end{aligned}$$

where e denotes the m-vector $(1, 1, \ldots, 1)^T$, and a vector inequality of the form $u \geq 0$ is interpreted component-wise. $\square$

2

Background

This chapter contains background information pertinent to the remaining chapters. Section 2.1 provides a relatively extensive coverage of optimality conditions for three problem formats: a general equality constrained problem (problem NEP), a general equality and inequality constrained problem (problem GNP), and finally, a simplified version of GNP that will be referred to as problem GNPs. Many well-known results will be given, but proofs will not be included. Section 2.2 gives background on penalty functions and introduces a number of primal-dual penalty functions. These functions are the focus of this thesis.

2.1 Optimality Conditions

2.1.1 Nonlinear equality constrained problems (NEP)

This section considers the optimality conditions for a nonlinear equality constrained problem. This problem format will be referred to as problem NEP and is given by

NEP
$$\begin{array}{ll} \underset{x \in \mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = 0. \end{array} \tag{2.1}$$

Definition 2.1.1. *A point* x^* *is a* first-order KKT point (Karush-Kuhn-Tucker point) *for problem* (2.1) *if there exists a Lagrange multiplier vector* y^**, such that the following are true:*

$$\text{(i) } c(x^*) = 0; \qquad \text{(ii) } g(x^*) = J(x^*)^T y^*.$$

It would be convenient if being a KKT point was a necessary condition for being a local constrained minimizer for problem (2.1). However, this is only the case if a certain regularity condition holds; this condition is known as a *constraint qualification.*

Definition 2.1.2 (Constraint qualification for equality constraints)**.** *The constraint qualification with respect to the equality constraints c(x) =0 holds at x if x is feasible and every nonzero vector p satisfying J(x)p = 0 is tangent to a differentiable feasible path emanating from x.*

It is now possible to state first-order necessary conditions for a local solution of problem NEP.

Theorem 2.1.1. *Let the constraint qualification hold at* x^**. Then* x^* *is a local solution of problem* NEP *only if there exists a Lagrange multiplier vector* y^* *such that*

$$g(x^*) = J(x^*)^T y^* = \sum_{i=1}^{m} y_i^* \nabla c_i(x^*). \tag{2.2}$$

Equivalently, if $Z(x^*)$ *denotes a matrix whose columns form a basis for the null space of* $J(x^*)$*, then*

$$Z(x^*)^T g(x^*) = 0. \ \square$$

The vector $Z(x)^T g(x)$ is known as the *reduced gradient* of f at x. The first-order condition $Z(x^*)^T g(x^*) = 0$ is analogous to the first-order condition $g(x^*) = 0$ in the unconstrained case.

To study second-order necessary conditions, it is convenient to define the function

$$\mathcal{L}(x, y) = f(x) - c(x)^T y, \tag{2.3}$$

which is called the *Lagrangian.* The gradient and Hessian of the Lagrangian are given by

$$\nabla\mathcal{L}(x, y) = \begin{pmatrix} g(x) - J(x)^T y \\ -c(x) \end{pmatrix} \triangleq \begin{pmatrix} g(x, y) \\ -c(x) \end{pmatrix}, \quad \text{and}$$

$$\nabla^2\mathcal{L}(x, y) = \begin{pmatrix} H(x) - \sum_{i=1}^m y_i \nabla^2 c_i(x) & -J(x)^T \\ -J(x) & 0 \end{pmatrix} \triangleq \begin{pmatrix} H(x, y) & -J(x)^T \\ -J(x) & 0 \end{pmatrix},$$

where $H(x)$ denotes the Hessian of the objective function f. To derive second-order optimality conditions, one must examine the second-order behavior of f along feasible paths emanating from x^*. This examination leads to the following second-order necessary conditions.

Theorem 2.1.2 (Second-order necessary conditions for problem NEP)**.** *If the constraint qualification holds at x^*, then x^* is a local solution of problem* NEP *only if:*

(a) $c(x^*) = 0$*;*

(b) *there exists a vector y^* such that $g(x^*) = J(x^*)^T y^*$; and*

(c) *for the y^* of part* (b)*, it holds that $p^T H(x^*, y^*) p \geq 0$ for every vector p satisfying $J(x^*) p = 0$.* $\square$

A point satisfying the criteria of the above theorem is called a *second-order KKT point.* Condition (c) is equivalent to the statement that $Z(x^*)^T H(x^*, y^*) Z(x^*)$

is positive semi-definite, where $Z(x^*)$ is a matrix whose columns form a basis for $\text{null}\big(J(x^*)\big)$. Given arbitrary vectors x and y, the matrix $Z(x)^T H(x,y) Z(x)$ is known as the *reduced Hessian* of the Lagrangian. The condition that the reduced Hessian is positive semi-definite at (x^*, y^*) is analogous to the condition that $H(x^*)$ be positive semi-definite in the *unconstrained* case.

It is now possible to state first- and second-order sufficient conditions for a constrained minimizer of problem NEP. These conditions are stronger than the second-order necessary conditions given in Theorem 2.1.2 because the curvature of $H(x^*, y^*)$ in the null space of $J(x^*)$ is bounded away from zero.

Theorem 2.1.3 (Second-order sufficient conditions for a strict local solution of problem NEP)**.** *A point x^* is a strict local minimizer of problem* NEP (2.1) *if:*

(a) $c(x^*) = 0$*;*

(b) *there exists a Lagrange multiplier vector y^* such that $g(x^*) = J(x^*)^T y^*$; and*

(c) *for the y^* of part* (b)*, the strict inequality $p^T H(x^*, y^*) p > 0$ holds for all nonzero p such that $J(x^*)p = 0$.* □

Theorem 2.1.4 (Second-order sufficient conditions for an isolated local solution of problem NEP)**.** *A point x^* is an isolated local minimizer of problem* NEP (2.1) *if:*

(a) $c(x^*) = 0$*;*

(b) *there exists a Lagrange multiplier vector y^* such that $g(x^*) = J(x^*)^T y^*$;*

(c) *for the y^* of part* (b)*, the strict inequality $p^T H(x^*, y^*) p > 0$ holds for all nonzero p such that $J(x^*)p = 0$; and*

(d) *the constraint gradients at x^* are linearly independent.* □

2.1.2 General nonlinear problem (GNP)

This section considers the optimality conditions for a general nonlinear constrained problem. This problem will be referred to as problem GNP and is given by

$$\text{GNP} \qquad \begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c_i(x) = 0 \quad \text{for} \quad i \in \mathcal{E}, \\ & c_i(x) \geq 0 \quad \text{for} \quad i \in \mathcal{I}, \end{array} \tag{2.4}$$

where $\mathcal{E} = \{1, 2, \ldots, m_{\mathcal{E}}\}$ is the set of indices corresponding to equality constraints and $\mathcal{I} = \{m_{\mathcal{E}} + 1, \ldots, m_{\mathcal{E}} + m_{\mathcal{I}}\}$ is the set of indices corresponding to inequality constraints ($m_{\mathcal{E}} + m_{\mathcal{I}} = m$).

Definition 2.1.3 (First-order KKT point for problem GNP)**.** *The point x^* is a first-order KKT point for problem* GNP*, if there exists an m-vector y^*, called a Lagrange multiplier vector, such that*

(i) $c_{\mathcal{E}}(x^*) = 0$ *and* $c_{\mathcal{I}}(x^*) \geq 0$ (feasibility),

(ii) $g(x^*) = J(x^*)^T y^*$ (stationarity),

(iii) $y^*_{\mathcal{I}} \geq 0$ (non-negativity of multipliers associated with inequalities), *and*

(iv) $c(x^*) \cdot y^* = 0$ (complementarity).

The complementarity condition given above as (iv), implies that when an inequality constraint is *inactive*, then its associated Lagrange multiplier must be zero.

Since the Lagrange multiplier vector above is not unique when J does not have full row rank, notation to describe all of the possible Lagrange multiplier vectors is introduced.

Definition 2.1.4 (Acceptable Lagrange multipliers)**.** *Given a KKT point x^* for problem* GNP (2.4)*, the set of acceptable Lagrange multipliers is defined as*

$$\mathcal{M}_y(x^*) = \{\, y \in \mathbb{R}^m : g(x^*) = J(x^*)^T y,\ y_{\mathcal{I}} \geq 0,\ c(x^*) \cdot y = 0 \,\}. \tag{2.5}$$

The complementarity condition $c(x^*) \cdot y = 0$ forces y_i to be zero when constraint c_i is inactive. However, it is still possible that both c_i and y_i are zero at the same time. The concept of *strict complementarity* rules out this possibility.

Definition 2.1.5 (Strict complementarity)**.** *Strict complementarity holds at the KKT point x^* if there exists a Lagrange multiplier vector $y^* \in \mathcal{M}_y(x^*)$ such that $y_i^* > 0$ for all $i \in \mathcal{A}_\mathcal{I}$.*

It would be convenient if being a KKT point was a necessary condition for being a local constrained minimizer for problem (2.4). However, this is only the case if a certain regularity condition holds; this condition is known as a *constraint qualification.* If the constraint qualification holds then it is true that being a KKT point is a necessary condition for optimality.

Definition 2.1.6 (First-order constraint qualification (FOCQ) for problem GNP)**.** *The first-order constraint qualification with respect to the set of constraints $c_i(x) = 0$ for $i \in \mathcal{E}$ and $c_i(x) \geq 0$ for $i \in \mathcal{I}$ holds at a feasible point x if every nonzero vector p such that $J_\mathcal{E}(x)p = 0$ and $J_{\mathcal{A}_\mathcal{I}}(x)p \geq 0$ is a tangent to a differentiable feasible path emanating from x.*

Each of the following conditions is sufficient to ensure that the constraint qualification holds at a point $\bar{x}$:

(i) The active constraints are linear at $\bar{x}$.

(ii) The active constraint gradients, $\{\nabla c_i(\bar{x}) : i \in \mathcal{A}(\bar{x})\}$ are linearly independent. This condition is referred to as the *linear independence constraint qualification* (LICQ).

(iii) The gradients of the equality constraints at $\bar{x}$ are linearly independent and there exists a nonzero vector p such that $J_\mathcal{E}(\bar{x})p = 0$ and $J_{\mathcal{A}_\mathcal{I}}(\bar{x})p > 0$, i.e., p is a "strictly interior" direction for the active inequality constraints. This condition is known as the *Mangasarian-Fromovitz Constraint Qualification* (MFCQ).

A few facts should be mentioned:

Fact 1: If the LICQ holds at a KKT point x^*, then the Lagrange multiplier vector is unique.

Fact 2: The MFCQ is a weaker condition than the LICQ.

Fact 3: If the MFCQ is satisfied at a KKT point x^*, then the set of acceptable Lagrange multipliers defined in (2.5) is bounded.

Fact 4: The LICQ is more practical than the MFCQ in the sense that verification of the LICQ is much easier.

Necessary conditions for problem GNP may now be discussed.

Lemma 2.1.1 (First-order necessary conditions for problem GNP)**.** *If x^* is a local minimizer of problem* GNP *and the MFCQ holds at x^*, then x^* is a KKT point.* $\square$

Similar to the nonlinear equality constrained problem (NEP), the use of the Lagrangian function in developing second-order conditions for problem GNP is paramount. Recall that the Lagrangian and its derivatives are given by

$$\nabla\mathcal{L}(x,y) = \begin{pmatrix} g(x) - J(x)^T y \\ -c(x) \end{pmatrix} \triangleq \begin{pmatrix} g(x,y) \\ -c(x) \end{pmatrix} \quad \text{and}$$

$$\nabla^2\mathcal{L}(x,y) = \begin{pmatrix} H(x) - \sum_{i=1}^m y_i \nabla^2 c_i(x) & -J(x)^T \\ -J(x) & 0 \end{pmatrix} \triangleq \begin{pmatrix} H(x,y) & -J(x)^T \\ -J(x) & 0 \end{pmatrix}.$$

In order to derive second-order conditions for optimality, the curvature of f must be considered only in directions for which f is stationary. This set of suitable directions at a feasible point x is defined as

$$\mathcal{S}_L(x) = \{\, p : p \neq 0,\ g(x)^T p = 0,\ J_{\mathcal{E}}(x)p = 0 \text{ and } J_{\mathcal{A}_{\mathcal{I}}}(x)p \geq 0 \,\}. \tag{2.6}$$

However, to ensure that these directions are tangents to an appropriate feasible path starting at x, another regularity condition is needed; this condition is a *second-order constraint qualification.*

In order to formulate this constraint qualification, it is useful to write (2.6) in a different but equivalent form. Given a KKT point x, choose any $y \in \mathcal{M}_y(x)$ and then define $\mathcal{A}_+(x)$ to be the set of indices of active inequality constraints with positive Lagrange multipliers and define $J_+(x)$ to be the corresponding rows of the Jacobian. Next, define $\mathcal{A}_0(x)$ to be the set of indices of active inequality constraints with zero Lagrange multipliers and define $J_0(x)$ to be the corresponding rows of the Jacobian. Note that $\mathcal{A}_+(x)$ and $\mathcal{A}_0(x)$ are functions of the specific y chosen. It can be seen from the short calculation

$$g(x)^T p = y_{\mathcal{E}}^T J_{\mathcal{E}}(x)p + y_+^T J_+(x)p + y_0^T J_0(x)p = y_{\mathcal{E}}^T J_{\mathcal{E}}(x)p + y_+^T J_+(x)p$$

that the set of suitable second-order directions can be described as

$$\mathcal{S}_L(x) = \{\, p : p \neq 0,\; J_+(x)p = 0,\; J_{\mathcal{E}}(x)p = 0 \text{ and } J_0(x)p \geq 0 \,\}. \tag{2.7}$$

Given this definition, it is possible to formulate the following second-order constraint qualification.

Definition 2.1.7 (Second-order constraint qualification (SOCQ))**.** *The second-order constraint qualification for problem* GNP (2.4) *holds at a KKT point x if, for all $y \in \mathcal{M}_y(x)$, every nonzero p satisfying $J_+(x)p = 0$, $J_0(x)p \geq 0$, and $J_{\mathcal{E}}(x)p = 0$, is a tangent to a twice-differentiable path $x(\alpha)$ such that $c_+\big(x(\alpha)\big) = 0$, $c_0\big(x(\alpha)\big) \geq 0$, and $c_{\mathcal{E}}\big(x(\alpha)\big) = 0$ for all $0 < \alpha \leq \hat{\alpha}$ for some $\hat{\alpha} > 0$.*

Fact1: If the active constraints are linear, then both the first- and second-order constraint qualifications hold.

Fact2: The LICQ implies that both the first- and second-order constraint qualifications are satisfied.

Fact3: The FOCQ does not imply the SOCQ nor does the SOCQ imply the FOCQ.

Second-order necessary conditions for problem GNP may now be stated. They require satisfaction of both the first- and second-order constraint qualification.

Theorem 2.1.5 (Second-order necessary conditions for problem GNP)**.** *Let the first- and second-order constraint qualifications hold at a point x^*. If x^* is a local solution of* GNP *then*

(1) *x^* is a KKT point; and*

(2) *for some $y \in \mathcal{M}_y(x^*)$, it is true that for all nonzero p satisfying $J_+(x)p = 0$, $J_0(x)p \geq 0$, and $J_\mathcal{E}(x^*)p = 0$, it holds that $p^T H(x^*, y)p \geq 0$.* □

Two different second-order sufficient conditions are now given.

Definition 2.1.8 (First second-order sufficient condition for problem GNP (SSC1))**.** *Let x^* be a KKT point as defined in Definition* 2.1.3 *with associated Lagrange multiplier vector y^*. Then condition* SSC1 *is said to hold at (x^*, y^*) if there exists $\omega > 0$ such that*

$$p^T H(x^*, y^*)p \geq \omega \|p\|^2$$

for all $p \neq 0$ satisfying $g(x^*)^T p = 0$, $J_{\mathcal{A}_\mathcal{I}}(x^*)p \geq 0$, and $J_\mathcal{E}(x^*)p = 0$.

A more demanding second-order condition places a requirement on *all* acceptable Lagrange multiplier vectors.

Definition 2.1.9 (Second second-order sufficient condition for problem GNP (SSC2))**.** *Let x^* be a KKT point as defined in Definition* 2.1.3. *Then the* SSC2 *holds at x^*, if for every Lagrange multiplier vector $y \in \mathcal{M}_y(x^*)$, there exists $\omega > 0$ such that*

$$p^T H(x^*, y^*)p \geq \omega \|p\|^2$$

for all $p \neq 0$ satisfying $g(x^*)^T p = 0$, $J_{\mathcal{A}_\mathcal{I}}(x^*)p \geq 0$, and $J_\mathcal{E}(x^*)p = 0$.

Conditions for a *strict* local constrained minimizer may now be given.

Theorem 2.1.6 (Sufficient conditions for a strict minimizer)**.** *The point x^* is a strict local constrained minimizer for problem* GNP *if*

(1) *x^* is a KKT point; and*

(2) *condition* SSC1 *holds at* (x^*, y) *for some* $y \in \mathcal{M}_y(x^*)$ *(see Definition* 2.1.8*).* □

Verifying part (2) for all p such that $g(x^*)^T p = 0$, $J_{\mathcal{A}_\mathcal{I}}(x^*)p \geq 0$ and $J_\mathcal{E}(x^*)p = 0$ requires finding the global minimizer of a possibly indefinite quadratic form over a cone, which is an NP-hard problem. Computational friendly sufficient conditions may be stated by making use of the fact that the set $\mathcal{S}_L(x)$ is the intersection of the sets $\{\, p : J_+(x)p = 0 \,\}$, $\{\, p : J_0(x)p \geq 0 \,\}$ and $\{\, p : J_\mathcal{E}(x)p = 0 \,\}$. Working with only the intersection of the sets $\{\, p : J_+(x)p = 0 \,\}$ and $\{\, p : J_\mathcal{E}(x)p = 0 \,\}$, which is a larger set, imposes conditions that are more strict. This leads to computationally friendly sufficient conditions for a strict local solution.

Theorem 2.1.7 (Computational second-order sufficient conditions)**.** *The point* x^* *is a strict minimizer of problem* GNP (2.4) *if the following conditions hold:*

(i) x^* *is a KKT point as defined in Definition* 2.1.3 *on page* 20 *with Lagrange multiplier vector* y^**;*

(ii) *if* y^*_+ *is the vector of strictly positive elements of the* y^* *corresponding to the inequalities from part* (i)*, and* $J_+(x^*)$ *is the associated matrix of constraint gradients, then there exists an* $\omega > 0$ *such that*

$$p^T H(x^*, y^*)p \geq \omega \|p\|^2$$

for all $p \neq 0$ *satisfying* $J_+(x^*)p = 0$ *and* $J_\mathcal{E}(x^*)p = 0$*.* □

This theorem gives conditions that guarantee that x^* is a *strict* local minimizer. Constraint qualifications are needed to prove that x^* is an *isolated* local solution of problem GNP.

Theorem 2.1.8 (Sufficient conditions for an isolated local constrained minimizer of problem GNP)**.** *The point* x^* *is an isolated local constrained minimizer of problem* GNP (2.4) *if:*

(i) *x^* is a KKT point as defined in Definition* 2.1.3 *on page* 20*;*

(ii) *the MFCQ holds at x^*, i.e., $J_{\mathcal{E}}(x^*)$ has linearly independent rows and there exists a vector p such that $J_{\mathcal{E}}(x^*)p = 0$ and $J_{\mathcal{A}_{\mathcal{I}}}(x^*)p > 0$; and*

(iii) *for all $y \in \mathcal{M}_y(x^*)$ there exists an $\omega > 0$ such that $p^T H(x^*, y)p \geq \omega \|p\|^2$ for and all nonzero vectors p satisfying $g(x^*)^T p = 0$, $J_{\mathcal{A}_{\mathcal{I}}}(x^*)p \geq 0$ and $J_{\mathcal{E}}(x^*)p = 0$.* □

Finally, computationally friendly sufficient conditions for an isolated solution of problem GNP are given.

Theorem 2.1.9 (Strong sufficient conditions for an isolated solution of problem GNP)**.** *The point x^* is an isolated local constrained minimizer of problem* GNP (2.4) *if:*

(i) *the LICQ holds at x^*, i.e., $J_{\mathcal{A}}(x^*)$ has full row rank;*

(ii) *x^* is a KKT point and strict complementarity holds, i.e., the necessarily unique Lagrange multiplier vector y^* has the property that $y_i^* > 0$ for all $i \in \mathcal{A}_{\mathcal{I}}(x^*)$; and*

(iii) *there exists an $\omega > 0$ such that $p^T H(x^*, y^*)p \geq \omega \|p\|^2$ for all nonzero vectors p satisfying $J_{\mathcal{A}}(x^*)p = 0$.* □

Part (iii) of this theorem only considers vectors p in the null space of the active constraints. This is a consequence of strict complementarity holding at x^*.

2.1.3 A simplified general nonlinear problem (GNPs)

This section considers the optimality conditions for a simplified version of problem GNP. This problem form will be referred to as problem GNPs and is given by

$$\text{GNPs} \qquad \begin{array}{ll} \underset{x \in \mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = 0, \;\; x \geq 0. \end{array} \tag{2.8}$$

In a general setting, there may be both upper and lower bounds on the vector x.

Problem GNPs is a special case of problem GNP. However, since most of the future analysis is done on problem GNPs, it is convenient to state the analogous definitions and theorems. First, a KKT point for problem GNPs is defined.

Definition 2.1.10 (First-order KKT point for problem GNPs)**.** *The point x^* is a first order KKT point for problem* GNPs*, if there exists a Lagrange multiplier vector $(y^*, z^*) \in \mathbb{R}^{m+n}$, such that*

(i) $c(x^*) = 0$*;*

(ii) $x^* \geq 0$*;*

(iii) $g(x^*) = J(x^*)^T y^* + z^*$*;*

(iv) $z^* \geq 0$*; and*

(v) $z^* \cdot x^* = 0$*.*

Since the Lagrange multiplier vector is not unique when the Jacobian of the active constraints does not have full row rank, it is convenient to define a set of acceptable Lagrange multiplier vectors for problem GNPs.

Definition 2.1.11 (Acceptable Lagrange multiplier vectors for problem GNPs)**.** *Given a KKT point x^* for problem* GNPs (2.8)*, the set of acceptable Lagrange multiplier vectors is defined as*

$$\mathcal{M}_{y,z}(x^*) = \{\, (y, z) \in \mathbb{R}^{m+n} : g(x^*) = J(x^*)^T y + z,\ z \geq 0,\ \textit{and}\ x^* \cdot z = 0 \,\}.$$

Complementarity forces z_i to be zero when $x_i^* > 0$, i.e., when the ith bound constraint is inactive. However, it is possible that x_i^* and z_i are both zero. *Strict complementarity* rules out this possibility.

Definition 2.1.12 (Strict complementarity for problem GNPs)**.** *Strict complementarity holds at the KKT point x^* if there exists a Lagrange multiplier vector $(y^*, z^*) \in \mathcal{M}_{y,z}(x^*)$ such that $z_i^* > 0$ whenever $x_i^* = 0$.*

The constraint qualification for problem GNPs may now be stated.

Definition 2.1.13 (First-order constraint qualification (FOCQ) for problem GNPs)**.** *The first-order constraint qualification with respect to the set of constraints* $c(x) = 0$ *and* $x \geq 0$ *holds at a feasible point* x *if every nonzero vector* p *that satisfies* $J(x)p = 0$ *and* $E_{\mathcal{A}}(x)p = p_{\mathcal{A}} \geq 0$ *is a tangent vector to a differentiable feasible path emanating from* x*.*

Lemma 2.1.2 (First-order necessary conditions for problem GNPs)**.** *If* x^* *is a local minimizer of problem* GNPs *and the* FOCQ *holds at* x^**, then* x^* *is a KKT point as defined by Definition* 2.1.10*.* $\square$

The Lagrangian function is used to develop second-order conditions. For problem GNPs, the Lagrangian function and its derivatives are given by

$$\mathcal{L}(x, y, z) = f(x) - c(x)^T y - x^T z,$$

$$\nabla\mathcal{L}(x, y, z) = \begin{pmatrix} g(x) - J(x)^T y - z \\ -c(x) \\ -x \end{pmatrix} \triangleq \begin{pmatrix} g(x, y, z) \\ -c(x) \\ -x \end{pmatrix},$$

$$\nabla^2\mathcal{L}(x, y, z) = \begin{pmatrix} H(x) - \sum_{i=1}^m y_i \nabla^2 c_i(x) & -J(x)^T & -I \\ -J(x) & 0 & 0 \\ -I & 0 & 0 \end{pmatrix}$$

$$\triangleq \begin{pmatrix} H(x, y) & -J(x)^T & -I \\ -J(x) & 0 & 0 \\ -I & 0 & 0 \end{pmatrix}.$$

Definition 2.1.14 (Second-order constraint qualification for problem GNPs (SOCQ))**.** *The second-order constraint qualification for problem* GNPs (2.8) *holds at a KKT point* x *if, for all* $(y, z) \in \mathcal{M}_{y,z}(x)$*, every nonzero* p *satisfying* $E_+(x)p = p_+ = 0$*,* $E_0(x)p = p_0 \geq 0$*, and* $J(x)p = 0$*, is a tangent to a twice-differentiable path* $x(\alpha)$ *such that* $x_+(\alpha) = 0$*,* $x_0(\alpha) \geq 0$ *and* $c\big(x(\alpha)\big) = 0$ *for all* $0 < \alpha \leq \hat{\alpha}$ *for some*

$\hat{\alpha} > 0$, where p_+ are the components of p that correspond to the bound variables with strictly positive Lagrange multipliers and p_0 are the components of p that correspond to the bound variables with zero Lagrange multipliers.

The following three facts pertain to the constraint qualifications.

Fact1: If the active constraints are linear, then both the first- and second-order constraint qualifications hold.

Fact2: The LICQ implies that both the first- and second-order constraint qualifications are satisfied.

Fact3: The FOCQ does not imply the SOCQ nor does the SOCQ imply the FOCQ.

Theorem 2.1.10 (Second-order necessary conditions for problem GNPs)**.** *Let the first- and second-order constraint qualifications hold at a point x^*. If x^* is a local solution of problem* GNPs *then*

(1) *x^* is a KKT point; and*

(2) *for some $(y, z) \in \mathcal{M}_{y,z}(x^*)$, it is true that $p^T H(x^*, y)p \geq 0$ for all nonzero p satisfying $g(x^*)^T p = 0$, $p_{\mathcal{A}} \geq 0$, and $J(x^*)p = 0$.* $\square$

Sufficient conditions for problem GNPs are now given.

Definition 2.1.15 (First second-order sufficient condition for GNPs (SSC1))**.** *Let x^* be a KKT point as defined in Definition* 2.1.10 *with associated Lagrange multiplier vector (y^*, z^*). Then condition* SSC1 *is said to hold at (x^*, y^*, z^*) if there exists $\omega > 0$ such that*

$$p^T H(x^*, y^*)p \geq \omega \|p\|^2$$

for all $p \neq 0$ satisfying $g(x^*)^T p = 0$, $p_{\mathcal{A}} \geq 0$, and $J(x^*)p = 0$.

A more demanding second-order condition places a requirement on *all* possible Lagrange multiplier vectors.

Definition 2.1.16 (Second second-order sufficient condition for GNPs (SSC2))**.** *Let* x^* *be a KKT point as defined in Definition* 2.1.10*. Condition* SSC2 *is said to hold at* x^**, if for every acceptable Lagrange multiplier vector* $(y, z) \in \mathcal{M}_{y,z}(x^*)$*, there exists* $\omega > 0$ *such that*

$$p^T H(x^*, y)p \geq \omega \|p\|^2$$

for all $p \neq 0$ *satisfying* $g(x^*)^T p = 0$*,* $p_{\mathcal{A}} \geq 0$*, and* $J(x^*)p = 0$*.*

Sufficient conditions for a *strict* local constrained minimizer for problem GNPs are now given.

Theorem 2.1.11 (Sufficient conditions for a strict minimizer for problem GNPs)**.** *The point* x^* *is a strict local constrained minimizer of problem* GNPs *if*

(1) x^* *is a KKT point; and*

(2) *condition* SSC1 *holds at* (x^*, y, z) *for some* $(y, z) \in \mathcal{M}_{y,z}(x^*)$*.* $\square$

Verifying part (2) for all p such that $g(x^*)^T p = 0$, $p_{\mathcal{A}} \geq 0$ and $J(x^*)p = 0$ requires finding the global minimizer of a possibly indefinite quadratic form over a cone, which is an NP-hard problem. Computationally friendly sufficient conditions may be formulated by using a set of feasible directions analogous to that defined by equation (2.7) on page 23 for problem GNP.

Theorem 2.1.12 (Computational second-order sufficient conditions for problem GNPs)**.** *The point* x^* *is a strict minimizer of problem* GNPs *if:*

(i) x^* *is a KKT point with Lagrange multiplier vector* (y^*, z^*) *as defined in Definition* 2.1.10*; and*

(ii) *if* z_+^* *is the vector of strictly positive elements of* z^* *from part* (i)*, then there has to exist an* $\omega > 0$ *such that*

$$p^T H(x^*, y^*)p \geq \omega \|p\|^2$$

for all nonzero p *satisfying* $p_+ = 0$*, and* $J(x^*)p = 0$*.* $\square$

Constraint qualifications are needed to guarantee that a point x^* is an *isolated* local solution of problem GNPs.

Theorem 2.1.13 (Sufficient conditions for an isolated local constrained minimizer of problem GNPs)**.** *The point x^* is an isolated local constrained minimizer of problem* GNPs (2.8) *if:*

(i) *x^* is a KKT point as defined in Definition* 2.1.10*;*

(ii) *the MFCQ holds at x^*, i.e., $J(x^*)$ has linearly independent rows and there exists a nonzero vector p such that $p_{\mathcal{A}} > 0$ and $J(x^*)p = 0$; and*

(iii) *for all $(y, z) \in \mathcal{M}_{y,z}(x^*)$, there exists an $\omega > 0$ such that $p^T H(x^*, y)p \geq \omega \|p\|^2$ for all nonzero vectors p satisfying $g(x^*)^T p = 0$, $p_{\mathcal{A}} \geq 0$ and $J(x^*)p = 0$.* □

Stronger sufficient conditions for an isolated solution of problem GNPs are now given.

Theorem 2.1.14 (Strong sufficient conditions for an isolated solution of problem GNPs)**.** *The point x^* is an isolated local constrained minimizer of problem* GNPs (2.8) *if:*

(i) *the LICQ holds at x^*, i.e.,*

$$\begin{pmatrix} J(x^*) \\ E_{\mathcal{A}}(x^*) \end{pmatrix}$$

has full row rank;

(ii) *x^* is a KKT point and strict complementarity holds, i.e., the necessarily unique Lagrange multiplier vector (y^*, z^*) has the property that $z_i^* > 0$ if $x_i^* = 0$; and*

(iii) *there exists an $\omega > 0$ such that $p^T H(x^*, y^*)p \geq \omega \|p\|^2$ for all nonzero vectors p satisfying $J(x^*)p = 0$ and $p_{\mathcal{A}} = 0$.* □

The following lemma gives a condition that is equivalent to item (i) above.

Lemma 2.1.3. *The matrix*

$$\begin{pmatrix} J(x) \\ E_{\mathcal{A}}(x) \end{pmatrix} \tag{2.9}$$

has linearly independent rows if and only if $\widehat{J}(x)$ *has linearly independent rows, where the matrix* $\widehat{J}(x)$ *contains the columns of* $J(x)$ *corresponding to bounds that are* inactive *at* x *and the matrix* $E_{\mathcal{A}}(x)$ *contains the rows of the identity matrix corresponding to bounds that are* active *at* x*.*

Proof. Note that there exists a nonsingular permutation matrix P, such that

$$\begin{pmatrix} J(x) \\ E_{\mathcal{A}}(x) \end{pmatrix} P = \begin{pmatrix} \widehat{J}(x) & \widetilde{J}(x) \\ 0 & I \end{pmatrix} \triangleq B, \tag{2.10}$$

where $\widehat{J}(x)$ is defined in the statement of the theorem and where $\widetilde{J}(x)$ contains the columns of $J(x)$ corresponding to *active* bounds at x. Since multiplication on the right by a nonsingular matrix does not change row rank, it is sufficient to show that B has full row rank if and only if $\widehat{J}(x)$ has full row rank.

($\Rightarrow$) For a contrapositive proof, assume $\widehat{J}(x)$ has dependent rows. This means that $\widehat{J}(x)^T$ has dependent columns and that there exists a vector $z_1 \neq 0$ that satisfies $\widehat{J}(x)^T z_1 = 0$. Define $z_2 = -\widetilde{J}(x)^T z_1$. It follows that

$$B^T \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} \widehat{J}(x)^T & 0 \\ \widetilde{J}(x)^T & I \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} \widehat{J}(x)^T z_1 \\ \widetilde{J}(x)^T z_1 + z_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Since $z_1 \neq 0$, this implies that B^T has dependent columns and that B has dependent rows.

($\Leftarrow$) For another contrapositive proof, assume B has dependent rows. This implies that B^T has dependent columns and that there exists a vector $(z_1, z_2)^T \neq 0$ such that

$$B^T \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} \widehat{J}(x)^T & 0 \\ \widetilde{J}(x)^T & I \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} \widehat{J}(x)^T z_1 \\ \widetilde{J}(x)^T z_1 + z_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{2.11}$$

Suppose $z_1 = 0$. Then the previous equation implies that $z_2 = 0$. This is a contradiction and implies that $z_1 \neq 0$. However, equation (2.11) gives $\widehat{J}(x)^T z_1 = 0$. Since $z_1 \neq 0$, this means $\widehat{J}(x)^T$ has dependent columns. Thus, $\widehat{J}(x)$ has dependent rows. □

Finally, Lemma 2.1.3 may be used to give sufficient conditions for an isolated constrained minimizer for problem GNPs that are equivalent to Theorem 2.1.14.

Theorem 2.1.15 (Strong sufficient conditions for an isolated solution of problem GNPs)**.** *The point x^* is an isolated local constrained minimizer of problem* GNPs (2.8) *if:*

(i) *the LICQ holds at x^*, i.e., $\widehat{J}(x^*)$ has full row rank;*

(ii) *x^* is a KKT point and strict complementarity holds, i.e., the necessarily unique Lagrange multiplier vector (y^*, z^*) has the property that $z_i^* > 0$ if $x_i^* = 0$; and*

(iii) *there exists an $\omega > 0$ such that $p^T H(x^*, y^*) p \geq \omega \|p\|^2$ for all nonzero vectors p satisfying $J(x^*)p = 0$ and $p_{\mathcal{A}} = 0$.* □

2.2 Primal-Dual Penalty Functions

This section serves as an introduction to a class of primal-dual penalty functions. The first subsection considers penalty functions, while the second subsection considers *shifted* penalty functions. The augmented Lagrangian function is derived by applying the penalty function to a shifted problem. The final subsection considers the introduction of inequalities and is the ultimate focus of this thesis.

2.2.1 Penalty functions

This subsection considers the following nonlinear equality constrained problem:

$$\text{NEP} \qquad \begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = 0. \end{array} \tag{2.12}$$

The quadratic penalty function is the basis for handling problem NEP and is given by

$$\mathcal{P}(x;\mu) = f(x) + \frac{1}{2\mu}\|c(x)\|^2. \tag{2.13}$$

A primal-dual pair $\big(x(\mu), y(\mu)\big)$ can be defined such that $x(\mu)$ minimizes $\mathcal{P}(x;\mu)$ and $y(\mu)$ is a vector of approximate Lagrange multipliers for problem NEP. The point $\big(x(\mu), y(\mu)\big)$ is a solution to the perturbed problem

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = c\big(x(\mu)\big), \end{array} \tag{2.14}$$

and satisfies the equations

$$\nabla f(x) - \sum_i y_i \nabla c_i(x) = 0 \;\text{ and }\; y_i = -c_i(x)/\mu.$$

These equations may be rewritten as

$$g(x) - J(x)^T y = 0, \tag{2.15a}$$

$$c(x) + \mu y = 0. \tag{2.15b}$$

Under standard assumptions on problem (2.12), Fiacco and McCormick in [10] show the existence of continuously differentiable functions $\big(x(\mu), y(\mu)\big)$ that satisfy the above equations; these points trace out a *trajectory of minimizers*. Using the notation $(x_\mu, y_\mu) \triangleq \big(x(\mu), y(\mu)\big)$, these points satisfy

$$g(x_\mu) - J(x_\mu)^T y_\mu = 0, \tag{2.16a}$$

$$c(x_\mu) + \mu y_\mu = 0. \tag{2.16b}$$

Furthermore, they show

$$\|\big(x(\mu), y(\mu)\big) - (x^*, y^*)\| = \Omega(\mu). \tag{2.17}$$

The *primal-dual* penalty function has $\big(x(\mu), y(\mu)\big)$ as a local minimizer and is defined as

$$\mathcal{P}(x, y; \mu) \triangleq f(x) + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x) + \mu y\|^2 \tag{2.18}$$

for a positive penalty parameter μ. This function may be interpreted as penalizing the constraint violation $c(x)$ *and* penalizing deviation from the trajectory of minimizers, where $c(x) + \mu y = 0$. This can be seen from (2.15b).

It is known that the quadratic penalty function is not ideal for handling equality constraints for the following reasons:

(i) Because of (2.17), it is necessary to drive μ towards zero to achieve a good approximation to (x^*, y^*). Moreover, because (2.17) is an estimate of type $\Omega(\cdot)$, rather than $O(\cdot)$, the solution $\big(x(\mu), y(\mu)\big)$ is guaranteed to be in error by at least some multiple of μ.

(ii) While it is possible to use an approximation to $\big(x(\mu_0), y(\mu_0)\big)$ associated with penalty parameter μ_0 as a starting point for computing $\big(x(\mu), y(\mu)\big)$ for a reduced penalty parameter μ, there is no obvious way to use prior knowledge about the solution to increase the accuracy of $\big(x(\mu), y(\mu)\big)$ as an approximation to (x^*, y^*).

(iii) An analysis like that leading to (2.17) shows that

$$\|\big(x(\mu), y(\mu)\big) - \big(x(\mu_0), y(\mu_0)\big)\| = \Omega\big(|\mu - \mu_0|\big).$$

Hence, if an approximation to $\big(x(\mu_0), y(\mu_0)\big)$ is used as the initial guess for computing $\big(x(\mu), y(\mu)\big)$, one would be starting a distance $\Omega\big(|\mu - \mu_0|\big)$ from the minimizer. Since $\nabla^2\mathcal{P}(x; \mu)$ is increasingly ill conditioned as $\mu \downarrow 0$, this systematic error could be significant. It would be nice if prior knowledge, etc., allowed us to find a starting point closer to the minimizer of the merit function (for this value of μ).

The next subsection considers the augmented Lagrangian function, which is a generalization of the quadratic penalty function (2.13) that allows prior information of the multipliers y to be introduced into the function. Use of this additional information allows for estimates (x_μ, y_μ) for a given μ that are much closer to (x^*, y^*) than is possible with (2.13).

2.2.2 Shifted penalty functions

In Powell's derivation of the "classical" augmented Lagrangian method, the solution of problem NEP (2.12) is found by repeatedly minimizing the quadratic penalty function for the "shifted" problem

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) - \mu y_e = 0, \end{array} \tag{2.19}$$

where y_e is an estimate of the optimal Lagrange multipliers y^*. This method is based on the observation that for sufficiently small μ, x^* is a minimizer for the quadratic penalty function applied to (2.19) with the choice $y_e = y^*$.

The quadratic penalty function applied to (2.19) is given by

$$f(x) + \frac{1}{2\mu}\|c(x) - \mu y_e\|^2,$$

which after rearrangement is equivalent to

$$f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{\mu}{2}\|y_e\|^2.$$

This function has the same minimizers as

$$\mathcal{L}_{\mathcal{A}}(x; y_e, \mu) \triangleq f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 \tag{2.20}$$

and is known as the augmented Lagrangian function.

A primal-dual pair $\big(x(\mu), y(\mu)\big)$ can be defined such that $x(\mu)$ minimizes $\mathcal{L}_\mathcal{A}(x; y_e, \mu)$ and $y(\mu)$ is the vector of associated Lagrange multipliers. This point satisfies the equations

$$\nabla f(x) - \sum_i y_i \nabla c_i(x) = 0 \ \text{ and } \ y_i = -\left(\frac{c_i(x)}{\mu} - [y_e]_i\right),$$

which may be rewritten as

$$\begin{aligned} g(x) - J(x)^T y &= 0, \\ c(x) + \mu(y - y_e) &= 0. \end{aligned}$$

The *primal-dual* penalty function for (2.19) is obtained by substituting $c(x) - \mu y_e$ for $c(x)$ in (2.18), which yields

$$f(x) + \frac{1}{2\mu}\|c(x) - \mu y_e\|^2 + \frac{1}{2\mu}\|c(x) + \mu(y - y_e)\|^2.$$

After rearrangement, this is equivalent to

$$f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x) + \mu(y - y_e)\|^2 + \frac{\mu}{2}\|y_e\|^2.$$

This function has the same minimizers as

$$\mathcal{M}(x, y; y_e, \mu) \triangleq f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x) + \mu(y - y_e)\|^2, \qquad (2.22)$$

and will be called the *primal-dual augmented Lagrangian function*. The primal-dual augmented Lagrangian function penalizes the constraint violation $c(x)$ *and* deviation from the trajectory for the perturbed problem; points on this perturbed trajectory satisfy $c(x) + \mu(y - y_e) = 0$. Note that $\mathcal{M}(x, y; 0, \mu) \equiv \mathcal{P}(x, y; \mu)$, i.e., the primal-dual penalty function is obtained from the primal-dual augmented Lagrangian function by setting $y_e \equiv 0$.

2.2.3 Handling inequalities

The primal-dual penalty function and primal-dual augmented Lagrangian function may be applied to problem NEP (2.12) in a relatively straightforward way.

The introduction of general inequality constraints give rise to further challenges. One technique for dealing with inequalities is to introduce them into the objective function via a barrier term. This idea makes particular sense in the primal-dual *penalty* context since both the penalty and barrier parameters must be driven to zero in order to obtain convergence. This technique has already been studied by Forsgren and Gill [12]. An alternative approach to handling general inequalities is by converting them to equality constraints through the use of slack variables. This converts the general inequality problem into a general equality problem with bounds on the slack variables. The equality constraints may then be handled by the primal-dual augmented Lagrangian function, while the bounds on the slacks are kept explicit. Active-set strategies may then be employed to handle these explicit bounds. This technique is the primary focus of this thesis and may be particularly advantageous when bounds on the primal variables already exist.

3

The Primal-Dual Augmented Lagrangian

In this chapter two primal-dual functions are considered: a primal-dual penalty function and a primal-dual augmented Lagrangian function. Most of the results, however, will be stated in terms of the primal-dual augmented Lagrangian. It will be shown that, in most cases, the results are trivially adapted to the primal-dual penalty function. The chapter is organized as follows. Section 3.1 considers the derivatives of the primal-dual penalty function and primal-dual augmented Lagrangian function. Section 3.2 discusses the inertia of the Hessian matrix associated with the primal-dual functions and relates them to standard optimality conditions. Section 3.3 gives properties of the primal-dual functions with a bias towards displaying their usefulness as merit functions in optimization algorithms. Section 3.4 discusses trajectories that are perturbations of the classical trajectory of minimizers. Section 3.5 considers the consequences of imposing explicit bounds on the dual variables. If any explicit bounds are active at a solution, it dictates that a different problem is being solved than "intended". Section 3.6 compares the systems that are solved in a primal-dual framework to the systems solved in "classical" SQP algorithms. Finally, Section 3.7 gives a *generalized* primal-dual function for which the primal-dual penalty, the primal-dual augmented Lagrangian, the proximal-point Lagrangian (see, for example, [27] and [26]), and others, are specific instances.

