An interior-point ℓ_1-penalty method for nonlinear optimization

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Abstract

A mixed interior/exterior-point method for nonlinear programming is described, that handles constraints by an ℓ_1-penalty function. A suitable decomposition of the penalty terms and embedding of the problem into a higher-dimensional setting leads to an equivalent, surprisingly regular, reformulation as a smooth penalty problem only involving inequality constraints. The resulting problem may then be tackled using interior-point techniques as finding a strictly feasible initial point is trivial. The reformulation relaxes the shape of the constraints, promoting larger steps and easing the nonlinearity of the strictly feasible set in the neighbourhood of a solution. If finite multipliers exist, exactness of the penalty function eliminates the need to drive the corresponding penalty parameter to infinity. Global and fast local convergence of the proposed scheme are established and practical aspects of the method are discussed.

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1 Introduction

A typical nonlinear programming problem is to

$$\begin{aligned} \underset{x\in\mathbb{R}^n}{\text{minimize}} \quad & f(x) && (1.1a)\\ \text{such that} \quad & c_{\mathcal{E}}(x) = 0 && (1.1b)\\ \text{and} \quad & c_{\mathcal{I}}(x) \geq 0, && (1.1c) \end{aligned}$$

involving a mixture of smooth, general, possibly nonlinear and nonconvex, equality and inequality constraints. Here $f\colon \mathbb{R}^n \to \mathbb{R}$, $c_{\mathcal{E}}\colon \mathbb{R}^n \to \mathbb{R}^{n_{\mathcal{E}}}$ and $c_{\mathcal{I}}\colon \mathbb{R}^n \to \mathbb{R}^{n_{\mathcal{I}}}$, where $\mathcal{E} = \{1,\ldots,n_{\mathcal{E}}\}$ and $\mathcal{I} = \{n_{\mathcal{E}}+1,\ldots,n_{\mathcal{E}}+n_{\mathcal{I}}\}$.

In this paper, we propose an interior-point approach for (1.1). At first sight, two difficulties emerge. Firstly, since we allow equality constraints, this might appear to preclude a interior approach. Secondly, a feasible initial point is not necessarily easily or efficiently found. To circumvent these difficulties, we embed the set of variables into a higher dimensional space for which the constraints have a nonempty and easily locatable interior. The resulting interior-point method has therefore an infeasible flavour.

A common way of attempting to solve (1.1) is build the corresponding ℓ_1-penalty function and to

$$\underset{x\in\mathbb{R}^n}{\text{minimize}} \quad \phi^{\mathrm{P}}(x,\nu) \stackrel{\text{def}}{=} f(x) + \nu\sum_{i\in\mathcal{E}}|c_i(x)| + \nu\sum_{i\in\mathcal{I}}\max[-c_i(x),0] \tag{1.2}$$

for some sufficiently-large penalty parameter, ν. However (1.2) is not smooth, and it might appear that sophisticated tools are needed to handle the derivative discontinuities in such a minimization. This is not the case. For, as we will see in Section 2, (1.2) is equivalent to the *smooth* problem

$$\begin{aligned} \underset{x\in\mathbb{R}^n,\ s\in\mathbb{R}^{n_{\mathcal{C}}}}{\text{minimize}} \quad & \phi^{\mathrm{S}}(x,s;\nu) \stackrel{\text{def}}{=} f(x) + \nu\sum_{i\in\mathcal{E}}[c_i(x)+2s_i] + \nu\sum_{i\in\mathcal{I}}s_i \\ \text{subject to} \quad & c(x)+s \geq 0 \quad \text{and} \quad s \geq 0, \end{aligned} \tag{1.3}$$

involving $n_{\mathcal{C}}$ additional so-called “elastic” variables s, where $\mathcal{C} \stackrel{\text{def}}{=} \mathcal{E}\cup\mathcal{I}$ and $n_{\mathcal{C}} \stackrel{\text{def}}{=} n_{\mathcal{E}}+n_{\mathcal{I}}$. This problem only involves *inequality* constraints, and it is trivial to pick s sufficiently large so that (x,s) is strictly feasible for (1.3).

Having embedded (1.1) in a higher-dimensional space involving only inequalities, an immediate possibility is to apply an interior-point method to the resulting problem (1.3). Thus, one might (approximately)

$$\underset{x\in\mathbb{R}^n,\ s\in\mathbb{R}^{n_{\mathcal{C}}}}{\text{minimize}} \quad \phi^{\mathrm{B}}(x,s;\mu,\nu) \stackrel{\text{def}}{=} \phi^{\mathrm{S}}(x,s;\nu) - \mu\sum_{i\in\mathcal{C}}\log(c_i(x)+s_i) - \mu\sum_{i\in\mathcal{C}}\log s_i. \tag{1.4}$$

for a sequence of barrier parameters, $\{\mu^k\}$, converging to zero from above. A theoretical investigation of the properties of ϕ^{B} and the problem (1.4) form the basis of Section 2 and Section 2.3. The global and local convergence properties of two standard trust-region methods for solving (1.4), both for fixed (μ,ν) and as they are modified are considered in Section 3. Algorithmic improvements, and extensions are described in Section 5 and Section 7, and conclusions drawn in Section 8.

The use of the transformation to the ℓ_1-penalty function to solve (1.1) is, of course, well known. The equivalence between the optimality conditions for nonconvex nonlinear programming problems and related penalty functions was first reported by Pietrzykowski (1969), and the results subsequently strengthened by Charalambous (1978), Han and Mangasarian (1979), Coleman and Conn (1980), Bazaraa and Goode (1982) and Huang and Ng (1994). See also Fletcher (1987, Chapters 12 and 14). In Section 2, we shall see how this equivalence is inherited by the problem (1.3).

The approach taken in this paper has its genesis in the work of Mayne and Polak (1976), more recently extended by Herskovits (1986), Lawrence and Tits (1996) and Tits, Wächter, Bakhtiari, Urban and Lawrence (2002), all of whom also reformulate (1.1) so as only to involve inequality constraints. Indeed, our basic approach coincides with theirs on setting s to zero. However, we prefer not to do this, as the resulting problem then has no obvious initial feasible point. More recently, Armand, Gilbert and Jan-Jégou (2002) investigated the reformulation

$$\underset{x \in \mathbb{R}^n,\, s \in \mathbb{R}^{n_\mathcal{I}}}{\text{minimize}} \quad f(x) \ \text{ such that } \ c_\mathcal{I}(x) + s \geq 0 \ \text{ and } \ s = 0, \tag{1.5}$$

for convex, inequality-constrained problems in which the resulting equality constraints $s = 0$ are handled by penalization. This idea was refined by Armand (2002) to give (1.3) in the convex, inequality-constrained case, which he then solved by minimizing a sequence of (convex) barrier functions like (1.4).

The present approach is also related to the so-called *elastic mode* used in the SNOPT package (Gill, Murray and Saunders 2002) and in Boman (1999), where it is used in a sequential quadratic programming framework as a fallback strategy to relax the constraints in case the current quadratic subproblem appears to be infeasible, unbounded or to have unbounded multipliers. In such a case, once the elastic mode has been triggered, it persists until convergence.

2 Equivalent smooth reformulations of the exact penalty function

2.1 Possible reformulations

As mentioned in Section 1, one way to treat the nonlinear constraints