3.1 Derivatives

Section 2.2 defined the primal-dual penalty function and the primal-dual augmented Lagrangian function as well as motivated their definitions. This section gives their first and second derivatives since any algorithm using these functions for continuous minimization must make use of them. By defining special auxiliary vectors, relatively concise derivatives may be written.

The definition and derivatives of the primal-dual penalty function (2.18) on page 35 are given by

$$\mathcal{P}(x,y;\mu) = f(x) + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x)+\mu y\|^2, \tag{3.1a}$$

$$\begin{aligned}\nabla\mathcal{P}(x,y;\mu) &= \begin{pmatrix} g(x) - J(x)^T(2\pi_p(x)-y) \\ c(x)+\mu y \end{pmatrix} \\ &= \begin{pmatrix} g(x) - J(x)^T(2\pi_p(x)-y) \\ \mu\big(y-\pi_p(x)\big) \end{pmatrix},\end{aligned} \tag{3.1b}$$

$$\nabla^2\mathcal{P}(x,y;\mu) = \begin{pmatrix} H\big(x, 2\pi_p(x)-y\big) + \frac{2}{\mu}J(x)^TJ(x) & J(x)^T \\ J(x) & \mu I \end{pmatrix}, \tag{3.1c}$$

where $\pi_p(x) \triangleq -c(x)/\mu$. The equation

$$2\pi_p(x) - y = y + 2\big(\pi_p(x)-y\big)$$

shows that $2\pi_p(x)-y$ is equal to y plus a multiple of the difference between $\pi_p(x)$ and y. For example, if x is on the classical trajectory given by (2.16b) on page 34, then $\pi_p(x) = y$ and $2\pi_p(x) - y = y$.

The primal-dual penalty function is used, for example, by Forsgren and Gill in [12]. In this paper they study problems with both general equality and inequality constraints. They "move" the general equality constraints and the general inequality constraints into the objective function of the subproblem via the primal-dual penalty function and primal-dual barrier term, respectively.

Next consider the primal-dual augmented Lagrangian function (2.22) on page 37, whose definition and derivatives are given by

$$\mathcal{M}(x,y;y_e,\mu) = f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x)+\mu(y-y_e)\|^2, \tag{3.2a}$$

$$\begin{aligned} \nabla\mathcal{M}(x,y;y_e,\mu) &= \begin{pmatrix} g(x) - J(x)^T(2\pi_a(x)-y) \\ c(x)+\mu(y-y_e) \end{pmatrix} \\ &= \begin{pmatrix} g(x) - J(x)^T(2\pi_a(x)-y) \\ \mu\big(y-\pi_a(x)\big) \end{pmatrix}, \end{aligned} \tag{3.2b}$$

$$\nabla^2\mathcal{M}(x,y;y_e,\mu) = \begin{pmatrix} H\big(x, 2\pi_a(x)-y\big) + \frac{2}{\mu}J(x)^TJ(x) & J(x)^T \\ J(x) & \mu I \end{pmatrix}, \tag{3.2c}$$

where $\pi_a(x) \triangleq y_e - c(x)/\mu$. Note that if $y_e = 0$, then $\pi_p(x) = \pi_a(x)$. The only difference between (3.1) and (3.2) is in the definition for π. Thus, one may often analyze properties of the primal-dual functions at the same time by relying on two facts:

- the primal-dual penalty function can be recovered from the primal-dual augmented Lagrangian function by setting $y_e = 0$.
- the "structure" of the derivatives are the same; the only difference arises in the definition of the "π" term.

The following section discusses the inertia of the Hessian of the primal-dual augmented Lagrangian function (3.2c). However, a similar result holds for the primal-dual penalty function with an appropriate switch of π_a to π_p. In fact, the primal-dual augmented Lagrangian function will henceforth be the focus of discussion since this is the primary concern of this thesis. However, as previously stated, most of the properties to be discussed apply either directly, or with a small change, to the primal-dual penalty function.

3.2 Inertia

As discussed in Section 2.1, optimality conditions may be partitioned into first- and second-order conditions. A primary objective of all algorithms discussed in this thesis is convergence to points satisfying certain second-order conditions. For problem NEP, Theorem 2.1.3 in Section 2.1 shows that verification of second-order conditions requires knowledge of the curvature of the Hessian of the Lagrangian restricted to the null space of $J(x^*)$, i.e., the reduced Hessian. This means that any potential algorithm *must* be able to deduce, either directly or indirectly, the inertia of the reduced Hessian. With this in mind, the inertia of the Hessian of the primal-dual augmented Lagrangian will now be discussed. For the rest of this section the following notation is used: $J = J(x)$, $\pi = \pi(x)$, and $H = H(x, 2\pi(x) - y)$ where $\pi(x) = y_e - \frac{1}{\mu}c(x)$.

Lemma 3.2.1. *For a given $\mu > 0$, the inertia of the primal-dual augmented Lagrangian is given by*

$$\operatorname{In}\big(\nabla^2\mathcal{M}(x, y; y_e, \mu)\big) = (m, 0, 0) \, + \operatorname{In}\Big(H + \frac{1}{\mu}J^TJ\Big).$$

Proof. The Hessian of the primal-dual augmented Lagrangian is given by

$$\nabla^2\mathcal{M}(x, y; y_e, \mu) = \begin{pmatrix} H + \frac{2}{\mu}J^TJ & J^T \\ J & \mu I_m \end{pmatrix}.$$

Define the nonsingular matrix S as

$$S = \begin{pmatrix} I_n & 0 \\ -J/\mu & I_m \end{pmatrix}.$$

Sylvester's law of inertia implies

$$\mathrm{In}\left(\nabla^2\mathcal{M}(x,y;y_e,\mu)\right) = \mathrm{In}\begin{pmatrix} H + \frac{1}{\mu}J^TJ & 0 \\ 0 & \mu I_m \end{pmatrix}.$$

Since μ is positive and inertia is additive along diagonal blocks of a block-diagonal matrix, it follows that

$$\mathrm{In}\left(\nabla^2\mathcal{M}(x,y;y_e,\mu)\right) = (m,0,0) + \mathrm{In}\left(H + \frac{1}{\mu}J^TJ\right).$$

□

This lemma indicates that the usefulness of $\mathcal{M}$ as a merit function capable of finding points satisfying second-order conditions is contingent on knowing the inertia of $H + (1/\mu)J^TJ$. Debreu's Lemma 1.5.1 implies the existence a finite $\bar{\mu} > 0$ such that this matrix is positive definite at points satisfying the second-order sufficient conditions to problem NEP for all $0 < \mu < \bar{\mu}$.

The optimization package SNOPT is an SQP algorithm that uses the augmented Lagrangian as a merit function. Typically, the augmented Lagrangian is considered a function of x for fixed y_e. However, SNOPT performs a line-search in both the x and y variables since it views the augmented Lagrangian as a function of both x *and* y. One could consider implementing an analogous idea for the primal-dual augmented Lagrangian, i.e., consider it as a function of (x, y, y_e). The following lemma shows that this is not possible.

Lemma 3.2.2. *Consider the following function*

$$f(x,y,y_e) = f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x) + \mu(y - y_e)\|^2,$$

i.e., $f(x,y,y_e)$ is the primal-dual augmented Lagrangian considered as a function of (x,y,y_e). Then the following holds

$$\mathrm{In}\left(\nabla^2 f(x,y,y_e)\right) = \mathrm{In}\left(Z^T H Z\right) + \left(m+r, r, m-r\right)$$

where r is the rank of the $m \times n$ matrix J and the columns of Z form a basis for the null space of J.

Proof. The Hessian of $f(x, y, y_e)$ is given by

$$\nabla^2 f(x, y, y_e) = \begin{pmatrix} H + \frac{2}{\mu} J^T J & J^T & -2J^T \\ J & \mu I_m & -\mu I_m \\ -2J & -\mu I_m & \mu I_m \end{pmatrix}.$$

Define the nonsingular matrix T as

$$T = \begin{pmatrix} I_n & -\frac{1}{\mu} J^T & \frac{1}{\mu} J^T \\ 0 & I_m & I_m \\ 0 & 0 & I_m \end{pmatrix}.$$

Then Sylvester's law of inertia implies $\text{In}\left(\nabla^2 f(x, y, y_e)\right) = \text{In}(B)$, where B is given by

$$B = \begin{pmatrix} H & -J^T & 0 \\ -J & 0 & 0 \\ 0 & 0 & \mu I_m \end{pmatrix}.$$

Therefore, $\text{In}\left(\nabla^2 f(x, y, y_e)\right) = (m, 0, 0) + \text{In}(C)$, where C is given by

$$C = \begin{pmatrix} H & -J^T \\ -J & 0 \end{pmatrix}.$$

Next, define the nonsingular matrix S as

$$S = \begin{pmatrix} I_m & 0 \\ 0 & -I_n \end{pmatrix}.$$

Sylvester's law of inertia implies

$$\text{In}\left(C\right) = \text{In}\left(SCS^T\right) = \text{In}\begin{pmatrix} H & J^T \\ J & 0 \end{pmatrix}.$$

Theorem 1.5.1 then implies $\text{In}(C) = \text{In}(Z^T H Z) + (r, r, m - r)$, where r is the rank of J. Putting this all together means

$$\text{In}\left(\nabla^2 f(x, y, y_e)\right) = \text{In}(Z^T H Z) + (m + r, r, m - r).$$

□

Note that this result shows that as a function of (x, y, y_e), the Hessian of the primal-dual augmented Lagrangian is *always* indefinite when $J \neq 0$.

3.3 Properties

The plan is to use the primal-dual augmented Lagrangian as the basis for new active-set algorithms. In order to develop an effective algorithm, a sound understanding of the properties of the underlying functions is essential. This section considers properties of the primal-dual augmented Lagrangian and shows that it is well suited for optimization methods.

Before discussing the primal-dual augmented Lagrangian, a brief discussion of the classical augmented Lagrangian is given. The first result displays the rational behind using the augmented Lagrangian.

Theorem 3.3.1. *If x^* satisfies the second-order sufficient conditions for a solution of problem* NEP (2.12) *on page* 34*, then there exists a $\bar{\mu}$ such that for all $0 < \mu < \bar{\mu}$, the point x^* satisfies the second-order sufficient conditions for a solution of the unconstrained problem*

$$\underset{x\in\mathbb{R}^n}{\text{minimize}} \;\; \mathcal{L}_{\mathcal{A}}(x; y^*, \mu) = f(x) - c(x)^T y^* + \frac{1}{2\mu}\|c(x)\|^2. \tag{3.3}$$

Proof. The second-order sufficient conditions for x to be an unconstrained minimizer of (3.3) are:

U1. $g(x) - J(x)^T(y^* - \frac{1}{\mu}c(x)) = 0$; and

U2. $H(x, y^* - \frac{1}{\mu}c(x)) + \frac{1}{\mu}J(x)^T J(x)$ is positive definite.

By assumption, x^* satisfies the second-order sufficient conditions given by Theorem 2.1.3 and thus

C1. $c(x^*) = 0$,

C2. $g(x^*) - J(x^*)^T y^* = 0$, and

C3. there exists $\omega > 0$ such that $p^T H(x^*, y^*) p \geq \omega \|p\|^2$ for all p satisfying $J(x^*)p = 0$.

It must be shown that x^* satisfies U1 and U2. It is easy to see that C1 and C2 imply x^* satisfies U1. Since $c(x^*) = 0$, it remains to show that $H(x^*, y^*) + (1/\mu)J(x^*)^T J(x^*)$ is positive definite for all positive μ sufficiently small. However, Debreu's Lemma 1.5.1 and C3 imply the existence of a finite $\bar{\mu} > 0$ such that

$$H(x^*, y^*) + \frac{1}{\mu} J(x^*)^T J(x^*)$$

is positive definite for all $0 < \mu < \bar{\mu}$. Therefore, for all $0 < \mu < \bar{\mu}$, the point x^* satisfies U1–U2 and must be an unconstrained minimizer of the augmented Lagrangian (3.3). □

There are two important points to note about this lemma.

(i) It has *not* been shown that all local minimizers of the augmented Lagrangian are local solutions of the constrained problem. The next example illustrates this point.

Example 3.3.1. *Consider the following problem*

$$\underset{x \in \mathbb{R}}{\text{minimize}} \;\; x + 1 \quad \text{subject to} \;\; \frac{1}{3}x^3 - \frac{3}{2}x^2 + 2x = 0, \tag{3.4}$$

which has a unique solution $(x^*, y^*) = (0, 1/2)$. For all $\mu < 1/6$, the augmented Lagrangian for this problem has a local minimizer $\bar{x} = 2 - O(\mu)$ at which $c(\bar{x}) \neq 0$ (see Figure 3.1).

(ii) Condition C3 cannot be relaxed to allow a semidefinite reduced Hessian.

Example 3.3.2. *Consider the problem where*

$$H = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \; J = \begin{pmatrix} 1 & 1 \end{pmatrix}, \; \textit{and} \; Z = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

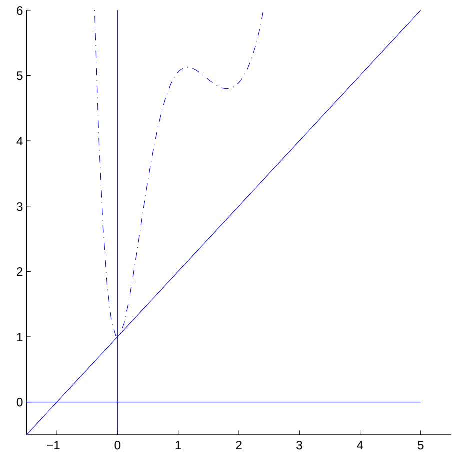

Fig. 3.1: This figure depicts the objective function and augmented Lagrangian for the one-dimensional problem given by Example 3.3.1. The constrained problem has a unique solution $(x^*, y^*) = (0, 1/2)$. However, for all $\mu < 1/6$, the augmented Lagrangian has a local minimizer $\bar{x} = 2 - O(\mu)$ such that $c(\bar{x}) \neq 0$.

> *Note that Z forms a basis for the null space of J. Thus,* C3 *is equivalent to $Z^T H Z$ being positive definite. In this case, $Z^T H Z$ is singular and $H + (1/\mu) J^T J$ is indefinite for all positive μ.*

Theorem 3.3.1 suggests an algorithm in which y^* is approximated by y_e and the augmented Lagrangian

$$\mathcal{L}_{\mathcal{A}}(x) \triangleq \mathcal{L}_{\mathcal{A}}(x; y_e, \mu) = f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2$$

is minimized. This problem may be solved using a sequence of subproblems of the form

$$\underset{\Delta x \in \mathbb{R}^n}{\text{minimize}} \;\; \nabla \mathcal{L}_{\mathcal{A}}(x)^T \Delta x + \frac{1}{2} \Delta x^T \nabla^2 \mathcal{L}_{\mathcal{A}}(x) \Delta x.$$

If $\nabla^2 \mathcal{L}_{\mathcal{A}}(x)$ is positive definite, then Δx is the unique solution of the Newton equations $\nabla^2 \mathcal{L}_{\mathcal{A}}(x) \Delta x = -\nabla \mathcal{L}_{\mathcal{A}}(x)$. In terms of the m-vector $\pi(x) = y_e - c(x)/\mu$, the gradient and Hessian of $\mathcal{L}_{\mathcal{A}}(x)$ are given by

$$\nabla \mathcal{L}_{\mathcal{A}}(x) = g(x) - J(x)^T \pi(x) \;\; \text{and} \;\; \nabla^2 \mathcal{L}_{\mathcal{A}}(x) = H\big(x, \pi(x)\big) + \frac{1}{\mu} J(x)^T J(x),$$

and the Newton equations are simply

$$\Big(H\big(x,\pi(x)\big) + \frac{1}{\mu}J(x)^TJ(x)\Big)\Delta x = -\big(g(x) - J(x)^T\pi(x)\big). \tag{3.5}$$

The elements of $\pi(x)$ may be viewed as approximate Lagrange multipliers. They are sometimes known as *first-order primal multiplier estimates.*

The next result shows that the Newton direction satisfies a "primal-dual" system. This system will be used later.

Lemma 3.3.1. *Assume that $J(x)$ has full row rank. If y is an <u>arbitrary</u> m-vector, then the augmented Lagrangian direction Δx satisfies the system*

$$\begin{pmatrix} H(x,\pi(x)) & J(x)^T \\ J(x) & -\mu I_m \end{pmatrix}\begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = -\begin{pmatrix} g(x) - J(x)^Ty \\ c(x) + \mu(y - y_e) \end{pmatrix}. \tag{3.6}$$

Proof. Define $J = J(x)$, $g = g(x)$, $c = c(x)$, $H = H(x,\pi)$, and $\pi = \pi(x)$. Then the Newton equations may be written as

$$\big(H + \frac{1}{\mu}J^TJ\big)\Delta x = -\big(g - J^T\pi\big).$$

The vector $-(1/\mu)J^TJ\Delta x - (1/\mu)J^Tc - J^T(y - y_e)$ lies in the column space of J^T, and hence there exists a vector Δy such that

$$J^T\Delta y = -\frac{1}{\mu}J^TJ\Delta x - \frac{1}{\mu}J^Tc - J^T(y - y_e). \tag{3.7}$$

Using this expression in conjunction with (3.5) and simplifying yields

$$H\Delta x - J^T\Delta y = -(g - J^Ty). \tag{3.8}$$

Equation (3.7) and full row rank of J implies

$$\mu\Delta y = -J\Delta x - \big(c + \mu(y - y_e)\big). \tag{3.9}$$

Equations (3.8) and (3.9) give the required result. □

Note that although Δx is independent of y, the vector Δy depends on the choice of y.

The primal-dual augmented Lagrangian is now considered. First, a theorem analogous to Theorem 3.3.1 is given.

Theorem 3.3.2. *If (x^*, y^*) satisfies the second-order sufficient conditions for a solution of problem* NEP (2.12) *on page* 34*, then there exists a positive $\bar{\mu}$ such that for all $0 < \mu < \bar{\mu}$, the point (x^*, y^*) is a solution of the unconstrained minimization problem*

$$\underset{x\in\mathbb{R}^n,\, y\in\mathbb{R}^m}{\text{minimize}} \qquad \mathcal{M}(x, y; y^*, \mu), \tag{3.10}$$

where $\mathcal{M}(x, y; y^*, \mu) = f(x) - c(x)^T y^* + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x) + \mu(y - y^*)\|^2$ is the primal-dual augmented Lagrangian.

Proof. Since x^* satisfies the second-order sufficient conditions for problem NEP, Theorem 2.1.3 implies that x^* satisfies

C1. $c(x^*) = 0$,

C2. $g(x^*) - J(x^*)^T y^* = 0$, and

C3. there exists $\omega > 0$ such that $p^T H(x^*, y^*) p \geq \omega\|p\|^2$ for all p satisfying $J(x^*)p = 0$.

In order to show that (x^*, y^*) is an unconstrained minimizer of (3.10), it must be shown that $\nabla\mathcal{M}(x^*, y^*; y^*, \mu) = 0$ and that $\nabla^2\mathcal{M}(x^*, y^*; y^*, \mu)$ is positive definite. As given by equation (3.2) on page 41, the gradient and Hessian are given by

$$\nabla\mathcal{M}(x, y; y^*, \mu) = \begin{pmatrix} g - J^T\big(2\pi(x) - y\big) \\ c + \mu(y - y^*) \end{pmatrix}$$

and

$$\nabla^2\mathcal{M}(x, y; y^*, \mu) = \begin{pmatrix} H\big(x, 2\pi(x) - y\big) + \dfrac{2}{\mu} J(x)^T J(x) & J(x)^T \\ J(x) & \mu I \end{pmatrix}$$

where $\pi(x) = y^* - c(x)/\mu$. Evaluation at x^* and the use of C1 shows that $\pi(x^*) = y^*$. Using this fact, C1 and C2, it follows that

$$\nabla \mathcal{M}(x^*, y^*; y^*, \mu) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and

$$\nabla^2 \mathcal{M}(x^*, y^*; y^*, \mu) = \begin{pmatrix} H(x^*, y^*) + \dfrac{2}{\mu} J(x^*)^T J(x^*) & J(x^*)^T \\ J(x^*) & \mu I \end{pmatrix}.$$

Lemma 3.2.1 shows that

$$\text{In}\left(\nabla^2 \mathcal{M}(x^*, y^*; y^*, \mu)\right) = \left(m, 0, 0\right) + \text{In}\left(H(x^*, y^*) + \frac{1}{\mu} J(x^*)^T J(x^*)\right)$$

Finally, C3 and Debreu's Lemma 1.5.1 imply that there exists a $\bar{\mu} > 0$ such that the matrix

$$H(x^*, y^*) + \frac{1}{\mu} J(x^*)^T J(x^*)$$

is positive definite for all $0 < \mu \leq \bar{\mu}$. Thus,

$$\text{In}(\nabla^2 \mathcal{M}(x^*, y^*; y^*, \mu)) = (m, 0, 0) + (n, 0, 0) = (m + n, 0, 0),$$

which implies that $\nabla^2 \mathcal{M}(x^*, y^*; y^*, \mu)$ is positive definite for all $0 < \mu \leq \bar{\mu}$. Thus, (x^*, y^*) is an unconstrained minimizer of problem (3.10) for all $0 < \mu \leq \bar{\mu}$. □

This result suggests that given an approximate multiplier, say y_e, one may define the primal-dual augmented Lagrangian

$$\mathcal{M}(x, y; y_e, \mu) = f(x) - c(x)^T y_e + \frac{1}{2\mu} \|c(x)\|^2 + \frac{1}{2\mu} \|c(x) + \mu(y - y_e)\|^2,$$

and then solve the unconstrained minimization problem

$$\underset{x \in \mathbb{R}^n,\, y \in \mathbb{R}^m}{\text{minimize}} \quad \mathcal{M}(x, y; y_e, \mu). \tag{3.11}$$

This would be followed by an appropriate update to y_e and another solve of the form (3.11). This process can then be repeated. Note that this is an unconstrained problem in both the primal *and* dual variables (x, y).

If v denotes the $(n+m)$ vector of primal-dual variables $v = (x, y)$, then problem (3.11) may be solved using a sequence of subproblems of the form

$$\underset{\Delta v \in \mathbb{R}^{n+m}}{\text{minimize}} \quad \nabla\mathcal{M}(v)^T \Delta v + \frac{1}{2}\Delta v^T \nabla^2\mathcal{M}(v)\Delta v \tag{3.12}$$

where $\Delta v = (\Delta x, \Delta y)$. If $\nabla^2\mathcal{M}(v)$ is positive definite, then Δv is the unique solution of the Newton equations

$$\nabla^2\mathcal{M}(v)\Delta v = -\nabla\mathcal{M}(v).$$

Substitution of the expressions for $\nabla\mathcal{M}$ and $\nabla^2\mathcal{M}$ yields the Newton system

$$\begin{pmatrix} H + \dfrac{2}{\mu}J^T J & J^T \\ J & \mu I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = -\begin{pmatrix} g - J^T\big(2\pi - y\big) \\ c + \mu(y - y_e) \end{pmatrix}, \tag{3.13}$$

where $H = H\big(x, 2\pi(x) - y\big)$, $g = g(x)$, $c = c(x)$, $\pi = \pi(x)$, and $J = J(x)$. It can be shown that this system becomes ill-conditioned as $\mu \to 0$. In fact, m eigenvalues approach zero, m eigenvalues approach infinity, and $n - m$ eigenvalues are bounded as $\mu \to 0$. For methods such as classical penalty and primal-dual penalty methods this is a potential problem. It was thought that this ill-conditioning was the primary cause of failure for classical penalty methods. However, it has been shown that these difficulties persist even when the Newton system is solved exactly. The true cause of failure was due to the first generated Newton direction immediately following a decrease in the penalty parameter. This issue was resolved by use of the primal-dual penalty function. This will be discussed in more detail shortly.

Classical augmented Lagrangian methods do not require $\mu \to 0$. However, augmented Lagrangian methods may still suffer from the two issues just discussed. First, although Lagrangian methods do not typically require μ to go to zero, they often require several reductions in μ. Thus, augmented Lagrangian methods behave the same way as classical penalty functions when the penalty parameter is decreased (in particular when μ is quite small). It will soon be shown that as the primal-dual penalty method solved this problem for the classical penalty method, so has the primal-dual augmented Lagrangian method solved this problem for the classical Lagrangian method. Second, typical augmented Lagrangian algorithms (see for example [8] and [13]) have a fall-back plan to ensure convergence. This typically consists of driving μ towards zero and ultimately causing the algorithm to behave like a penalty method. Thus, although a "typical" augmented Lagrangian method run has μ fixed when approaching a solution, there still exist problems for which μ is driven very small. This means that ill-conditioning is still a potential issue. The next lemma shows that the Newton equations given by (3.13) are equivalent to another system whose conditioning is as good (or as bad) as problem NEP.

Lemma 3.3.2. *The following two systems are equivalent:*

$$\begin{pmatrix} H(x, 2\pi - y) + \frac{2}{\mu}J^TJ & J^T \\ J & \mu I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = - \begin{pmatrix} g - J^T(2\pi - y) \\ c + \mu(y - y_e) \end{pmatrix} \tag{3.14}$$

and

$$\begin{pmatrix} H(x, 2\pi - y) & J^T \\ J & -\mu I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = - \begin{pmatrix} g - J^T y \\ c + \mu(y - y_e) \end{pmatrix}. \tag{3.15}$$

In other words, $(\Delta x, \Delta y)$ is a solution of the first system if and only if $(\Delta x, \Delta y)$ is a solution of the second system.

Proof. Multiplying both sides of (3.14) by the *non-singular* matrix

$$N = \begin{pmatrix} I & -\frac{2}{\mu}J^T \\ 0 & I_m \end{pmatrix},$$

and scaling the last m columns by -1 gives

$$\begin{pmatrix} H(x, 2\pi - y) & J^T \\ J & -\mu I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = - \begin{pmatrix} g - J^T y \\ c + \mu(y - y_e) \end{pmatrix}.$$

□

This lemma shows that the better conditioned system (3.15) may be used when solving for a search direction $\Delta v = (\Delta x, \Delta y)$ satisfying (3.13). System (3.15) bears a striking resemblance to system (3.6) on page 48 associated with the classical augmented Lagrangian method. The next lemma makes this precise.

Lemma 3.3.3. *If J has full row rank and π is substituted for y in the Hessian associated with the primal-dual augmented Lagrangian system* (3.15)*, then the vector Δx associated with the solution of the resulting modified Newton system*

$$\begin{pmatrix} H(x,\pi) & J^T \\ J & -\mu I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = - \begin{pmatrix} g - J^T y \\ c + \mu(y - y_e) \end{pmatrix},$$

is the conventional augmented Lagrangian direction given by (3.5) *on page* 48.

Proof. This follows directly from Lemma 3.3.1. □

The quality of the first Newton search direction following a decrease in the penalty parameter μ is now considered. Fiacco and McCormick [10] show that under certain standard assumptions and for μ sufficiently small, there exists a continuously differentiable path of solutions parameterized by μ, say $(x_\mu, y_\mu) \triangleq \big(x(\mu), y(\mu)\big)$, such that (x_μ, y_μ) is a minimizer to the primal-dual penalty function

$$\underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} \;\; \mathcal{P}(x, y; \mu) \; . \tag{3.16}$$

One of the principal benefits of the primal-dual penalty and primal-dual augmented Lagrangian occurs in the definition of the step immediately following a decrease in the penalty parameter μ. When using the primal-dual augmented Lagrangian in an optimization routine, one typically expects μ to stay bounded away from zero and for the Lagrange multiplier vector estimate y_e to converge to the Lagrange multiplier vector. However, if y_e is *fixed*, there exists a trajectory of minimizers (x_μ, y_μ) for the following problem for μ sufficiently small:

$$\underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} \;\; \mathcal{M}(x, y; y_e, \mu). \tag{3.17}$$

These minimizers have the property that $(x_\mu, y_\mu) \to (x^*, y^*)$ as $\mu \to 0$. Also, for a given value of μ, the point (x_μ, y_μ) satisfies the following equations:

$$g(x_\mu) - J(x_\mu)^T y_\mu = 0 \quad \text{and} \quad c(x_\mu) + \mu(y_\mu - y_e) = 0. \tag{3.18}$$

To clarify the goal of future analysis, consider the following situation. Suppose that a minimizer (x_μ, y_μ) has been calculated during an implementation of a primal-dual augmented Lagrangian method. However, the constraint violation, i.e., the norm of $c(x_\mu)$, has not decreased as much as desired. The current point is then kept, the penalty parameter is decreased to say $\bar{\mu}$, and y_e is kept fixed (in practice, the Lagrange multiplier estimate y_e may be updated, but this current scenario is applicable for other reasons and is the situation of interest). The next step is to find a point on the trajectory for the reduced penalty parameter $\bar{\mu}$. What is the quality of the first Newton direction?

Of particular interest in answering this question is the tangent vector to the trajectory of minimizers at (x_μ, y_μ). The following definitions are used: $c_\mu = c(x_\mu)$, $J_\mu = J(x_\mu)$, $\pi_\mu = \pi(x_\mu)$, and $g_\mu = g(x_\mu)$. Since (x_μ, y_μ) is a minimizer of the primal-dual augmented Lagrangian it satisfies the following equations:

$$g(x_\mu) - J(x_\mu)^T\big(2\pi(x_\mu) - y_\mu\big) = 0 \ \text{ and } \ c(x_\mu) + \mu(y_\mu - y_e) = 0. \tag{3.19}$$

Differentiation of these equations with respect to μ shows that the tangent vector (x'_μ, y'_μ) satisfies the following system

$$\begin{pmatrix} H\big(x_\mu, 2\pi(x_\mu) - y_\mu\big) + \dfrac{2}{\mu} J_\mu^T J_\mu & J_\mu^T \\ J_\mu & \mu I \end{pmatrix} \begin{pmatrix} x'_\mu \\ y'_\mu \end{pmatrix} = - \begin{pmatrix} \dfrac{2}{\mu^2} J_\mu^T c_\mu \\ y_\mu - y_e \end{pmatrix}.$$

Multiplication on the left by the nonsingular matrix

$$N \triangleq \begin{pmatrix} I & -\dfrac{2}{\mu} J_\mu^T \\ 0 & I \end{pmatrix}$$

followed by symmetrization and simplification of the right-hand side yields

$$\begin{pmatrix} H\big(x_\mu, 2\pi(x_\mu) - y_\mu\big) & J_\mu^T \\ J_\mu & -\mu I \end{pmatrix} \begin{pmatrix} x'_\mu \\ -y'_\mu \end{pmatrix} = - \begin{pmatrix} -\dfrac{2}{\mu} J_\mu^T(y_\mu - \pi_\mu) \\ y_\mu - y_e \end{pmatrix}.$$

Since $y_\mu = \pi_\mu$ on the trajectory, the tangent vector (x'_μ, y'_μ) satisfies the following system:

$$\begin{pmatrix} H(x_\mu, y_\mu) & J_\mu^T \\ J_\mu & -\mu I \end{pmatrix} \begin{pmatrix} x'_\mu \\ -y'_\mu \end{pmatrix} = - \begin{pmatrix} 0 \\ y_\mu - y_e \end{pmatrix}. \tag{3.20}$$

Taylor expansion centered at μ gives

$$x_{\bar\mu} = x_\mu + (\bar\mu - \mu)x'_\mu + O\left((\bar\mu - \mu)^2\right),$$
$$y_{\bar\mu} = y_\mu + (\bar\mu - \mu)y'_\mu + O\left((\bar\mu - \mu)^2\right),$$

and thus

$$x_{\bar\mu} - x_\mu \approx (\bar\mu - \mu)x'_\mu\ ,$$
$$y_{\bar\mu} - y_\mu \approx (\bar\mu - \mu)y'_\mu\ .$$

This implies that

$$(\bar\mu - \mu) \begin{pmatrix} x'_\mu \\ y'_\mu \end{pmatrix} \tag{3.21}$$

is a good search direction for computing $(x_{\bar\mu}, y_{\bar\mu})$, i.e., $\bar\mu - \mu$ times the tangent to the trajectory is a good search direction for computing $(x_{\bar\mu}, y_{\bar\mu})$.

The aim is to compare the direction given by (3.21) with the direction generated by the primal-dual augmented Lagrangian function. It will be shown that the first Newton direction generated by the primal-dual augmented Lagrangian is an excellent direction; it is known that the first direction generated by the classical augmented Lagrangian is not a good direction.

The first Newton system for the primal-dual augmented Lagrangian function with parameter $\bar\mu$ is given by

$$\begin{pmatrix} H\big(x_\mu, 2\bar\pi(x_\mu) - y_\mu\big) + \dfrac{2}{\bar\mu} J_\mu^T J_\mu & J_\mu^T \\ J_\mu & \bar\mu I \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \begin{pmatrix} g_\mu - J_\mu^T\big(2\bar\pi(x_\mu) - y_\mu\big) \\ c_\mu + \bar\mu(y_\mu - y_e) \end{pmatrix},$$

where $\bar{\pi}(x) \triangleq y_e - c(x)/\bar{\mu}$. Multiplication by the nonsingular matrix

$$N_2 \triangleq \begin{pmatrix} I & -\dfrac{2}{\bar{\mu}} J_\mu^T \\ 0 & I \end{pmatrix},$$

followed by symmetrization and simplification leads to

$$\begin{pmatrix} H\big(x_\mu, 2\bar{\pi}(x_\mu) - y_\mu\big) & J_\mu^T \\ J_\mu & -\bar{\mu} I \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = - \begin{pmatrix} g_\mu - J_\mu^T y_\mu \\ c_\mu + \bar{\mu}(y_\mu - y_e) \end{pmatrix}.$$

Since (x_μ, y_μ) is on the trajectory, the previous system simplifies to

$$\begin{pmatrix} H\big(x_\mu, y_\mu + \frac{2(\bar{\mu}-\mu)}{\bar{\mu}}(y_\mu - y_e)\big) & J_\mu^T \\ J_\mu & -\bar{\mu} I \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = - \begin{pmatrix} 0 \\ (\bar{\mu} - \mu)(y_\mu - y_e) \end{pmatrix}. \tag{3.22}$$

Using (3.20) and (3.22), it can be shown that

$$\begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = (\bar{\mu} - \mu) \begin{pmatrix} x'_\mu \\ y'_\mu \end{pmatrix} + O\big(|\bar{\mu} - \mu|^2\big). \tag{3.23}$$

Thus for a fixed y_e, (3.21) and (3.23) imply that the first primal-dual augmented Lagrangian direction following a decrease in the penalty parameter is an excellent direction.

The previous argument has shown that if

1. a point (x_μ, y_μ) *on* the trajectory of minimizers is found for a given value of the penalty parameter μ,
2. the penalty parameter is then *decreased*, to say $\bar{\mu}$, and
3. y_e is kept *fixed*,

then to first-order, the first Newton direction for the primal-dual augmented Lagrangian function (using $\bar{\mu}$) agrees with the tangent to the trajectory of minimizers at μ. This result is very specific and begs the question: If we only have an approximation to (x_μ, y_μ), then does there exist a "perturbed trajectory" leading to $(x_{\bar{\mu}}, y_{\bar{\mu}})$? The next section answers this question.

3.4 A Perturbed Trajectory

This section discusses the existence of a perturbed trajectory. It is known that under certain assumptions, there exists a continuously differentiable path of minimizers for the primal-dual augmented Lagrangian function for μ sufficiently small and y_e fixed. It was also shown in Section 3.3 that when an *exact* minimizer of the primal-dual augmented Lagrangian function for a given value of μ is found, then the first Newton direction following a decrease in μ is tangent to the curve of minimizers parameterized by μ (assuming y_e is kept fixed). In fact, it was shown that the first Newton step is identical to the step predicted by a first-order Taylor series approximation. However, due to numerical error an exact minimizer is rarely found. More importantly, it is often advantageous to only *approximately* solve subproblems and only require high accuracy near a solution to the given problem. Is the first Newton direction for minimizing the primal-dual augmented Lagrangian following a decrease in μ related to some nearby trajectory emanating from the current *approximation* to (x_μ, y_μ)? The following theorem addresses this question.

Theorem 3.4.1 (A Wedge of Perturbed Trajectories)**.** *Consider problem* NEP*. Let* (x^*, y^*) *satisfy the second-order sufficient conditions given by Theorem* 2.1.3 *and let* (x_μ, y_μ) *represent a point on the classical trajectory of minimizers associated with the primal-dual augmented Lagrangian for* y_e *fixed and* $\mu > 0$*. Then there exists an open ball* $B\big((x_\mu, y_\mu), r_1\big)$ *centered at* (x_μ, y_μ) *of radius* r_1 *such that for each* $(x_0, y_0) \in B\big((x_\mu, y_\mu), r_1\big)$ *there exists a positive number* $r_2 \triangleq r_2(x_0, y_0)$ *and an interval* $(r_2, \mu]$ *such that if* $\bar{\mu} \in (r_2, \mu]$ *then there exists a positive number* r_3 *and an open neighborhood* $B_\alpha(0, r_3)$ *centered at zero of radius* r_3*, and a unique continuously differentiable function* $v(\alpha) \triangleq \big(x(\alpha), y(\alpha)\big)$ *defined on* $B_\alpha(0, r_3)$ *such that*

$$v(0) = \begin{pmatrix} x(0) \\ y(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \tag{3.24}$$

and if $1 \in B_\alpha(0, r_3)$*, then*

$$v(1) = \begin{pmatrix} x(1) \\ y(1) \end{pmatrix} = \begin{pmatrix} x_{\bar{\mu}} \\ y_{\bar{\mu}} \end{pmatrix}. \tag{3.25}$$

Moreover, if $(\Delta x, \Delta y)$ *is the solution to the first Newton system for minimizing the primal-dual augmented Lagrangian with* $\bar{\mu}$*, then* $(\Delta x, \Delta y) \equiv v'(0)$ *and* $(x_0, y_0) + (\Delta x, \Delta y)$ *is the first-order Taylor approximation to* $(x_{\bar{\mu}}, y_{\bar{\mu}})$ *(see Figure* 3.2 *on page* 61*).*

Proof. Since (x_μ, y_μ) is a strict minimizer of the primal-dual augmented Lagrangian, the matrix

$$\begin{pmatrix} H\big(x_\mu, 2\pi(x_\mu) - y_\mu\big) + \frac{2}{\mu} J(x_\mu)^T J(x_\mu) & J(x_\mu)^T \\ J(x_\mu) & \mu I_m \end{pmatrix}$$

is positive definite. This means that there exists an open ball $B\big((x_\mu, y_\mu), r_1\big)$ centered at (x_μ, y_μ) of radius r_1 such that if $(x, y) \in B\big((x_\mu, y_\mu), r_1\big)$ then the matrix

$$\begin{pmatrix} H\big(x, 2\pi(x) - y\big) + \frac{2}{\mu} J(x)^T J(x) & J(x)^T \\ J(x) & \mu I_m \end{pmatrix}$$

is positive definite, where $\pi(x) = y_e - c(x)/\mu$. Let $(x_0, y_0) \in B\big((x_\mu, y_\mu), r_1\big)$. Then the matrix

$$\begin{pmatrix} H\big(x_0, 2\pi(x_0) - y_0\big) + \frac{2}{\mu} J(x_0)^T J(x_0) & J(x_0)^T \\ J(x_0) & \mu I_m \end{pmatrix}$$

is positive definite and there must exist a positive number $r_2 < \mu$ and an interval $(r_2, \mu]$ such that if $\widehat{\mu} \in (r_2, \mu]$ then

$$\begin{pmatrix} H\big(x_0, 2\widehat{\pi}(x_0) - y_0\big) + \frac{2}{\widehat{\mu}} J(x_0)^T J(x_0) & J(x_0)^T \\ J(x_0) & \widehat{\mu} I_m \end{pmatrix}$$

is positive definite, where $\widehat{\pi}(x) = y_e - c(x)/\widehat{\mu}$. Let $\bar{\mu} \in (r_2, \mu]$ and therefore

$$\begin{pmatrix} H\big(x_0, 2\bar{\pi}(x_0) - y_0\big) + \frac{2}{\bar{\mu}} J(x_0)^T J(x_0) & J(x_0)^T \\ J(x_0) & \bar{\mu} I_m \end{pmatrix} \tag{3.26}$$

is positive definite, where $\bar{\pi}(x) = y_e - c(x)/\bar{\mu}$. Define the function

$$F_\alpha(x,y) = \begin{pmatrix} g(x) - J(x)^T\big(2\bar{\pi}(x) - y\big) - (1-\alpha)\Big(g(x_0) - J(x_0)^T\big(2\bar{\pi}(x_0) - y_0\big)\Big) \\ c(x) + \bar{\mu}(y - y_e) - (1-\alpha)\big(c(x_0) + \bar{\mu}(y_0 - y_e)\big) \end{pmatrix}.$$

Differentiation with respect to (x,y) gives

$$\nabla_{xy} F_\alpha(x,y) = \begin{pmatrix} H\big(x, 2\bar{\pi}(x) - y\big) + \frac{2}{\bar{\mu}} J(x)^T J(x) & J(x)^T \\ J(x) & \bar{\mu} I_m \end{pmatrix}. \tag{3.27}$$

Evaluation at (x_0, y_0) for $\alpha = 0$ yields

$$F_0(x_0, y_0) = 0 \quad \text{and} \tag{3.28a}$$

$$\nabla_{xy} F_0(x_0, y_0) = \begin{pmatrix} H\big(x_0, 2\bar{\pi}(x_0) - y_0\big) + \frac{2}{\bar{\mu}} J(x_0)^T J(x_0) & J(x_0)^T \\ J(x_0) & \bar{\mu} I_m \end{pmatrix}. \tag{3.28b}$$

Equation (3.26) shows that $\nabla_{xy} F_0(x_0, y_0)$ is positive definite and therefore nonsingular. Use of the Implicit Function Theorem implies the existence of an open neighborhood $B_\alpha(0, r_3)$ centered at zero of radius r_3, and a unique continuously differentiable function $v(\alpha) = \big(x(\alpha), y(\alpha)\big)$ defined on $B_\alpha(0, r_3)$ such that $v(0) = (x_0, y_0)$ and $F_\alpha\big(x(\alpha), y(\alpha)\big) = 0$ for all $\alpha \in B_\alpha(0, r_3)$.

If $1 \in B_\alpha(0, r_3)$, then definition of F_α implies

$$0 = F_1\big(x(1), y(1)\big) = \begin{pmatrix} g(x_1) - J(x_1)^T\big(2\bar{\pi}(x_1) - y_1\big) \\ c(x_1) + \bar{\mu}(y_1 - y_e) \end{pmatrix},$$

where $(x_1, y_1) \triangleq \big(x(1), y(1)\big)$. Uniqueness of $v(\alpha)$ implies

$$v(1) = \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} x_{\bar{\mu}} \\ y_{\bar{\mu}} \end{pmatrix}. \tag{3.29}$$

Use of the definition $(x_\alpha, y_\alpha) = \big(x(\alpha), y(\alpha)\big)$, the following holds for all $\alpha \in B_\alpha(0, r_3)$:

$$g(x_\alpha) - J(x_\alpha)^T\big(2\bar{\pi}(x_\alpha) - y_\alpha\big) - (1-\alpha)\Big(g(x_0) - J(x_0)^T\big(2\bar{\pi}(x_0) - y_0\big)\Big) = 0,$$
$$c(x_\alpha) + \bar{\mu}(y_\alpha - y_e) - (1-\alpha)\big(c(x_0) + \bar{\mu}(y_0 - y_e)\big) = 0.$$

Differentiation with respect to α shows that (x'_α, y'_α) satisfies

$$\begin{pmatrix} H\big(x_\alpha, 2\bar{\pi}(x_\alpha) - y_\alpha\big) + \frac{2}{\bar{\mu}} J(x_\alpha)^T J(x_\alpha) & J(x_\alpha)^T \\ J(x_\alpha) & \bar{\mu} I_m \end{pmatrix} \begin{pmatrix} x'_\alpha \\ y'_\alpha \end{pmatrix} = -\begin{pmatrix} g(x_0) - J(x_0)^T\big(2\bar{\pi}(x_0) - y_0\big) \\ c(x_0) + \bar{\mu}(y_0 - y_e) \end{pmatrix}.$$

Evaluation at $\alpha = 0$ gives

$$\begin{pmatrix} H\big(x_0, 2\bar{\pi}(x_0) - y_0\big) + \frac{2}{\bar{\mu}} J(x_0)^T J(x_0) & J(x_0)^T \\ J(x_0) & \bar{\mu} I_m \end{pmatrix} \begin{pmatrix} x'_0 \\ y'_0 \end{pmatrix} = -\begin{pmatrix} g(x_0) - J(x_0)^T\big(2\bar{\pi}(x_0) - y_0\big) \\ c(x_0) + \bar{\mu}(y_0 - y_e) \end{pmatrix}. \quad (3.30)$$

The first Newton system for minimizing the primal-dual augmented Lagrangian $\mathcal{M}(x, y; y_e, \bar{\mu})$ is given by

$$\begin{pmatrix} H\big(x_0, 2\bar{\pi}(x_0) - y_0\big) + \frac{2}{\bar{\mu}} J(x_0)^T J(x_0) & J(x_0)^T \\ J(x_0) & \bar{\mu} I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = -\begin{pmatrix} g(x_0) - J(x_0)^T\big(2\bar{\pi}(x_0) - y_0\big) \\ c(x_0) + \bar{\mu}(y_0 - y_e) \end{pmatrix}. \quad (3.31)$$

Equation (3.26) and systems (3.30) and (3.31) imply

$$\begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} \equiv \begin{pmatrix} x'_0 \\ y'_0 \end{pmatrix} = v'(0).$$

A first-order Taylor approximation of $v(1)$ centered at $\alpha = 0$ gives

$$v(1) \approx v(0) + v'(0).$$

Since $v(0) = (x_0, y_0)$ and $v'(0) = (\Delta x, \Delta y)$, the final part of the proof is complete. $\square$

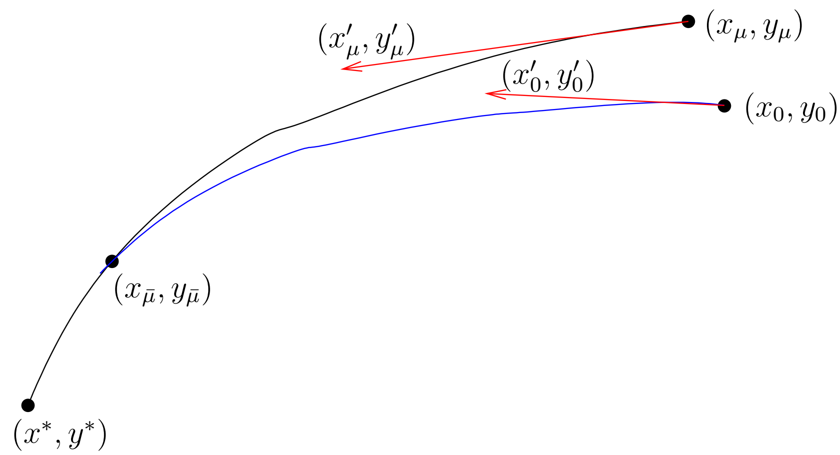

Fig. 3.2: The point (x^*, y^*) is a solution to problem NEP. The points (x_μ, y_μ) and $(x_{\bar{\mu}}, y_{\bar{\mu}})$ are points on the "classical" trajectory of minimizers (black) corresponding to μ and $\bar{\mu}$ respectively. The point (x_0, y_0) is an approximation to (x_μ, y_μ) and lies on the blue trajectory which is the so called perturbed trajectory. The vector (x'_μ, y'_μ) is tangent to the classical trajectory at (x_μ, y_μ), while (x'_0, y'_0) is tangent to the perturbed trajectory at (x_0, y_0).

3.5 Imposing Explicit Bounds on the Dual Variables

The subproblem for solving problem NEP (2.12) on page 34, takes the form

$$\underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} \;\; \mathcal{M}(x, y; y_e, \mu), \tag{3.32}$$

which is an unconstrained problem in both the primal and dual variables. Although problem NEP has been the focus of discussion to this point, an obvious modification to the subproblem can be made when considering problem GNPs (2.8) on page 26. The subproblem associated with problem GNPs takes the form

$$\begin{aligned} &\underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} && \mathcal{M}(x, y; y_e, \mu) \\ &\text{subject to} && x \geq 0, \end{aligned} \tag{3.33}$$

where minimization occurs over the primal and dual variables, but the dual variables are always unconstrained. Every convergence proof must deal with multipliers that may become unbounded as $\mu \to 0$. Ultimately, it must be shown that certain quantities are bounded or in some cases that these quantities converge to zero if μ converges to zero. For example, in [8] and [13] it is not assumed that the multipliers are bounded, but instead it is shown that if the penalty parameter μ converges to zero, then the quantity $\mu\|y_k\| \to 0$. One immediate feature of subproblems (3.32) and (3.33) is that explicit "artificial" bounds may easily be imposed on the dual variables. This ensures boundedness of the dual variables, which is an attractive feature. Two examples will now be given, followed by two theorems that concern the effects of imposing explicit "artificial" bounds on the dual variables.

Example 3.5.1. *Consider the simple example problem*

$$\begin{array}{ll} \underset{x\in\mathbb{R}}{\text{minimize}} & \tfrac{1}{2}x^2 \\ \text{subject to} & x-1=0, \end{array}$$

which has solution $(x^*,y^*)=(1,1)$. *The primal-dual augmented Lagrangian function for this problem is given by*

$$\mathcal{M}(x,y;y_e,\mu)=\tfrac{1}{2}x^2-y_e(x-1)+\frac{1}{2\mu}(x-1)^2+\frac{1}{2\mu}\big(x-1+\mu(y-y_e)\big)^2,$$

for which

$$\nabla\mathcal{M}(x,y;y_e,\mu)=\begin{pmatrix} x-y_e+\frac{1}{\mu}(x-1)+\frac{1}{\mu}\big(x-1+\mu(y-y_e)\big) \\ x-1+\mu(y-y_e) \end{pmatrix}.$$

Hence, minimizing $\mathcal{M}(x,y;y_e,\mu)$ *gives*

$$x(\mu)=\frac{1+\mu y_e}{1+\mu},\quad y(\mu)=\frac{1+\mu y_e}{1+\mu}.$$

Notice that $\big(x(\mu),y(\mu)\big)\to(x^*,y^*)$ *as* $\mu\to 0$ *as expected. Also, it is easy to see that if the Lagrange multiplier* y^* *is substituted for* y_e *then* $x(\mu)=x^*$ *and* $y(\mu)=y^*$ *for all* μ.

Now consider what happens if bounds $-b \le y \le b$ are added. The above solution is optimal if $|(1+\mu y_e)/(1+\mu)| \le b$ because then $y(\mu)$ still satisfies its bounds. However, if $|(1+\mu y_e)/(1+\mu)| > b$, then y becomes active at the solution.

<u>*Case 1: $(1+\mu y_e)/(1+\mu) > b$*</u>

The optimal solution is given by

$$\begin{pmatrix} x - y_e + \frac{1}{\mu}(x-1) + \frac{1}{\mu}(x - 1 + \mu(y - y_e)) \\ x - 1 + \mu(y - y_e) \end{pmatrix} - \begin{pmatrix} 0 \\ -1 \end{pmatrix} \eta = 0, \quad y - b = 0,$$

where the second equation highlights that the dual variable is active at its upper bound, b, at a solution. The solution is then

$$x(\mu) = \frac{2 - \mu b + 2\mu y_e}{2+\mu}, \quad y(\mu) = b, \quad \eta(\mu) = \frac{\mu\big(1 - (1+\mu)b + \mu y_e\big)}{2+\mu} > 0.$$

Notice that if $\mu \to 0$ then

$$x(\mu) \to 1, \quad y(\mu) = b, \quad \eta(\mu) \to 0.$$

<u>*Case 2: $(1+\mu y_e)/(1+\mu) < -b$*</u>

The optimal solution is given by

$$\begin{pmatrix} x - y_e + \frac{1}{\mu}(x-1) + \frac{1}{\mu}(x - 1 + \mu(y - y_e)) \\ x - 1 + \mu(y - y_e) \end{pmatrix} - \begin{pmatrix} 0 \\ -1 \end{pmatrix} \eta = 0, \quad y + b = 0,$$

where the second equation highlights that the dual variable is active at its lower bound, $-b$, at a solution. The solution is then

$$x(\mu) = \frac{2 + \mu b + 2\mu y_e}{2+\mu}, \quad y(\mu) = -b, \quad \eta(\mu) = \frac{\mu\big(1 + (1+\mu)b + \mu y_e\big)}{2+\mu}.$$

Notice that if $\mu \to 0$ then

$$x(\mu) \to 1, \quad y(\mu) = -b, \quad \eta(\mu) \to 0. \tag{3.34}$$

The linear independent constraint qualification (LICQ) was satisfied for the previous problem. This fact guaranteed the existence and uniqueness of Lagrange multipliers. In the next two-dimensional example the LICQ does not hold and Lagrange multipliers *do not* exist.

Example 3.5.2. *Consider the example problem*

$$\begin{array}{ll} \underset{x\in\mathbb{R}^2}{\text{minimize}} & \tfrac{1}{2}(x_1+1)^2 \\ \text{subject to} & x_1^2 - x_2 = 0, \quad x_2 = 0, \end{array}$$

which has solution $x^* = (0,0)$. *The primal-dual augmented Lagrangian function for this problem is given by*

$$\mathcal{M}(x,y;y_e,\mu) = f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x)+\mu(y-y_e)\|^2, \tag{3.35}$$

where

$$f(x) = \tfrac{1}{2}(x_1+1)^2, \qquad g(x) = \begin{pmatrix} x_1+1 \\ 0 \end{pmatrix}, \tag{3.36}$$

$$c(x) = \begin{pmatrix} x_1^2 - x_2 \\ x_2 \end{pmatrix}, \quad J(x) = \begin{pmatrix} 2x_1 & -1 \\ 0 & 1 \end{pmatrix}. \tag{3.37}$$

Thus, $J(x^*)$ *has linearly dependent rows and the following equation shows that Lagrange multipliers do not exist:*

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = g(x^*) \neq J(x^*)^T y = \begin{pmatrix} 0 \\ y_2 - y_1 \end{pmatrix}.$$

Table 3.1 *gives the minimizer* $\big(x(\mu), y(\mu)\big)$ *to*

$$\underset{x\in\mathbb{R}^2, y\in\mathbb{R}^2}{\text{minimize}} \ \mathcal{M}(x,y;y_e,\mu)$$

with $y_e = (0,0)$ *and for decreasing values of* μ. *Notice that* $x(\mu) \to (0,0)$ *and* $y(\mu) \to (-\infty,-\infty)$. *If artificial bounds are enforced, then the subproblem takes the following form:*

$$\begin{array}{ll} \underset{x\in\mathbb{R}^2, y\in\mathbb{R}^2}{\text{minimize}} & \mathcal{M}(x,y;y_e,\mu) \\ \text{subject to} & -\gamma e \le y \le \gamma e, \end{array} \tag{3.38}$$

for some positive scalar γ. *Table* 3.2 *gives the solution to problem* (3.38) *with* $\gamma = 1000$, *and for decreasing values of* μ. *Moreover, the choice* $y_e = (-1000,-1000)$ *was made because the Lagrange multipliers diverge to negative infinity when no artificial bounds are enforced.*

Table 3.1: Minimizers of the primal-dual augmented Lagrangian *without* artificial bounds on y.

μ	x_1	x_2	y_1	y_2
1	−0.6823278	0.2327856	−0.2327856	−0.2327856
10^{-1}	−0.3990027	0.0772256	−0.7722558	−0.7722558
10^{-3}	−0.0966679	0.0046724	−4.6723455	−4.6723455
10^{-5}	−0.0213896	0.0002288	−22.875813	−22.875813
10^{-7}	−0.0046344	0.0000107	−107.38866	−107.38866
10^{-9}	−0.0009997	0.0000005	−499.66667	−499.66667
10^{-11}	−0.0002154	0.0000000	−2320.6861	−2320.6861
10^{-13}	−0.0000466	0.0000000	−10847.567	−10847.567

These examples show that when artificial bounds on the dual variables are imposed, the quantities $x(\mu)$ still may converge to x^* as $\mu \to 0$. Example 3.2 shows that this is reasonable even when the LICQ did not hold and Lagrange multipliers did not exist.

Theorem 3.5.1. *Let* (x^*, y^*, z^*) *be a solution to problem* GNPs (2.8) *on page* 26. *Assume that* $\widehat{J}(x^*)$ *has full row rank, where* $\widehat{J}(x^*)$ *are the columns of* $J(x^*)$ *corresponding to inactive bounds at* x^*. *If* $y^* \notin [-\gamma e, \gamma e]$, *then there does not exist a solution* $(x^*, \bar{y}, \bar{z}, \bar{w})$ *to any problem of the form*

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} & \mathcal{M}(x, y; y_e, \mu) \\ \text{subject to} & x \geq 0, \quad -\gamma e \leq y \leq \gamma e, \end{array} \tag{3.39}$$

for any finite μ *and any* $y_e \in [-\gamma e, \gamma e]$, *where* $\bar{z}$ *are the multipliers for the constraints* $x \geq 0$ *and* $\bar{w}$ *are the multipliers for the constraints* $-\gamma e \leq y \leq \gamma e$.

Proof. A solution of problem (3.39) satisfies

$$\begin{pmatrix} g(x) - J(x)^T(2y_e - \frac{2}{\mu}c(x) - y) \\ c(x) + \mu(y - y_e) \end{pmatrix} = \begin{pmatrix} z \\ w \end{pmatrix}. \tag{3.40}$$

Table 3.2: Minimizers of the primal-dual augmented Lagrangian *with* artificial bounds on y.

μ	x_1	x_2	y_1	y_2	w_1	w_2
1	−0.0004998	0.0000002	−1000.0	−1000.0	0.0000002	0.0000002
10^{-1}	−0.0004998	0.0000002	−1000.0	−1000.0	0.0000002	0.0000002
10^{-3}	−0.0004998	0.0000001	−1000.0	−1000.0	0.0000001	0.0000001
10^{-5}	−0.0004997	0.0000001	−1000.0	−1000.0	0.0000001	0.0000001
10^{-7}	−0.0004996	0.0000001	−1000.0	−1000.0	0.0000001	0.0000001
10^{-9}	−0.0004881	0.0000001	−1000.0	−1000.0	0.0000001	0.0000001
10^{-11}	−0.0002801	0.0000000	−1000.0	−1000.0	0.0000000	0.0000000
10^{-13}	−0.0000752	0.0000000	−1000.0	−1000.0	0.0000000	0.0000000

For a contrapositive proof assume that $(x^*, \bar{y}, \bar{z}, \bar{w})$ is a solution to (3.39) as given by (3.40). Thus, it satisfies

$$\begin{pmatrix} g(x^*) \\ \mu(\bar{y} - y_e) \end{pmatrix} = \begin{pmatrix} J(x^*)^T(2y_e - \bar{y}) + \bar{z} \\ \bar{w} \end{pmatrix} \tag{3.41}$$

since $c(x^*) = 0$. The full row rank assumption implies uniqueness of the Lagrange multipliers and thus

$$y^* = 2y_e - \bar{y} \quad \text{and} \quad z^* = \bar{z}. \tag{3.42}$$

First assume that $y_i^* > \gamma$. Then $\bar{w}_i \neq 0$ since if it was, then (3.41) would imply that $\bar{y}_i = [y_e]_i$ and (3.42) then implies $\bar{y}_i = y_i^* > \gamma$. This is a contradiction since $\bar{y} \in [-\gamma e, \gamma e]$. Since $\bar{w}_i \neq 0$, it must hold that $\bar{y}_i$ is equal to one of its bounds. Suppose that $\bar{y}_i = -\gamma$. This would imply that $\bar{w}_i > 0$ (since $\bar{w}_i = 0$ has already been ruled out). However, the following then holds:

$$\bar{w}_i = \mu\big(\bar{y}_i - [y_e]_i\big) = -\mu\big(\gamma + [y_e]_i\big) \leq 0.$$

This is a contradiction so $\bar{y}_i = \gamma$. However, this implies that $\bar{w}_i < 0$ (since $\bar{w}_i = 0$ has already been ruled out). But then it follows that

$$\bar{w}_i = \mu\big(\bar{y}_i - [y_e]_i\big) = \mu\big(\gamma - [y_e]_i\big) \geq 0,$$

which is another contradiction. Thus no component of y^* can be greater than γ.

A similar argument shows that no component of y^* can be less than $-\gamma$. Thus $y^* \in [-\gamma e, \gamma e]$ and the proof is complete. □

This theorem shows how certain algorithms may proceed when artificial bounds are imposed on y. For example, in the framework of a bound constrained Lagrangian (BCL) method, a sequence of subproblems of the form (3.39) may be solved with appropriate updates made to μ_k and y_k^e. The previous theorem may be used to show that if the artificial bounds placed on the subproblems restrict their solutions, then μ_k will necessarily be forced to zero to obtain convergence. Chapter 4 discusses a BCL method that makes use of artificial bounds in the subproblem.

If the artificial bounds do not restrict the subproblem solution, then the solution lies on the trajectory of minimizers. However, when components of y become active it becomes unclear which problem is being solved. Intuitively, this behavior seems related to exact penalty functions since for γ large enough the exact solution to the intended subproblem is found. This turns out to be true, as the next theorem shows.

Theorem 3.5.2. *Let $\gamma > 0$. If $(\bar{x}, \bar{y}, \bar{w})$ is a solution of*

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} & \mathcal{M}(x, y; y_e, \mu) \\ \text{subject to} & -\gamma e \le y \le \gamma e, \end{array} \tag{3.43}$$

where $\bar{w}$ are the multipliers for the constraints $-\gamma e \le y \le \gamma e$, then there exists a positive diagonal scaling matrix P such that $\bar{x}$ is a solution to

$$\underset{x\in\mathbb{R}^n}{\text{minimize}} \;\; f(x) + \|P\big(c(x) + \mu(\bar{y} - y_e)\big)\|_1. \tag{3.44}$$

Proof. Define $\bar{\pi} \triangleq \bar{y} - \frac{2}{\mu}\bar{w}$. The diagonal scaling matrix $P \triangleq \operatorname{diag}(\rho_1, \ldots, \rho_m)$ is then defined as

$$\rho_i = \begin{cases} \bar{\pi}_i & \text{if } \bar{w}_i < 0, \\ -\bar{\pi}_i & \text{if } \bar{w}_i > 0, \\ |\bar{\pi}_i| + \epsilon & \text{if } \bar{w}_i = 0, \end{cases} \tag{3.45}$$

where ϵ is any positive real number. It will be shown that the diagonals of P are strictly positive. Using Lemma 1.5.4, the non-smooth problem (3.44) is equivalent to the following smooth problem

$$\begin{aligned} \underset{x\in\mathbb{R}^n, u\in\mathbb{R}^m, v\in\mathbb{R}^m}{\text{minimize}} \quad & f(x) + \sum_{i=1}^{m} \rho_i(u_i + v_i) \\ \text{subject to} \quad & c(x) + \mu(\bar{y} - y_e) - u + v = 0, \quad u \geq 0, \quad v \geq 0. \end{aligned} \tag{3.46}$$

Define the following:

$$\bar{u}_i = \begin{cases} 0 & \text{if } \bar{w}_i \leq 0, \\ \bar{w}_i & \text{if } \bar{w}_i > 0, \end{cases} \tag{3.47a}$$

$$\bar{v}_i = \begin{cases} 0 & \text{if } \bar{w}_i \geq 0, \\ -\bar{w}_i & \text{if } \bar{w}_i < 0, \end{cases} \tag{3.47b}$$

$$\bar{z}_u = Pe + \bar{\pi}, \tag{3.47c}$$

$$\bar{z}_v = Pe - \bar{\pi}. \tag{3.47d}$$

It will be shown that $(\bar{x}, \bar{u}, \bar{v}, \bar{\pi}, \bar{z}_u, \bar{z}_v)$ is a solution to (3.46), where $\bar{\pi}$ is the Lagrange multiplier vector for the general equality constraint, $\bar{z}_u$ is the Lagrange multiplier vector for $u \geq 0$, and $\bar{z}_v$ is the Lagrange multiplier vector for $v \geq 0$.

The solution $(\bar{x}, \bar{y}, \bar{w})$ satisfies the following optimality condition:

$$J(\bar{x})^T\big(2\pi(\bar{x}) - \bar{y}\big) = g(\bar{x}), \tag{3.48a}$$

$$c(\bar{x}) + \mu(\bar{y} - y_e) = \bar{w}, \tag{3.48b}$$

$$-\gamma e \le \bar{y} \le \gamma e, \tag{3.48c}$$

$$\min(\gamma e - \bar{y}, \bar{y} + \gamma e, |\bar{w}|) = 0, \tag{3.48d}$$

$$\bar{w} \cdot (\gamma e + \bar{y}) \le 0, \tag{3.48e}$$

$$\bar{w} \cdot (-\gamma e + \bar{y}) \le 0, \tag{3.48f}$$

where $\pi(x) \triangleq y_e - c(x)/\mu$. The conditions that must be verified for the point $(\bar{x}, \bar{u}, \bar{v}, \bar{\pi}, \bar{z}_u, \bar{z}_v)$ are:

C1. $\bar{u} \ge 0,\ \bar{v} \ge 0,\ \bar{z}_u \ge 0,\ \bar{z}_v \ge 0,\ \ \bar{u} \cdot \bar{z}_u = 0,\ \bar{v} \cdot \bar{z}_v = 0;$

C2. $c(\bar{x}) + \mu(\bar{y} - y_e) - \bar{u} + \bar{v} = 0;$

C3. $g(\bar{x}) = J(\bar{x})^T\bar{\pi};$

C4. $Pe = \bar{z}_u - \bar{\pi};$

C5. $Pe = \bar{z}_v + \bar{\pi}.$

(proof of C2): Note that $\bar{w} = \bar{u} - \bar{v}$. Thus C2 follows directly from (3.48b).

(proof of C3): By definition of $\bar{\pi}$ and $\pi(x)$ and use of (3.48b), the following equality holds:

$$\bar{\pi} = \bar{y} - \frac{2}{\mu}\bar{w} = 2y_e - \frac{2}{\mu}c(\bar{x}) - \bar{y} = 2\pi(\bar{x}) - \bar{y}. \tag{3.49}$$

C3 follows from this equality and (3.48a).

(proof of C4): Follows by definition (3.47c).

(proof of C5): Follows by definition (3.47d).

(proof of C1): $\bar{u} \ge 0$ and $\bar{v} \ge 0$ by definition.

Next it is shown that $\bar{u} \cdot \bar{z}_u = 0$. The result is trivial if $\bar{u}_i = 0$. So suppose that $\bar{u}_i \ne 0$. This implies that $\bar{w}_i > 0$ and thus $\rho_i = -\bar{\pi}_i$. It follows that $[\bar{z}_u]_i \triangleq \rho_i + \bar{\pi}_i = 0$.

Now it is shown that $\bar{v}\cdot\bar{z}_v = 0$. The result is trivial if $\bar{v}_i = 0$. So suppose that $\bar{v}_i > 0$. This implies that $\bar{w}_i < 0$ and thus $\rho_i = \bar{\pi}_i$. It follows that $[\bar{z}_v]_i \triangleq \rho_i - \bar{\pi}_i = 0$.

Next consider the following three cases:

1. Suppose $\bar{w}_i = 0$. Then $\rho_i = |\bar{\pi}_i| + \epsilon > 0$ and $[\bar{z}_v]_i = |\bar{\pi}_i| + \epsilon - \bar{\pi}_i > 0$. Similarly, $[\bar{z}_u]_i = |\bar{\pi}_i| + \epsilon + \bar{\pi}_i > 0$.

2. Suppose $\bar{w}_i > 0$. Then $\bar{y}_i = -\gamma$ and $\bar{\pi}_i = \bar{y}_i - \frac{2}{\mu}\bar{w}_i = -\gamma - \frac{2}{\mu}\bar{w}_i < 0$. This implies that $\rho_i = -\bar{\pi}_i > 0$ and that $[\bar{z}_v]_i = \rho_i - \bar{\pi}_i = -2\bar{\pi}_i > 0$. Likewise, $[\bar{z}_u]_i = \rho_i + \bar{\pi}_i = 0$.

3. Suppose $\bar{w}_i < 0$. Then $\bar{y}_i = \gamma$ and $\bar{\pi}_i = \bar{y}_i - \frac{2}{\mu}\bar{w}_i = \gamma - \frac{2}{\mu}\bar{w}_i > 0$. This implies that $\rho_i = \bar{\pi}_i > 0$ and that $[\bar{z}_v]_i = \rho_i - \bar{\pi}_i = 0$. Likewise, $[\bar{z}_u]_i = \rho_i + \bar{\pi}_i = 2\bar{\pi}_i > 0$.

The proof is complete since in all cases $\bar{z}_u \geq 0$, $\bar{z}_v \geq 0$, and $\rho_i > 0$. □

3.6 Relationship to Classical SQP

Much of the previous analysis has concerned the subproblem

$$\underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} \ \mathcal{M}(x, y; y_e, \mu),$$

where $\mathcal{M}$ is the primal-dual augmented Lagrangian. In practice, this subproblem is not always solved to a very high accuracy; high accuracy is required only as a solution to the underlying problem is approached. An extreme case of this situation is to restrict each subproblem to one iteration. This strategy is the basis for sequential quadratic programming (SQP) methods. Two of the more well known of these methods are SNOPT, [14] by Gill, Murray and Saunders, and the Sℓ_1-QP method by Fletcher [11].

This section discusses the relationship between the Newton equations for the primal-dual augmented Lagrangian function and the equations associated with the "classical" SQP approach. The discussion takes place in the context of problem NEP (2.12) on page 34. The classical SQP subproblem is given by

$$\underset{\Delta x \in \mathbb{R}^n}{\text{minimize}} \;\; g_k^T \Delta x + \frac{1}{2}\Delta x^T H_k \Delta x \quad \text{subject to} \;\; c_k + J_k \Delta x = 0. \tag{3.50}$$

where (x_k, y_k) is the current point, $H_k = H(x_k, y_k)$ is the Hessian of the Lagrangian (or an approximation of the Hessian of the Lagrangian), $g_k = g(x_k)$, $c_k = c(x_k)$, and $J_k = J(x_k)$. The solution to this QP is then used in a line-search with an appropriate merit function. The solution satisfies the following KKT system

$$\begin{pmatrix} H(x_k, y_k) & J_k^T \\ J_k & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = - \begin{pmatrix} g_k - J_k^T y_k \\ c_k \end{pmatrix}. \tag{3.51}$$

The transformed Newton system for the primal-dual augmented Lagrangian is given by (3.15) on page 52 as

$$\begin{pmatrix} H\big(x_k, \underline{2\pi_k - y_k}\big) & J_k^T \\ J_k & \underline{-\mu I_m} \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = - \begin{pmatrix} g_k - J_k^T y_k \\ c_k + \underline{\mu(y_k - y_e)} \end{pmatrix}, \tag{3.52}$$

where $\pi(x) = y_e - c(x)/\mu$ and $\pi_k = \pi(x_k)$. The differences between the classical SQP system (3.51) and the transformed primal-dual system (3.52) have been underlined.

Next we show that system (3.52) is closely related to another obtained by "primal-dualizing" the SQP subproblem (3.50). The phrase "primal-dualizing" refers to the process of moving the constraints into the objective via two quadratic penalty functions; one penalizes the constraint violation while the other penalizes deviation from the trajectory. Primal-dualizing (3.50) results in the function

$$\begin{aligned} f(\Delta x, y) = g_k^T \Delta x + \frac{1}{2}\Delta x^T H_k \Delta x - (c_k + J_k \Delta x)^T y_e \\ + \frac{1}{2\mu}\|c_k + J_k \Delta x\|_2^2 + \frac{1}{2\mu}\|c_k + J_k \Delta x + \mu(y - y_e)\|_2^2. \end{aligned}$$

The derivatives of $f(\Delta x, y)$ are given by

$$\nabla f(\Delta x, y) = \begin{pmatrix} g_k + H_k \Delta x + \frac{2}{\mu} J_k^T (c_k + J_k \Delta x + \frac{\mu}{2} y - \mu y_e) \\ c_k + J_k \Delta x + \mu (y - y_e) \end{pmatrix}, \quad \text{and}$$

$$\nabla^2 f(\Delta x, y) = \begin{pmatrix} H_k + \dfrac{2}{\mu} J_k^T J_k & J_k^T \\ J_k & \mu I_m \end{pmatrix}.$$

By setting the gradient equal to zero and using the definition $\Delta y \triangleq y - y_k$, it follows that the solution to

$$\underset{\Delta x \in \mathbb{R}^n, \Delta y \in \mathbb{R}^m}{\text{minimize}} \quad f(\Delta x, y_k + \Delta y)$$

satisfies the following system

$$\begin{pmatrix} H_k + \dfrac{2}{\mu} J_k^T J_k & J_k^T \\ J_k & \mu I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = - \begin{pmatrix} g_k + \frac{2}{\mu} J_k^T (c_k + \dfrac{\mu}{2} y_k - \mu y_e) \\ c_k + \mu (y_k - y_e) \end{pmatrix}.$$

Multiplying on the left by

$$N = \begin{pmatrix} I_n & -\dfrac{2}{\mu} J_k^T \\ 0 & I_m \end{pmatrix}$$

yields

$$\begin{pmatrix} H_k & -J_k^T \\ J_k & \mu I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = - \begin{pmatrix} g_k - J_k^T y_k \\ c_k + \mu (y_k - y_e) \end{pmatrix}.$$

Restoring symmetry gives

$$\begin{pmatrix} \underline{H_k} & J_k^T \\ J_k & -\mu I_m \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta y \end{pmatrix} = - \begin{pmatrix} g_k - J_k^T y_k \\ c_k + \mu (y_k - y_e) \end{pmatrix}. \tag{3.54}$$

Note that (3.52) and (3.54) are identical except for the underlined $(1,1)$ block. Thus, finding a solution to the Newton equations for the primal-dual augmented Lagrangian function applied to problem NEP, is equivalent to finding a stationary point of the primal-dualized classical SQP subproblem with $H(x_k, y_k)$ replaced by $H(x_k, 2\pi(x_k) - y_k)$. A mnemonic phrase for remembering this idea is given by:

$$(\text{Primal-Dualize} + \text{Linearize}) \equiv (\text{Linearize} + \text{Primal-Dualize})_{\text{mod}(2\pi - y)}.$$

It should be emphasized that this phrase is not intended to be rigorous.

3.7 A Generalization

Section 2.2 motivated the definition of the primal-dual penalty and primal-dual augmented Lagrangian functions. The rest of the previous sections have focused on the primal-dual augmented Lagrangian function and its properties. As discussed previously, the properties of the primal-dual augmented Lagrangian also hold for the primal-dual penalty function either directly or with a small change in argument. This observation was due to the following two facts, which are stated again for convenience:

- the primal-dual penalty function can be recovered from the primal-dual augmented Lagrangian function by setting $y_e = 0$.

- the structure of the derivatives are the same; the only difference arises in the definition of the "π" term.

Although these properties are listed separately, the first item implies the second item since the "π" terms are identical upon setting $y_e = 0$.

This does not mean, however, that the primal-dual penalty function and the primal-dual augmented Lagrangian function possess *all* of the same properties. In particular, a primal-dual penalty method *requires* the penalty parameter to be driven to zero in order to obtain convergence, while a primal-dual augmented Lagrangian method requires this only when things appear to be going "badly". Thus, although much of the analysis for one carries over to the other, they are still different functions with different properties.

A *generalized* primal-dual function parameterized by ν is now given. It will be shown that various primal-dual functions, including the ones already discussed, may be obtained from this generalized primal-dual function by choosing particular values for the parameter ν.

Given an approximate Lagrange multiplier vector y_e, consider the generalized primal-dual function

$$\mathcal{M}(x,y;y_e,\mu,\nu) = f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{\nu}{2\mu}\|c(x)+\mu(y-y_e)\|^2, \quad (3.55)$$

where ν and μ are constant scalars with $\mu > 0$. This may be derived as a shifted-constraint version of the Forsgren-Gill merit function. Using the the m-vector $\pi(x) = y_e - c(x)/\mu$, the gradient and Hessian for $\mathcal{M}(x,y;y_e,\mu,\nu)$ may be written as

$$\nabla\mathcal{M}(x,y;y_e,\mu,\nu) = \begin{pmatrix} g - J^T\big((1+\nu)\pi - \nu y\big) \\ \nu\big(c + \mu(y-y_e)\big) \end{pmatrix} \quad (3.56a)$$

$$= \begin{pmatrix} g - J^T\big(\pi(x) + \nu(\pi - y)\big) \\ \nu\mu(y-\pi) \end{pmatrix}, \quad (3.56b)$$

and

$$\nabla^2\mathcal{M}(x,y;y_e,\mu,\nu) = \begin{pmatrix} H\big(x,(1+\nu)\pi - \nu y\big) + \dfrac{1+\nu}{\mu}J^TJ & \nu J^T \\ \nu J & \nu\mu I \end{pmatrix}, \quad (3.56c)$$

where J, g, c, and π denote $J(x)$, $g(x)$, $c(x)$, and $\pi(x)$, respectively.

The primal-dual augmented Lagrangian function

$$\mathcal{M}(x,y;y_e,\mu) = f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x)+\mu(y-y_e)\|^2$$

is obtained from the generalized primal-dual function by setting $\nu = 1$. The classical augmented Lagrangian function

$$\mathcal{L}_{\mathcal{A}}(x;y_e,\mu) = f(x) - c(x)^T y_e + \frac{1}{2\mu}\|c(x)\|^2$$

is obtained from the generalized primal-dual function by setting $\nu = 0$. The "proximal-point" Lagrangian function

$$\mathcal{L}_{\mathcal{P}}(x,y) \triangleq f(x) - c(x)^T y - \frac{\mu}{2}\|y-y_e\|^2$$

is obtained from the generalized primal-dual function by setting $\nu = -1$. This makes the dual function quadratic in y instead of linear.

By making further choices for y_e, more functions may be obtained. The primal-dual penalty function

$$\mathcal{P}(x, y; \mu) \triangleq f(x) + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x) + \mu y\|^2$$

is obtained from the generalized primal-dual function by setting $\nu = 1$ and $y_e = 0$. The classical penalty function

$$\mathcal{P}(x; \mu) \triangleq f(x) + \frac{1}{2\mu}\|c(x)\|^2$$

is obtained from the generalized primal-dual function by setting $\nu = 0$ and $y_e = 0$. Finally, the "proximal-point" penalty function

$$\mathcal{P}_{\mathcal{P}}(x, y) \triangleq f(x) - c(x)^T y - \frac{\mu}{2}\|y\|^2$$

is obtained from the generalized primal-dual function by setting $\nu = -1$ and $y_e = 0$.

To summarize, Table 3.3 gives certain functions obtained from the generalized primal-dual function (3.55) by setting ν and y_e to specific values.

Table 3.3: Special cases of the generalized primal-dual function.

Function	ν	y_e
Primal-Dual Augmented Lagrangian Function	1	y_e
Augmented Lagrangian Function	0	y_e
Proximal-Point Lagrangian Function	-1	y_e
Primal-Dual Penalty Function	1	0
Classical Penalty Function	0	0
Proximal-Point Penalty Function	-1	0

It is important to mention that Sections 3.1–3.3 could have been discussed in terms of the *generalized* primal-dual function. Sections 3.4–3.6 could then have been discussed by specializing to the case $\nu = 1$. One advantage of this approach is that it may have shed some light on the "mysterious" appearance of the "2π" in the derivatives of the primal-dual functions. A second advantage is that it would have emphasized the generalized primal-dual function. A sufficient understanding of the potential use and benefits of varying ν inside an optimization algorithm has still not been realized and deserves more study.

There are advantages of immediately specializing to the primal-dual penalty function and the primal-dual augmented Lagrangian function. First, there was the hope that a more thorough derivation and justification could be made for these special cases. Justification for the generalized primal-dual function could have been made, but it may have been less clear to the "average" reader. Second, it seemed more natural to specialize initially since very little is understood about the potential benefits of varying ν.

The following theorem is given as an example of how the generalized primal-dual function could have been discussed in Sections 3.1–3.3. In fact, Theorem 3.3.2 of Section 3.3 is a corollary to Theorem 3.7.1 below.

Theorem 3.7.1. *If* (x^*, y^*) *satisfies the second-order sufficient conditions for a solution of problem* NEP (2.12)*, then there exists a* $\bar{\mu}$ *such that for all* $0 < \mu < \bar{\mu}$ *and all* $\nu > 0$*, the point* (x^*, y^*) *is a solution of the unconstrained minimization problem*

$$\underset{x \in \mathbb{R}^n,\, y \in \mathbb{R}^m}{\text{minimize}} \qquad \mathcal{M}(x, y; y^*, \mu, \nu), \tag{3.57}$$

where $\mathcal{M}(x, y; y^*, \mu, \nu) = f(x) - c(x)^T y^* + \frac{1}{2\mu}\|c(x)\|^2 + \frac{\nu}{2\mu}\|c(x) + \mu(y - y^*)\|^2$ *is the generalized primal-dual function.*

Proof. By assumption, x^* satisfies the second-order sufficient conditions for problem NEP. Therefore, Theorem 2.1.3 implies that x^* satisfies

C1. $c(x^*) = 0$,

C2. $g(x^*) - J(x^*)^T y^* = 0$, and

C3. there exists $\omega > 0$ such that $p^T H(x^*, y^*)p \geq \omega\|p\|^2$ for all p satisfying $J(x^*)p = 0$.

To show that (x^*, y^*) is an unconstrained minimizer of (3.57), the following must be shown: $\nabla\mathcal{M}(x^*, y^*; y^*, \mu, \nu) = 0$ and $\nabla^2\mathcal{M}(x^*, y^*; y^*, \mu, \nu)$ is positive definite. Condition C1 and the definition $\pi(x) = y^* - c(x)/\mu$ shows that $\pi(x^*) = y^*$. This fact, (3.56b), (3.56c) and C2, imply

$$\nabla\mathcal{M}(x^*, y^*; y^*, \mu, \nu) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and

$$\nabla^2\mathcal{M}(x^*, y^*; y^*, \mu, \nu) = \begin{pmatrix} H(x^*, y^*) + \dfrac{1+\nu}{\mu} J(x^*)^T J(x^*) & \nu J(x^*)^T \\ \nu J(x^*) & \nu\mu I_m \end{pmatrix}.$$

An argument similar to that used in Lemma 3.2.1 shows that

$$\text{In}\big(\nabla^2\mathcal{M}(x^*, y^*; y^*, \mu, \nu)\big) = \big(m, 0, 0\big) + \text{In}\Big(H(x^*, y^*) + \frac{1}{\mu} J(x^*)^T J(x^*)\Big)$$

for all $\nu > 0$. Finally, C3 and Debreu's Lemma 1.5.1 imply that there exists a $\bar{\mu} > 0$ such that the matrix

$$H(x^*, y^*) + \frac{1}{\mu} J(x^*)^T J(x^*)$$

is positive definite for all $0 < \mu \leq \bar{\mu}$. Thus,

$$\text{In}\big(\nabla^2\mathcal{M}(x^*, y^*; y^*, \mu, \nu)\big) = \big(m, 0, 0\big) + \big(n, 0, 0\big) = \big(m + n, 0, 0\big),$$

which means that $\nabla^2\mathcal{M}(x^*, y^*; y^*, \mu, \nu)$ is positive definite for all $0 < \mu \leq \bar{\mu}$ and all $\nu > 0$. Therefore, (x^*, y^*) is an unconstrained minimizer of problem (3.57). $\square$

4

A Primal-Dual Bound Constrained Lagrangian (BCL) Method

This chapter considers an algorithm for finding local constrained minimizers of the following problem:

$$\text{GNPs} \qquad \begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x)=0, \quad x\geq 0, \end{array} \tag{4.1}$$

where $c:\mathbb{R}^n\rightarrow\mathbb{R}^m$ and $f:\mathbb{R}^n\rightarrow\mathbb{R}$. This choice of problem format assumes that all general inequality constraints $c_i(x)\geq 0$ have been converted to general equality constraints by the introduction of slack variables. One should note that the analysis to be done for this problem format easily carries over to the more general setting with $l\leq x\leq u$.

Problem GNPs will be solved by solving a sequence of bound constrained problems of the form

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} & \mathcal{M}(x,y;y_k^e,\mu_k) \\ \text{subject to} & -\gamma_k e\leq y\leq \gamma_k e, \quad x\geq 0, \end{array} \tag{4.2}$$

where $\mathcal{M}(x, y; y_k^e, \mu_k)$ is the primal-dual augmented Lagrangian function introduced in Chapter 3, $\{\gamma_k\}$ is a sequence of constants, $\{y_k^e\}$ is a sequence of estimates of the Lagrange multiplier vector satisfying $y_k^e \in [-\gamma_k e, \gamma_k e]$, and $\{\mu_k\}$ is a sequence of positive penalty parameters. An approximate solution to this problem will be denoted by $(x_k^*, y_k^*, z_k^*, w_k^*)$ where z_k^* is the reduced cost vector for $x \geq 0$ and w_k^* is the reduced cost vector for $-\gamma_k e \leq y \leq \gamma_k e$. Note that the following analysis carries over to the more realistic setting where each constraint is given its own penalty parameter.

The rest of this chapter is organized as follows. Section 4.1 discusses some basic concepts as well as introduces necessary notation and terminology. Section 4.2 states the primal-dual BCL method. Section 4.3 shows that the algorithm is globally convergent, while section Section 4.4 studies local convergence properties. Section 4.5 considers what occurs when the primal-dual BCL algorithm is applied to an infeasible problem. Section 4.6 considers the existence of subproblem solutions in the neighborhood of a solution to problem GNPs. Furthermore, identification of the optimal active set by the subproblem is studied. Section 4.7 considers the implications of imposing certain second-order conditions on the subproblem solutions. Finally, Section 4.8 discusses higher-order updating schemes.

4.1 Notation

This section introduces notation and terminology. The following definition of a first-order KKT for problem GNPs is an alternative but equivalent definition to Definition 2.1.10 on page 27.

Definition 4.1.1. *A point* (x, y, z) *is a first-order KKT point (Karush-Kuhn-*

Tucker point) for problem (4.1) *if it satisfies the following conditions:*

$$c(x) = 0, \tag{4.3a}$$

$$g(x) - J(x)^T y = z, \tag{4.3b}$$

$$\min(x, z) = 0. \tag{4.3c}$$

The vector y is the Lagrange multiplier vector for the constraint $c(x) = 0$ and z is the Lagrange multiplier vector (reduced cost vector) for the constraint $x \geq 0$. Condition (4.3c) is a concise formulation of conditions (ii), (iv), and (v) in Definition 2.1.10.

Given primal and dual convergence tolerances, η_* and ω_* respectively, the point (x, y, z) will be considered an acceptable solution to problem GNPs if it satisfies the following criteria:

$$\|c(x)\| \leq \eta_*, \tag{4.4a}$$

$$g(x) - J(x)^T y = z, \tag{4.4b}$$

$$\|\min(x, z)\|_\infty \leq \omega_*. \tag{4.4c}$$

Given a point x, we define the index set $\mathcal{I}(x) = \{\, j \in 1\!:\!n \mid [x]_j > 0 \,\}$ associated with the inactive bounds at x. With this definition in hand, further notation is listed below. This list also summarizes notation introduced previously.

- (x^*, y^*, z^*) is an optimal solution for problem GNPs.
- (x_k, y_k, z_k) is the kth estimate of (x^*, y^*, z^*).
- $(x_k^*, y_k^*, z_k^*, w_k^*)$ is an approximate solution of the kth subproblem.
- x_* is a limit point of $\{x_k^*\}$.
- $g(x)$ is the gradient of $f(x)$ evaluated at x.
- $J(x)$ is the $m \times n$ Jacobian of $c(x)$ evaluated at x.

- $\hat{g}(x)$ is the vector of components of $g(x)$ associated with the indices in $\mathcal{I}(x_*)$.
- $\widehat{J}(x)$ are the columns of $J(x)$ associated with the indices in $\mathcal{I}(x_*)$.
- $\mathcal{M}(x, y; y_k^e, \mu_k)$ is the kth primal-dual augmented Lagrangian evaluated at (x, y).
- $H(x)$ is the Hessian of $f(x)$ evaluated at x.
- $H_i(x)$ is the Hessian of $c_i(x)$ evaluated at x.
- $L(x, y) = f(x) - c(x)^T y$ is the Lagrangian.
- $H(x, y)$ is the Hessian of the Lagrangian with respect to x evaluated at (x, y).
- $\pi(x; y_e, \mu) = y_e - c(x)/\mu$ is the vector of primal first-order multiplier estimates.
- $\pi_k = \pi(x_k^*; y_k^e, \mu_k)$ is the kth vector of primal first-order multiplier estimates.
- $\widetilde{y}(x, y; y_e, \mu) = 2\pi(x; y_e, \mu) - y$ is the vector of primal-dual first-order multiplier estimates.
- $\widetilde{y}_k = \widetilde{y}(x_k^*, y_k^*; y_k^e, \mu_k)$ is the kth vector of primal-dual first-order multiplier estimates.
- $\widehat{y}(x)$ is the least-squares multiplier estimate as described in (4.5) below.

At all points x for which $\widehat{J}(x)$ has full row rank, the least-squares multiplier estimate is defined as:

$$\widehat{y}(x) \triangleq \underset{y}{\operatorname{argmin}} \|\hat{g}(x) - \widehat{J}(x)^T y\|_2^2. \tag{4.5}$$

It is not possible to calculate $\widehat{y}(x)$ since x^* is not known in advance. The quantity $\widehat{y}(x)$ is used only as a theoretical tool and is never required by the algorithm.

The following assumptions are used:

(AS1a) The functions $f(x)$ and $\{c_i(x)\}$ are twice continuously differentiable for all $x \geq 0$.

(AS1b) The second derivative of the functions $f(x)$ and $\{c_i(x)\}$ are locally Lipschitz continuous at all points within the compact set $\mathcal{B}_x \subset \mathbb{R}^n$ given in assumption AS2a.

(AS2a) The sequence $\{x_k^*\}$ is contained in the compact set $\mathcal{B}_x \subset \mathbb{R}^n$.

(AS2b) If K is a subsequence of the integers such that $\lim_{k\in K} x_k^* = x_*$, then $\{y_k^*\}_K$ is contained in the compact set $\mathcal{B}_y \subset \mathbb{R}^m$.

(AS3) The matrix $\widehat{J}(x_*)$ has full row rank at every limit point x_* of the sequence $\{x_k^*\}$ $\big($at least one limit point is guaranteed by assumption AS2a$\big)$.

Using notation and assumptions defined above, the following three lemmas are now stated.

Lemma 4.1.1. *If assumption* AS1a *holds and* $\widehat{J}(x)$ *has full row rank, then* $\widehat{y}(x)$ *is differentiable and its derivative is given by*

$$\frac{d}{dx}\widehat{y}(x) = \big(\widehat{J}(x)^\dagger\big)^T H\big(x, \widehat{y}(x)\big) + \big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1} B(x),$$

where $\widehat{J}(x)^\dagger \triangleq \widehat{J}(x)^T\big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}$ *and the* i*th row of* $B(x)$ *is given by* $\big(\hat{g}(x) - \widehat{J}(x)^T\widehat{y}(x)\big)^T H_i(x)$.

Proof. The vector $\widehat{y}(x)$ is a solution to (4.5) if and only if $\widehat{y}(x)$ satisfies $\widehat{J}(x)r(x) = 0$ and $r(x) = \hat{g}(x) - \widehat{J}(x)^T\widehat{y}(x)$. Differentiation of the first equation yields $\widehat{J}(x)r'(x) + B(x) = 0$, while differentiation and rearrangement of the definition of $r(x)$ yields $r'(x) = H\big(x, \widehat{y}(x)\big) - \widehat{J}(x)^T\widehat{y}'(x)$. Elimination of $r'(x)$ from these equations and use of the non-singularity of $\widehat{J}(x)\widehat{J}(x)^T$ gives the desired result. □

Lemma 4.1.2. *If assumption* AS1 *holds and* $\widehat{J}(x)$ *has full row rank, then the least-squares estimate* $\widehat{y}(x)$ *is Lipschitz continuous in a neighborhood of* x.

Proof. From the integral Mean-Value Theorem it follows that

$$\widehat{y}(z) - \widehat{y}(x) = \int_0^1 \widehat{y}'\big(z(\xi)\big) \cdot (z - x)\, d\xi,$$

where $z(\xi) = x + \xi(z - x)$ and $\widehat{y}'$ is defined as in Lemma 4.1.1. Since the right-hand side is bounded in a neighborhood of x, the inequality

$$\|\widehat{y}(z) - \widehat{y}(x)\| \leq \alpha \|z - x\|$$

holds for some $\alpha > 0$ and for all z in some neighborhood of x. □

Lemma 4.1.3. *Assume that $\widehat{J}(x)$ has full row rank. Then there exists a constant $\alpha > 0$ such that for all y*

$$\|\widehat{y}(x) - y\| \leq \alpha \|\hat{g}(x) - \widehat{J}(x)^T y\|.$$

Proof. By assumption, $\widehat{J}(x)$ has full row rank and the least-squares solution may be written as

$$\widehat{y}(x) = (\widehat{J}(x)\widehat{J}(x)^T)^{-1}\widehat{J}(x)\hat{g}(x).$$

The following now holds

$$\begin{aligned} \|\widehat{y}(x) - y\| &= \|\big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}\widehat{J}(x)\hat{g}(x) - y\| \\ &= \|\big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}\widehat{J}(x)\hat{g}(x) - \big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}\big(\widehat{J}(x)\widehat{J}(x)^T\big)y\| \\ &\leq \|\big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}\widehat{J}(x)\|\|\hat{g}(x) - \widehat{J}(x)^T y\|. \end{aligned}$$

Let $\alpha \triangleq \|\big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}\widehat{J}(x)\|$. At this point it is only clear that $\alpha \geq 0$. Assume $\alpha = 0$. This implies that $\big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}\widehat{J}(x) = 0$ and thus that

$$\big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}\widehat{J}(x)e_j = 0 \ \text{ for all } j.$$

Since $\big(\widehat{J}(x)\widehat{J}(x)^T\big)^{-1}$ is nonsingular, this implies that

$$\widehat{J}(x)e_j = \widehat{J}_j(x) = 0 \ \text{ for all } j,$$

where $\widehat{J}_j(x)$ is the jth column of $\widehat{J}(x)$. Thus, $\widehat{J}(x)$ is the zero matrix. This is a contradiction since $\widehat{J}(x)$ was assumed to have full row rank. It follows that $\alpha > 0$ and the proof is complete. □

4.2 Statement of the Algorithm

Classical bound-constrained Lagrangian (BCL) methods are known to be locally convergent if the penalty parameter is sufficiently small and if the sequence of subproblems are solved exactly. Bertsekas [1] extends this result by showing that the BCL subproblems need only be minimized approximately. In both cases it may be necessary to drive the penalty parameter to zero to guarantee global convergence. In this case, the BCL subproblems are close to those of the quadratic penalty method. Algorithm 4.2.1 below is similar to the algorithm proposed by Conn, Gould, and Toint [8], which is the basis for the well-known code LANCELOT (see [7]).

Based on the primal infeasibility, each iterate is regarded as either "successful" or "unsuccessful". In the "successful" case, if y_k^* is "close" to the boundary, then μ_k is decreased. This results in a larger "artificial" bound γ_k, which encourages the dual variables to be inactive during the next iteration. In the "unsuccessful" case, the parameter μ_k is decreased and the "artificial" bound γ_k is increased. Again, large "artificial" bounds encourage the dual variables in the subproblem to be inactive; when approaching a solution it is highly desirable for the dual variables to be inactive. Next, the penalty parameter μ_k is decreased in order to drive convergence. As described in [1], convergence of the multiplier method depends critically on the size of μ_k and $\|y_k^e - y^*\|$. The strategy of decreasing μ_k in order to drive convergence is based on the assumption that if μ_k is decreased enough then the iterates will eventually enter a "cone of convergence". Once this "cone of convergence" has been entered, the penalty parameter will no longer need to be decreased and the algorithm will converge.

Algorithm 4.2.1. Primal-Dual BCL Algorithm (pdBCL)

INPUT: (x_0, y_0)

Set constants μ_0, η_0, ω_0, η_*, ω_*, τ_*, μ_c, τ_f, k_τ, ν, α_η, α_ω, β_η, β_ω, α_γ, and α_τ.

Set $y_0^e = y_0$; $\quad \nu = (\|y_0^e\|_\infty + 1)\mu_0^{\alpha_\gamma}$; $\quad \gamma_0 = \nu\mu_0^{-\alpha_\gamma}$; $\quad \tau_0 = \min(\mu_0\omega_0, k_\tau\mu_0^{\alpha_\tau})$;

converged $\leftarrow$ **false**;

while not *converged* **do**

  Find $(x_k^*, y_k^*, z_k^*, w_k^*)$, a solution to (4.2) as given by condition (4.6).

  if $(x_k^*, \widetilde{y}_k, z_k^*)$ satisfies (4.4) **then** *converged* $\leftarrow$ **true** **end if**

  Compute (x_{k+1}^s, y_{k+1}^s) to increase the convergence rate.

  if $\|c(x_k^*)\| \le \max(\eta_*, \eta_k)$ [successful]

    if $\|y_k^*\|_\infty > \gamma_k - \tau_f$ **then** [approaching boundary]

      $\mu_{k+1} \leftarrow \mu_c\mu_k$; $\quad \gamma_{k+1} \leftarrow \nu\mu_{k+1}^{-\alpha_\gamma}$;

    end if

    $\eta_{k+1} \leftarrow \eta_k\mu_{k+1}^{\beta_\eta}$; $\quad \omega_{k+1} \leftarrow \omega_k\mu_{k+1}^{\beta_\omega}$; [decrease η_k and ω_k]

    $\tau_{k+1} \leftarrow \min(\mu_{k+1}\omega_{k+1}, k_\tau\mu_{k+1}^{\alpha_\tau})$;

  else [unsuccessful]

    $\mu_{k+1} \leftarrow \mu_c\mu_k$; $\quad \gamma_{k+1} \leftarrow \nu\mu_{k+1}^{-\alpha_\gamma}$;

    $\eta_{k+1} \leftarrow \eta_0\mu_{k+1}^{\alpha_\eta}$; $\quad \omega_{k+1} \leftarrow \omega_0\mu_{k+1}^{\alpha_\omega}$; [increase or decrease η_k and ω_k]

    $\tau_{k+1} \leftarrow \min(\mu_{k+1}\omega_{k+1}, k_\tau\mu_{k+1}^{\alpha_\tau})$;

  end if

$$y_{k+1}^e = \begin{cases} y_{k+1}^s & \text{if } \|y_{k+1}^s\|_\infty \le \gamma_{k+1}; & \text{[higher-order]} \\ \widetilde{y}_k & \text{if } \|y_{k+1}^s\|_\infty > \gamma_{k+1} \text{ and } \|\widetilde{y}_k\|_\infty \le \gamma_{k+1}\ ; & \text{[first-order]} \\ y_k^e & \text{otherwise.} \end{cases}$$

  $k \leftarrow k + 1$;

end do

OUTPUT: $(x^*, y^*, z^*) \leftarrow (x_k^*, \widetilde{y}_k, z_k^*)$

The parameters associated with Algorithm 4.2.1 are defined as follows:

- μ_0 $(0 < \mu_0 < 1)$ is the initial penalty parameter.
- η_0 $(\eta_* \leq \eta_0 < \frac{1}{2})$ is the initial primal infeasibility tolerance.
- ω_0 $(\omega_* \leq \omega_0 < \frac{1}{2})$ is the initial dual infeasibility tolerance for the x-variables.
- η_* $(0 < \eta_* \ll 1)$ is the primal convergence tolerance.
- ω_* $(0 < \omega_* \ll 1)$ is the dual convergence tolerance for the x-variables.
- τ_* $(0 < \tau_* \ll 1)$ is the dual convergence tolerance for the y-variables.
- μ_c $(0 < \mu_c < 1)$ is the contraction factor for μ_k.
- τ_f $(1 \geq \tau_f > 0)$ is the boundary "fudge-factor" for the y-variables.
- k_τ $(k_\tau > 0)$ is a positive constant used in the update to τ_k. This parameter is required for the proof of Lemma 4.3.4.
- ν $(\nu > 0)$ is a positive constant used in the definition of γ_k. Given μ_0 and y_0^e, ν is set to $\nu = (\|y_0^e\|_\infty + 1)\mu_0^{\alpha_\gamma}$, which implies that $\gamma_0 = \|y_0^e\|_\infty + 1$. This update guarantees that $y_0^e \in [-\gamma_0 e, \gamma_0 e]$. Moreover, if (x_0, y_0) is optimal, then the algorithm will exit on the first iteration.
- α_η $(0 < \alpha_\eta < \min(1, \alpha_\omega))$ is a constant used to update η_k in the "unsuccessful" case. The condition $\alpha_\eta > 0$ ensures that $\eta_k < \eta_0$ for all $k > 0$ in the "unsuccessful" case. The condition $\alpha_\eta < \min(1, \alpha_\omega)$ is required for the proof of Theorem 4.4.2.
- α_ω $(\alpha_\omega > 0)$ is a constant used in the update to ω_k in the "unsuccessful" case. This parameter ensures that $\{\omega_k\}$ converges to zero and that $\omega_k < \omega_0$ for all $k > 0$.

- β_η ($0 < \beta_\eta < \min(1, \beta_\omega)$) is a constant used in the update to η_k in the "successful" case. The condition $\beta_\eta > 0$ ensures that $\eta_{k+1} < \eta_k$ in the "successful" case. The condition $\beta_\eta < \min(1, \beta_\omega)$ is required for the proof of Theorem 4.4.2.

- β_ω ($\beta_\omega > 0$) is a constant used in the update to ω_k in the "successful" case. This parameter ensures that $\omega_{k+1} < \omega_k$ in the "successful" case.

- α_γ ($0 < \alpha_\gamma < 1$) is a constant used in the update to γ_k. The condition $\alpha_\gamma > 0$ is required for the proof of Lemma 4.3.2. The condition $\alpha_\gamma < 1$ is required for the proof of Lemma 4.3.3.

- α_τ ($\alpha_\tau > 1$) is a constant used in the update to τ_k. This value is required for the proof of Lemma 4.3.4 to hold.

During each iteration the point $(x_k^*, y_k^*, z_k^*, w_k^*)$ is accepted as a solution to problem (4.2) if it satisfies the following:

$$x_k^* \geq 0, \tag{4.6a}$$

$$\| \min(x_k^*, z_k^*)\|_\infty \leq \omega_k, \tag{4.6b}$$

$$-\gamma_k e \leq y_k^* \leq \gamma_k e, \tag{4.6c}$$

$$\| \min(\gamma_k e - y_k^*, y_k^* + \gamma_k e, |w_k^*|)\|_\infty \leq \tau_k, \tag{4.6d}$$

$$\text{If } [\gamma_k e - y_k^*]_j \leq \tau_k, \text{ then } [w_k^*]_j \leq \tau_k, \tag{4.6e}$$

$$\text{If } [y_k^* + \gamma_k e]_j \leq \tau_k, \text{ then } [w_k^*]_j \geq -\tau_k, \tag{4.6f}$$

$$\nabla \mathcal{M}(x_k^*, y_k^*; y_k^e, \mu_k) = \begin{pmatrix} z_k^* \\ w_k^* \end{pmatrix}. \tag{4.6g}$$

Condition (4.6b) is equivalent to $[x_k^*]_i \geq -\omega_k$ and $[z_k^*]_i \geq -\omega_k$ holding in addition to either $[x_k^*]_i \leq \omega_k$ or $[z_k^*]_i \leq \omega_k$ holding for $i = 1\!:\!n$. A similar statement holds for condition (4.6d).

4.3 Global Convergence

In this section the pdBCL algorithm is shown to be globally convergent. The first result gives information about points that are produced by the algorithm. With this result in hand, the global convergence proof is relatively straight forward.

Lemma 4.3.1. *Suppose that assumptions* AS1a*,* AS2a*, and* AS3 *hold. Let* $\{\mu_k\}$*,* $\{\gamma_k\}$*,* $\{\tau_k\}$*, and* $\{\omega_k\}$ *be given sequences of positive numbers such that* $\{\omega_k\} \to 0$*, and let* $\{y_k^e\}$ *be any sequence of vectors in* $\mathbb{R}^m$*. Let* $(x_k^*, y_k^*, z_k^*, w_k^*)$ *be a sequence of points satisfying conditions* (4.6a), (4.6b), and (4.6g). Also let K be a subsequence of the integers such that $\lim_{k\in K} x_k^* = x_*$, a limit point of $\{x_k^*\}$. Define $\widetilde{y}_k = 2\pi_k - y_k^* = 2y_k^e - \frac{2}{\mu_k}c(x_k^*) - y_k^*$, and set $y_* = \widehat{y}(x_*)$ and $z_* = g(x_*) - J(x_*)^T y_*$. The following properties then hold:

1. There are positive constants α_1 and α_2 such that for $k \in K$ sufficiently large,

   a) $\|\widetilde{y}_k - y_*\| \le \beta_1 \triangleq \alpha_1\omega_k + \alpha_2\|x_k^* - x_*\|$

   b) $2\|c(x_k^*)\| \le \mu_k\|\widetilde{y}_k - y_*\| + 2\mu_k\|y_k^e - y_*\| + \mu_k\|y_k^* - y_*\|$

   c) $\|c(x_k^*)\| \le \mu_k\|\widetilde{y}_k - y_*\| + \mu_k\|y_k^e - y_*\| + \|w_k^*\|$

   d) $\|y_k^* - y_*\| \le \|\widetilde{y}_k - y_*\| + (2/\mu_k)\|w_k^*\|$

   e) $\|y_k^* - y_*\| \le \frac{2}{\mu_k}\|c(x_k^*)\| + 2\|y_k^e - y_*\| + \|\widetilde{y}_k - y_*\|$

   Moreover; parts b), c), d), and e) hold for all k.

2. $\lim_{k\in K} \widetilde{y}_k = y_*$

3. $\lim_{k\in K} z_k^* = g(x_*) - J(x_*)^T y_* = z_*$

4. For all $k \in K$ sufficiently large,

   a) $2\|w_k^*\| \le \mu_k\|\widetilde{y}_k - y_*\| + 4\mu_k\|y_k^e - y_*\| + 3\mu_k\|y_k^* - y_*\|$

   b) $2\|w_k^*\| \le \mu_k\beta_1 + 4\mu_k\|y_k^e - y_*\| + 3\mu_k\|y_k^* - y_*\|$

Moreover; part a) holds for all k.

5. If $c(x_*) = 0$, then (x_*, y_*, z_*) is a first-order KKT point for problem GNPs.

Proof. Assumption AS3 and the fact that $\lim_{k\in K} x_k^* = x_*$, implies that $\widehat{J}(x_k^*)$ has full row rank for $k \in K$ sufficiently large. Thus, Lemma 4.1.3 implies that there exists a number $\alpha_1 > 0$ such that

$$\|\widehat{y}(x_k^*) - \widetilde{y}_k\| \le \frac{\alpha_1}{\sqrt{n}} \|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T \widetilde{y}_k\| \text{ for } k \in K \text{ sufficiently large.} \tag{4.7}$$

Now to proceed with bounding the right-hand side. First note that since $\lim_{k\in K} x_k^* = x_*$ and $[x_*]_{\mathcal{I}} > 0$, it must be the case that for $k \in K$ sufficiently large $[x_k^*]_{\mathcal{I}} > 0$. Condition (4.6b) and the fact that $\{\omega_k\} \to 0$, gives

$$\min\left([x_k^*]_{\mathcal{I}}, [z_k^*]_{\mathcal{I}}\right) = [z_k^*]_{\mathcal{I}} \text{ for } k \in K \text{ sufficiently large.}$$

This implies the following

$$\begin{aligned} \|[z_k^*]_{\mathcal{I}}\| &\le \|\min(x_k^*, z_k^*)\| \\ &= \left(\sum_{j=1}^{n} \min([x_k^*]_j, [z_k^*]_j)^2\right)^{1/2} \\ &\le \left(\sum_{j=1}^{n} \omega_k^2\right)^{1/2} = \sqrt{n}\omega_k \text{ for } k \in K \text{ sufficiently large.} \end{aligned}$$

Condition (4.6g) and the definition of $\widetilde{y}_k$, implies that the following holds for all $k \in K$ sufficiently large:

$$\sqrt{n}\omega_k \ge \|[z_k^*]_{\mathcal{I}}\| = \|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T\left(2\pi_k - y_k^*\right)\| = \|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T \widetilde{y}_k\|.$$

Thus,

$$\|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T \widetilde{y}_k\| \le \sqrt{n}\omega_k \text{ for } k \in K \text{ sufficiently large.} \tag{4.8}$$

This bound and (4.7) yields

$$\|\widehat{y}(x_k^*) - \widetilde{y}_k\| \le \alpha_1\omega_k \text{ for } k \in K \text{ sufficiently large.} \tag{4.9}$$

Use of (4.9), Lipschitz continuity of the least-squares multiplier estimate in a neighborhood of x_* $\big($recall that $y_* = \widehat{y}(x_*)\big)$, and the triangle inequality imply the existence of a number $\alpha_2 > 0$ such that

$$\begin{aligned}\|\widetilde{y}_k - y_*\| &= \|\widetilde{y}_k - \widehat{y}(x_k^*) + \widehat{y}(x_k^*) - y_*\| \\ &\leq \|\widetilde{y}_k - \widehat{y}(x_k^*)\| + \|\widehat{y}(x_k^*) - y_*\| \\ &\leq \alpha_1\omega_k + \alpha_2\|x_k^* - x_*\| = \beta_1 \text{ for } k \in K \text{ sufficiently large.}\end{aligned} \tag{4.10}$$

This proves 1a). Also, since $\{\omega_k\} \to 0$ and $\lim_{k\in K} x_k^* = x_*$, both terms on the right-hand side of (4.10) go to zero implying

$$\lim_{k\in K} \widetilde{y}_k = y_*.$$

This proves 2.

Next, using (4.6g) and taking limits for $k \in K$ leads to

$$\begin{aligned}\lim_{k\in K} z_k^* &= \lim_{k\in K} g(x_k^*) - J(x_k^*)^T\widetilde{y}_k \\ &= g(x_*) - J(x_*)^T y_* = z_*.\end{aligned}$$

This proves 3.

By definition $\widetilde{y}_k = 2y_k^e - \frac{2}{\mu_k}c(x_k^*) - y_k^*$. Rearrangement and introduction of y_* leads to

$$\frac{2}{\mu_k}c(x_k^*) = 2y_k^e - 2y_* + y_* - \widetilde{y}_k + y_* - y_k^*.$$

Applying norms and the triangle inequality gives

$$2\|c(x_k^*)\| \leq \mu_k\|\widetilde{y}_k - y_*\| + 2\mu_k\|y_k^e - y_*\| + \mu_k\|y_k^* - y_*\|.$$

This proves 1b).

Substitution of $c(x_k^*)$ from condition (4.6g) into the definition of $\widetilde{y}_k$ shows

$$\widetilde{y}_k = 2y_k^e - \frac{2}{\mu_k}c(x_k^*) - y_k^* = y_k^* - \frac{2}{\mu_k}w_k^*. \tag{4.11}$$

Rearrangement, introduction of y_* and the triangle inequality gives

$$\|y_k^* - y_*\| = \|\widetilde{y}_k + \frac{2}{\mu_k} w_k^* - y_*\| \le \|\widetilde{y}_k - y_*\| + \frac{2}{\mu_k}\|w_k^*\|,$$

which proves 1d).

Application of the bound given in part 1d) to the third term of part 1b) implies

$$\|c(x_k^*)\| \le \mu_k \|\widetilde{y}_k - y_*\| + \mu_k \|y_k^e - y_*\| + \|w_k^*\|,$$

which proves part 1c).

Definition of $\widetilde{y}_k$, introduction of y_*, and the triangle inequality gives

$$\|y_k^* - y_*\| \le \frac{2}{\mu_k}\|c(x_k^*)\| + 2\|y_k^e - y_*\| + \|\widetilde{y}_k - y_*\|,$$

which proves part 1e).

Now part 4 is proved. Condition (4.6g), the triangle inequality, and part 1b) gives

$$\begin{aligned} 2\|w_k^*\| &= 2\|c(x_k^*) + \mu_k(y_k^* - y_k^e)\| \\ &\le 2\|c(x_k^*)\| + 2\mu_k\|y_k^* - y_*\| + 2\mu_k\|y_* - y_k^e\| \\ &\le \mu\|\widetilde{y}_k - y_*\| + 4\mu_k\|y_k^e - y_*\| + 3\mu_k\|y_k^* - y_*\|. \end{aligned}$$

This proves 4a). Applying the bound given in 1a) to 4a) gives 4b).

It remains to show part 5. To this end, assume that $c(x_*) = 0$. To show that (x_*, y_*, z_*) is a first-order KKT point, it remains to show that $\min(x_*, z_*) = 0$. From (4.6b)

$$\|\min(x_k^*, z_k^*)\|_\infty \le \omega_k.$$

Since $\{\omega_k\} \to 0$, the following holds

$$\lim_{k\in K} \|\min(x_k^*, z_k^*)\|_\infty \le \lim_{k\in K} \omega_k = 0,$$

which implies that $\lim_{k\in K} \|\min(x_k^*, z_k^*)\|_\infty = 0$. Continuity of norms and the fact that $\lim_{k\in K}(x_k^*, z_k^*) = (x_*, z_*)$ implies

$$\min(x_*, z_*) = 0.$$

This proves part 5. □

Note that these results were independent of the sequences $\{\mu_k\}$, $\{\gamma_k\}$, $\{\tau_k\}$, and $\{y_k^e\}$.

This result motivates the definition of Algorithm 4.2.1. Convergence to first-order points occurs provided the constraint violation is forced to zero. This is an explanation for the "*successful/unsuccessful*" terminology.

The following lemma shows that Algorithm 4.2.1 generates sequences $\{\gamma_k\}$ and $\{y_k^e\}$ such that $y_k^e \in [-\gamma_k e, \gamma_k e]$.

Lemma 4.3.2. *Algorithm* 4.2.1 *generates sequences* $\{\gamma_k\}$ *and* $\{y_k^e\}$ *such that* $y_k^e \in [-\gamma_k e, \gamma_k e]$ *for all* $k \geq 0$*.*

Proof. Inspection of Algorithm 4.2.1 reveals that $\gamma_k = \nu\mu_k^{-\alpha_\gamma}$ for all k, and that γ_0 is chosen to satisfy $y_0^e \in [\gamma_0 e, \gamma_0 e]$. The result is now established by induction. Suppose that the following holds for k:

$$\|y_k^e\|_\infty \leq \gamma_k = \nu\mu_k^{-\alpha_\gamma}.$$

If either $\|y_{k+1}^s\|_\infty \leq \gamma_{k+1}$ or $\|\widetilde{y}_k\|_\infty \leq \gamma_{k+1}$, then the result holds for $k+1$ by definition of y_{k+1}^e. Therefore assume that these cases do not hold, i.e., assume that $y_{k+1}^e = y_k^e$. The following two cases must be considered:

1. $\mu_{k+1} \leftarrow \mu_k$,

2. $\mu_{k+1} \leftarrow \mu_c\mu_k$.

For case 1, the following inequality suffices:

$$\|y_{k+1}^e\|_\infty = \|y_k^e\|_\infty \leq \gamma_k = \gamma_{k+1}. \tag{4.12}$$

For the second case, the following holds:

$$\|y_{k+1}^e\|_\infty = \|y_k^e\|_\infty \leq \gamma_k = \nu\mu_k^{-\alpha_\gamma} = \frac{\nu\mu_{k+1}^{-\alpha_\gamma}\mu_k^{-\alpha_\gamma}}{\mu_{k+1}^{-\alpha_\gamma}}.$$

Since $\mu_{k+1} = \mu_c \mu_k$, $\gamma_{k+1} = \nu \mu_{k+1}^{-\alpha_\gamma}$, $0 < \mu_c < 1$, and $0 < \alpha_\gamma$, it follows that

$$\|y_{k+1}^e\|_\infty \leq \gamma_{k+1} \frac{\mu_k^{-\alpha_\gamma}}{(\mu_c \mu_k)^{-\alpha_\gamma}} = \mu_c^{\alpha_\gamma} \gamma_{k+1} < \gamma_{k+1}. \tag{4.13}$$

Equations (4.12) and (4.13) give the desired result for each case. □

The following lemma provides information about a certain quantity associated with Algorithm 4.2.1 in the case that $\{\mu_k\} \to 0$.

Lemma 4.3.3. *Suppose that* $\{\mu_k\} \to 0$ *as Algorithm* 4.2.1 *is executed. Then the quantity* $\{\mu_k \gamma_k\} \to 0$.

Proof. Note that at every step $\gamma_k = \nu \mu_k^{-\alpha_\gamma}$. Since $\alpha_\gamma < 1$ and $\{\mu_k\} \to 0$, the following holds:

$$\{\mu_k \gamma_k\} = \{\mu_k \nu \mu_k^{-\alpha_\gamma}\} = \{\nu \mu_k^{1-\alpha_\gamma}\} \to 0.$$

□

Corollary 4.3.1. *Suppose that* $\{\mu_k\} \to 0$ *as Algorithm* 4.2.1 *is executed. Then the quantity* $\{\mu_k \|y_k^*\|\} \to 0$.

Proof. Since $y_k^* \in [-\gamma_k e, \gamma_k e]$ the following holds:

$$\mu_k \|y_k^*\| \leq \sqrt{m} \mu_k \|y_k^*\|_\infty \leq \sqrt{m} \mu_k \gamma_k.$$

The result is proved since Lemma 4.3.3 implies that the right-hand side goes to zero. □

The following is another immediate corollary to Lemma 4.3.3.

Corollary 4.3.2. *Suppose that* $\{\mu_k\} \to 0$ *as Algorithm* 4.2.1 *is executed. Then the quantity* $\{\mu_k \|y_k^e\|\} \to 0$.

Proof. Use of Lemma 4.3.2 gives

$$\mu_k \|y_k^e\| \leq \sqrt{m} \mu_k \|y_k^e\|_\infty \leq \sqrt{m} \mu_k \gamma_k. \tag{4.14}$$

The result is proved since Lemma 4.3.3 implies that the right-hand side goes to zero. □

The first convergence result for Algorithm 4.2.1 may now be stated. The following theorem shows that the subproblem solutions converge to a first-order KKT point.

Theorem 4.3.1 (Global Convergence of Subproblem Solutions). *Suppose assumptions* AS1a, AS2a *and* AS3 *hold. Let* $(x_k^*, y_k^*, z_k^*, w_k^*)$ *be the sequence of vectors produced by Algorithm* 4.2.1 *with tolerances* $\omega_* = \eta_* = 0$*. Then all parts of Lemma* 4.3.1 *hold, thus* (x_*, y_*, z_*) *as defined in Lemma* 4.3.1 *is a first-order KKT point.*

Proof. Algorithm 4.2.1 generates sequences $\{\mu_k\}$, $\{\tau_k\}$, and $\{\omega_k\}$ such that $\{\omega_k\} \to 0$. It also generates a sequence of positive numbers $\{\gamma_k\}$, vectors $\{y_k^e\}$ such that $y_k^e \in [-\gamma_k e, \gamma_k e]$ (see Lemma 4.3.2), and points $(x_k^*, y_k^*, z_k^*, w_k^*)$ satisfying (4.6) on page 87. Thus, properties 1–4 of Lemma 4.3.1 on page 88 hold.

It remains to show $c(x_*) = 0$. There are two cases to consider:

1. $\{\mu_k\}$ is bounded away from zero;
2. $\{\mu_k\} \to 0$.

Consider case 1. Since $\{\mu_k\}$ stays bounded away from zero, there exists an integer k_1 such that all iterations are *successful* from iteration k_1 onward. This implies that $\|c(x_k^*)\| \le \max(\eta_k, \eta_*) = \eta_k$ for all $k \ge k_1$. Since $\{\eta_k\} \to 0$, this implies that $\lim_{k\in K} \|c(x_k^*)\| = 0$. Continuity of $c(x)$ and of norms gives $c(x_*) = 0$ as desired.

Next consider case 2. Note that part 2 of Lemma 4.3.1 shows that $\lim_{k\in K} \widetilde{y}_k = y_*$. Part 1b) of Lemma 4.3.1 gives

$$2\|c(x_k^*)\| \le \mu_k \|\widetilde{y}_k - y_*\| + 2\mu_k \|y_k^e - y_*\| + \mu_k \|y_k^* - y_*\|$$

for all k. Use of Corollary 4.3.1, Corollary 4.3.2, and $\lim_{k\in K} \widetilde{y}_k = y_*$, implies that the ride-hand side goes to zero on K. Thus, $\{\|c(x_k^*)\|\}_K \to 0$. Continuity of $c(x)$ and $\|\cdot\|$ implies that $c(x_*) = 0$ as desired. □

The previous result is independent of tolerance τ_* and the choice of $\{\tau_k\}$. The choice of $\{\tau_k\}$ becomes important when considering convergence of the sequence $\{y_k^*\}$. The following lemma makes this precise.

Lemma 4.3.4. *Let the assumptions and tolerances from Theorem* 4.3.1 *hold. Additionally, assume that* AS2b *holds. Let* $\tau_* = 0$ *and let* $(x_k^*, y_k^*, z_k^*, w_k^*)$ *be the sequence of vectors produced by Algorithm* 4.2.1. *Then all parts of Lemma* 4.3.1 *hold, thus* (x_*, y_*, z_*) *as defined in Lemma* 4.3.1 *is a first-order KKT point. Moreover*

$$\lim_{k \in K} y_k^* = y_*.$$

Proof. Theorem 4.3.1 gives that (x_*, y_*, z_*) as defined in Lemma 4.3.1 is a first-order KKT point. It remains to show that $\lim_{k \in K} y_k^* = y_*$. First note that $\{\tau_k\} \to 0$ since $\{\omega_k\} \to 0$. Part 1d) of Lemma 4.3.1 says

$$\|y_k^* - y_*\| \leq \|\widetilde{y}_k - y_*\| + (2/\mu_k)\|w_k^*\| \tag{4.15}$$

for all $k \in K$. Since $\lim_{k \in K} \widetilde{y}_k = y_*$ by Theorem 4.3.1, it is sufficient to show $\lim_{k \in K}(1/\mu_k)\|w_k^*\| = 0$. Consider the two cases:

1. $\{\mu_k\}$ bounded away from zero,
2. $\{\mu_k\} \to 0$.

First consider case 1. Since $\{\mu_k\}$ is bounded away from zero, there exists an integer k_1 such that $\|y_k^*\|_\infty \leq \gamma_k - \tau_f$ for all $k \geq k_1$. Since $\{\tau_k\} \to 0$, condition (4.6d) implies that there exists a $k_2 \geq k_1$ such that $\|w_k^*\|_\infty \leq \tau_k$ for all $k \geq k_2$. Thus,

$$\|w_k^*\| \leq \sqrt{m}\|w_k^*\|_\infty \leq \sqrt{m}\,\tau_k.$$

Since $\{\tau_k\} \to 0$ this implies

$$\lim_k \|w_k^*\| = 0,$$

and since $\{\mu_k\}$ is bounded away from zero, it follows that

$$\lim_k \frac{1}{\mu_k}\|w_k^*\| = 0.$$

This completes case 1. In addition, since $\{\, c(x_k^*) \,\}_K \to 0$, $\{\mu_k\}$ is bounded away from zero, and $\{\, y_k^* \,\}_K \to y_*$, condition (4.6g) implies that $\{\, y_k^e \,\}_K \to y_*$.

Now consider case 2. First note that $\{\gamma_k\} \to \infty$ since $\{\mu_k\} \to 0$. Condition (4.6d) then implies that there exists an integer k_3 such that $\|w_k^*\|_\infty \le \tau_k$ for all $k \in K$ and $k \ge k_3$. This can be seen as follows. Define the set

$$S = \{\, k \in K : \|y_k^*\|_\infty \ge \gamma_k - \tau_f \,\}.$$

If S were infinite then there would exist a subsequence $K_S \subset K$ such that

$$\|y_k^*\|_\infty \ge \gamma_k - \tau_f \;\text{ for all } k \in K_S.$$

This implies that $\{\|y_k^*\|_\infty\} \to \infty$ on K_S since $\{\gamma_k\} \to \infty$ on K_S. This contradicts the assumed boundedness of $\{y_k^*\}_K$ and therefore S is finite. Thus, for all $k \in K$ sufficiently large, $\|y_k^*\|_\infty < \gamma_k - \tau_f$, i.e., the vector y_k^* is "τ_f free" from its bounds. Then condition (4.6d) implies that for $k \in K$ sufficiently large, $\|w_k^*\|_\infty \le \tau_k$. Hence,

$$\frac{1}{\mu_k}\|w_k^*\| \le \frac{1}{\mu_k}\sqrt{m}\,\|w_k^*\|_\infty \le \frac{1}{\mu_k}\sqrt{m}\,\tau_k \le k_\tau\sqrt{m}\,\mu_k^{\alpha_\tau - 1} \quad \text{for } k \in K \text{ sufficiently large.}$$

Since $\{\mu_k\} \to 0$ and $\alpha_\tau > 1$, it follows that

$$\lim_{k \in K} \frac{1}{\mu_k}\|w_k^*\| = 0,$$

and case 2 is proved. □

Note that in case 1, convergence of $\|w_k^*\|$ to zero was over *all* k not just $k \in K$.

4.4 Local Convergence

Since $(x, y, z, w) = (x^*, y^*, z^*, 0)$ is a minimizer for the primal-dual BCL subproblem (4.2) on page 78 for μ_k sufficiently small, $\gamma_k > \|y^*\|_\infty$, and with the choice $y_k^e = y^*$, it seems possible to bound the error in the subproblem solutions in terms of the error in y_k^e. The next result makes this precise. First, additional assumptions are stated.

(AS4a) Strict complementarity holds at the solution (x^*, y^*, z^*) under consideration, i.e., $\max(x^*, z^*) > 0$.

(AS4b) If (x^*, y^*, z^*) is a KKT point for problem GNPs, then the following matrix is nonsingular:

$$\begin{pmatrix} H^*_{FR,FR} & (J^*_{FR})^T \\ J^*_{FR} & 0 \end{pmatrix},$$

where $H^*_{FR,FR}$ represents the rows and columns of $H(x^*, y^*)$ corresponding to components of x^* that are free, and J^*_{FR} represents the columns of $J(x^*)$ corresponding to components of x^* that are free.

If the LICQ holds at x^* and the point (x^*, y^*) satisfied the standard second-order sufficient conditions of being a minimizer, then AS4b holds. This can be shown by using Corollary 1.5.1.

The following theorem is similar to Lemma 5.1 in [8].

Theorem 4.4.1. *Let the following assumptions hold:* AS1a, AS1b, AS2a, AS2b, AS3, AS4a, *and* AS4b. *Let K be a subsequence of integers such that $\{x_k^*\}_K \to x^*$, a KKT point for problem* GNPs *with associated Lagrange multiplier vector (y^*, z^*). Assume $\{y_k^e\}_K$ is any sequence of vectors and that $\{\mu_k\}$ is a sequence of positive scalars such that $\lim_{k\in K} \mu_k \|y_k^e - y^*\| = 0$ and $\lim_{k\in K} \mu_k \|y_k^* - y^*\| = 0$. Furthermore, assume that the sequence of vectors $(x_k^*, y_k^*, z_k^*, w_k^*)$ are solutions to the pdBCL subproblem* (4.6) *on page* 87 *with tolerances $\{\omega_k\} \to 0$ and $\{\tau_k\} \to 0$ such that $\tau_k \le \max(\mu_k\omega_k, k_\tau \mu_k^{\alpha_\tau})$ for constants $\alpha_\tau > 1$ and $k_\tau > 0$. Then there exist positive constants c_{11}, c_{12}, c_{13}, c_{14}, c_{15}, c_{16}, c_{17}, $\bar{\mu}$, $\bar{\omega}$ and a positive integer $\bar{k}$, such that*

1. $\|y_k^* - y^*\| \le c_{16}\omega_k + c_{14}\mu_k\|y_k^e - y^*\|$,
2. $\|x_k^* - x^*\| \le c_{15}\omega_k + c_{14}\mu_k\|y_k^e - y^*\|$,

3. $\|\widetilde{y}_k - y^*\| \le c_{13}\omega_k + c_{14}\mu_k\|y_k^e - y^*\|$,

4. $\|c(x_k^*)\| \le c_{17}\mu_k\omega_k + (\mu_k + c_{14}\mu_k^2)\|y_k^e - y^*\|$,

for all $k \ge \bar{k}$, $k \in K$, $\omega_k \le \bar{\omega}$, *and* $\mu_k \le \bar{\mu}$.

Proof. The assumptions are sufficient for the results of Lemma 4.3.1 to hold. Parts 2 and 3 of that theorem imply that $\{\widetilde{y}_k\}_K \to y_*$ and $\{z_k^*\}_K \to z_*$ for some y_* and z_*. Furthermore, under the given assumptions above, part 1b) of Lemma 4.3.1 shows that $\{\|c(x_k^*)\|\}_K \to 0$. Thus, $c(x^*) = 0$ and part 5 then implies that (x^*, y_*, z_*) is a KKT point. Therefore, $(x^*, y^*, z^*) = (x^*, y_*, z_*)$ since assumption AS3 guarantees a unique Lagrange multiplier vector. Since they are equal, reference will now only be made to (x^*, y^*, z^*). Let the integer $k_0 \in K$ be defined such that for all $k \in K$, $k \ge k_0$, the estimates in Lemma 4.3.1 hold.

A Taylor series expansion at x^* gives

$$c(x_k^*) = J(x^*)(x_k^* - x^*) + r_3, \tag{4.16}$$

where

$$\|r_3\| \le c_3\|x_k^* - x^*\|^2 \ \text{ for some constant } c_3. \tag{4.17}$$

Next, condition (4.6g) on page 87 and the Taylor-series expansion of g and J at x^* give

$$z_k^* = g(x^*) + H(x^*)(x_k^* - x^*) - J(x^*)^T\widetilde{y}_k - \Big(\sum H_i(x^*)[\widetilde{y}_k]_i\Big)(x_k^* - x^*) + r_1, \tag{4.18}$$

where

$$r_1 = r_1(x_k^*, x^*, \widetilde{y}_k) = \int_0^1 \Big(H\big(x^* + s(x_k^* - x^*), \widetilde{y}_k\big) - H(x^*, \widetilde{y}_k)\Big)(x_k^* - x^*)\, ds. \tag{4.19}$$

Boundedness and Lipschitz continuity of the Hessians of f and $\{c_i(x)\}$ in a neighborhood of x^* imply

$$\|r_1\| \le c_1\|x_k^* - x^*\|^2 \ \text{ for some positive constant } c_1. \tag{4.20}$$

By adding and subtracting the terms $J(x^*)^T y^*$ and $\sum H_i(x^*)y_i^*(x_k^* - x^*)$, equation (4.18) is equivalent to

$$z_k^* = g(x^*, y^*) + H(x^*, y^*)(x_k^* - x^*) + J(x^*)^T(y^* - \widetilde{y}_k) + r_1 + r_2, \tag{4.21}$$

where

$$r_2 = r_2(x_k^*, x^*, \widetilde{y}_k, y^*) = \sum_i H_i(x^*)\big([y^* - \widetilde{y}_k]_i\big)(x_k^* - x^*). \tag{4.22}$$

Norm inequalities imply

$$\|r_2\| \le c_2 \|x_k^* - x^*\| \|y^* - \widetilde{y}_k\| \text{ for some positive constant } c_2. \tag{4.23}$$

Equations (4.16) and (4.21) may be expressed in terms of one system:

$$\begin{pmatrix} H(x^*, y^*) & J(x^*)^T \\ J(x^*) & 0 \end{pmatrix} \begin{pmatrix} x_k^* - x^* \\ y^* - \widetilde{y}_k \end{pmatrix} = \begin{pmatrix} z_k^* - g(x^*, y^*) \\ c(x_k^*) \end{pmatrix} - \begin{pmatrix} r_1 + r_2 \\ r_3 \end{pmatrix}.$$

Partitioning the previous system according to the free and fixed components of x^* yields

$$\begin{pmatrix} H^*_{FR,FR} & H^*_{FR,FX} & (J^*_{FR})^T \\ H^*_{FX,FR} & H^*_{FX,FX} & (J^*_{FX})^T \\ J^*_{FR} & J^*_{FX} & 0 \end{pmatrix} \begin{pmatrix} [x_k^* - x^*]_{FR} \\ [x_k^* - x^*]_{FX} \\ y^* - \widetilde{y}_k \end{pmatrix} = \begin{pmatrix} [z_k^* - g(x^*, y^*)]_{FR} \\ [z_k^* - g(x^*, y^*)]_{FX} \\ c(x_k^*) \end{pmatrix} - \begin{pmatrix} [r_1 + r_2]_{FR} \\ [r_1 + r_2]_{FX} \\ r_3 \end{pmatrix},$$

where $H^* = H(x^*, y^*)$ and $J^* = J(x^*)$. Elimination of the second row, second column, and use of $[g(x^*, y^*)]_{FR} = 0$ leads to

$$\begin{pmatrix} H^*_{FR,FR} & (J^*_{FR})^T \\ J^*_{FR} & 0 \end{pmatrix} \begin{pmatrix} [x_k^* - x^*]_{FR} \\ y^* - \widetilde{y}_k \end{pmatrix} = \begin{pmatrix} [z_k^*]_{FR} - H^*_{FR,FX}[x_k^*]_{FX} \\ c(x_k^*) - J^*_{FX}[x_k^*]_{FX} \end{pmatrix} - \begin{pmatrix} [r_1 + r_2]_{FR} \\ r_3 \end{pmatrix}. \tag{4.24}$$

Define the matrix on the left-hand side of the previous equation as S, i.e.,

$$S = \begin{pmatrix} H^*_{FR,FR} & (J^*_{FR})^T \\ J^*_{FR} & 0 \end{pmatrix}.$$

Assumption AS4b implies that S is nonsingular and therefore the following definition is made:

$$M = \|S^{-1}\|. \tag{4.25}$$

Since $[x^*]_{FR} > 0$, condition (4.6b) on page 87 shows that there exists an integer k_1 such that

$$\|[z^*_k]_{FR}\|_\infty \le \omega_k \text{ for all } k \in K,\ k \ge k_1. \tag{4.26}$$

Also, since $[x^*]_{FX} = 0$, assumption AS4a and condition (4.6b) imply that there exists an integer k_2 such that

$$\|[x^*_k]_{FX}\|_\infty \le \omega_k \text{ for all } k \in K,\ k \ge k_2. \tag{4.27}$$

This further implies

$$\|x^*_k - x^*\| \le \|[x^*_k - x^*]_{FR}\| + \|[x^*_k - x^*]_{FX}\| \le \|[x^*_k - x^*]_{FR}\| + \sqrt{n}\,\omega_k, \tag{4.28}$$

for all $k \in K$, $k \ge k_2$. For convenience, the following notation is introduced:

$$\Delta x_{FR} \triangleq \|[x^*_k - x^*]_{FR}\|, \quad \Delta y \triangleq \|y^* - \widetilde{y}_k\|, \quad \Delta v \triangleq \left\| \begin{pmatrix} [x^*_k - x^*]_{FR} \\ y^* - \widetilde{y}_k \end{pmatrix} \right\|. \tag{4.29}$$

Using this notation, (4.17), (4.20), (4.23), and (4.28) imply

$$\left\| \begin{pmatrix} [r_1 + r_2]_{FR} \\ r_3 \end{pmatrix} \right\| \le c_5 \Delta x^2_{FR} + c_6 \omega_k^2 + c_2 \Delta x_{FR} \Delta y + c_7 \Delta x_{FR} \omega_k + c_8 \omega_k \Delta y \tag{4.30}$$

for all $k \in K$, $k \ge \max(k_0, k_2)$, where $c_5 = c_1 + c_3$, $c_6 = 2n$, $c_7 = 4\sqrt{n}$, and $c_8 = c_2\sqrt{n}$.

Similarly, part 1c) of Lemma 4.3.1, equation (4.26) and equation (4.27) yield

$$\left\| \begin{pmatrix} [z_k^*]_{FR} - H^*_{FR,FX}[x_k^*]_{FX} \\ c(x_k^*) - J^*_{FX}[x_k^*]_{FX} \end{pmatrix} \right\| \le c_9\omega_k + \mu_k\|\widetilde{y}_k - y^*\| + \mu_k\|y_k^e - y^*\| + \|w_k^*\| \quad (4.31)$$

for all $k \in K$, $k \ge \max(k_0, k_1, k_2)$, where

$$c_9 = \sqrt{n} + \sqrt{n}\left\| \begin{pmatrix} H^*_{FR,FX} \\ J^*_{FX} \end{pmatrix} \right\|. \quad (4.32)$$

Note that $\{\mu_k\} \to 0$ implies $\{\gamma_k\} \to \infty$. Therefore, assumption AS2b and condition (4.6d) imply the existence of $\bar{\mu}_1 > 0$ such that if $\mu_k < \bar{\mu}_1$ then $\|w_k^*\|_\infty \le \tau_k$. Since $\tau_k \le \omega_k$ by construction, this implies that $\|w_k^*\|_\infty \le \omega_k$. Use of this bound in equation (4.31) gives

$$\left\| \begin{pmatrix} [z_k^*]_{FR} - H^*_{FR,FX}[x_k^*]_{FX} \\ c(x_k^*) - J^*_{FX}[x_k^*]_{FX} \end{pmatrix} \right\| \le c_{10}\omega_k + \mu_k\|\widetilde{y}_k - y^*\| + \mu_k\|y_k^e - y^*\| \quad (4.33)$$

for all $k \in K$, $k \ge \max(k_0, k_1, k_2)$, and $\mu_k \le \bar{\mu}_1$, where $c_{10} = c_9 + \sqrt{m}$.

Since $\Delta x_{FR} \le \Delta v$ and $\Delta y \le \Delta v$, it follows from equations (4.24), (4.30), (4.33), definition of M, and norm inequalities that

$$\Delta v \le M\big(c_{11}\Delta v^2 + c_6\omega_k^2 + c_{12}\omega_k\Delta v + c_{10}\omega_k + \mu_k\Delta v + \mu_k\|y_k^e - y^*\|\big) \quad (4.34)$$

for all $k \in K$, $k \ge \max(k_0, k_1, k_2)$ and $\mu_k \le \bar{\mu}_1$, where $c_{11} = c_2 + c_5$ and $c_{12} = c_7 + c_8$. Define the following quantities:

$$\bar{\mu} = \min(\tfrac{1}{4}, \bar{\mu}_1) \quad \text{and} \quad \bar{\omega} = \min\left(1, \frac{1}{4Mc_{12}}\right). \quad (4.35)$$

Since $\{(x_k^*, \widetilde{y}_k\}_K \to (x^*, y^*)$, there exists an integer k_3 such that

$$\Delta v \le \frac{1}{4Mc_{11}} \text{ for all } k \in K,\ k \ge k_3. \quad (4.36)$$

Define $\bar{k} = \max(k_0, k_1, k_2, k_3)$ and then define

$$K^* = \{\, k \in K : k \ge \bar{k},\ \mu_k \le \bar{\mu}, \text{ and } \omega_k \le \bar{\omega} \,\}. \quad (4.37)$$

Using (4.34), (4.35), (4.36), and (4.37), it follows that

$$\Delta v \le \tfrac{1}{4}\Delta v + \tfrac{1}{4}\Delta v + \tfrac{1}{4}\Delta v + Mc_6\omega_k + Mc_{10}\omega_k + M\mu_k\|y_k^e - y^*\| \ \text{ for all } k \in K^*.$$

Grouping terms and simplifying gives

$$\Delta v \le c_{13}\omega_k + c_{14}\mu_k\|y_k^e - y^*\| \ \text{ for all } k \in K^*, \tag{4.38}$$

where $c_{13} = 4Mc_6 + 4Mc_{10}$ and $c_{14} = 4M$. This trivially implies

$$\|\widetilde{y}_k - y^*\| \le c_{13}\omega_k + c_{14}\mu_k\|y_k^e - y^*\| \ \text{ for all } k \in K^*, \tag{4.39}$$

which proves part 3. Use of (4.28) and (4.38) gives

$$\|x_k^* - x^*\| \le c_{15}\omega_k + c_{14}\mu_k\|y_k^e - y^*\| \ \text{ for all } k \in K^*, \tag{4.40}$$

where $c_{15} = \sqrt{n} + c_{13}$. This proves part 2. Part 1 is now proved. First note that the update to τ_k ensures the following:

$$\frac{1}{\mu_k}\|w_k^*\| \le \frac{\sqrt{m}}{\mu_k}\|w_k^*\|_\infty \le \frac{\sqrt{m}}{\mu_k}\tau_k \le \sqrt{m}\,\omega_k \quad \text{if } \mu_k \le \bar{\mu}_1.$$

This inequality, part 1d) of Lemma 4.3.1 and part 3 of this theorem imply

$$\|y_k^* - y^*\| \le c_{16}\omega_k + c_{14}\mu_k\|y_k^e - y^*\| \ \text{ for all } k \in K^*, \tag{4.41}$$

where $c_{16} = c_{13} + 2\sqrt{m}$. This proves part 1. Finally, part 1b) of Lemma 4.3.1 and parts 1 and 3 of this theorem imply

$$\|c(x_k^*)\| \le c_{17}\mu_k\omega_k + (\mu_k + c_{14}\mu_k^2)\|y_k^e - y^*\| \ \text{ for all } k \in K^*, \tag{4.42}$$

where $c_{17} = \frac{1}{2}(c_{13} + c_{16})$. This proves part 4. □

The next corollary gives a condition for an "arbitrary" Lagrange multiplier vector estimate that guarantees convergence of the estimate. It is similar to Corollary 5.2 in [8].

Corollary 4.4.1. *Suppose that the same conditions as those in Theorem* 4.4.1 *hold and that y^s_{k+1} is any Lagrange multiplier estimate for which*

$$\|y^s_{k+1} - y^*\| \le c_{18}\omega_k + c_{19}\|x^*_k - x^*\| \tag{4.43}$$

for positive constants c_{18} and c_{19} and for all $k \in K$ sufficiently large. Then there exist positive constants c_{13}, c_{14}, c_{15}, c_{16}, c_{17}, c_{18}, c_{20}, c_{21}, $\widehat{\mu}$, $\widehat{\omega}$, and $\widehat{k}$ such that the following hold

$$\|y^*_k - y^*\| \le c_{16}\omega_k + c_{14}\mu_k\|y^e_k - y^*\|, \tag{4.44a}$$

$$\|x^*_k - x^*\| \le c_{15}\omega_k + c_{14}\mu_k\|y^e_k - y^*\|, \tag{4.44b}$$

$$\|\widetilde{y}_k - y^*\| \le c_{13}\omega_k + c_{14}\mu_k\|y^e_k - y^*\|, \tag{4.44c}$$

$$2\|c(x^*_k)\| \le c_{17}\mu_k\omega_k + (2\mu_k + c_{14}\mu_k^2)\|y^e_k - y^*\|, \tag{4.44d}$$

$$\|y^s_{k+1} - y^*\| \le c_{20}\omega_k + c_{21}\mu_k\|y^e_k - y^*\|, \tag{4.44e}$$

for all $k \in K$, $k \ge \widehat{k}$, $\omega_k \le \widehat{\omega}$, and $\mu_k \le \widehat{\mu}$, and where $c_{20} = c_{18} + c_{15}c_{19}$ and $c_{21} = c_{14}c_{19}$.

Proof. Equations (4.44a), (4.44b), (4.44c), (4.44d) and definitions of $\bar{\mu}$, $\bar{\omega}$, and $\bar{k}$ follow from Theorem 4.4.1. By assumption, there must exist $\widehat{k} \ge \bar{k}$ such that (4.43) holds for all $k \in K$ and $k \ge \widehat{k}$. Define $\widehat{\omega} = \bar{\omega}$ and $\widehat{\mu} = \bar{\mu}$. Then equation (4.44e) follows by applying the bound given by (4.44b) to inequality (4.43). □

It is now shown that under certain assumptions, the penalty parameter μ_k is bounded away from zero. This is an important result because the subproblems become more difficult to solve as μ_k decreases to zero. Ideally, μ_k should be as large as possible to ensure well-conditioned subproblems, but small enough to ensure convergence and the correct inertia of $\nabla^2\mathcal{M}$. The next theorem is similar to Theorem 5.3 in [8] with a nearly identical proof.

Theorem 4.4.2. *Suppose that the iterates $\{x^*_k\}$ of Algorithm* 4.2.1 *converge to the* single *limit point x^*. Let assumptions* AS1a, AS1b*,* AS2a*,* AS2b*,* AS3*,* AS4a*, and*

AS4b *hold. Let* α_η *and* β_η *satisfy*

$$\alpha_\eta < \min(1, \alpha_\omega), \tag{4.45}$$

$$\beta_\eta < \min(1, \beta_\omega), \tag{4.46}$$

and suppose (4.43) *holds for all* k *sufficiently large. Then there is a positive constant* μ *such that* $\mu_k \geq \mu$ *for all* k.

Proof. The proof given by Conn, Gould, and Toint for Theorem 5.3 in [8] is by contradiction. They assume that $\{\mu_k\} \to 0$ and this implies that infinitely many "unsuccessful" steps were performed. This does not follow immediately in Algorithm 4.2.1 since $\{\mu_k\}$ may decrease during "successful" *and* "unsuccessful" iterations. However, assume that infinitely many "successful" iterations decrease μ_k. This implies $\|y_k^*\|_\infty > \gamma_k - \tau_f$ on a subsequence of the natural numbers. Since $\{\gamma_k\} \to \infty$, this implies that $\{\|y_k^*\|_\infty\} \to \infty$ on the same subsequence. This contradicts assumption AS2b and hence, only finitely many "successful" iterations decrease μ_k. Since $\{\mu_k\} \to 0$ by assumption, it must be the case that infinitely many "unsuccessful" iterations occurred (the same statement as in [8]).

The remainder of the proof is identical. □

The final result of this section shows that Algorithm 4.2.1 is at least R-linearly convergent. The result is analogous to Theorem 5.5 in [8].

Theorem 4.4.3. *Under the assumptions given in Theorem* 4.4.2*, the iterates* x_k^**,* y_k^**,* $\widetilde{y}_k$ *and any* y_k^s *satisfying inequality* (4.43) *are at least R-linearly convergent with R-factor at most* $\widehat{\mu}^{\min(\beta_\omega, \beta_\eta)}$*, where* $\widehat{\mu}$ *is the smallest value of the penalty parameter generated by Algorithm* 4.2.1.

Proof. Theorem 4.4.2 shows that $\{\mu_k\}$ is bounded away from zero and therefore there exists a number $\widehat{\mu}$ such that for k sufficiently large $\mu_k \equiv \widehat{\mu}$. Consider only these values of k for the rest of the proof. Examination of Algorithm 4.2.1 implies

$$\omega_{k+1} = \omega_k \widehat{\mu}^{\beta_\omega}, \quad \eta_{k+1} = \eta_k \widehat{\mu}^{\beta_\eta}, \quad \|c(x_k^*)\| \leq \eta_k. \tag{4.47}$$

This allows the following bound to be used in equation (4.31) on page 101:

$$\left\| \begin{pmatrix} [z_k^*]_{FR} - H^*_{FR,FX}[x_k^*]_{FX} \\ c(x_k^*) - J^*_{FX}[x_k^*]_{FX} \end{pmatrix} \right\| \le c_9\omega_k + \eta_k. \tag{4.48}$$

This leads to the following bound on Δv:

$$\Delta v \le M\big(c_9\omega_k + c_6\omega_k^2 + \eta_k + (c_2 + c_5)\Delta v^2 + (c_7 + c_8)\omega_k\Delta v\big). \tag{4.49}$$

Pick k sufficiently large that

$$\Delta v \le \frac{1}{3M(c_2 + c_5)} \quad \text{and} \quad \omega_k \le \min\left(1, \frac{1}{3M(c_7 + c_8)}\right). \tag{4.50}$$

It follows that

$$\Delta v \le c_{22}\omega_k + 3\eta_k \tag{4.51}$$

where $c_{22} = 3c_6 + 3c_9$. It immediately follows that

$$\|\widetilde{y}_k - y^*\| \le c_{22}\omega_k + 3\eta_k \quad \text{and} \quad \|[x_k^* - x^*]_{FR}\| \le c_{22}\omega_k + 3\eta_k. \tag{4.52}$$

Next, equation (4.28) on page 100 and equation (4.52) imply

$$\|x_k^* - x^*\| \le c_{23}\omega_k + 3\eta_k \tag{4.53}$$

where $c_{23} = \sqrt{n} + c_{22}$.

As in Theorem 4.4.1, it may be shown that

$$\frac{1}{\mu_k}\|w_k^*\| \le \sqrt{m}\,\omega_k.$$

This fact, equation (4.52) and part 1d) of Lemma 4.3.1, imply

$$\|y_k^* - y^*\| \le c_{24}\omega_k + 3\eta_k \tag{4.54}$$

where $c_{24} = c_{22} + 2\sqrt{m}$.

Finally, equation (4.43) and (4.53) imply

$$\|y_{k+1}^s - y^*\| \le c_{25}\omega_k + c_{26}\eta_k \tag{4.55}$$

where $c_{25} = c_{18} + c_{22} + \sqrt{n}$ and $c_{26} = 3c_{19}$.

Inequality (4.47) and equations (4.52), (4.53), (4.54), and (4.55) complete the proof. □

4.5 Infeasible Problems

Not every optimization problem is well-defined. It is possible that the user of an optimization routine may formulate a set of nonlinear constraints $c(x) = 0$ for which no non-negative solution to $c(x) = 0$ exists. Detecting this situation is difficult and is equivalent to showing that the *global* minimum of

$$\begin{aligned} &\underset{x\in\mathbb{R}^n}{\text{minimize}} \quad \tfrac{1}{2}\|c(x\|^2 \\ &\text{subject to } \ x \geq 0 \end{aligned} \tag{4.56}$$

is strictly positive. This is a very difficult problem. It is of interest to study the behavior of the primal-dual BCL algorithm in this situation. The next theorem shows that when Algorithm 4.2.1 is applied to an infeasible problem, the subproblem solutions converge to a first-order KKT point of problem (4.56). A point (x, z) is a first-order KKT point for problem (4.56) if it satisfies

$$J(x)^T c(x) = z, \tag{4.57a}$$

$$\min(x, z) = 0. \tag{4.57b}$$

Theorem 4.5.1. *Assume* AS1a *and* AS2a *hold. Suppose* GNPs *is infeasible and that Algorithm* 4.2.1 *is applied with tolerances* $\omega_* = \eta_* = 0$. *Let* $\lim_{k\in K} x_k^* = x_*$. *Then* (x_*, z_*) *is a first-order KKT point for problem* (4.56), *where* $z_* \triangleq J(x_*)^T c(x_*)$.

Proof. Condition (4.6a) on page 87 implies $x_k^* \geq 0$ for all k, and since $\lim_{k\in K} x_k^* = x_*$ it follows that

$$x_* \geq 0. \tag{4.58}$$

Since problem GNPs is infeasible, there exists an $\eta > 0$ such that if $x \geq 0$ then $\|c(x)\| > \eta$. Since $\{\eta_k\} \to 0$ as $k \to \infty$, there exists an integer k_2 such that $\|c(x_k^*)\| > \eta_k$ for all $k \geq k_2$. In other words, from iteration k_2 onward, all iterates are "*unsuccessful*" and that $\{\mu_k\} \to 0$.

Condition (4.6g) implies

$$g(x_k^*) - J(x_k^*)^T(2y_k^e - \frac{2}{\mu_k}c(x_k^*) - y_k^*) = z_k^*.$$

Multiplication by μ_k and use of condition (4.6b) shows

$$2J(x_k^*)^T c(x_k^*) \geq \underbrace{-\mu_k \omega_k e}_{(a)} - \underbrace{\mu_k g(x_k^*)}_{(b)} + \underbrace{\mu_k J(x_k^*)^T(2y_k^e - y_k^*)}_{(c)}. \tag{4.59}$$

Term (a) goes to zero since $\{\mu_k\} \to 0$ and $\{\omega_k\} \to 0$. Term (b) goes to zero on K because $\{\mu_k\} \to 0$ and $\{\, g(x_k^*)\,\}_K \to g(x_*)$. Term (c) goes to zero on K by Corollary 4.3.1 and Corollary 4.3.2. Therefore, assumption AS1a and convergence of $\{x_k^*\}_K \to x_*$ imply

$$z_* = J(x_*)^T c(x_*) = \lim_{k \in K} J(x_k^*)^T c(x_k^*) \geq 0. \tag{4.60}$$

It remains to show that $[z_*]_{\mathcal{I}} = 0$. Since $\lim_{k\in K} x_k^* = x_*$ and $[x_*]_{\mathcal{I}} > 0$, it is the case that $[x_k^*]_{\mathcal{I}} > 0$ for $k \in K$ sufficiently large. Condition (4.6b) and the fact that $\{\omega_k\} \to 0$ implies

$$\min([x_k^*]_{\mathcal{I}}, [z_k^*]_{\mathcal{I}}) = [z_k^*]_{\mathcal{I}} \text{ for all } k \in K \text{ sufficiently large.}$$

This implies

$$\begin{aligned} \|[z_k^*]_{\mathcal{I}}\| \leq \|\min(x_k^*, z_k^*)\| &= \Big(\sum_{j=1}^{n} \min([x_k^*]_j, [z_k^*]_j)^2\Big)^{\frac{1}{2}} \\ &\leq \Big(\sum_{j=1}^{n} \omega_k^2\Big)^{\frac{1}{2}} = \sqrt{n}\omega_k \text{ for all } k \in K \text{ sufficiently large.} \end{aligned}$$

Condition (4.6f) and the definition of $\widetilde{y}_k$ imply

$$\begin{aligned} \sqrt{n}\omega_k &\geq \|[z_k^*]_{\mathcal{I}}\| \\ &= \|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T(2\pi_k(x_k^*) - y_k^*)\| \\ &= \|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T\widetilde{y}_k\| \text{ for all } k \in K \text{ sufficiently large.} \end{aligned}$$

Definition of $\widetilde{y}_k$ and rearrangement gives

$$\|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T(2y_k^e - \frac{2}{\mu_k}c(x_k^*) - y_k^*)\| \leq \sqrt{n}\,\omega_k \text{ for all } k \in K \text{ sufficiently large.}$$

Use of the "reverse" triangle inequality followed by the classical triangle inequality gives

$$\begin{aligned}\|2\widehat{J}(x_k^*)^T c(x_k^*)\| &\leq \sqrt{n}\mu_k\omega_k + \mu_k\|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T(2y_k^e - y_k^*)\| \\ &\leq \underbrace{\sqrt{n}\mu_k\omega_k}_{(a)} + \underbrace{\mu_k\|\hat{g}(x_k^*)\|}_{(b)} + \underbrace{\mu_k\|\widehat{J}(x_k^*)^T(2y_k^e - y_k^*)\|}_{(c)}.\end{aligned}$$

Terms (a) and (b) go to zero on K since $\{\mu_k\} \to 0$, $\{\omega_k\} \to 0$ and $\{\hat{g}(x_k^*)\}_K \to \hat{g}(x_*)$. Since $\{\widehat{J}(x_k^*)\}_K \to \widehat{J}(x_*)$, Corollaries 4.3.1 and 4.3.2 imply that term (c) goes to zero on K. Combining this with assumption AS1a yields

$$[z_*]_{\mathcal{I}} = \widehat{J}(x_*)^T c(x_*) = \lim_{k\in K} \widehat{J}(x_k^*)^T c(x_k^*) = 0. \tag{4.61}$$

Equations (4.58), (4.60), and (4.61) complete the proof. □

Note that this theorem made no mention of the tolerance τ_* or the sequence $\{\tau_k\}$.

4.6 Existence of Subproblem Solutions

This section shows the existence and uniqueness of subproblem solutions in a neighborhood of a solution to GNPs under certain assumptions. Furthermore, it is shown that the subproblem solutions eventually identify the optimal active set.

The following additional assumption is used.

(AS5.) The following second-order sufficient condition holds at a solution (x^*, y^*, z^*) to problem GNPs: there exists a positive ω such that

$$p^T H(x^*, y^*)p \geq \omega\|p\|^2 \tag{4.62}$$

for all $p \neq 0$ such that $p_{FX} = 0$ and $J(x^*)p = 0$.

The next lemma is required for the proof of the main result of this section.

Lemma 4.6.1. *Assume* AS4a *and* AS5 *hold at a solution* (x^*, y^*, z^*) *of problem* GNPs. *Then there exists a positive* $\bar{\mu}$ *such that for all* $0 < \mu \leq \bar{\mu}$ *the following matrix is nonsingular*

$$S \triangleq \begin{pmatrix} H(x^*, y^*) + \frac{2}{\mu} J(x^*)^T J(x^*) & J(x^*)^T & -I \\ J(x^*) & \mu I & 0 \\ Z^* & 0 & X^* \end{pmatrix}. \tag{4.63}$$

Note that assumption AS3 *is not needed.*

Proof. By using the nonsingular transformation

$$N = \begin{pmatrix} I & -\frac{2}{\mu} J(x^*)^T & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix},$$

it is sufficient to prove that $S_1 \triangleq NS$ is nonsingular. Multiplication of S by N gives

$$S_1 = \begin{pmatrix} H(x^*, y^*) & -J(x^*)^T & -I \\ J(x^*) & \mu I & 0 \\ Z^* & 0 & X^* \end{pmatrix}.$$

Define $H^* = H(x^*, y^*)$ and $J^* = J(x^*)$. Let $p = (p_1, p_2, p_3)$ be a vector in the null space of S_1. Partitioning S_1 according to free and fixed variables leads to

$$\begin{pmatrix} H^*_{FR,FR} & H^*_{FR,FX} & -{J^*_{FR}}^T & -I_{FR,FR} & 0 \\ H^*_{FX,FR} & H^*_{FX,FX} & -{J^*_{FX}}^T & 0 & -I_{FX,FX} \\ J^*_{FR} & J^*_{FX} & \mu I & 0 & 0 \\ Z^*_{FR} & 0 & 0 & X^*_{FR} & 0 \\ 0 & Z^*_{FX} & 0 & 0 & X^*_{FX} \end{pmatrix} \begin{pmatrix} [p_1]_{FR} \\ [p_1]_{FX} \\ p_2 \\ [p_3]_{FR} \\ [p_3]_{FX} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

The fixed components of x satisfy $x^*_{FX} = 0$ and assumption AS4a implies $z^*_{FR} = 0$. Thus,

$$\begin{pmatrix} H^*_{FR,FR} & H^*_{FR,FX} & -J^{*\,T}_{FR} & -I_{FR,FR} & 0 \\ H^*_{FX,FR} & H^*_{FX,FX} & -J^{*\,T}_{FX} & 0 & -I_{FX,FX} \\ J^*_{FR} & J^*_{FX} & \mu I & 0 & 0 \\ 0 & 0 & 0 & X^*_{FR} & 0 \\ 0 & Z^*_{FX} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} [p_1]_{FR} \\ [p_1]_{FX} \\ p_2 \\ [p_3]_{FR} \\ [p_3]_{FX} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{4.64}$$

Since $x^*_{FR} > 0$, the fourth row of equations implies $[p_3]_{FR} = 0$. Since assumption AS4a implies $z^*_{FX} > 0$, the fifth row of equations implies $[p_1]_{FX} = 0$. System (4.64) simplifies to

$$\begin{pmatrix} H^*_{FR,FR} & -J^{*\,T}_{FR} & 0 \\ H^*_{FX,FR} & -J^{*\,T}_{FX} & -I_{FX,FX} \\ J^*_{FR} & \mu I & 0 \end{pmatrix} \begin{pmatrix} [p_1]_{FR} \\ p_2 \\ [p_3]_{FX} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \tag{4.65}$$

Therefore, $[p_1]_{FR}$ and p_2 satisfy

$$\begin{pmatrix} H^*_{FR,FR} & J^{*\,T}_{FR} \\ J^*_{FR} & -\mu I \end{pmatrix} \begin{pmatrix} [p_1]_{FR} \\ -p_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Assumption AS5, Debreu's Lemma 1.5.1, and Lemma 1.5.3 guarantee the existence of $\bar{\mu} > 0$ such that this matrix is nonsingular for $0 < \mu \leq \bar{\mu}$. For these values of μ, $[p_1]_{FR} = 0$ and $p_2 = 0$. Finally, (4.65) implies $[p_3]_{FX} = 0$ and the proof is complete. □

The following theorem shows the existence and uniqueness of subproblem solutions. It also shows that the subproblem solutions will eventually identify the optimal active set. This is important since identification of the optimal active set, in essence, converts the *inequality* constrained problem into an *equality* constrained problem.

Theorem 4.6.1. *Suppose that assumptions* AS4a *and* AS5 *hold at a solution* (x^*, y^*, z^*) *of problem* GNPs. *Then there exists* $\bar{\mu} > 0$ *such that for any* μ *fixed* *satisfying* $0 < \mu < \bar{\mu}$, *there exists an open neighborhood* $\mathcal{T}$ *of* y^* *and continuously differentiable functions* $\big(x(y_e), y(y_e), z(y_e)\big)$ *defined on* $\mathcal{T}$ *such that*

$$x(y_e) \to x^*, \quad y(y_e) \to y^*, \quad z(y_e) \to z^*. \tag{4.66}$$

Moreover, if $\gamma > \|y^*\|_\infty$ *then* $\big(x(y_e), y(y_e), z(y_e), 0\big)$ *is a* minimizer *to*

$$\begin{aligned} &\underset{x,y}{\text{minimize}} \quad \mathcal{M}(x, y; y_e, \mu) \\ &\text{subject to } -\gamma e \le y \le \gamma e, \quad x \ge 0. \end{aligned} \tag{4.67}$$

The vector $z(y_e)$ *is the Lagrange multiplier vector for* $x \ge 0$ *and the* m*-vector* 0 *is the Lagrange multiplier vector for* $-\gamma e \le y \le \gamma e$*. Also, the active set of* $x(y_e)$ *agrees with the active set at* x^**.*

Proof. An argument similar to that used in Theorem 3.3.2 gives the existence of a positive $\bar{\mu}$ such that $(x^*, y^*, z^*, w^*) = (x^*, y^*, z^*, 0)$ satisfies the second-order sufficient conditions for problem (4.67) for all $0 < \mu < \bar{\mu}$, with the choice $y_e = y^*$ and assuming that $\|y^*\|_\infty < \gamma$. Choose any μ satisfying this inequality. With this choice, the following holds

$$\nabla^2 \mathcal{M}(x^*, y^*; y^*, \mu)_{FR,FR} > 0, \tag{4.68}$$

i.e., the reduced Hessian of the primal-dual merit function is positive definite at (x^*, y^*) and with the choice $y_e = y^*$. The vector z^* is the multiplier vector for $x \ge 0$ and w^* is the multiplier vector for $-\gamma e \le y \le \gamma e$.

Define the function

$$F(x, y, z; y_e) = \begin{pmatrix} g(x) - J(x)^T\big(2y_e - \frac{2}{\mu}c(x) - y\big) - z \\ c(x) + \mu(y - y_e) \\ ZXe \end{pmatrix} \tag{4.69}$$

with derivative

$$F'(x, y, z; y_e) = \begin{pmatrix} H(x, 2\pi(x) - y) + \frac{2}{\mu}J(x)^T J(x) & J(x)^T & -I \\ J(x) & \mu I & 0 \\ Z & 0 & X \end{pmatrix}. \tag{4.70}$$

Evaluation at (x^*, y^*, z^*) for $y_e = y^*$ gives $F(x^*, y^*, z^*; y^*) = 0$ and

$$F'(x^*, y^*, z^*; y^*) = \begin{pmatrix} H(x^*, y^*) + \frac{2}{\mu} J(x^*)^T J(x^*) & J(x^*)^T & -I \\ J(x^*) & \mu I & 0 \\ Z^* & 0 & X^* \end{pmatrix}, \tag{4.71}$$

which is nonsingular by Lemma 4.6.1. The Implicit Function Theorem implies the existence of an open neighborhood $\mathcal{T}_1$ of y^*, and unique continuously differentiable functions $\big(x(y_e), y(y_e), z(y_e)\big)$ satisfying

1. $\big(x(y^*), y(y^*), z(y^*)\big) = (x^*, y^*, z^*)$,
2. $F\big(x(y_e), y(y_e), z(y_e)\big) = 0$,

for all y_e in $\mathcal{T}_1$. This means that $\big(x(y_e), y(y_e), z(y_e)\big)$ satisfies the *equality* optimality conditions for problem (4.67) (ignoring the bounds on the y-variables). Next, by possibly shrinking $\mathcal{T}_1$, there exists an open neighborhood $\mathcal{T}_2$ of y^* such that the following hold for all $y_e \in \mathcal{T}_2$:

a. if $[x^*]_i > 0$, then $[x(y_e)]_i > 0$,

b. if $[z^*]_i > 0$, then $[z(y_e)]_i > 0$,

c. $\|y(y_e)\|_\infty < \gamma$.

Use of 2 above shows that if $[x(y_e)]_i > 0$ then $[z(y_e)]_i = 0$. Also, if $x_i^* = 0$, then assumption AS4a implies $z_i^* > 0$. Part b above then implies that $[z(y_e)]_i > 0$, which part 2 above then implies $[x(y_e)]_i = 0$. Thus, the following hold for all $y_e \in \mathcal{T}_2$:

- $\big(x(y_e), y(y_e), z(y_e), 0\big)$ satisfies the first-order optimality conditions for problem (4.67),
- Strict complementarity holds at $\big(x(y_e), y(y_e), z(y_e), 0\big)$,
- The active set at $x(y_e)$ is identical to the active set at x^*,

- The vector $y(y_e)$ is free from its bounds.

It is only left to show that $\big(x(y_e), y(y_e), z(y_e), 0\big)$ satisfies the *second-order* sufficient conditions. Since $\big(x(y_e), y(y_e), z(y_e), 0\big) \to (x^*, y^*, z^*, 0)$ as $y_e \to y^*$, statement (4.68) implies that there exists an open neighborhood $\mathcal{T}$ of y_e (possibly smaller than $\mathcal{T}_2$) such that

$$\nabla^2 \mathcal{M}\big(x(y_e), y(y_e); y_e, \mu\big)_{FR,FR} > 0$$

for all $y_e \in \mathcal{T}$. Therefore, $\big(x(y_e), y(y_e), z(y_e), 0\big)$ is a *minimizer* for problem (4.67). This completes the proof. □

4.7 Second-Order Points

The proposed primal-dual BCL method requires solving subproblem (4.2) on page 78 at every iteration. Solutions to these subproblems satisfy the conditions given by (4.6) on page 87. These are first-order conditions and, therefore, only convergence to *first-order* points can be proved. It is reasonable to believe that if certain second-order conditions are enforced at each subproblem solution, then convergence to points satisfying certain second-order conditions may follow. To this end, the following definition and additional assumption are used.

Definition 4.7.1 (Second-order sufficiency)**.** *The first-order KKT point* (x^*, y^*, z^*) *satisfies the second-order sufficiency conditions for problem* GNPs *if it satisfies strict complementarity (see* AS4a*) and if*

$$p^T H(x^*, y^*) p > 0$$

for all $p \neq 0$ *such that* $p_{FX} = 0$ *and* $J(x^*)p = 0$*.*

(AS6). Let $(x_k^*, y_k^*, z_k^*, w_k^*)$ be a sequence of solutions to subproblem (4.2), and let $\{x_k^*\}_K \to x^*$. For all $k \in K$ large enough let the following conditions hold for some positive constants δ_1 and δ_2 independent of k:

a. (Strict Complementarity)

$$\max(x_k^*, z_k^*) > \delta_1 e, \tag{4.72}$$

$$\max(\gamma_k e - y_k^*, |w_k^*|) \geq \delta_2 e, \tag{4.73}$$

$$\max(\gamma_k e + y_k^*, |w_k^*|) \geq \delta_2 e \tag{4.74}$$

b. (Second-order condition)

$$\Delta v^T \nabla^2 \mathcal{M}(x_k^*, y_k^*; y_k^e, \mu_k) \Delta v \geq \delta_1 \|\Delta v\|^2,$$

for all $\Delta v \neq 0$ such that $\Delta x_{FX} = 0$ and where $\Delta v = (\Delta x,\ \Delta y)^T$.

Certain methods that use second-derivatives may be able to guarantee that

$$\Delta v^T \nabla^2 \mathcal{M}(x_k^*, y_k^*; y_k^e, \mu_k) \Delta v \geq 0 \tag{4.75}$$

for all $\Delta v \neq 0$ such that $\Delta v_{FX} = 0$ (see e.g., [6]). Thus, part b of AS6 is a stronger condition than (4.75). Part b implies that for $k \in K$ sufficiently large, the sequence of minimum eigenvalues of the reduced Hessian of the primal-dual augmented Lagrangian is positive and bounded away from zero.

Theorem 4.7.1. *Assume* AS3 *holds. Let* $(x_k^*, y_k^*, z_k^*, w_k^*)$ *be a sequence satisfying* AS6. *Let* $\lim_{k \in K} x_k^* = x^*$, *and let*

$$(x^*, y^*, z^*) = \lim_{k \in K} (x_k^*, \widetilde{y}_k, z_k^*)$$

be a first-order KKT point of problem GNPs. *Then* (x^*, y^*, z^*) *satisfies the second-order sufficient conditions given by Definition* 4.7.1.

Proof. Assumption AS6 gives $\max(x_k^*, z_k^*) > \delta_1 e$. Taking limits shows $\max(x^*, z^*) \geq \delta_1 e > 0$ so that (x^*, z^*) satisfies strict complementarity. Conditions (4.73) and (4.74) imply that y_k^* is "uniformly free" from its bound for all $k \in K$ sufficiently large. This implies that the y-variables also satisfy strict complementarity and that the optimal active-set is identified for $k \in K$ sufficiently large.

Let $\Delta\bar{x} \neq 0$ such that $\Delta\bar{x}_{FX} = 0$ and $J(x^*)\Delta\bar{x} = 0$. Assumption AS3 implies that for $k \in K$ sufficiently large, $J(x_k^*)$ has full row rank. Continuity of null space basis' for a full row rank matrix (see [16]) implies that for $k \in K$ sufficiently large there exist vectors $\Delta v_k = (\Delta x_k, \Delta y_k)^T$ such that $\Delta y_k = 0$, $[\Delta x_k]_{FX} = 0$, $J_{FR}(x_k^*)[\Delta x_k]_{FR} = 0$, and $\{\Delta v_k\}_{k\in K} \to (\Delta\bar{x}, 0)^T$. With this choice, part b of AS6 implies

$$\delta_1 \|[\Delta x_k]_{FR}\|^2 = \delta_1 \|\Delta v_k\|^2 \tag{4.76}$$

$$\leq \Delta v_k \nabla^2 \mathcal{M}(x_k^*, y_k^*; y_k^e, \mu_k)\Delta v_k \tag{4.77}$$

$$= [\Delta x_k]_{FR}^T \big(H_{FR,FR}(x_k^*, \widetilde{y}_k) + \frac{2}{\mu_k} J_{FR}(x_k^*)^T J_{FR}(x_k^*)\big)[\Delta x_k]_{FR} \tag{4.78}$$

$$= [\Delta x_k]_{FR}^T H_{FR,FR}(x_k^*, \widetilde{y}_k)[\Delta x_k]_{FR}. \tag{4.79}$$

Taking limits on $k \in K$ implies

$$\Delta\bar{x}_{FR}^T H_{FR,FR}(x^*, y^*)\Delta\bar{x}_{FR} \geq \delta_1 \|\Delta\bar{x}_{FR}\|^2, \tag{4.80}$$

which implies

$$\Delta\bar{x}^T H(x^*, y^*)\Delta\bar{x} \geq \delta_1 \|\Delta\bar{x}\|^2 > 0. \tag{4.81}$$

Thus, (x^*, y^*, z^*) satisfies the second-order sufficient conditions given by Definition 4.7.1. □

4.8 Higher-Order Updates

Algorithm 4.2.1 contains a step for computing the vector (x_{k+1}^s, y_{k+1}^s). This vector is intended to increase the rate of convergence of $\{y_k^e\} \to y^*$. This section discusses options available for updating y_k^e that may lead to faster convergence than both the first-order primal-dual multiplier estimate $\widetilde{y}_k$, and the least-squares multiplier estimate $\widehat{y}(x_k^*)$.

4.8.1 A second-order update

This subsection considers three derivations of the same second-order update to y_k^e. Although, the update to y_k^e is the same, the different derivations supply different auxiliary vectors that may be used to update the x and/or y-variables. These derivations will be described in the context of problem NEP. Obvious modifications may be used for problem GNPs.

Problem NEP

The first derivation is analogous to that of Bertsekas' in [1]. Key to this analysis is the following dual functional

$$d_\mu(y_e) = \mathcal{M}\big(x(y_e), y(y_e); y_e, \mu\big), \tag{4.82}$$

where $\big(x(y_e), y(y_e)\big)$ is the minimizer of the primal-dual augmented Lagrangian function for a given value of y_e. Tacitly, it is assumed that these minimizers exist and that everything is local to a solution of problem NEP. It will be shown that (x^*, y^*) is a *maximizer* of $d_\mu(y^*)$ for μ sufficiently small. Consider the gradient of $d_\mu(y_e)$, which is given by

$$\begin{aligned}\nabla d_\mu(y_e) = x'(y_e)^T\Big(\big(x(y_e)\big) - J\big(x(y_e)\big)^T\Big(2\pi\big(x(y_e)\big) - y(y_e)\Big)\Big) \\ + y'(y_e)^T\Big(c\big(x(y_e)\big) + \mu\big(y(y_e) - y_e\big)\Big) \\ - c\big(x(y_e)\big) - \Big(c\big(x(y_e)\big) + \mu\big(y(y_e) - y_e\big)\Big).\end{aligned}$$

Since $\big(x(y_e), y(y_e)\big)$ is a minimizer of the primal-dual augmented Lagrangian, it satisfies

$$g\big(x(y_e)\big) - J\big(x(y_e)\big)^T\big(2\pi\big(x(y_e)\big) - y\big(y_e\big)\big) = 0 \text{ and} \tag{4.83}$$

$$c\big(x(y_e)\big) + \mu\big(y(y_e) - y_e\big) = 0. \tag{4.84}$$

This implies that

$$\nabla d_\mu(y_e) = -c\big(x(y_e)\big).$$

Evaluation at $y_e = y^*$ gives

$$\nabla d_\mu(y^*) = -c(x^*) = 0,$$

which implies that $y_e = y^*$ is a stationary point of d_μ.

Now it is shown that y^* is a *maximizer* of d_μ. Differentiation of ∇d_μ gives

$$\nabla^2 d_\mu(y_e) = -J\big(x(y_e)\big)x'(y_e). \tag{4.85}$$

Differentiation of (4.83) and (4.84) shows that $x'(y_e)$ satisfies the following system

$$\begin{pmatrix} H\big(x(y_e),y(y_e)\big) + \frac{2}{\mu}J\big(x(y_e)\big)^T J\big(x(y_e)\big) & J\big(x(y_e)\big)^T \\ J\big(x(y_e)\big) & \mu I \end{pmatrix} \begin{pmatrix} x'(y_e) \\ y'(y_e) \end{pmatrix} = \begin{pmatrix} 2J\big(x(y_e)\big)^T \\ \mu I \end{pmatrix}$$

Block elimination of this system gives

$$x'(y_e) = \Big(H\big(x(y_e),y(y_e)\big) + \frac{1}{\mu}J\big(x(y_e)\big)^T J\big(x(y_e)\big)\Big)^{-1} J\big(x(y_e)\big)^T.$$

Equation (4.85) may then be written as

$$\nabla^2 d_\mu(y_e) = -J\big(x(y_e)\big)\Big(H\big(x(y_e),y(y_e)\big) + \frac{1}{\mu}J\big(x(y_e)\big)^T J\big(x(y_e)\big)\Big)^{-1} J\big(x(y_e)\big)^T.$$

Evaluation at $y_e = y^*$ gives

$$\nabla^2 d_\mu(y^*) = -J(x^*)\Big(H(x^*,y^*) + \frac{1}{\mu}J(x^*)^T J(x^*)\Big)^{-1} J(x^*)^T.$$

Under the second-order sufficiency assumption AS5, Debreu's Lemma 1.5.1 guarantees the existence of $\bar{\mu} > 0$ such that $H(x^*,y^*) + \frac{1}{\mu}J(x^*)^T J(x^*)$ is positive definite for all $0 < \mu \le \bar{\mu}$. Thus, for these values of μ the matrix $d_\mu(y^*)$ is *negative* definite. Thus, $d_\mu(y_e)$ is *maximized* at $y_e = y^*$.

An obvious choice for updating y_e is to performing one step of Newton's method for *maximizing* $d_\mu(y_e)$. The relevant Newton system is given by

$$\Big(J\big(x(y_e)\big)\Big(H\big(x(y_e),y(y_e)\big) + \frac{1}{\mu}J\big(x(y_e)\big)^T J\big(x(y_e)\big)\Big)^{-1} J\big(x(y_e)\big)^T\Big)\Delta y_e = -c\big(x(y_e)\big). \tag{4.86}$$

Thus, the update to y_e is given by

$$y_e \leftarrow y_e + \Delta y_e, \tag{4.87}$$

where Δy_e is the solution of (4.86).

This previous description offers a plausible update to y_e, but suffers from two drawbacks. First, although an update to y_e is made, no improvement (update) in the x-variables and y-variables is achieved. Secondly, the update is clear when *exact* minimization is used, i.e., when points on the trajectory are calculated exactly, however, it becomes less clear what system should be solved when only approximate solutions are found. The following derivation of the same update to y_e partly remedies both deficiencies.

Consider applying Newton's method to

$$F_1(x, y) = \begin{pmatrix} g(x) - J(x)^T\big(y - \frac{1}{\mu}c(x)\big) \\ c(x) \end{pmatrix}.$$

The second component of F_1 is a feasibility requirement, while the first component is a stationarity requirement of the classical augmented Lagrangian function. The derivative of F_1 is given by

$$F_1'(x, y) = \begin{pmatrix} H\big(x, y - \frac{1}{\mu}c(x)\big) + \frac{1}{\mu}J(x)^TJ(x) & -J(x)^T \\ J(x) & 0 \end{pmatrix},$$

Newton's equations are

$$\begin{pmatrix} H\big(x, y - \frac{1}{\mu}c(x)\big) + \frac{1}{\mu}J(x)^TJ(x) & -J(x)^T \\ J(x) & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y_e \end{pmatrix} = -\begin{pmatrix} g(x) - J(x)^T\big(y - \frac{1}{\mu}c(x)\big) \\ c(x) \end{pmatrix}. \tag{4.88}$$

Evaluation at the point $(x, y) = \big(x(y_e), y_e\big)$, where $x(y_e)$ is the point on the classical trajectory associated with a fixed μ, gives

$$\begin{pmatrix} H + \frac{1}{\mu}J^TJ & -J^T \\ J & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y_e \end{pmatrix} = -\begin{pmatrix} g - J^T(y_e - \frac{1}{\mu}c) \\ c \end{pmatrix},$$

where $J = J\big(x(y_e)\big)$, $c = c\big(x(y_e)\big)$, $g = g\big(x(y_e)\big)$, and $H = H\left(x(y_e), y_e - \frac{1}{\mu}c\big(x(y_e)\big)\right)$. Block elimination gives the solution as

$$\Delta y_e = \Big(J(H + \frac{1}{\mu}J^TJ)^{-1}J^T\Big)^{-1}\Big(-c + J\Big(H + \frac{1}{\mu}J^TJ\Big)^{-1}\Big(g - J^T(y_e - \frac{1}{\mu}c)\Big)\Big),$$
$$\Delta x = (H + \frac{1}{\mu}J^TJ)^{-1}\Big(J^T\Delta y - \Big(g - J^T(y_e - \frac{1}{\mu}c)\Big)\Big).$$

Since $g - J^T(y_e - \frac{1}{\mu}c) = 0$ on the trajectory, the above equations simplify to

$$\Delta y_e = -\Big(J(H + \frac{1}{\mu}J^TJ)^{-1}J^T\Big)^{-1}c \ \text{ and} \tag{4.89}$$

$$\Delta x = (H + \frac{1}{\mu}J^TJ)^{-1}J^T\Delta y. \tag{4.90}$$

Comparison of (4.86) and (4.89) shows that the updates to y_e are identical. Equation (4.90) gives the additional vector Δx which is a sensible update in the x-variables. Also note that system (4.88) can be solved for any $(x, y) \approx \big(x(y_e), y_e\big)$.

The previous discussion partly remedies the deficiencies of the first derivation. However, it may be considered unnatural since the primal-dual augmented Lagrangian function is minimized to generate points near the trajectory, but yet stationary conditions of the classical augmented Lagrangian function is used in the definition of F_1. Also, the primal-dual augmented Lagrangian function is minimized over x *and* y, but no update to y is made. The following derivation may be considered more natural and does offer an update to the y-variables. Consider applying Newton's method for zero-finding to

$$F_2(x, y, y_e) = \begin{pmatrix} g(x) - J(x)^T\big(2\pi(x) - y\big) \\ c(x) + \mu(y - y_e) \\ c(x) \end{pmatrix}. \tag{4.91}$$

The derivative of F_2 with respect to (x, y, y_e) is

$$F_2'(x, y, y_e) = \begin{pmatrix} \bar{H} + \frac{2}{\mu}J(x)^TJ(x) & J(x)^T & -2J(x)^T \\ J(x) & \mu I & -\mu I \\ J(x) & 0 & 0 \end{pmatrix},$$

where $\bar{H} = H\big(x, 2\pi(x) - y\big)$. The Newton equations are

$$\begin{pmatrix} \bar{H} + \frac{2}{\mu}J(x)^TJ(x) & J(x)^T & -2J(x)^T \\ J(x) & \mu I & -\mu I \\ J(x) & 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \\ \Delta y_e \end{pmatrix} = - \begin{pmatrix} g(x) - J(x)^T\big(2\pi(x) - y\big) \\ c(x) + \mu(y - y_e) \\ c(x) \end{pmatrix}.$$

For convenience, define $\Delta v = (\Delta x, \Delta y, \Delta y_e)$. Also define the following nonsingular matrix

$$N = \begin{pmatrix} I & -\frac{1}{\mu}J(x)^T & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix}$$

and consider the following equivalent system:

$$NF_2'(x, y, y_e)N^T\Delta\bar{v} = -NF_2(x, y, y_e),$$

where

$$\Delta\bar{v} = N^{-T}\Delta v = \begin{pmatrix} \Delta x \\ \Delta y + \frac{1}{\mu}J(x)\Delta x \\ \Delta y_e \end{pmatrix} \triangleq \begin{pmatrix} \Delta\bar{x} \\ \Delta\bar{y} \\ \Delta\bar{y}_e \end{pmatrix}. \tag{4.92}$$

Multiplication yields the following system

$$\begin{pmatrix} \bar{H} + \frac{1}{\mu}J(x)^TJ(x) & 0 & -J(x)^T \\ 0 & \mu I & -\mu I \\ J & 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta\bar{x} \\ \Delta\bar{y} \\ \Delta\bar{y}_e \end{pmatrix} = - \begin{pmatrix} g(x) - J(x)^T\big(y_e - \frac{1}{\mu}c(x)\big) \\ c(x) + \mu(y - y_e) \\ c(x) \end{pmatrix}. \tag{4.93}$$

Block elimination gives the solution as

$$\begin{aligned} \Delta\bar{y}_e &= \Big(J(\bar{H} + \frac{1}{\mu}J^TJ)^{-1}J^T\Big)^{-1}\Big(-c + J\big(\bar{H} + \frac{1}{\mu}J^TJ\big)^{-1}\big(g - J^T(y_e - \frac{1}{\mu}c)\big)\Big), \\ \Delta\bar{x} &= (\bar{H} + \frac{1}{\mu}J^TJ)^{-1}\Big(J^T\Delta\bar{y}_e - \big(g - J^T(y - \frac{1}{\mu}c)\big)\Big), \\ \Delta\bar{y} &= \Delta\bar{y}_e - \frac{1}{\mu}\big(c + \mu(y - y_e)\big), \end{aligned}$$

where $J = J(x)$, $c = c(x)$, and $g = g(x)$. The solution Δv now follows from equation (4.92):

$$\Delta y_e = \Big(J(\bar{H} + \frac{1}{\mu}J^TJ)^{-1}J^T\Big)^{-1}\Big(-c + J\big(\bar{H} + \frac{1}{\mu}J^TJ\big)^{-1}\big(g - J^T(y_e - \frac{1}{\mu}c)\big)\Big), \tag{4.94}$$

$$\Delta x = (\bar{H} + \frac{1}{\mu}J^TJ)^{-1}\Big(J^T\Delta y_e - \big(g - J^T(y_e - \frac{1}{\mu}c)\big)\Big), \tag{4.95}$$

$$\Delta y = \Delta y_e + y_e - y. \tag{4.96}$$

Note that on the trajectory, equations (4.89), (4.90), (4.94), and (4.95) show that Δy_e and Δx are identical for both derivations. Also, equation (4.96) implies that $y + \Delta y = y_e + \Delta y_e$. Therefore, $y_e + \Delta y_e$ is a good update for both y_e *and* y.

Three additional points should be made:

1. When not on the trajectory, system (4.93) is the appropriate system to be solved. Therefore, this updating method is appropriate when *approximate* subproblem minimizers are found.

2. System (4.93) is $(n + 2m)$ by $(n + 2m)$. However, it may be solved by first solving an $(n + m)$ by $(n + m)$ system for $(\Delta x, \Delta y_e)$ followed by the use of (4.96) to define Δy.

3. This derivation seems more natural since it is based on applying Newton's method to a function containing quantities pertinent to the *primal-dual augmented Lagrangian*; this is in contrast to the previous discussion which made use of stationarity conditions associated with the classical augmented Lagrangian.

4.8.2 A trajectory-following update

The following updating scheme focuses on the properties of the trajectory of minimizers. It is based on the fact that the first Newton direction generated by the primal-dual augmented Lagrangian function following a decrease in the penalty parameter is a good direction. For more details see Chapter 3.

Problem NEP

Consider problem NEP For simplicity assume that an *exact* subproblem solution $\big(x(\mu), y(\mu), \widetilde{y}(\mu)\big)$ has been found for a given value of the penalty parameter μ. The point $\big(x(\mu), y(\mu), \widetilde{y}(\mu)\big)$ satisfies the following set of equations:

$$g\big(x(\mu)\big) - J\big(x(\mu)\big)^T \widetilde{y}(\mu) = 0, \tag{4.97a}$$

$$c\big(x(\mu)\big) + \mu\big(y(\mu) - y_e\big) = 0, \tag{4.97b}$$

$$c\big(x(\mu)\big) + \tfrac{1}{2}\mu\big(\widetilde{y}(\mu) - y_e\big) + \tfrac{1}{2}\mu\big(y(\mu) - y_e\big) = 0. \tag{4.97c}$$

Consider minimization of the primal-dual augmented Lagrangian for a smaller value of the penalty parameter, say $\bar{\mu}$. A solution $\big(x(\bar{\mu}), y(\bar{\mu}), \widetilde{y}(\bar{\mu})\big)$ to this problem satisfies the following equations

$$\begin{aligned} g(x) - J(x)^T \widetilde{y} &= 0, \\ c(x) + \bar{\mu}(y - y_e) &= 0, \\ c(x) + \tfrac{1}{2}\bar{\mu}(\widetilde{y} - y_e) + \tfrac{1}{2}\bar{\mu}(y - y_e) &= 0. \end{aligned}$$

Defining $(x_\mu, y_\mu, \widetilde{y}_\mu) = \big(x(\mu), y(\mu), \widetilde{y}(\mu)\big)$ and writing Newton's equations linearized at $(x, y, \widetilde{y}) = (x_\mu, y_\mu, \widetilde{y}_\mu)$ yields

$$\begin{pmatrix} H(x_\mu, \widetilde{y}_\mu) & -J_\mu^T & 0 \\ J_\mu & 0 & \bar{\mu} I \\ J_\mu & \frac{\bar{\mu}}{2} I & \frac{\bar{\mu}}{2} I \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta \widetilde{y} \\ \Delta y \end{pmatrix} = - \begin{pmatrix} g_\mu - J_\mu^T \widetilde{y}_\mu \\ c_\mu + \bar{\mu}(y_\mu - y_e) \\ c_\mu + \frac{1}{2}\bar{\mu}(\widetilde{y}_\mu - y_e) + \frac{1}{2}\bar{\mu}(y_\mu - y_e) \end{pmatrix}, \tag{4.98}$$

where $c_\mu = c\big(x(\mu)\big)$, $g_\mu = g\big(x(\mu)\big)$, and $J_\mu = J\big(x(\mu)\big)$. This shows that the choice of $\bar{\mu}$ is important. If $\bar{\mu}$ is chosen to small, the right-hand side may not be close to zero and one step of classical Newton's Method will most likely not be productive. In fact, equation (4.97b) shows that the right-hand side is equivalent to

$$= -\begin{pmatrix} 0 \\ (\bar{\mu} - \mu)(y_\mu - y_e) \\ (\bar{\mu} - \mu)(y_\mu - y_e) \end{pmatrix}. \tag{4.99}$$

To expect progress, $\bar{\mu}$ should be chosen to ensure that $(\bar{\mu} - \mu)(y_\mu - y_e)$ is "small". One choice is the following:

$$\bar{\mu} = \left(\frac{\|y_\mu - y_e\|}{1 + \|y_\mu - y_e\|} \right)^\alpha \mu, \quad \text{for } \alpha > 0. \tag{4.100}$$

Note that if $\|y_\mu - y_e\|$ is large then $\bar{\mu} \approx \mu$, and if $\|y_\mu - y_e\| \approx 0$, then $\bar{\mu} \approx 0$.

Once $\bar{\mu}$ has been chosen, system (4.98) must be solved. Multiplying the second block of equations by -1, adding it to the third block of equations, and then replacing the third block, followed by symmetrization yields

$$\begin{pmatrix} H(x_\mu, \widetilde{y}_\mu) & J_\mu^T & 0 \\ J_\mu & 0 & \bar{\mu} I \\ 0 & -\frac{\bar{\mu}}{2} I & -\frac{\bar{\mu}}{2} I \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta \widetilde{y} \\ \Delta y \end{pmatrix} = -\begin{pmatrix} g_\mu - J_\mu^T \widetilde{y}_\mu \\ c_\mu + \bar{\mu}(y_\mu - y_e) \\ \frac{\bar{\mu}}{2}(\widetilde{y}_\mu - y_\mu) \end{pmatrix}. \tag{4.101}$$

Block elimination gives

$$\begin{pmatrix} H(x_\mu, \widetilde{y}_\mu) & J_\mu^T \\ J_\mu & -\bar{\mu} I \end{pmatrix} \begin{pmatrix} \Delta x \\ -\Delta \widetilde{y} \end{pmatrix} = -\begin{pmatrix} g_\mu - J_\mu^T \widetilde{y}_\mu \\ c_\mu + \bar{\mu}(\widetilde{y}_\mu - y_e) \end{pmatrix}, \quad \text{and} \tag{4.102}$$

$$\Delta y = \widetilde{y}_\mu + \Delta \widetilde{y} - y_\mu. \tag{4.103}$$

Two points should be noted. First, Δy may be defined by equation (4.103) once $\Delta \widetilde{y}$ is computed from equation (4.102). Second, the updated value of the y-vector is equivalent to the updated value of the $\widetilde{y}$-vector, i.e., $y_\mu + \Delta y = \widetilde{y}_\mu + \Delta \widetilde{y}$.

5

A Primal-Dual ℓ_1- Linearly Constrained Lagrangian (LCL) Method

5.1 Background

In this chapter we consider algorithms based on solving a sequence of linearly constrained subproblems. As in previous chapters, the underlying constrained problem will be written in the form:

$$\text{GNPs} \qquad \underset{x\in\mathbb{R}^n}{\text{minimize}} \quad f(x) \qquad \text{subject to} \quad c(x)=0, \quad x\geq 0, \tag{5.1}$$

where $c:\mathbb{R}^n \to \mathbb{R}^m$ and $f:\mathbb{R}^n \to \mathbb{R}$. Let $\mathcal{L}_{\mathcal{A}}(x;y_e,\mu)$ denote the function

$$\mathcal{L}_{\mathcal{A}}(x;y_e,\rho) = f(x) - c(x)^T y_e + \tfrac{1}{2}\rho\|c(x)\|^2,$$

which is the standard augmented Lagrangian function with $\mu = 1/\rho$. If $\bar{c}_k(x) = c(x_k) + J(x_k)(x-x_k)$ denotes the linearization of the general constraint vector $c(x)$ at the point x_k, then problem GNPs may be solved as a sequence of linearly constrained Lagrangian (LCL) subproblems of the form

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} & \mathcal{L}_{\mathcal{A}}(x; y_k^e, \rho_k) \\ \text{subject to} & \bar{c}_k(x) = 0, \quad x \geq 0, \end{array} \tag{5.2}$$

where y_k^e is an estimate of the Lagrange multiplier vector. This LCL method is the basis for the nonlinear optimization package MINOS of Murtagh and Saunders [21, 22].

Algorithm 5.1.1. Basic LCL Algorithm
INPUT: (x_0, y_0^e, z_0)
Set $\rho_0 = \bar{\rho} \geq 0$;
$k \leftarrow 0$;
converged ← **false**;
while not *converged* **do**
  Find a solution $(x_k^*, \Delta y_k^*, z_k^*)$ of the subproblem:

$$\underset{x\in\mathbb{R}^n}{\text{minimize}} \;\; \mathcal{L}_{\mathcal{A}}(x; y_k^e, \rho_k) \quad \text{subject to} \;\; \bar{c}_k(x) = 0, \quad x \geq 0.$$

  $x_{k+1} \leftarrow x_k^*; \quad y_{k+1}^e \leftarrow y_k^e + \Delta y_k^*; \quad z_{k+1} \leftarrow z_k^*;$
  Set *converged*; $\rho_{k+1} \leftarrow \bar{\rho}$;
  $k \leftarrow k + 1$;
end do
OUTPUT: $(x^*, y^*, z^*) \leftarrow (x_k, y_k^e, z_k)$

For details of the convergence criteria, see the MINOS User's Guide [23].

The basic LCL method of Algorithm 5.1.1 has two major deficiencies. First, the constraints $\bar{c}_k(x) = 0$ and $x \geq 0$ may be infeasible, in which case the subproblem has no solution. Second, the distance from the point of linearization to the subproblem solution may be arbitrarily large, i.e., the quantity $\|x_k^* - x_k\|$ may be arbitrarily large. These problems are addressed by Friedlander and Saunders [13], who regularize the standard LCL subproblem by introducing an ℓ_1 penalty term of the linearized constraint violations. The analogous approach for the primal-dual augmented Lagrangian function gives the so-called *elastic subproblem*:

$$\begin{array}{ll} \underset{x,u,v}{\text{minimize}} & \mathcal{L}_{\mathcal{A}}(x; y_k^e, \rho_k) + \sigma_k e^T(u+v) \\ \text{subject to} & \bar{c}_k(x) + u - v = 0, \quad x, u, v \geq 0. \end{array} \tag{5.3}$$

It is well known that the objective term $\sigma_k e^T(u+v)$ and elastic constraints $\bar{c}_k(x) + u - v = 0$, $u \geq 0$, and $v \geq 0$ of problem (5.3) define an alternative formulation of the ℓ_1 penalization of the linearized constraints. In particular, problem (5.6) is equivalent to

$$\begin{array}{ll} \underset{x,u,v}{\text{minimize}} & \mathcal{L}_{\mathcal{A}}(x; y_k^e, \rho_k) + \sigma_k \|\bar{c}_k(x)\|_1 \\ \text{subject to} & x \geq 0. \end{array} \tag{5.4}$$

In [13], Friedlander and Saunders observe that this subproblem unifies the BCL and the LCL approaches. If $\sigma_k \equiv 0$, then subproblem (5.4) is equivalent to the primal BCL subproblem. BCL methods are known to be globally convergent, but the *rate* of convergence is only R-linear unless a higher-order updating scheme is used for the multipliers y_k^e. Therefore, it is desirable to solve the LCL subproblem (5.2) near a solution since it will be shown that this recovers the R-quadratic convergence established by Robinson [25] for the basic LCL Algorithm 5.1.1 with $\bar{\rho} = 0$. The ℓ_1 penalty function is exact, which implies that if the linearization $\bar{c}_k(x) = 0$ is feasible and σ_k is sufficiently large, then u_k^* and v_k^* are likely to be zero and the minimizers of subproblem (5.4) will coincide with the minimizers of subproblem (5.2).

The discussion of this chapter loosely follows that of Friedlander and Saunders in [13]. The main difference is that here we consider the use of the primal-dual augmented Lagrangian rather than the standard primal augmented Lagrangian. In addition, since the objective function of the primal-dual variant of the subproblem (5.3) is a function of both the primal and dual variables, explicit bounds may be imposed on the dual variables.

5.2 A Primal-Dual Approach

The analogous LCL approach for the primal-dual augmented Lagrangian function involves the function

$$\mathcal{M}(x, y; y_e, \rho) = f(x) - c(x)^T y_e + \tfrac{1}{2}\rho\|c(x)\|^2 + \tfrac{1}{2}\rho\|c(x) + (y - y_e)/\rho\|^2,$$

which is identical to the primal-dual augmented Lagrangian function (3.2a) of page 41, with $\mu = 1/\rho$. As in the primal LCL method, Problem GNPs may be solved as a sequence of linearly constrained subproblems. In the primal-dual case we define the subproblem

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} & \mathcal{M}(x, y; y_k^e, \rho_k) \\ \text{subject to} & \bar{c}_k(x) = 0, \\ & x \ge 0, \quad -\gamma_k e \le y \le \gamma_k e, \end{array} \tag{5.5}$$

where γ_k is a positive constant and y_k^e is an estimate of the Lagrange multiplier vector. The associated *elastic subproblem* is

$$\begin{array}{ll} \underset{x,y,u,v}{\text{minimize}} & \mathcal{M}(x, y; y_k^e, \rho_k) + \sigma_k e^T(u + v) \\ \text{subject to} & \bar{c}_k(x) + u - v = 0, \\ & x, u, v \ge 0, \quad -\gamma_k e \le y \le \gamma_k e. \end{array} \tag{5.6}$$

Let z_k denote the reduced-cost vector for $x \ge 0$, and w_k the reduced-cost vector for $-\gamma_k e \le y \le \gamma_k e$. Similarly, let Δy_k denote the Lagrange multiplier vector for the elastic linearized constraint $\bar{c}_k(x) + u - v = 0$. The point (x_k^*, y_k^*, u_k^*, v_k^*, Δy_k^*, z_k^*,

$w_k^*)$ is regarded as an approximate solution of the subproblem (5.6) if it satisfies

$$x_k^* \geq 0, \tag{5.7a}$$

$$\| \min(x_k^*, z_k^*)\|_\infty \leq \omega_k, \tag{5.7b}$$

$$-\gamma_k e \leq y_k^* \leq \gamma_k e, \tag{5.7c}$$

$$\| \min(\gamma_k e - y_k^*, y_k^* + \gamma_k e, |w_k^*|)\|_\infty \leq \tau_k, \tag{5.7d}$$

$$\text{If } [\gamma_k e - y_k^*]_j \leq \tau_k, \text{ then } [w_k^*]_j \leq \tau_k, \tag{5.7e}$$

$$\text{If } [y_k^* + \gamma_k e]_j \leq \tau_k, \text{ then } [w_k^*]_j \geq -\tau_k, \tag{5.7f}$$

$$\begin{pmatrix} \nabla \mathcal{M}_x(x_k^*, y_k^*; y_k^e, \rho_k) - J(x_k)^T \Delta y_k^* \\ \nabla \mathcal{M}_y(x_k^*, y_k^*; y_k^e, \rho_k) \end{pmatrix} = \begin{pmatrix} z_k^* \\ w_k^* \end{pmatrix}, \tag{5.7g}$$

$$\bar{c}_k(x_k^*) + u_k^* - v_k^* = 0, \tag{5.7h}$$

$$\| \min(u_k^*, \, \sigma_k e - \Delta y_k^*)\|_\infty \leq \omega_k, \tag{5.7i}$$

$$\| \min(v_k^*, \, \sigma_k e + \Delta y_k^*)\|_\infty \leq \omega_k. \tag{5.7j}$$

Note that the inequalities (5.7i) and (5.7j) imply that

$$\|\Delta y_k^*\|_\infty \leq \sigma_k + \omega_k. \tag{5.8}$$

Note that the following analysis carries over to the more realistic setting where each constraint is given its own penalty parameter.

The chapter is organized as follows. Section 5.3 introduces necessary notation, terminology and assumptions. Section 5.4 supplies the statement of a primal-dual ℓ_1-LCL algorithm. Section 5.5 shows that the algorithm is globally convergent, while Sections 5.6–5.8 discuss finite termination and asymptotic equivalence to the classical LCL algorithm given by Robinson in [25]. Section 5.9 concerns the second-order properties of solutions when certain second-order properties are satisfied by the subproblem solutions. Section 5.10 considers local convergence properties. In particular, it is shown that the primal-dual ℓ_1-LCL algorithm inherits the fast convergence properties of Robinson's method (see [25]). Finally, Section 5.11 considers the properties of limit points generated by the the primal-dual ℓ_1 algorithm when applied to an *infeasible* problem.

5.3 Notation

The following definition of a first-order KKT for problem GNPs is an alternate, but equivalent, version of Definition 2.1.10 on page 27.

Definition 5.3.1. *A point* (x, y, z) *is a first-order Karush-Kuhn-Tucker (KKT) point for problem* GNPs (5.1) *if it satisfies the following conditions:*

$$c(x) = 0, \tag{5.9a}$$

$$g(x) - J(x)^T y = z, \tag{5.9b}$$

$$\min(x, z) = 0. \tag{5.9c}$$

The vector y is the Lagrange multiplier vector for the nonlinear constraint $c(x) = 0$. The nonnegative vector z is the reduced-cost (i.e., Lagrange multiplier) vector for the nonnegativity constraint $x \geq 0$. Condition (5.9c) is a concise statement of conditions (ii), (iv), and (v) in Definition 2.1.10.

Given primal and dual convergence tolerances η_* and ω_*, the point (x, y, z) will be regarded as an acceptable solution to problem GNPs if it satisfies the following criteria:

$$\|c(x)\| \leq \eta_*, \tag{5.10a}$$

$$g(x) - J(x)^T y = z, \tag{5.10b}$$

$$\|\min(x, z)\|_\infty \leq \omega_*. \tag{5.10c}$$

Given a point $x \geq 0$, the index set $\mathcal{I}(x) = \{\, j \in 1\!:\!n \mid [x]_j > 0 \,\}$ associated with the inactive bounds at x will occur frequently in the analysis. Given this definition, additional notation is listed below. (The list also summarizes notation introduced in previous sections).

- (x^*, y^*, z^*) is an optimal solution of problem GNPs.
- (x_k, y_k, z_k), is the kth estimate of (x^*, y^*, z^*).
- $(x_k^*,\ y_k^*,\ u_k^*,\ v_k^*,\ \Delta y_k^*,\ z_k^*,\ w_k^*)$ denotes an approximate solution of the kth subproblem.
- x_* is a limit point of $\{x_k^*\}$.
- $g(x)$ is the gradient of $f(x)$ evaluated at x.
- $J(x)$ is the $m \times n$ Jacobian of $c(x)$ evaluated at x.
- $\hat{g}(x) = [g(x)]_{\mathcal{I}}$ is the vector of components of $g(x)$ corresponding to indices in $\mathcal{I}(x_*)$.
- $\widehat{J}(x)$ is the matrix of columns of $J(x)$ with indices in $\mathcal{I}(x_*)$.
- $\mathcal{M}_k(x, y) = \mathcal{M}(x, y; y_k^e, \rho_k)$ is the kth primal-dual augmented Lagrangian evaluated at (x, y).
- $L(x, y) = f(x) - c(x)^T y$ is the Lagrangian evaluated at (x, y).
- $H(x, y)$ is the Hessian of the Lagrangian with respect to x evaluated at (x, y).
- $\pi(x; y_e, \rho) = y_e - \rho c(x)$ is the *primal first-order estimate* of y^*.
- $\pi_k = \pi(x_k^*; y_k^e, \rho_k)$ is the kth primal first-order estimate of y^*.
- $\widetilde{y}(x, y, \Delta y; y_e, \rho) = 2\pi(x; y_e, \rho) - y + \Delta y$ is the *primal-dual second-order estimate* of y^*.
- $\widetilde{y}_k = \widetilde{y}(x_k^*, y_k^*, \Delta y_k^*; y_k^e, \rho_k)$ is the kth primal-dual second-order estimate of y^*.
- $\widehat{y}(x)$ is the least-squares multiplier estimate as described in (5.11) below.

At all points x for which $\widehat{J}(x)$ has full row rank, the least-squares multiplier estimate is defined as

$$\widehat{y}(x) = \operatorname*{argmin}_y \|\hat{g}(x) - \widehat{J}(x)^T y\|_2^2. \tag{5.11}$$

It is not possible to calculate $\widehat{y}(x)$ since x_* is not known in advance. The quantity $\widehat{y}(x)$ is used only as a theoretical tool and is never required by the algorithm.

The following assumptions are also made about the problem:

(AS1a) The functions $f(x)$ and $\{c_i(x)\}$ are twice continuously differentiable for all $x \geq 0$.

(AS2a) The sequence $\{x_k^*\}$ is contained in the compact set $\mathcal{B}_x \subset \mathbb{R}^n$.

(AS2b) If K is a subsequence of the integers such that $\lim_{k\in K} x_k^* = x_*$, then $\{y_k^*\}_K$ is contained in the compact set $\mathcal{B}_y \subset \mathbb{R}^m$.

(AS3) The matrix $\widehat{J}(x_*)$ has full row rank at every limit point x_* of the sequence $\{x_k^*\}$ $\big($at least one limit point is guaranteed by assumption AS2a$\big)$.

5.4 Statement of the Algorithm

Algorithm 5.4.1 given below is very similar to the *stabilized* LCL algorithm proposed by Friedlander and Saunders [13]. The principal differences are as follows: (i) Algorithm 5.4.1 uses the *primal-dual* augmented Lagrangian instead of the classical augmented Lagrangian; (ii) explicit "artificial" bounds are imposed on the dual variables of the subproblem; and (iii) an alternative update for σ_k may be used in the situation where an iterate is labeled as "successful" (see below).

Based on the current degree of infeasibility, each pdℓ_1-LCL iterate is regarded as either "successful" or "unsuccessful". In the successful case, the solution estimates are updated by using information from the current subproblem solution.

Next an optimality check is performed, followed by a decrease in the primal infeasibility parameter η_k. The penalty parameter σ_k may also be decreased if Δy_k^* is "too large". Finally, the index j, which represents the number of consecutive successful iterations, is incremented by one. In the case of an unsuccessful iteration, first, the subproblem solutions are discarded. The penalty parameter ρ_k is then increased in an attempt to decrease the primal infeasibility at the next iteration. Next, the "artificial" bound γ_k on the dual variables is increased; the η_k is reset, and σ_k is decreased. Decreasing σ_k is appropriate because small values of σ_k encourage deviation from the linearized constraints, which may necessary in order to decrease primal infeasibility.

Algorithm 5.4.1. Primal-Dual ℓ_1-LCL Algorithm (pdℓ_1-LCL)

INPUT: (x_0, y_0)

Set ρ_0, σ_0, η_*, η_0, ω_*, τ_*, α_η, β_η, τ_ρ, τ_σ, α_γ, α_τ, k_τ, and δ;

Set $y_0^e = y_0$; $\quad z_0 = g(x_0) - J(x_0)^T y_0$; $\quad w_0 = 0$; $\quad \nu = (\|y_0^e\|_\infty + 1)\rho_0^{-\alpha_\gamma}$; $\quad \gamma_0 = \nu\rho_0^{\alpha_\gamma}$;

Set *converged* $\leftarrow$ **false**, $k \leftarrow 0$, $j \leftarrow 0$.

while not *converged* **do**

  Choose τ_k, $\omega_k > 0$ so that $\lim_{k\to\infty} \tau_k \le \tau_*$, $\tau_k \le k_\tau \rho_k^{\alpha_\tau}$, and $\lim_{k\to\infty} \omega_k \le \omega_*$;

  Find $(x_k^*, y_k^*, u_k^*, v_k^*, \Delta y_k^*, z_k^*, w_k^*)$, a solution to (5.6) as given by conditions (5.7).

  If multiple solutions exists, choose $(x_k^*, y_k^*, \Delta y_k^*, z_k^*, w_k^*)$ closest to (x_k, y_k, z_k, w_k);

  if $\|c(x_k^*)\| \le \max(\eta_*, \eta_k)$ **then** [successful]

    $x_{k+1} \leftarrow x_k^*$; $\quad y_{k+1} \leftarrow y_k^*$; $\quad z_{k+1} \leftarrow z_k^*$; $\quad y_{k+1}^e \leftarrow \widetilde{y}_k$;

    if $(x_{k+1}, y_{k+1}^e, z_{k+1})$ satisfies (5.10) **then** *converged* $\leftarrow$ **true end if**

    $\rho_{k+1} \leftarrow \rho_k$, $\quad \gamma_{k+1} \leftarrow \gamma_k$

    $\eta_{k+1} \leftarrow \eta_k/(1 + \rho_{k+1}^{\beta_\eta})$; [decrease η_k]

    if $\|\Delta y_k^*\|_\infty \ge \delta(\frac{1}{2})^j$ **then** $\sigma_{k+1} \leftarrow \sigma_k/\tau_\sigma$ **end if** [decrease σ_k]

    $j \leftarrow j + 1$;

  else [unsuccessful]

    $x_{k+1} \leftarrow x_k$; $\quad y_{k+1} \leftarrow y_k$; $\quad z_{k+1} \leftarrow z_k$; $\quad y_{k+1}^e \leftarrow y_k^e$;

$\rho_{k+1} \leftarrow \tau_\rho \rho_k$; $\quad \gamma_{k+1} \leftarrow \nu \rho_{k+1}^{\alpha_\gamma}$; [increase ρ_k, increase γ_k]

$\eta_{k+1} \leftarrow \eta_0/(1+\rho_{k+1}^{\alpha_\eta})$; [increase or decrease η_k]

$\sigma_{k+1} \leftarrow \sigma_k/\tau_\sigma$; [decrease σ_k]

$j \leftarrow 0$;

end if

$k \leftarrow k+1$;

end do

OUTPUT: $(x^*, y^*, z^*) \leftarrow (x_k, y_k^e, z_k)$;

The parameters associated with Algorithm 5.4.1 are defined as follows:

- ρ_0 ($\rho_0 \geq 0$) is the initial penalty parameter;
- σ_0 ($\sigma_0 \geq 0$) is the initial ℓ_1 penalty parameter for the linearized constraints;
- η_* ($0 < \eta_* \ll 1$) is the limiting primal convergence tolerance;
- η_0 ($\eta_* \leq \eta_0$) is the initial primal infeasibility tolerance;
- ω_* ($0 < \eta_* \ll 1$) is the limiting dual convergence tolerance for the x-variables;
- ω_0 ($\omega_* \leq \omega_0 < 1$) is the initial dual infeasibility tolerance for the x-variables;
- τ_* ($0 < \eta_* \ll 1$) is the dual convergence tolerance for the y-variables;
- α_η ($0 < \alpha_\eta < 1$) is the constant used in the update to η_k in the unsuccessful case. The condition $\alpha_\eta > 0$ ensures that $\{\eta_k\} \to 0$ as $k \to \infty$ in the event that infinitely many unsuccessful iterations occur;
- β_η ($0 < \beta_\eta$) is the constant used in the update to η_k in the successful case;
- τ_ρ ($\tau_\rho > 1$) is the expansion factor for ρ_k;
- τ_σ ($\tau_\sigma > 1$) is the scale-factor for σ_k;

- α_γ $(0 < \alpha_\gamma < 1)$ is the constant used in the definition of γ_k. The condition $\alpha_\gamma > 0$ is needed to ensure that $\{\gamma_k\} \to \infty$ if $\{\rho_k\} \to \infty$. The condition $\alpha_\gamma < 1$ is needed for Lemma 5.5.2 to hold;

- α_τ $(\alpha_\tau < -1)$ is the constant used in the definition of τ_k;

- k_τ $(k_\tau > 0)$ is used in the definition of τ_k;

- δ $(\delta > 0)$ is another positive constant;

- ν $(\nu > 0)$ is used in definition of γ_k. Given ρ_0 and y_0^e, the parameter ν is set to $\nu = (\|y_0^e\|_\infty + 1)\rho_0^{-\alpha_\gamma}$. As $\gamma_0 = \nu\alpha_0^{\alpha_\gamma}$, it follows that $\gamma_0 = \|y_0^e\|_\infty + 1$. Therefore, y_0^e will be in the interior of $[-\gamma_0 e, \gamma_0 e]$. This is not good if the user inputs a large inaccurate value of y_0. In practice, an *a priori* limit on the size of γ_0 should be enforced.

5.5 Global Convergence

In this section we establish the global convergence of Algorithm 5.4.1. The method of proof is similar to that of Friedlander and Saunders [13]. The first result gives properties of any limit point generated by Algorithm 5.4.1. It is similar to Lemma 5.2 of [13] and Lemma 4.4 of [5].

Lemma 5.5.1. *Suppose that assumptions* AS1a, AS2a, *and* AS3 *hold. Let* $\{\omega_k\}$, $\{\tau_k\}$, $\{\gamma_k\}$, *and* $\{\rho_k\}$ *be positive sequences such that* $\{\omega_k\} \to 0$. *Let* $\{x_k\}$ *be a sequence of vectors in* $\mathcal{B}_x$, $\{y_k^e\}$ *be any sequence of vectors, and* $\{(x_k^*, y_k^*, \Delta y_k^*, z_k^*)\}$ *be a sequence of vectors satisfying conditions* (5.7a), (5.7b), *and* (5.7g). *Let* K *be a subsequence of integers such that* $\lim_{k\in K} x_k^* = x_*$. *Let* $\widetilde{y}_k = \widetilde{y}(x_k^*, y_k^*, \Delta y_k^*; y_k^e, \rho_k)$, $y_* = \widehat{y}(x_*)$, *and* $z_* = g(x_*) - J(x_*)^T y_*$. *Then the following properties hold:*

1. *There are positive constants* α_1, α_2, *and* M *such that, for* $k \in K$ *sufficiently large,*

a) $\|\widetilde{y}_k - y_*\| \le \beta_1 \triangleq \alpha_1\omega_k + M\|x_k^* - x_k\|\|\Delta y_k^*\| + \alpha_2\|x_k^* - x_*\|$

b) $\rho_k\|c(x_k^*)\| \le \frac{1}{2}\|\widetilde{y}_k - y_*\| + \|y_k^e - y_*\| + \frac{1}{2}\|y_k^* - y_*\| + \frac{1}{2}\|\Delta y_k^*\|$

c) $\rho_k\|c(x_k^*)\| \le \|\widetilde{y}_k - y_*\| + \|\Delta y_k^*\| + \|y_k^e - y_*\| + \rho_k\|w_k^*\|$

d) $\|y_k^* - y_*\| \le \|\widetilde{y}_k - y_*\| + \|\Delta y_k^*\| + 2\rho_k\|w_k^*\|$

e) $\|y_k^* - y_*\| \le 2\rho_k\|c(x_k^*)\| + \|\Delta y_k^*\| + 2\|y_k^e - y_*\| + \|\widetilde{y}_k - y_*\|.$

Moreover; parts b), c), d), *and* e) *hold for all* k*.*

2. *If* $\lim_{k\in K}\|\Delta y_k^*\| = 0$*, or* $\{\|\Delta y_k^*\|\}_{k\in K}$ *is bounded above with* $\lim_{k\in K}\|x_k^* - x_k\| = 0$*, then* $\lim_{k\in K}\widetilde{y}_k = y_*$ *and* $\lim_{k\in K} z_k^* = z_*$

3. *For all* $k \in K$ *sufficiently large,*

   a) $\rho_k\|w_k^*\| \le \frac{1}{2}\|\widetilde{y}_k - y_*\| + 2\|y_k^e - y_*\| + \frac{3}{2}\|y_k^* - y_*\| + \frac{1}{2}\|\Delta y_k^*\|$

   b) $\rho_k\|w_k^*\| \le \frac{1}{2}\beta_1 + 2\|y_k^e - y_*\| + \frac{3}{2}\|y_k^* - y_*\| + \frac{1}{2}\|\Delta y_k^*\|$

   Moreover; part a) *holds for all* k*.*

4. *If* $c(x_*) = 0$*, then* (x_*, y_*, z_*) *is a first-order KKT point for problem* GNPs.

Proof. Assumption AS3 and the fact that $\lim_{k\in K} x_k^* = x_*$, implies that $\widehat{J}(x_k^*)$ has full row rank for $k \in K$ sufficiently large. Thus, Lemma 4.1.3 and the fact that $\|\big(J(x)J(x)^T\big)^{-1}J(x)\|$ is bounded in a neighborhood of x_* implies that there exists an $\alpha_1 > 0$ such that

$$\|\widehat{y}(x_k^*) - \widetilde{y}_k\| \le \frac{\alpha_1}{\sqrt{n}}\|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T\widetilde{y}_k\| \ \text{ for } k \in K \text{ sufficiently large.} \tag{5.12}$$

Now we bound the right-hand side. First note that since $\lim_{k\in K} x_k^* = x_*$ and $[x_*]_{\mathcal{I}} > 0$, it must be the case that for $k \in K$ sufficiently large $[x_k^*]_{\mathcal{I}} > 0$. Using (5.7b) and the fact that $\{\omega_k\} \to 0$, gives

$$\min\big([x_k^*]_{\mathcal{I}}, [z_k^*]_{\mathcal{I}}\big) = [z_k^*]_{\mathcal{I}} \ \text{ for } k \in K \text{ sufficiently large.}$$

This implies the following

$$
\begin{aligned}
\|[z_k^*]_{\mathcal{I}}\| &\le \|\min(x_k^*, z_k^*)\| \\
&= \Big(\sum_{j=1:n} \big(\min([x_k^*]_j, [z_k^*]_j)\big)^2 \Big)^{1/2} \\
&\le \Big(\sum_{j=1:n} \omega_k^2 \Big)^{1/2} = \sqrt{n}\,\omega_k \;\text{ for } k \in K \text{ sufficiently large.}
\end{aligned}
$$

Thus,

$$
\|[z_k^*]_{\mathcal{I}}\| \le \sqrt{n}\,\omega_k, \quad \text{for } k \in K \text{ sufficiently large.} \tag{5.13}
$$

The condition (5.7g) and the definitions of $\widetilde{y}_k$ and π_k, allow us to derive the following expression for all $k \in K$ sufficiently large:

$$
\begin{aligned}
z_k^* &= g(x_k^*) - J(x_k^*)^T(2\pi_k - y_k^*) - J(x_k)^T \Delta y_k^* \\
&= g(x_k^*) - J(x_k^*)^T(2\pi_k - y_k^* + \Delta y_k^*) + \big(J(x_k^*) - J(x_k)\big)^T \Delta y_k^* \\
&= g(x_k^*) - J(x_k^*)^T \widetilde{y}_k + \big(J(x_k^*) - J(x_k)\big)^T \Delta y_k^*.
\end{aligned} \tag{5.14}
$$

Under the assumption that $c(x)$ is twice continuously differentiable on $\mathcal{B}_x$, it holds that $J(x)$ is Lipschitz continuous on $\mathcal{B}_x$ and there must exist a positive M such that $\|J(x_k^*) - J(x_k)\| \le M\frac{\sqrt{n}}{\alpha_1}\|x_k^* - x_k\|$. Using this result in conjunction with the triangle-inequality and equations (5.13) and (5.14), yields

$$
\begin{aligned}
\|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T \widetilde{y}_k\| &= \|[z_k^*]_{\mathcal{I}} - \big(\widehat{J}(x_k^*) - \widehat{J}(x_k)\big)^T \Delta y_k^*\| \\
&\le \|[z_k^*]_{\mathcal{I}}\| + \|\big(\widehat{J}(x_k^*) - \widehat{J}(x_k)\big)^T \Delta y_k^*\| \\
&\le \sqrt{n}\omega_k + M\frac{\sqrt{n}}{\alpha_1}\|x_k^* - x_k\|\|\Delta y_k^*\|.
\end{aligned}
$$

This last inequality and equation (5.12) imply the bound

$$
\|\widehat{y}(x_k^*) - \widetilde{y}_k\| \le \alpha_1\omega_k + M\|x_k^* - x_k\|\|\Delta y_k^*\|, \quad \text{for } k \in K \text{ sufficiently large.} \tag{5.15}
$$

Using (5.15), the Lipschitz continuity of the least-squares multiplier estimate in a neighborhood of x_* $\big($recall that $y_* = \widehat{y}(x_*)\big)$, and the triangle inequality, we may infer the existence of a positive α_2 such that

$$\begin{aligned} \|\widetilde{y}_k - y_*\| &= \|\widetilde{y}_k - \widehat{y}(x_k^*) + \widehat{y}(x_k^*) - y_*\| \\ &\le \|\widetilde{y}_k - \widehat{y}(x_k^*)\| + \|\widehat{y}(x_k^*) - y_*\| \\ &\le \underbrace{\alpha_1\omega_k}_{(a)} + \underbrace{M\|x_k^* - x_k\|\|\Delta y_k^*\|}_{(b)} + \underbrace{\alpha_2\|x_k^* - x_*\|}_{(c)} = \beta_1, \end{aligned} \tag{5.16}$$

for $k \in K$ sufficiently large. This proves part 1a).

To prove part 2, consider (5.16). First, suppose that $\{\|\Delta y_k^*\|\}_{k\in K} \to 0$. The term (a) goes to zero since $\{\omega_k\} \to 0$. Similarly, the term (b) goes to zero on K because $\|x_k^* - x_k\|$ is bounded from AS2a and because $\{\|\Delta y_k^*\|\}_{k\in K} \to 0$. The term (c) goes to zero since $\lim_{k\in K} x_k^* = x_*$. This implies that $\lim_{k\in K} \widetilde{y}_k = y_*$. As J is continuous on the compact set $\mathcal{B}_x$, the set $\{\|J(x_k^*) - J(x_k)\|\}$ is bounded, giving

$$\lim_{k\in K} \|\big(J(x_k^*) - J(x_k)\big)^T \Delta y_k^*\| = 0. \tag{5.17}$$

On the other hand, suppose that $\{\|\Delta y_k^*\|\}_{k\in K}$ is bounded and $\lim_{k\in K} \|x_k^* - x_k\| = 0$. The term (a) goes to zero since $\{\omega_k\} \to 0$. The term (b) goes to zero because $\{\|\Delta y_k^*\|\}_{k\in K}$ is bounded and $\lim_{k\in K} \|x_k^* - x_k\| = 0$. Moreover, the term (c) goes to zero since $\lim_{k\in K} x_k^* = x_*$. This implies that $\lim_{k\in K} \widetilde{y}_k = y_*$. Also, as $\{\|\Delta y_k^*\|\}_{k\in K}$ is bounded and $\lim_{k\in K} \|x_k^* - x_k\| = 0$, it must hold that

$$\lim_{k\in K} \|\big(J(x_k^*) - J(x_k)\big)^T \Delta y_k^*\| = 0. \tag{5.18}$$

Taking the limit of equation (5.14) for $k \in K$ and using equations (5.17) and (5.18) yields

$$\begin{aligned} \lim_{k\in k} z_k^* &= \lim_{k\in k} \Big(g(x_k^*) - J(x_k^*)^T \widetilde{y}_k + \big(J(x_k^*) - J(x_k)\big)^T \Delta y_k^*\Big) \\ &= g(x_*) - J(x_*)^T y_* = z_*, \end{aligned}$$

which proves part 2.

By definition, $\widetilde{y}_k = 2y_k^e - 2\rho_k c(x_k^*) - y_k^* + \Delta y_k^*$. Introducing y_* and performing some rearrangement leads to

$$2\rho_k c(x_k^*) = 2y_k^e - 2y_* + y_* - \widetilde{y}_k + y_* - y_k^* + \Delta y_k^*.$$

Taking norms and using the triangle inequality gives

$$2\rho_k\|c(x_k^*)\| \le \|\widetilde{y}_k - y_*\| + 2\|y_k^e - y_*\| + \|y_k^* - y_*\| + \|\mathit{\Delta} y_k^*\|.$$

Dividing this equation through by 2 proves part 1b).

Substituting $c(x_k^*)$ from condition (5.7g) into the definition of $\widetilde{y}_k$ gives

$$\widetilde{y}_k = 2y_k^e - 2\rho_k c(x_k^*) - y_k^* + \mathit{\Delta} y_k^* = y_k^* + \mathit{\Delta} y_k^* - 2\rho_k w_k^*. \tag{5.19}$$

Introducing y_*, rearranging, taking norms and using the triangle inequality yields

$$\begin{aligned}\|y_k^* - y_*\| &= \|\widetilde{y}_k - y_* - \mathit{\Delta} y_k^* + 2\rho_k w_k^*\| \\ &\le \|\widetilde{y}_k - y_*\| + \|\mathit{\Delta} y_k^*\| + 2\rho_k\|w_k^*\|,\end{aligned}$$

which proves part 1d). Applying the bound given by part 1d) to part 1b) gives 1c).

Introducing y_* in the definition of $\widetilde{y}_k$ and using the triangle inequality gives

$$\|y_k^* - y_*\| \le 2\rho_k\|c(x_k^*)\| + \|\mathit{\Delta} y_k^*\| + 2\|y_k^e - y_*\| + \|\widetilde{y}_k - y_*\|,$$

which proves part 1e).

For part 3, we note that condition (5.7g), the triangle inequality, and the introduction of y_*, and the result of part 1b) lead to

$$\begin{aligned}\rho_k\|w_k^*\| &= \|\rho_k c(x_k^*) + (y_k^* - y_k^e)\| \\ &\le \rho_k\|c(x_k^*)\| + \|y_k^* - y_*\| + \|y_* - y_k^e\| \\ &\le \tfrac{1}{2}\|\widetilde{y}_k - y_*\| + 2\|y_k^e - y_*\| + \frac{3}{2}\|y_k^* - y_*\| + \tfrac{1}{2}\|\mathit{\Delta} y_k^*\|,\end{aligned}$$

which proves part 3a). Applying the bound from part 1a) to part 3a) gives part 3b).

It remains to verify part 4. To this end, assume that $c(x_*) = 0$. To show that (x_*, y_*, z_*) is a first-order KKT point, it must be shown that $\min(x_*, z_*) = 0$. From condition (5.7b) we have

$$\|\min(x_k^*, z_k^*)\|_\infty \le \omega_k.$$

As $\{\omega_k\} \to 0$, it must holds that

$$\lim_{k \in k} \| \min(x_k^*, z_k^*) \|_\infty \le \lim_{k \in k} \omega_k = 0,$$

which implies that $\lim_{k \in k} \| \min(x_k^*, z_k^*) \|_\infty = 0$. The continuity of norms and the fact that $\lim_{k \in k}(x_k^*, z_k^*) = (x_*, z_*)$ gives $\min(x_*, z_*) = 0$, which proves part 4. □

Note that these results are independent of the choice of sequences $\{\rho_k\}$, $\{\gamma_k\}$, $\{\tau_k\}$, and $\{y_k^e\}$.

As in Chapter 4, the quantity $\|y_k^e\|/\rho_k$ plays an important role in the proof of global convergence. This quantity must converge to zero if the penalty parameter ρ_k converges to infinity. This implies that $\{y_k^e\}$ need not remain bounded, but must not grow too fast compared to ρ_k. First, we show that the sequence $\{\|y_k^*\|\}$ does not grow too fast relative to the penalty parameter. The following result makes this idea precise.

Lemma 5.5.2. *Suppose that Algorithm* 5.4.1 *gives* $\{\rho_k\} \to \infty$ *as* $k \to \infty$. *Then* $\{\|y_k^*\|/\rho_k\} \to 0$.

Proof. Since $y_k^* \in [-\gamma_k e, \gamma_k e]$ and $\gamma_k = \nu \rho_k^{\alpha_\gamma}$ for all k, it follows that

$$\frac{\|y_k^*\|}{\rho_k} \le \frac{\sqrt{m}\,\|y_k^*\|_\infty}{\rho_k} \le \frac{\sqrt{m}\,\gamma_k}{\rho_k} = \frac{\sqrt{m}\,\nu \rho_k^{\alpha_\gamma}}{\rho_k} = \sqrt{m}\,\nu \rho_k^{\alpha_\gamma - 1} \tag{5.20}$$

Since $\alpha_\gamma < 1$ and $\{\rho_k\} \to \infty$, the right-hand side goes to zero. This implies that if $\{\rho_k\} \to \infty$ as $k \to \infty$, then $\{\|y_k^*\|/\rho_k\} \to 0$. □

The next lemma is adapted from Lemma 5.3 in [13].

Lemma 5.5.3. *Suppose that Algorithm* 5.4.1 *gives* $\{\rho_k\} \to \infty$ *as* $k \to \infty$. *Then* $\{\|y_k^e\|/\rho_k\} \to 0$.

Proof. Let $\{k_1, k_2, \dots\}$ denote the indices of iterates that are labeled as unsuccessful by Algorithm 5.4.1. Similarly, let $\{l_1, l_2, \dots\}$ denote the associated indices for which the *last* successful iteration was performed. With these definitions,

$$y_{k_i+1}^e = \widetilde{y}_{l_i} \;\text{ and }\; \rho_{k_i+1} = \tau_\rho^{k_i - l_i} \rho_{l_i}\,. \tag{5.21}$$

The parameter ρ_k increases if and only if an unsuccessful iteration is executed. As y_k^e is not updated during unsuccessful iterations, it is sufficient to show that $\{\|y_{k_i+1}^e\|/\rho_{k_i+1}\} \to 0$ as $i \to \infty$.

If there are only finitely many (possibly zero) successful iterations, then from some point on, the multiplier estimate y_k^e is kept fixed. As $\{\rho_k\} \to \infty$, it must hold that $\{\|y_{k_i+1}^e\|/\rho_{k_i+1}\} \to 0$.

Therefore, assume that there are infinitely many successful iterations. Using the definition of $\widetilde{y}_k$, the triangle inequality, the equation (5.21), and the bound $\tau_\rho^{k_i - l_i} \geq 1$, it holds that

$$\begin{aligned} \frac{\|y_{k_i+1}^e\|}{\rho_{k_i+1}} = \frac{\|\widetilde{y}_{l_i}\|}{\tau_\rho^{(k_i-l_i)}\rho_{l_i}} \leq \frac{\|\widetilde{y}_{l_i}\|}{\rho_{l_i}} &= \frac{\|2y_{l_i}^e - 2\rho_{l_i}c(x_{l_i}^*) - y_{l_i}^* + \Delta y_{l_i}^*\|}{\rho_{l_i}} \\ &\leq \underbrace{\frac{\|\Delta y_{l_i}^*\|}{\rho_{l_i}}}_{(a)} + 2\underbrace{\frac{\|y_{l_i}^e - \rho_{l_i}c(x_{l_i}^*)\|}{\rho_{l_i}}}_{(b)} + \underbrace{\frac{\|y_{l_i}^*\|}{\rho_{l_i}}}_{(c)}. \end{aligned} \tag{5.22}$$

Equation (5.8) on page 128 shows that $\|\Delta y_{l_i}^*\|$ is bounded, and therefore the term (a) goes to zero as $\{\rho_k\} \to \infty$. The definition of the forcing sequence $\{\eta_k\}$ is analogous to that in [8] and therefore Lemma 4.1 from [8] implies that (b) goes to zero as $\{\rho_k\} \to \infty$. Finally, Lemma 5.5.2 implies that the term (c) goes to zero as $\{\rho_k\} \to \infty$. Thus, equation (5.22) implies that $\{\|y_{k_i+1}^e\|/\rho_{k_i+1}\} \to 0$. □

The previous two lemmas may now be used to prove global convergence of the subproblem solutions. Algorithm 5.5.1 gives the update used by Friedlander and Saunders for η_k in the successful case.

Algorithm 5.5.1. Update to η_k in the successful case (single limit point).

$\sigma_{k+1} \leftarrow \frac{1}{1+\rho_k}\min(1 + \|\Delta y_k^*\|_\infty, \bar{\sigma})$

Using this update, Friedlander and Saunders prove global convergence of the subproblem solutions under the assumption that there is a *single* limit point. In addition, they suggest the following alternative update to handle the case where there are *multiple* limit points.

Algorithm 5.5.2. Update to η_k in the successful case (multiple limit points).

if $\|\Delta y_k^*\|_\infty \le \delta(\frac{1}{2})^j$

$\sigma_{k+1} \leftarrow \frac{1}{1+\rho_k}\min(1 + \|\Delta y_k^*\|_\infty,\, \bar{\sigma});$ [reset σ_k]

else

$\sigma_{k+1} = \sigma_k/\tau_\sigma;$ [decrease σ_k]

end if

The primal-dual ℓ_1-LCL Algorithm 5.4.1 uses neither of the updates given above. The reason for this is made clear after the next result. Theorem 5.5.1 says that the subproblem solutions generated by Algorithm 5.4.1 are globally convergent.

Theorem 5.5.1 (Global convergence of subproblem solutions)**.** *Suppose assumptions* AS1a, AS2a *and* AS3 *hold. Let* $\{(x_k^*, y_k^*, \Delta y_k^*, z_k^*)\}$ *be the sequence of vectors generated by Algorithm* 5.4.1 *with tolerances* $\omega_* = 0$ *and* $\eta_* = 0$*. Let* K *be a subsequence of the integers such that* $\lim_{k\in K} x_k^* = x_*$*. Then all parts of Lemma* 5.5.1 *hold. Therefore,* (x_*, y_*, z_*) *as defined in Lemma* 5.5.1 *is a first-order KKT point.*

Proof. Algorithm 5.4.1 generates scalar sequences $\{\omega_k\}$, $\{\tau_k\}$, $\{\gamma_k\}$, and $\{\rho_k\}$ such that $\{\omega_k\} \to 0$. It also generates a sequence $(x_k^*, y_k^*, \Delta y_k^*, z_k^*)$ that satisfies (5.7) for each k. Therefore, the hypotheses of Lemma 5.5.1 hold, and parts 1 and 3 of that lemma follow immediately.

Since each $x_k^* \ge 0$ by condition (5.7b), it follows that $x_* = \lim_{k\in K} x_k^* \ge 0$. Examination of Algorithm 5.4.1 shows that one of the following four cases must occur:

1. $\{\rho_k\}$ is uniformly bounded, and $\{\sigma_k\} \to 0$;

2. $\{\rho_k\}$ is uniformly bounded, and $\{\sigma_k\} \nrightarrow 0$;

3. $\{\rho_k\} \rightarrow \infty$, and $\{\sigma_k\} \rightarrow 0$;

4. $\{\rho_k\} \rightarrow \infty$, and $\{\sigma_k\} \nrightarrow 0$.

Case 4 can not occur, since if $\rho_k \rightarrow \infty$ then $\sigma_k \rightarrow 0$.

Consider case 1. Since $\{\sigma_k\} \rightarrow 0$ and $\{\omega_k\} \rightarrow 0$, equation (5.8) implies the $\{\Delta y_k^*\} \rightarrow 0$. This shows that part 2 of Lemma 5.5.1 holds. As $\{\rho_k\}$ is uniformly bounded, it must be true that for k sufficiently large every iteration is successful and that $\|c(x_k^*)\| \leq \eta_k$. Since $\{\eta_k\} \rightarrow 0$, c is continuous, norms are continuous, and $\{x_k^*\}_{k\in K} \rightarrow x_*$, it follows that $c(x_*) = 0$. Thus, part 4 of Lemma 5.5.1 holds.

Consider case 2. Since $\{\rho_k\}$ is uniformly bounded, every iteration is successful for k sufficiently large. It also follows that $j \rightarrow \infty$ as $k \rightarrow \infty$. The argument used in case 1 shows that $c(x_*) = 0$. Thus, part 4 of Lemma 5.5.1 holds. Furthermore, since $\{\sigma_k\} \nrightarrow 0$ it follows that $\|\Delta y_k^*\|_\infty < \delta(\frac{1}{2})^j$ for k sufficiently large. Since $j \rightarrow \infty$ as $k \rightarrow \infty$, it follows that $\lim_{k\rightarrow\infty} \Delta y_k^* = 0$. Thus, part 2 of Lemma 5.5.1 holds.

Finally, consider case 3. Since $\{\sigma_k\} \rightarrow 0$, equation (5.8) on page 128 implies the $\{\Delta y_k^*\} \rightarrow 0$. This shows that part 2 of Lemma 5.5.1 holds, and therefore $\lim_{k\in K} \widetilde{y}_k = y_*$. Part 1b) of Lemma 5.5.1 implies

$$2\|c(x_k^*)\| \leq \underbrace{\frac{\|\widetilde{y}_k - y_*\|}{\rho_k}}_{(a)} + 2\underbrace{\frac{\|y_k^e - y_*\|}{\rho_k}}_{(b)} + \underbrace{\frac{\|y_k^* - y_*\|}{\rho_k}}_{(c)} + \underbrace{\frac{\|\Delta y_k^*\|}{\rho_k}}_{(d)} \tag{5.23}$$

Terms (a) and (d) go to zero on K since $\{\rho_k\} \rightarrow \infty$, $\{\widetilde{y}_k\}_{k\in K} \rightarrow y_*$, and $\{\Delta y_k^*\} \rightarrow 0$. Lemma 5.5.2 and Lemma 5.5.3 imply that terms (b) and (c) go to zero. Therefore, equation (5.23) implies $\lim_{k\in K} c(x_k^*) = 0$. As $\lim_{k\in K} x_k^* = x_*$, the continuity of c and the continuity of norms imply that $c(x_*) = 0$. Thus, part 4 of Lemma 5.5.1 holds. □

Friedlander and Saunders use Algorithm 5.5.2 to update η_k in the successful case in order to account for multiple limit points. The integer j represents the number of consecutive successful major iterations and δ is a positive parameter. With this update, the authors claim global convergence without the single limit point assumption. They also note that any forcing sequence converging to zero may be used in the "if" part, but that requiring only a mild decrease in $\|\Delta y_k^*\|_\infty$ at each iteration should interfere less with the fast local convergence of the method since $\|\Delta y_k^*\|$ may be expected to decrease at a linear rate. However, Friedlander-Saunders proof of case 2 does not treat all the possible situations that may arise. If case 2 applies, $\{\rho_k\}$ is uniformly bounded and every iterate is successful for k sufficiently large. Clearly, in this case, $j \to \infty$. Friedlander and Saunders argue that if Δy_k^* does not satisfy the "if" part of Algorithm 5.5.2 infinitely often, then $\{\sigma_k\} \to 0$. However, this does not appear to be guaranteed since it is possible that both the "if" and "else" statements occur infinitely often—implying that σ_k alternates between being decreased and being reset.

However, it is true that if $\{x_k^*\}$ contains *finitely many* limit points, then there exists *some* subsequence, call it $\bar{K}$, say, such that $\lim_{k\in\bar{K}}(x_k^*, \widetilde{y}_k, z_k^*, \Delta y_k^*) = (x_*, y_*, z_*, 0)$ and that (x_*, y_*, z_*) is a KKT point. This can be seen as follows. Let K_1, K_2, ..., K_l be disjoint subsequences of the integers such that $\lim_{k\in K_i} x_k^* = x_*^i$, a limit point of $\{x_k^*\}$, for $i = 1 : l$. Therefore, $\{x_*^i\}$ for $i = 1 : l$ is the finite set of limit points of $\{x_k^*\}$. Since $\{\rho_k\}$ is assumed uniformly bounded, then all iterates are successful for k sufficiently large. If the "if" part happens *finitely* often, then $\{\sigma_k\} \to 0$ and part 2 of Lemma 5.2 by Friedlander and Saunders holds. If the "if" part occurs infinitely often, then it must be true that the "if" part occurs infinitely often on K_m for some $1 \le m \le l$. It could occur infinitely often on more than one subsequence, but one will suffice. This implies that there exists a sub-subsequence $K_{\bar{m}} \subseteq K_m$ such that $\{\Delta y_k^*\}_{K_{\bar{m}}} \to 0$ since $j \to \infty$. Since $\{x_k^*\}_{K_{\bar{m}}} \to x_*^m$, $\{\Delta y_k^*\}_{K_{\bar{m}}} \to 0$, and $c(x_*^m) = 0$, Lemma 5.2 by Friedlander and Saunders implies that (x_*^m, y_*^m, z_*^m) is a KKT point where $\lim_{k\in K_{\bar{m}}} \widetilde{y}_k = y_*^m$ and $z_*^m \triangleq g(x_*^m) - J(x_*^m)^T y_*^m$. Note that this is on the sub-subsequence $K_{\bar{m}}$, and not, as Lemma 5.2 of Friedlander and Saunders claim, on K_m.

So it appears that the update used by the sLCL algorithm to handle *multiple* limit points may not work as predicted. However, in practice it is unlikely to be a problem. First, the algorithm usually converges, which implies that a unique limit point exists. Even when multiple limit points exist, it seems unlikely that the case described above would occur. It seems more likely that σ_k would be driven to zero and begin to resemble the BCL method, which is know to be globally convergent. The possible ramifications of this observation on the sLCL algorithm is unclear at this point.

Corollary 5.5.1 (Convergence of Δy_k^* to zero). *Let* $\{(x_k^*, y_k^*, \Delta y_k^*, z_k^*)\}$ *be the sequence of vectors generated by Algorithm* 5.4.1. *Then*

$$\lim_{k\to\infty} \Delta y_k^* = 0.$$

Proof. See proof of Theorem 5.5.1. □

5.6 Termination in the Limit

This section follows the outline of Section 5.4 of [13]. Friedlander and Saunders note that the convergence test takes place during successful iterations only, i.e., since $\eta_* = 0$, when $\|c(x_k^*)\| \le \eta_k$. To guarantee that the algorithm eventually terminates as the iterates converge, successful iterates must be guaranteed to occur infinitely often. Friedlander and Saunders show that their definition of the forcing sequence η_k ensures this property. As a counter example, if $\eta_k \equiv 0$ for all k, then the algorithm tests for convergence only in the rare case that $c(x_k^*) = 0$. The forcing sequence used in Algorithm 5.4.1 is the same as that used by Friedlander and Saunders in [13]. This sequence was suggested originally by Conn et al. [5] and Conn, Gould, and Toint [8]. The following result is identical to Corollary 5.5 of [13].

Corollary 5.6.1 (Global convergence with a single limit point). *Let* $\{(x_k, y_k^e, z_k)\}$ *be the sequence of vectors generated by Algorithm* 5.4.1. *Let* x_* *be the single limit* *point of* $\{x_k^*\}$. *Suppose that assumptions* AS1a, AS2a *and* AS3 *hold. Then*

$$\lim_{k\to\infty}(x_k, y_k^e, z_k) = (x_*, y_*, z_*),$$

and (x_*, y_*, z_*) *is a first-order KKT point for problem* GNPs.

Proof. See Corollary 5.5 in [13]. □

The following theorem shows that $\{y_k^*\}$ converges to y_* under assumption AS2b.

Theorem 5.6.1. *Suppose assumptions* AS1a, AS2a, AS2b, *and* AS3 *hold. Let* $\{(x_k^*, y_k^*, \Delta y_k^*, z_k^*)\}$ *be the sequence of vectors generated by Algorithm* 5.4.1 *with tolerances* $\omega_* = 0$ *and* $\eta_* = 0$. *Let* x_* *be the single limit point of* $\{x_k^*\}$. *Then*

$$\lim_{k\to\infty}(x_k^*, y_k^*, \widetilde{y}_k, z_k^*) = (x_*, y_*, y_*, z_*)$$

and (x_*, y_*, z_*) *is a first-order KKT point as defined in Lemma* 5.5.1.

Proof. Theorem 5.5.1 shows that

$$\lim_{k\to\infty}(x_k^*, \widetilde{y}_k, z_k^*) = (x_*, y_*, z_*)$$

and that (x_*, y_*, z_*) is a first-order KKT point. It remains to establish that $\lim_{k\to\infty} y_k^* = y_*$. Two cases are considered:

1. $\{\rho_k\} \to \infty$,
2. $\{\rho_k\}$ is uniformly bounded.

First consider case 1. Part 1d) of Lemma 5.5.1 gives

$$\|y_k^* - y_*\| \le \underbrace{\|\widetilde{y}_k - y_*\|}_{(a)} + \underbrace{\|\Delta y_k^*\|}_{(b)} + \underbrace{2\rho_k\|w_k^*\|}_{(c)} \quad \text{for all } k \text{ sufficiently large.} \tag{5.24}$$

Note that $\{\sigma_k\} \to 0$ and $\{\gamma_k\} \to \infty$ since $\{\rho_k\} \to \infty$. Term (a) goes to zero because $\lim_{k\to\infty} \widetilde{y}_k = y_*$. Since $\{\omega_k\} \to 0$ and $\{\sigma_k\} \to 0$, equation (5.8) implies that term (b) goes to zero. Since $\{\gamma_k\} \to \infty$, assumption AS2b and condition (5.7d) imply that

$$\|w_k^*\|_\infty \le \tau_k \text{ for all } k \text{ sufficiently large.} \tag{5.25}$$

By construction, τ_k satisfies $\tau_k \le k_\tau \rho_k^{\alpha_\tau}$ for some positive constant k_τ and some number $\alpha_\tau < -1$. It follows that

$$\rho_k \|w_k^*\| \le \sqrt{m}\rho_k \|w_k^*\|_\infty \le \sqrt{m}\rho_k k_\tau \rho_k^{\alpha_\tau} = \sqrt{m} k_\tau \rho_k^{\alpha_\tau + 1} \text{ for all } k \text{ sufficiently large.}$$

The right-hand side goes to zero since $\{\rho_k\} \to \infty$ and $\alpha_\tau < -1$, which implies $\{\rho_k \|w_k^*\|\} \to 0$. Thus, term (c) goes to zero. Since terms (a), (b), and (c) go to zero, equation (5.24) shows that $\lim_{k\to\infty} y_k^* = y_*$.

Next, consider case 2. Since $\{\rho_k\}$ remains uniformly bounded it follows that all iterates are successful for k sufficiently large. Moreover, the condition $c(x_k^*) \le \eta_k$ is satisfied for all k sufficiently large. Since $\{\eta_k\} \to 0$, this implies

$$\lim_{k\to\infty} c(x_k^*) = 0. \tag{5.26}$$

Part 1e) of Lemma 5.5.1 gives

$$\|y_k^* - y_*\| \le \underbrace{2\rho_k \|c(x_k^*)\|}_{(a)} + \underbrace{\|\Delta y_k^*\|}_{(b)} + \underbrace{2\|y_k^e - y_*\|}_{(c)} + \underbrace{\|\widetilde{y}_k - y_*\|}_{(d)}. \tag{5.27}$$

Since $\{\rho_k\}$ is uniformly bounded, equation (5.26) implies that the term (a) goes to zero. Corollary 5.5.1 and Corollary 5.6.1 imply that the terms (b) and (c) go to zero. The term (d) goes to zero because $\{\widetilde{y}_k\} \to y_*$. Therefore, equation (5.27) implies that $\lim_{k\to\infty} y_k^* \to y_*$.

□

The proof of Corollary 5.6.1 requires showing that infinitely many successful iterations occur. Therefore, the following corollary is immediate and simply extends the result of Corollary 5.6.1 to include convergence of the sequence $\{y_k\}$.

Corollary 5.6.2 (Global convergence with a single limit point). *Let* $\{(x_k, y_k, y_k^e, z_k)\}$ *be the sequence of vectors generated by Algorithm* 5.4.1*. Let* x_* *be the single limit point of* $\{x_k^*\}$*. Suppose that assumptions* AS1a, AS2a*,* AS2b *and* AS3 *hold. Then*

$$\lim_{k\to\infty}(x_k, y_k, y_k^e, z_k) = (x_*, y_*, y_*, z_*),$$

and (x_*, y_*, z_*) *is a first-order KKT point for problem* GNPs. □

5.7 Asymptotic Equivalence to LCL

The efficiency of an LCL method relies on the following facts: 1) the subproblem eventually identifies the optimal active-set; and 2) the subproblem restricts its search to the linearized constraints, which can be very accurate near a solution. Friedlander and Saunders note that during early iterations, the ℓ_1 penalty term may allow great deviation from the linearized constraints. However, satisfaction of the linearized constraints must be enforced near a solution in order to recover the fast convergence properties of Robinson's original LCL method. The following result shows that, under certain assumptions, the linearized constraints will eventually be satisfied to within a multiple of the termination parameter ω_k.

Theorem 5.7.1 (Convergence to non-elastic subproblem solutions). *Let* (x_k, y_k, y_k^e, z_k) *and* $(\Delta y_k^*, u_k^*, v_k^*)$ *be the sequences generated by Algorithm* 5.4.1*. Let* x_* *be the single limit point of* $\{x_k^*\}$*. Suppose that assumptions* AS1a, AS2a*,* AS2b *and* AS3 *hold and that* $\{\rho_k\}$ *remains bounded. Then, if* $\sigma_k \ge \sigma_L > 0$ *for all* k*, and for some number* σ_L*, then*

$$\|u_k^*\|_\infty \le \omega_k \quad \text{and} \quad \|v_k^*\|_\infty \le \omega_k \tag{5.28}$$

for all k *sufficiently large.*

Proof. The assumptions are sufficient for Corollary 5.6.2 to hold. Therefore

$$\lim_{k\to\infty}(x_k, y_k, y_k^e, z_k) = (x_*, y_*, y_*, z_*),$$

and in particular $\lim_{k\to\infty} c(x_k^*) = c(x_*) = 0$. Also, since $\{\rho_k\}$ is bounded, there exists a positive integer k_1 such that $\rho_k \equiv \bar{\rho}$ for all $k \geq k_1$. Since $c(x_*) = 0$, $\{y_k^e\}$ is a Cauchy sequence, $\{y_k^*\} \to y_*$, and $\{\omega_k\} \to 0$, there exists a positive integer $k_2 \geq k_1$ such that

$$\|y_{k+1}^e - y_k^e\|_\infty < \sigma_L/3, \tag{5.29}$$

$$2\bar{\rho}\|c(x_k^*)\|_\infty < \sigma_L/3 - \omega_k, \tag{5.30}$$

$$\|y_k^* - y_k^e\|_\infty < \sigma_L/3, \tag{5.31}$$

for all $k \geq k_2$. The following equality holds since every iteration is successful for $k \geq k_2$:

$$y_{k+1}^e = 2y_k^e - 2\bar{\rho}c(x_k^*) - y_k^* + \Delta y_k^* \text{ for all } k \geq k_2.$$

Rearrangement leads to

$$\Delta y_k^* = \underbrace{y_{k+1}^e - y_k^e}_{(a)} + \underbrace{2\bar{\rho}c(x_k^*)}_{(b)} + \underbrace{y_k^* - y_k^e}_{(c)} \text{ for all } k \geq k_2.$$

Applying the bound given by (5.29) to term (a), the bound given by (5.30) to term (b), and the bound given by (5.31) to term (c) yields

$$-\sigma_L e + \omega_k e < \Delta y_k^* < \sigma_L e - \omega_k e \text{ for all } k \geq k_2.$$

Since $\sigma_L \leq \sigma_k$ for all k, it follows that

$$-\sigma_k e + \omega_k e < \Delta y_k^* < \sigma_k e - \omega_k e \text{ for all } k \geq k_2 \quad .$$

Therefore,

$$\sigma_k e - \Delta y_k^* > \omega_k$$

$$\sigma_k e + \Delta y_k^* > \omega_k$$

Comparison of these equations with conditions (5.7i) and (5.7j) on page 128 implies

$$\|u_k^*\|_\infty \leq \omega_k \text{ and } \|v_k^*\|_\infty \leq \omega_k.$$

□

This theorem shows that the linearized constraints are asymptotically satisfied provided $\{\sigma_k\}$ is bounded away from zero. The update used by Friedlander and Saunders for σ_k in the successful case *guarantees* that $\sigma_k \geq 1/(1+\bar{\rho})$ and hence that σ_k stays bounded away from zero. The updated used by the pdℓ_1-LCL Algorithm 5.4.1 is likely to generate smaller values of σ_k than those generated by the sLCL algorithm. As a result, the update proposed for σ_k for the successful case may be more stabile since convergence is guaranteed when *multiple* limit points exist, but at the expense of rate of convergence. In practice, it might be wise to allow σ_k to increase in the successful case a finite number of times. This will not affect the global convergence proof, but may help recover the fast local convergence rate of LCL methods. However, Friedlander and Saunders point out that $\|\Delta y_k^*\|$ is expected to decrease at a linear rate. If the forcing sequence used in the "if" part for the update to η_k in the successful case converges *sub*linearly, then σ_k would be expected to stay bounded away from zero. In this way, the fast local convergence of Robinson's LCL method is recovered.

5.8 Finite Termination

The following result follows from Corollary 5.6 in [13]. It says that Algorithm 5.4.1 will eventually terminate when ω_* and η_* are strictly positive, as they are in practice.

Corollary 5.8.1 (Finite Termination)**.** *Suppose the convergence tolerances ω_* and η_* are strictly positive. Then, under the conditions of Corollary* 5.6.1*, Algorithm* 5.4.1 *terminates after a finite number of iterations.* □

5.9 Second-Order Points

The proposed primal-dual ℓ_1 LCL algorithm requires a solution to subproblem (5.5) on page 127 at every iteration. Solutions to these subproblems satisfy the first-order conditions (5.7) on page 128. Since these are first-order conditions, only convergence to *first-order* points may be proved. It is reasonable to believe that if certain second-order conditions are enforced at each subproblem solution, then convergence to points satisfying certain second-order conditions may be obtained. To this end, the following definition and assumption are used.

Definition 5.9.1 (Second-order sufficiency). *The first-order KKT point* (x^*, y^*, z^*) *satisfies the second-order sufficiency conditions for problem* GNPs *if it satisfies strict complementarity and if*

$$\Delta x^T H(x^*, y^*)\Delta x > 0$$

for all $\Delta x \neq 0$ *such that* $\Delta x_{FX} = 0$ *and* $J(x^*)\Delta x = 0$, *where* Δx_{FX} *represents the components of* Δx *corresponding to those* x*-variables that are fixed at their bound.*

(AS4). Let $(x_k^*, y_k^*, \Delta y_k^*, z_k^*, w_k^*)$ be a sequence of solutions to subproblem (5.5) on page 127, and let $\{x_k^*\}_K \to x^*$. For all $k \in K$ large enough let the following conditions hold for some δ_1, $\delta_2 > 0$ independent of k:

a) (Strict complementarity)

$$\max(x_k^*, z_k^*) \geq \delta_1 e, \tag{5.32}$$

$$\max(\gamma_k e - y_k^*, |w_k^*|) \geq \delta_2 e, \tag{5.33}$$

$$\max(\gamma_k e + y_k^*, |w_k^*|) \geq \delta_2 e. \tag{5.34}$$

b) (Second-order condition)

$$\Delta w^T D_k \Delta w \geq \delta_1 \|\Delta w\|^2, \tag{5.35}$$

where

$$\Delta w = \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix},$$

$$D_k = \begin{pmatrix} H\big(x_k^*, 2y_k^e - 2\rho_k c(x_k^*) - y_k^*\big) + 2\rho_k J(x_k^*)^T J(x_k^*) & J(x_k^*)^T \\ J(x_k^*) & \frac{1}{\rho_k} I \end{pmatrix},$$

for all $\Delta w \neq 0$ such that $\Delta x_{FX} = 0$ and $J(x_k)\Delta x = 0$.

Condition (5.32) is the normal complementarity condition on the x-variables. Conditions (5.33) and (5.34) imply that the vector y_k^* is "free" from its bound for k sufficiently large. Condition (5.35) implies that the sequence of minimum eigenvalues of the reduced Hessian of the primal-dual augmented Lagrangian is eventually positive and bounded away from zero. These are reasonable conditions for the following reasons. First, Theorem 5.7.1 says that if $\{\rho_k\}$ remains uniformly bounded then for k sufficiently large u_k^* and v_k^* will be considered fixed by the subproblem solver. Second, it will be pointed out in Section 5.10 that $\{\rho_k\}$ usually will remain bounded.

Theorem 5.9.1 (Convergence to an isolated local minimizer)**.** *Let* $\{(x_k, y_k, y_k^e, z_k)\}$ *be the sequence of vectors generated by Algorithm* 5.4.1*. Let* x_* *be the single limit point of* $\{x_k^*\}$*. Suppose that assumptions* AS1a*,* AS2a*,* AS2b*,* AS3*, and* AS4 *hold, that* $\{\rho_k\}$ *remains uniformly bounded, and that* $\sigma_k \geq \sigma_L > 0$ *for all* k*. Then* (x_*, y_*, z_*) *is an isolated local minimizer.*

Proof. First note that $\rho_k \equiv \bar{\rho}$ for all k sufficiently large. This follows since $\{\rho_k\}$ is uniformly bounded and by examination of Algorithm 5.4.1.

Theorem 5.5.1 and Corollary 5.6.2 show that

$$\lim_{k\to\infty} (x_k^*, y_k^*, z_k^*) = (x_*, y_*, z_*)$$

and

$$\lim_{k\to\infty} (x_k, y_k, y_k^e, z_k) = (x_*, y_*, y_*, z_*)$$

and that (x_*, y_*, z_*) is a first-order KKT point. Assumption AS4 implies that $\max(x_k^*, z_k^*) \geq \delta_1 e$. Taking limits yields $\max(x^*, z^*) \geq \delta_1 e > 0$. Thus, (x^*, z^*) satisfies strict complementarity.

Part a) of AS4 ensures strict complementarity in the x- and y-variables. The reduced costs for u_k^* and v_k^* are given by $\sigma_k e - \Delta y_k^*$ and $\sigma_k e + \Delta y_k^*$, respectively. Strict complementarity holds in the u- and v-variables since $\sigma_k \geq \sigma_L > 0$ and since Corollary 5.5.1 implies that $\lim_{k\to\infty} \Delta y_k^* = 0$. Since strict complementarity holds in all variables, it follows that the optimal active set is identified by the subproblem in a neighborhood of a solution. Also note that

$$\lim_{k\to\infty} \left(2y_k^e - 2\rho_k c(x_k^*) - y_k^*\right) = y_* \tag{5.36}$$

since $\lim_{k\to\infty}(y_k^e, y_k^*) = (y_*, y_*)$, $\{\rho_k\}$ is uniformly bounded, and $\lim_{k\to\infty} c(x_k^*) = 0$.

Define the matrix

$$A_k = \begin{pmatrix} J(x_k) & 0 \\ E_{FX} & 0 \end{pmatrix},$$

where E_{FX} are the rows of the $n \times n$ identity matrix corresponding to components of x_k^* that are fixed. Taking limits leads to

$$A_* = \begin{pmatrix} J(x_*) & 0 \\ E_{FX} & 0 \end{pmatrix}.$$

The claim is that A_* has full row rank. This is proved by showing that A_*^T has full column rank. Let $(\zeta_1, \zeta_2) \neq 0$ be in the null-space of A_*^T so that

$$\begin{pmatrix} J(x_*)^T & E_{FX}^T \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

where E_{FX}^T are the columns of the $n \times n$ identity matrix corresponding to components of x_k^* that are fixed. The first set of equations gives $J(x_*)^T\zeta_1 + E_{FX}^T\zeta_2 = 0$. Since $[E_{FX}^T\zeta_2]_{FR} = 0$, this implies $[J(x_*)^T\zeta_1]_{FR} = J_{FR}(x_*)^T\zeta_1 = 0$. The full row rank assumption AS3 implies $\zeta_1 = 0$, and therefore $E_{FX}^T\zeta_2 = 0$. Examining the fixed components shows $[E_{FX}^T\zeta_2]_{FX} = \zeta_2 = 0$. Thus, $(\zeta_1, \zeta_2) = 0$ implying that A_*^T has full column rank.

Since A_k converges to the full row-rank matrix A_*, and since the optimal active set is identified for k sufficiently large, Gill et al. [16] give the existence of matrices Z_k and Z_* such that the columns of Z_k and Z_* form a basis for the null-space of A_k and A_*, respectively. Furthermore, $\lim_{k\to\infty} Z_k = Z_*$.

With this notation, part b) of AS4 is equivalent to $Z_k^T D_k Z_k \succeq \delta_1$. Taking limits, using equation (5.36), and continuity of the spectrum of a matrix, yields

$Z_*^T D_* Z_* \succeq \delta_1$, where

$$D_* = \begin{pmatrix} H(x_*, y_*) + 2\bar{\rho} J(x_*)^T J(x_*) & J(x_*)^T \\ J(x_k^*) & \frac{1}{\bar{\rho}} I \end{pmatrix}.$$

Now let $\Delta\bar{x}$ be any nonzero vector such that $J(x_*)\Delta\bar{x} = 0$ and $\Delta\bar{x}_{FX} = 0$. Then $(\Delta\bar{x}, 0)^T \in \text{null}(A_*)$ and thus there exists a *nonzero* vector q such that

$$\begin{pmatrix} \Delta\bar{x} \\ 0 \end{pmatrix} = Z_* q.$$

The following then holds

$$\begin{aligned} \Delta\bar{x}^T H(x_*, y_*) \Delta\bar{x} &= \Delta\bar{x}^T \big(H(x_*, y_*) + 2\bar{\rho} J(x_*)^T J(x_*) \big) \Delta\bar{x} \\ &= \begin{pmatrix} \Delta\bar{x} \\ 0 \end{pmatrix}^T \begin{pmatrix} H(x_*, y_*) + 2\bar{\rho} J(x_*)^T J(x_*) & J(x_*)^T \\ J(x_*) & \frac{1}{\bar{\rho}} I \end{pmatrix} \begin{pmatrix} \Delta\bar{x} \\ 0 \end{pmatrix} \\ &= q^T Z_*^T D_* Z_* q \\ &\geq \delta_1 \|q\|^2 > 0. \end{aligned}$$

The first equality follows since $\Delta\bar{x} \in \text{null}\big(J(x_*)\big)$. The second equality can be seen by multiplying the given matrices. The third equality follows from the definitions of q, Z_*, and D_*. The rest follows since $q \neq 0$ and $Z_*^T D_* Z_* \succeq \delta_1$.

This shows that (x_*, y_*, z_*) satisfies the second-order sufficiency conditions for problem GNPs and is therefore an isolated local minimizer. □

5.10 Local Convergence

This section considers the convergence properties of the pdℓ_1-LCL Algorithm 5.4.1. It is shown that the local convergence properties of Robinson's original LCL algorithm is maintained when exact subproblem solutions are found.

Bertsekas [2], Conn et al. [5], and Conn, Gould, and Toint in [8] show how to construct forcing sequences $\{\eta_k\}$ such that $\|c(x_k^*)\|$ will eventually always be true. This means that eventually the iterates are always updated and that ρ_k is no longer increased. This result follows since $\{\eta_k\}$ is decreased *sub*linearly and $\|c(x_k^*)\|$ decreases superlinearly as $\{\rho_k\} \to \infty$. Therefore, for the remainder of this section it is assumed that $\{\rho_k\}$ is uniformly bounded so that $\rho_k \equiv \bar{\rho}$ for all k greater than some positive integer $\bar{k}$.

The following assumption is used.

(AS5) The point (x_*, y_*, z_*) satisfies the second-order sufficiency conditions for problem GNPs as given by Definition 5.9.1.

Robinson in [25] shows that under assumptions AS1a, AS3, and AS5 that his algorithm exhibits R-quadratic convergence. Friedlander and Saunders show that Robinson's convergence analysis applies to their sLCL algorithm by noticing that the sLCL subproblem with $\rho_k \equiv \bar{\rho}$ is equivalent to Robinson's subproblem of a related problem with the same minimizers. Therefore, in a neighborhood of a solution, the only difference between Robinson's Algorithm and the sLCL Algorithm is the update to y_k^e. The different updates are given by:

$$y_{k+1}^e \leftarrow y_k^e + \Delta y_k^*, \qquad \text{[Robinson]} \tag{5.37}$$

$$y_{k+1}^e \leftarrow y_k^e + \Delta y_k^* - \bar{\rho} c(x_k^*). \qquad \text{[sLCL]} \tag{5.38}$$

Friedlander and Saunders viewed the term $\bar{\rho} c(x_k^*)$ as a perturbation of Robinson's update. They also noticed that this perturbation does not interfere with the rate of convergence since Robinson proved that $\{c(x_k^*)\}$ converges to zero at the same rate as $\{x_k^*\}$ converges to x_*.

The pdℓ_1-LCL Algorithm 5.4.1 inherits the convergence properties of the sLCL algorithm when *exact* subproblem solutions are computed and $y_* \in (-\bar{\gamma} e, \bar{\gamma} e)$, where $\bar{\gamma} = \nu(\bar{\rho})^{\alpha_\gamma}$. This can be seen as follows. Suppose that y_k^e is given. If the solution to subproblem (5.5) on page 127 satisfies $y_k^* \in (-\gamma_k e, \gamma_k e)$, then $w_k^* = 0$. Furthermore, the following may be shown

$$\big(x_k^*,\, y_k^*,\, z_k^*,\, \Delta y_k^*\big)_{\text{pd}\ell_1\text{LCL}} = \big(x_k^*,\, y_k^e - \bar{\rho} c(x_k^*),\, z_k^*,\, \Delta y_k^*\big)_{\text{sLCL}}. \tag{5.39}$$

This equation is not meant to be rigorous. The quantities on the left-hand side are quantities related to the solution of subproblem (5.5), while the quantities on the right-hand side are quantities related to the sLCL algorithm. What this means is that the sLCL subproblem solution $(x_k^*, z_k^*, \Delta y_k^*)$ is *identical* to the solution $(x_k^*, z_k^*, \Delta y_k^*)$ for subproblem (5.5). In addition, the first-order multiplier update $y_k^e - \bar{\rho} c(x_k^*)$ for the sLCL algorithm is precisely the vector y_k^* computed as part of the solution of subproblem (5.5). Since the steps executed by the two algorithms are the same, the only difference can occur in the update to y_k^e. The updates are given by:

$$y_{k+1}^e \leftarrow 2y_k^e - 2\bar{\rho} c(x_k^*) - y_k^* + \Delta y_k^*, \qquad [\text{pd}\ell_1\text{-LCL}] \tag{5.40}$$

$$y_{k+1}^e \leftarrow y_k^e - \bar{\rho} c(x_k^*) + \Delta y_k^*. \qquad [\text{sLCL}] \tag{5.41}$$

However, these are equivalent since

$$[x_k^*]_{\text{sLCL}} = [x_k^*]_{\text{pd}\ell_1\text{LCL}}, \tag{5.42}$$

$$[\Delta y_k^*]_{\text{sLCL}} = [\Delta y_k^*]_{\text{pd}\ell_1\text{LCL}}, \tag{5.43}$$

$$[y_k^e - \bar{\rho} c(x_k^*)]_{\text{sLCL}} = [y_k^*]_{\text{pd}\ell_1\text{LCL}}. \tag{5.44}$$

Therefore, with exact subproblem solves, the algorithms are identical and the pdℓ_1-LCL algorithm inherits the convergence properties of the sLCL algorithm. The convergence result is summarized in Theorem 5.10.1 below. For this theorem the following notation is used

$$r_k = \begin{pmatrix} x_k \\ y_k^e \\ z_k \end{pmatrix} \quad \text{and} \quad r_* = \begin{pmatrix} x_* \\ y_* \\ z_* \end{pmatrix}.$$

Theorem 5.10.1 (Robinson [25])**.** *Suppose assumptions* AS1a, AS3*, and* AS5 *hold at* r_**. Further assume that* $y_* \in (-\gamma_0 e, \gamma_0 e)$ *when Algorithm* 5.4.1 *executes. Then there exists a positive constant* δ *such that if* $\|r_0 - r_*\| < \delta$*, then the sequence* $\{r_k\}$

generated by Algorithm 5.4.1 *converges to* r_*. *Moreover, the sequence converges R-quadratically, so that for all* $k \geq 0$,

$$\|r_k - r_*\| \leq L(\tfrac{1}{2})^{2^k} \tag{5.45}$$

for some positive constant L. *Also, the difference between consecutive iterates converges at an R-linear rate:*

$$\|r_{k+1} - r_k\| \leq \delta(\tfrac{1}{2})^k. \ \square$$

Robinson does not state the R-linear rate of convergence of consecutive iterates as part of a result, but it is found in the proof of (5.45). Friedlander and Saunders noticed this and included it as part of Theorem 6.2 in [13].

Bräuninger later showed in [4] that the R-quadratic rate of convergence of Robinson's algorithm could be preserved with only *approximate* solutions of the subproblems. This is done by solving the subproblems to a tolerance that is tightened at a rate similar to the decrease in the square of the primal and dual infeasibilities. Since the sLCL is asymptotically equivalent to Robinson's method applied to a "similar" problem with identical solutions, it follows that Bräuninger's result holds for the sLCL algorithm. Therefore, the sLCL algorithm can maintain R-quadratic convergence under *approximate* solves. However, since the proof of R-quadratic convergence of the pdℓ_1-LCL algorithm is not tied directly to Robinson's method, it can not immediately be stated that Algorithm 5.4.1 is R-quadratically convergent under *approximate* solves. Another way of thinking about it is as follows: 1) the sLCL Algorithm is R-quadratically convergent; 2) Bräuninger showed how to maintain R-quadratic convergence with *approximate* solves; and 3) the *pd*ℓ_1-LCL Algorithm finds solutions that *approximate* the *approximate* solutions of the sLCL algorithm. Therefore, it seems likely that the pdℓ_1-LCL Algorithm is R-quadratically convergent under approximate solves as well.

5.11 Infeasible Problems

Not every optimization problem is well-defined. It is possible that the user of an optimization routine may formulate a set of nonlinear constraints $c(x) = 0$ for which no non-negative solution to $c(x) = 0$ exists. Detecting this situation is difficult and is equivalent to showing that the *global* minimum of

$$\begin{aligned} &\underset{x\in\mathbb{R}^n}{\text{minimize}} \quad \tfrac{1}{2}\|c(x\|^2 \\ &\text{subject to } \ x \geq 0 \end{aligned} \tag{5.46}$$

is strictly positive. This is a very difficult problem. It is of interest to study the behavior of the primal-dual ℓ_1 LCL algorithm in this situation. The next theorem shows that when Algorithm 5.4.1 is applied to an infeasible problem, the subproblem solutions converge to a first-order KKT point of problem (5.46). A point (x, z) is a first-order KKT point for problem (5.46) if it satisfies

$$J(x)^T c(x) = z, \tag{5.47a}$$

$$\min(x, z) = 0. \tag{5.47b}$$

Theorem 5.11.1. *Assume* AS1a *and* AS2a *hold. Suppose* GNPs *is infeasible and that Algorithm* 5.4.1 *is applied with tolerances* $\omega_* = \eta_* = 0$. *Let* $\lim_{k\in K} x_k^* = x_*$. *Then* (x_*, z_*) *is a first-order KKT point for problem* (5.46) *where* $z_* \triangleq J(x_*)^T c(x_*)$. *(Note: Nothing has been said about the sequence* $\{\tau_k\}$ *or the tolerance* τ_**.)*

Proof. Condition (5.7a) on p. 128 shows $x_k^* \geq 0$ for all k. Since $\lim_{k\in K} x_k^* = x_*$, this implies

$$x_* \geq 0. \tag{5.48}$$

Since problem GNPs is infeasible, there exists a positive η such that if $x \geq 0$ then $\|c(x)\| > \eta$. Since $\{\eta_k\} \to 0$ as $k \to \infty$, there exists an integer $k_1 \geq 0$ such that $\|c(x_k^*)\| > \eta_k$ for all $k \geq k_1$. In other words, from k_1 on, all iterates are "*unsuccessful*", which implies that $\{\rho_k\} \to \infty$ and $\{\sigma_k\} \to 0$. Furthermore, x_k and

y_k^e are no longer updated which means that there exists a vector $\bar{x}$ and a vector $\bar{y}$ such that

$$x_k \equiv \bar{x} \;\text{ and }\; y_k^e \equiv \bar{y} \;\text{ for all } k \geq K_1. \tag{5.49}$$

Conditions (5.7b) and (5.7g) on page 128 imply

$$g(x_k^*) - J(x_k^*)^T\big(2\bar{y} - 2\rho_k c(x_k^*) - y_k^*\big) - J(\bar{x})^T \mathit{\Delta} y_k^* \geq -\omega_k e.$$

Rearranging and dividing both sides by ρ_k leads to

$$2J(x_k^*)^T c(x_k^*) \geq \underbrace{-\frac{\omega_k}{\rho_k} e}_{(a)} - \underbrace{\frac{g(x_k^*)}{\rho_k}}_{(b)} + \underbrace{\frac{J(x_k^*)^T(2\bar{y} - y_k^*)}{\rho_k}}_{(c)} + \underbrace{\frac{J(\bar{x})^T \mathit{\Delta} y_k^*}{\rho_k}}_{(d)}. \tag{5.50}$$

Note that assumption AS1a and convergence of $\{x_k^*\}_K \to x_*$ imply

$$\lim_{k\in K} J(x_k^*)^T c(x_k^*) = J(x_*)^T c(x_*) = z_*. \tag{5.51}$$

Term (a) of equation (5.50) goes to zero since $\{\rho_k\} \to \infty$ and $\{\omega_k\} \to 0$. Term (b) goes to zero on K since $\{\rho_k\} \to \infty$ and since $\{g(x_k^*)\}_K \to g(x_*)$. Term (c) goes to zero on K by Lemma 5.5.2 and since $\{J(x_k^*)\}_{k\in K} \to J(x_*)$ and $\rho_k \to \infty$. Finally, term (d) goes to zero since $\bar{x}$ is constant and since equation (5.8) on page 128 shows that $\|\mathit{\Delta} y_k^*\| \to 0$. Equations (5.50) and (5.51) imply

$$z_* = J(x_*)^T c(x_*) \geq 0. \tag{5.52}$$

It is left to show $[z_*]_{\mathcal{I}} = 0$. Since $\lim_{k\in K} x_k^* = x_*$ and $[x_*]_{\mathcal{I}} > 0$, it is the case that $[x_k^*]_{\mathcal{I}} > 0$ for $k \in K$ sufficiently large. Condition (5.7b) and the fact that $\{\omega_k\} \to 0$, gives

$$\min([x_k^*]_{\mathcal{I}}, [z_k^*]_{\mathcal{I}}) = [z_k^*]_{\mathcal{I}} \;\text{ for all } k \in K \text{ sufficiently large.}$$

This implies

$$\begin{aligned}\|[z_k^*]_{\mathcal{I}}\| \leq \|\min(x_k^*, z_k^*)\| &= \Big(\sum_{j=1}^{n} \min([x_k^*]_j, [z_k^*]_j)^2\Big)^{\frac{1}{2}} \\ &\leq \Big(\sum_{j=1}^{n} \omega_k^2\Big)^{\frac{1}{2}} = \sqrt{n}\,\omega_k \;\text{ for all } k \in K \text{ sufficiently large.}\end{aligned}$$

Using condition (5.7f) and the definition of $\widetilde{y}_k$, the following holds

$$\begin{aligned}\sqrt{n}\,\omega_k &\geq \|[z_k^*]_{\mathcal{I}}\| \\ &= \|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T\big(2\bar{y} - 2\rho_k c(x_k^*) - y_k^*\big) - \widehat{J}(\bar{x})^T\Delta y_k^*\| \\ &= \|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T\big(2\bar{y} - 2\rho_k c(x_k^*) - y_k^* + \Delta y_k^*\big) + \big(\widehat{J}(x_k^*) - \widehat{J}(\bar{x})\big)^T\Delta y_k^*\|\end{aligned}$$

for all $k \in K$ sufficiently large. Use of the "reverse" triangle inequality, followed by the classical triangle inequality and Lipshitz continuity of J on $\mathcal{B}_x$ gives a constant M such that

$$\begin{aligned}&2\|\widehat{J}(x_k^*)^T c(x_k^*)\| \\ &\quad\leq \frac{\sqrt{n}\omega_k}{\rho_k} + \frac{\|\hat{g}(x_k^*) - \widehat{J}(x_k^*)^T(2\bar{y} - y_k^* + \Delta y_k^*) + \big(\widehat{J}(x_k^*) - \widehat{J}(\bar{x})\big)^T\Delta y_k^*\|}{\rho_k} \\ &\quad\leq \frac{\sqrt{n}\omega_k}{\rho_k} + \frac{\|\hat{g}(x_k^*)\|}{\rho_k} + \frac{\|\widehat{J}(x_k^*)^T(2\bar{y} - y_k^* + \Delta y_k^*)\|}{\rho_k} + \frac{\|\big(\widehat{J}(x_k^*) - \widehat{J}(\bar{x})\big)^T\Delta y_k^*\|}{\rho_k} \\ &\quad\leq \underbrace{\frac{\sqrt{n}\omega_k}{\rho_k}}_{(a)} + \underbrace{\frac{\|\hat{g}(x_k^*)\|}{\rho_k}}_{(b)} + \underbrace{\frac{\|\widehat{J}(x_k^*)^T(2\bar{y} - y_k^* + \Delta y_k^*)\|}{\rho_k}}_{(c)} + \underbrace{M\frac{\|x_k^* - \bar{x}\|\|\Delta y_k^*\|}{\rho_k}}_{(d)}\end{aligned} \tag{5.53}$$

Terms (a) and (b) go to zero on K since $\{\rho_k\} \to \infty$, $\{\omega_k\} \to 0$ and $\{\hat{g}(x_k^*)\}_K \to \hat{g}(x_*)$. Lemma 5.5.2, Corollary 5.5.1, and the fact that $\{\,\widehat{J}(x_k^*)\,\}_K \to \widehat{J}(x_*)$ shows that term (c) goes to zero on K. Term (d) goes to zero since $\{x_k^*\}$ and $\bar{x}$ are in the compact set $\mathcal{B}_x$ and since $\{\Delta y_k^*\} \to 0$ by Corollary 5.5.1. This means that the right-hand side of (5.53) goes to zero implying

$$\lim_{k\in K} \widehat{J}(x_k^*)^T c(x_k^*) = 0.$$

Combining this with assumption AS1a shows

$$[z_*]_{\mathcal{I}} = \widehat{J}(x_*)^T c(x_*) = \lim_{k\in K} \widehat{J}(x_k^*)^T c(x_k^*) = 0. \tag{5.54}$$

Equations (5.48), (5.52), and (5.54) complete the proof. □

6

Numerical Results

In this chapter we describe numerical experiments that are intended to illustrate the properties of the algorithms formulated and analyzed in Chapters 4 and 5. In particular, we consider a MATLAB [20] implementation of the primal-dual augmented Lagrangian algorithms pdBCL and pdℓ_1-LCL. Since the focus of this thesis has been on the theoretical properties of these methods, only a preliminary implementation is described here. Numerous modifications would be necessary before the software would be suitable for general distribution. The numerical results are intended only to show that the primal-dual approach is a reasonable approach; we expect the efficiency and robustness of the algorithms to be substantially improved in subsequent work.

Numerical results are given for nonlinearly constrained problems from the CUTEr test collection (see Bongartz et al. [3] and Gould, Orban and Toint [17]). The CUTEr problems are defined with the format

$$\begin{array}{ll} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to} & c_\ell \le c(x) \le c_u, \quad a_\ell \le Ax \le a_u, \quad x_\ell \le x \le x_u. \end{array} \tag{6.1}$$

The addition of slack variables gives the equivalent problem:

$$\begin{array}{ll} \underset{x,s_c,s_a}{\text{minimize}} & f(x) \\ \text{subject to} & \begin{pmatrix} c(x) - s_c \\ Ax - s_a \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \\ & \begin{pmatrix} c_\ell \\ a_\ell \end{pmatrix} \le \begin{pmatrix} s_c \\ s_a \end{pmatrix} \le \begin{pmatrix} c_u \\ a_u \end{pmatrix}, \quad x_\ell \le x \le x_u, \end{array}$$

which, for suitable definitions of x, f and c, is equivalent to the problem

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & c(x) = 0, \quad x_\ell \le x \le x_u, \end{array} \tag{6.2}$$

considered earlier in this thesis.

6.1 Test Problem Selection

The test set was constructed by using the CUTEr interactive `select` tool, which allows the identification of groups of problems with certain features. The input for the `select` tool was as follows:

```
Objective function type        : O
Constraints type               : O
Regularity                     : R
Degree of available derivatives : 2
Problem interest               : *
Explicit internal variables    : *
Number of variables            : in [   1,   50]
Number of constraints          : in [   1,   50]
```

These options are defined as follows:

- `Objective function type (O)`: There is a general objective function (i.e., the objective is not constant, linear, quadratic, or a sum of squares).

- `Constraints type (O)`: There are general nonlinear constraints (i.e., the constraints do not consist of only bound-, linear-, quadratic-, fixed-variable, or linear network constraints).
- `Regularity (R)`: The objective and constraint functions are twice-continuously differentiable.
- `Degree of available derivatives (2)`: Analytic second derivatives are available.
- `Number of variables (in [ 1, 50])`: The number of variables is between 1 and 50.
- `Number of constraints (in [ 1, 50])`: The number of constraints is between 1 and 50.

The `select` tool gives 44 problems with these attributes, 32 of which are problems from the Hock and Schittkowski test collection [19].

Four of the 44 problems were then eliminated from the test set. *hs103* and *launch* were omitted because SNOPT was unable to solve them in the slack-variable form (6.2). Problem *hs99exp* is sufficiently badly scaled that the use of *any* optimization method is problematic. Finally, *mesh* was removed because of the existence of feasible points at which the objective values is unbounded below. The final test set was composed of the following 40 problems: *allinitc*, *alsotame*, *bt11*, *bt6*, *cresc4*, *dipigri*, *hs100*, *hs100lnp*, *hs100mod*, *hs101*, *hs102*, *hs104*, *hs107*, *hs109*, *hs111*, *hs111lnp*, *hs26*, *hs40*, *hs46*, *hs47*, *hs56*, *hs60*, *hs64*, *hs68*, *hs69*, *hs7*, *hs71*, *hs74*, *hs75*, *hs77*, *hs78*, *hs79*, *hs80*, *hs81*, *hs93*, *hs99*, *synthes1*, *synthes2*, *synthes3*, and *twobars*.

6.2 Solving the subproblem

Both pdBCL and pdℓ_1-LCL define "outer" and "inner" iterations. The "outer" iterations are responsible for updating parameters and solution estimates, testing optimality, and forming the subproblems. The "inner" iterations are those of the subproblem solver, and the efficiency of this solver has a crucial effect on the overall efficiency of the method.

The software package SNOPT was used as the solver for both the pdBCL and pdℓ_1-LCL subproblem. SNOPT is a sequential quadratic programming (SQP) method that maintains a quasi-Newton approximation of the Hessian of the Lagrangian. An SQP method also generates inner and outer iterations, which we call major and minor iterations to distinguish them from the iterates of the primal-dual methods. In the context of pdBCL and pdℓ_1-LCL, the major iterations generate a sequence of points that converge to the solution of the subproblem. At each major iterate a QP subproblem is used to generate a search direction towards the next major iterate. Solving such a subproblem is itself an iterative procedure, with the minor iterations of an SQP method being the iterations of the QP method. As the outer iterates of the pdBCL and pdℓ_1-LCL methods converge, SNOPT solves a sequence of similar subproblems. This allows the use of the option `warm start` to increase efficiency. In the case of a warm start, the final working set of active constraints from the previous subproblem is used as the first working set of the next problem. SNOPT is available as a library of Fortran and C routines [15]. The package includes a MEX interface that allows SNOPT to be called directly from Matlab.

It must be emphasized that SNOPT may not always be the best solver for the subproblem. SNOPT is a first derivative method that is unable to exploit second derivatives when they are known. It is likely that a second-derivative solver would improve the efficiency of the methods significantly. However, the efficiency of second-derivative solvers is critically dependent on the method used to treat the occurrence of negative curvature in the Hessian of the subproblem. The choice of an appropriate second-derivative solver is an ongoing research issue that is beyond the scope of this thesis. The advantage of SNOPT is that it may be used easily as a "black-box" solver and provides a stable and consistent platform for comparing the pdBCL and pdℓ_1-LCL approaches.

Other issues, unrelated to the choice of solver, also affect the performance of the overall method. In particular, robustness and efficiency may depend on the choice of problem format. For example, if the SNOPT package is applied directly to the Hock-Schittkowski test problems defined in the CUTEr format (6.1) then all the problems are solved successfully. However, SNOPT failed on several of the problems given in the generic form (6.2) that does not distinguish between linear and nonlinear constraints. This observation leads us to the conclusion that the pdBCL and pdℓ_1-LCL approaches may also benefit from exploiting the properties of the constraint gradients. We expand on this topic below.

The purpose of the numerical results is to illustrate the properties of the algorithms formulated and analyzed in Chapters 4 and 5. In some cases, it is necessary to simplify the algorithms in order to simplify the corresponding analysis. Future implementations of the methods proposed here should necessarily incorporate specific improvements that will provide a more efficient and robust algorithm. Some possible improvements are proposed below.

Choice of penalty parameter. Instead of a single penalty parameter μ (or ρ), each constraint should have its own penalty parameter. This generalization would improve robustness on poorly scaled problems. Moreover, the penalty parameter μ should be allowed to *increase* as well as decrease. This property would not violate the theoretical analysis, provided that μ *eventually* goes to zero when infinitely many "unsuccessful" iterations occur. The BCL or LCL subproblems tend to be more difficult to solve for small values of μ. However, practical experience has also shown that a slow decrease in μ early on, may be quite expensive. In practice it is necessary to strike a balance between decreasing μ when things go wrong and increasing μ for later iterates in the neighborhood of the solution.

Exploiting linear constraints and bounds. As each subproblem is expressed in the generic form (6.2), the problem structure induced by the presence of linear constraints and simply-bounded slack variables is not communicated to the solver SNOPT. If the linear constraints are known, an initial point may be found that satisfies the linear constraints and bounds. For example, in the LCL subproblem, the linearly constrained subproblem has the form

$$\begin{array}{ll} \underset{x,y,s_c,s_a,u,v}{\text{minimize}} & \mathcal{M}(x,y;y_k^e,\rho_k) + \sigma e^T(u+v) \\ \text{subject to} & \begin{pmatrix} \bar{c}_k(x) - s_c + u - v \\ Ax - s_a \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \\ & \begin{pmatrix} c_\ell \\ a_\ell \end{pmatrix} \le \begin{pmatrix} s_c \\ s_a \end{pmatrix} \le \begin{pmatrix} c_u \\ a_u \end{pmatrix}, \quad u,v \ge 0, \\ & x_\ell \le x \le x_u, \quad -\gamma_k e \le y \le \gamma_k e. \end{array} \tag{6.3}$$

Thus, it is beneficial to define an initial point as the solution of one of the following *proximal-point problems*:

$$\text{PP1} \qquad \begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & \|x - \widehat{x}\|_1 \\ \text{subject to} & \begin{pmatrix} x_\ell \\ a_\ell \end{pmatrix} \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le \begin{pmatrix} x_u \\ a_u \end{pmatrix} \end{array} \tag{6.4}$$

or

$$\text{PP2} \qquad \begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & \tfrac{1}{2}\|x - \widehat{x}\|^2 \\ \text{subject to} & \begin{pmatrix} x_\ell \\ a_\ell \end{pmatrix} \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le \begin{pmatrix} x_u \\ a_u \end{pmatrix}, \end{array} \tag{6.5}$$

where $\widehat{x}$ is the initial value input by the user. Problems PP1 and PP2 compute a vector x "close" to $\widehat{x}$ that satisfies the linear constraints. If the solver returns that either PP1 or PP2 is infeasible, then the problem should be assumed infeasible.

There are additional benefits for LCL methods if the initial point is feasible with respect to the linear constraints. If x_0 is feasible for the linear constraints, then so are all subsequent iterates, which implies that the linear constraints need not be included in the augmented Lagrangian term of the objective function. This approach is used by Friedlander and Saunders in [13].

6.3 The pdBCL Method

The pdBCL subproblems for the problem format (6.2) take the form

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n, y\in\mathbb{R}^m}{\text{minimize}} & \mathcal{M}(x, y; y_k^e, \mu_k) \\ \text{subject to} & -\gamma_k e \le y \le \gamma_k e, \quad x_\ell \le x \le x_u. \end{array} \tag{6.6}$$

Table 6.1 lists the default parameter values used for the pdBCL method.

Table 6.1: Default parameter values used by pdBCL method.

Parameter	Value	Parameter	Value
μ_0	8.0e-1	η_0	8.0e-1
ω_0	1.0e+0	τ_*	1.0e-6
η_*	1.0e-6	ω_*	1.0e-6
μ_c	5.0e-1	τ_f	1.0e+0
α_γ	5.0e-1	k_τ	1.0e+0
α_η	1.0e-1	α_ω	1.0e+0
β_η	9.0e-1	β_ω	1.0e+0
		α_τ	1.5e+0

As discussed in Chapter 4, the primal-dual BCL Algorithm 4.2.1 provides a step for generating a higher-order update for y_e. Table 6.3 and Table 6.4 compare the following three alternatives: (i) a first-order update; (ii) a trajectory-following update; and (iii) the second-order Newton update. The first-order update modifies y_e by the primal-dual first-order update (see Section 4.1). The trajectory-following update was discussed in subsection 4.8.2; after an approximate point on the trajectory is found, one step of Newton's Method is performed for minimizing the primal-dual augmented Lagrangian function for a smaller value of the penalty parameter. This approach depends critically on how the smaller value of the penalty parameter is chosen. The second-order Newton update was discussed in subsection 4.8.1; it is one step of Newton's method for finding a zero of the function F_2 (see p. 119). Ideally, the second-order update to y_e should be "damped". It is well known that Newton's method is not globally convergent and additional safeguards are necessary to guarantee global convergence. A simple option is to use the Newton step in a line-search that guarantees sufficient decrease in $\|F_2\|$. Near a solution of the original problem, the Newton step would be accepted and the usual rapid convergence of Newton's method is expected. Far from a solution, the line search should greatly stabilize the algorithm. Preliminary testing indicates that the update to y_e leads to significant unwanted oscillation between first and second-order estimates, particularly when far from a solution.

In Tables 6.3 and 6.4 three statistics are reported: `Major`, `Minor`, and `QPits`. Column `Major` refers to the number of "outer" iterations. Therefore, the number reported is the number of bound constrained subproblems that were solved. Column `Minor` refers to the number of "inner" iterations, i.e., the number of quadratic programs solved by SNOPT. Thus, this column represents the number of function evaluations. Evaluation of f, g, c, J, and H is counted as a single function evaluation. Finally, column `QPits` refers to the number of QP iterations performed by SNOPT. Note that this is *not* the number of quadratic programs, but rather the number of total iterations used to solve every QP for that problem.

The first-order updating scheme requires the most iterates and function evaluations, while the Newton second-order method requires the fewest. It is also clear that the trajectory following update shows improvement over the first-order updating strategy, but is still inferior to the Newton second-order update.

6.4 The pdℓ_1-LCL Method

The pdℓ_1-LCL subproblems associated with the problem format (6.2) take the form

$$\begin{array}{ll} \underset{x,y,u,v}{\text{minimize}} & \mathcal{M}(x,y;y_k^e,\rho_k) + \sigma e^T(u+v) \\ \text{subject to} & \bar{c}_k(x) + u - v = 0, \\ & x_\ell \le x \le x_u, \quad -\gamma_k e \le y \le \gamma_k e, \quad u,v \ge 0. \end{array} \tag{6.7}$$

Table 6.2 lists the default parameter values used for the pdℓ_1-LCL method.

Table 6.2: Default parameter values used by pdℓ_1-LCL method.

Parameter	Value	Parameter	Value
ρ_0	`1.0e+0`	σ_0	`100`
ω_0	`1.0e+0`	τ_*	`1.0e-6`
η_*	`1.0e-6`	ω_*	`1.0e-6`
τ_ρ	`8.0e+0`	τ_σ	`5.0e+0`
k_τ	`1.0e+0`	α_γ	`5.0e-1`
α_η	`1.0e-1`	α_τ	`-1.2e+0`
β_η	`9.0e-1`	δ	`1.0e+0`

In Table 6.5 and 6.6 three statistics are reported: `Major`, `Minor`, and `QPits`. Column `Major` refers to the number of "outer" iterations. Therefore, the number reported is the number of linearly constrained subproblems that were solved. Column `Minor` refers to the number of "inner" iterations, i.e., the number of quadratic programs solved by SNOPT. Thus, this column represents the number of function evaluations. Evaluation of f, g, c, J, and H is counted as a single function evaluation. Finally, column `QPits` refers to the number of QP iterations performed by SNOPT. Note that this is *not* the number of quadratic programs, but rather the number of total iterations used to solve every QP for that problem.

As in the case of BCL, some simple changes to the algorithm will provide better performance. The LCL optimization package MINOS [23] is relatively reliable and exhibits good rates of convergence. Thus, a better algorithm would be obtained by simulating the use of MINOS by starting with the elastic variables u and v fixed at zero and not allow them to move. The Lagrange multipliers Δy of the linearized constraints may then be monitored and if the quantity $\|\Delta y\|_\infty$ ever exceeds the bound guaranteed if u and v were allowed to deviate, then "elastic" mode is entered. In other words, a primal-dual version of MINOS would be used, and only if things start going poorly would elastic mode be entered. This should give great improvement in the numerical results.

Table 6.3: Comparison of different pdBCL updates. (Problems 1–20)

	First-order			Trajectory			Second-order		
Problem	Major	Minor	QPits	Major	Minor	QPits	Major	Minor	QPits
allinitc	97	6463	7469	96	13294	14189	18	165	171
alsotame	58	90	112	24	47	59	4	10	10
bt11	55	107	121	30	380	395	6	20	28
bt6	59	286	376	29	228	255	8	38	54
cresc4	13	632	1017	19	1763	3341	10	538	972
dipigri	17	1091	1372	13	614	873	5	236	468
hs100	16	983	1277	12	539	811	4	230	474
hs100lnp	59	371	505	14	255	361	4	97	188
hs100mod	32	1390	2386	100	1413	2434	6	409	874
hs101	100	41347	86712	27	37501	78077	7	2410	5304
hs102	100	20624	43964	100	63604	139411	15	9034	19434
hs104	55	6115	11594	57	8196	15102	20	1918	3011
hs107	100	1228	2226	100	2468	3506	27	2086	3715
hs109	100	1304	3344	100	8654	20852	22	2427	5459
hs111	24	478	529	22	355	383	10	38	66
hs111lnp	24	478	529	22	355	383	10	38	66
hs26	62	97	168	25	86	96	18	39	49
hs40	28	72	112	21	401	698	5	5	18
hs46	61	180	253	22	171	187	18	21	34
hs47	63	199	276	16	161	177	13	17	32

Table 6.4: Comparison of different pdBCL updates. (Problems 21–40)

	First-order			Trajectory			Second-order		
Problem	Major	Minor	QPits	Major	Minor	QPits	Major	Minor	QPits
hs56	18	69	99	21	181	196	27	29	42
hs60	63	128	201	31	119	135	6	22	30
hs64	34	472	546	34	506	547	6	42	83
hs68	61	579	771	48	821	913	64	591	908
hs69	17	680	947	21	658	814	43	1419	2582
hs7	62	102	107	33	75	81	5	7	13
hs71	56	105	216	34	190	301	10	159	276
hs74	53	728	1244	100	1317	2326	4	171	384
hs75	100	2333	4995	100	4145	9047	5	110	245
hs77	57	305	389	24	247	274	6	37	54
hs78	56	87	158	15	131	151	5	12	29
hs79	62	181	257	18	218	237	6	12	27
hs80	57	85	214	25	128	231	5	10	28
hs81	53	91	249	27	195	306	5	7	25
hs93	21	1010	2009	21	1049	2038	22	683	1209
hs99	100	1199	4168	100	1411	5184	5	329	810
synthes1	17	231	292	23	473	531	9	291	639
synthes2	20	1133	1436	23	1489	1818	19	1146	1428
synthes3	11	1221	1849	13	1362	2011	14	2119	5686
twobars	59	91	117	27	186	228	7	11	29

Table 6.5: Primal-Dual ℓ_1-LCL Method. (Problems 1–20)

	pdℓ_1-LCL		
Problem	Major	Minor	QPits
allinitc	60	2505	2933
alsotame	6	6	26
bt11	23	126	460
bt6	9	76	140
cresc4	20	1605	3593
dipigri	19	315	643
hs100	18	331	648
hs100lnp	19	48	162
hs100mod	19	451	745
hs101	48	33159	65470
hs102	34	19359	37048
hs104	20	775	1756
hs107	14	1014	2207
hs109	20	7757	12634
hs111	21	348	784
hs111lnp	21	346	764
hs26	11	63	106
hs40	12	9	68
hs46	9	56	118
hs47	19	371	794

Table 6.6: Primal-Dual ℓ_1-LCL Method. (Problems 21–40)

	pdℓ_1-LCL		
Problem	Major	Minor	QPits
hs56	18	102	327
hs60	8	39	70
hs64	17	460	646
hs68	19	478	757
hs69	18	453	701
hs7	16	60	117
hs71	15	21	108
hs74	19	60	193
hs75	39	2159	3561
hs77	13	1454	2230
hs78	18	13	129
hs79	7	16	68
hs80	15	12	116
hs81	15	12	116
hs93	15	557	838
hs99	28	4817	9680
synthes1	23	12	221
synthes2	9	643	2434
synthes3	60	8247	60468
twobars	18	13	108

Bibliography

[1] D. P. Bertsekas. *Constrained optimization and Lagrange multiplier methods.* Academic Press, New York and London, 1982.

[2] D. P. Bertsekas. *Constrained optimization and Lagrange multiplier methods.* Computer Science and Applied Mathematics. Academic Press Inc. [Harcourt Brace Jovanovich Publishers], New York, 1982.

[3] I. Bongartz, A. R. Conn, N. I. M. Gould, and Ph. L. Toint. CUTE: Constrained and unconstrained testing environment. *ACM Trans. Math. Softw.*, 21(1):123–160, 1995.

[4] J. Bräuninger. A modification of Robinson's algorithm for general nonlinear programming problems requiring only approximate solutions of subproblems with linear equality const. In *Optimization techniques (Proc. 8th IFIP Conf., Würzburg, 1977), Part 2*, volume 7 of *Lecture Notes in Control and Information Sci.*, pages 33–41. Springer, Berlin, 1978.

[5] A. R. Conn, N. Gould, A. Sartenaer, and P. L. Toint. Convergence properties of an augmented Lagrangian algorithm for optimization with a combination of general equality and linear constraints. *SIAM J. Optim.*, 6(3):674–703, 1996.

[6] A. R. Conn, N. I. M. Gould, and Ph. L. Toint. Global convergence of a class of trust region algorithms for optimization with simple bounds. *SIAM J. Numer. Anal.*, 25:433–460, 1988.

[7] A. R. Conn, N. I. M. Gould, and Ph. L. Toint. A comprehensive description of LANCELOT. Technical Report 91/10, Département de Mathématique, Facultés Universitaires de Namur, 1991.

[8] A. R. Conn, N. I. M. Gould, and Ph. L. Toint. A globally convergent augmented Lagrangian algorithm for optimization with general constraints and simple bounds. *SIAM J. Numer. Anal.*, 28:545–572, 1991.

[9] A. R. Conn, N. I. M. Gould, and Ph. L. Toint. *Trust-Region Methods*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2000.

[10] A. V. Fiacco and G. P. McCormick. *Nonlinear Programming: Sequential Unconstrained Minimization Techniques*. John Wiley and Sons, Inc., New York-London-Sydney, 1968.

[11] R. Fletcher. An ℓ_1 penalty method for nonlinear constraints. In P. T. Boggs, R. H. Byrd, and R. B. Schnabel, editors, *Numerical Optimization 1984*, pages 26–40, Philadelphia, 1985.

[12] A. Forsgren and P. E. Gill. Primal-dual interior methods for nonconvex nonlinear programming. *SIAM J. Optim.*, 8:1132–1152, 1998.

[13] M. P. Friedlander and M. A. Saunders. A globally convergent linearly constrained Lagrangian method for nonlinear optimization. *SIAM J. Optim.*, 15(3):863–897 (electronic), 2005.

[14] P. E. Gill, W. Murray, and M. A. Saunders. SNOPT: An SQP algorithm for large-scale constrained optimization. *SIAM Rev.*, 47:99–131, 2005.

[15] P. E. Gill, W. Murray, and M. A. Saunders. User's guide for SNOPT Version 7: Software for large-scale nonlinear programming. Numerical Analysis Report 2006-2, Department of Mathematics, University of California, San Diego, La Jolla, CA, 2006.

[16] P. E. Gill, W. Murray, M. A. Saunders, G. W. Stewart, and M. H. Wright. Properties of a representation of a basis for the null space. *Math. Program.*, 33:172–186, 1985.

[17] N. I. M. Gould, D. Orban, and Ph. L. Toint. CUTEr and SifDec: A constrained and unconstrained testing environment, revisited. *ACM Trans. Math. Softw.*, 29(4):373–394, 2003.

[18] M. R. Hestenes. Multiplier and gradient methods. *J. Optim. Theory Appl.*, 4:303–320, 1969.

[19] W. Hock and K. Schittkowski. *Test Examples for Nonlinear Programming Codes*. Lecture Notes in Economics and Mathematical Systems 187. Springer Verlag, Berlin, Heidelberg and New York, 1981.

[20] MathWorks Inc., Natick, Massachusetts. *Matlab User's Guide*, 1992.

[21] B. A. Murtagh and M. A. Saunders. Large-scale linearly constrained optimization. *Math. Program.*, 14:41–72, 1978.

[22] B. A. Murtagh and M. A. Saunders. A projected Lagrangian algorithm and its implementation for sparse nonlinear constraints. *Math. Program.*, 16:84–117, 1982.

[23] B. A. Murtagh and M. A. Saunders. MINOS 5.5 User's Guide. Report SOL 83-20R, Department of Operations Research, Stanford University, Stanford, CA, Revised 1998.

[24] M. J. D. Powell. A method for nonlinear constraints in minimization problems. In R. Fletcher, editor, *Optimization*, pages 283–298, London and New York, 1969. Academic Press.

[25] S. M. Robinson. A quadratically-convergent algorithm for general nonlinear programming problems. *Math. Program.*, 3:145–156, 1972.

[26] R. T. Rockafellar. Augmented Lagrangians and applications of the proximal point algorithm in convex programming. *Math. Oper. Res.*, 1(2):97–116, 1976.

[27] R. T. Rockafellar. Monotone operators and the proximal-point algorithm. *SIAM J. Control Optim.*, 14:877–898, 1976.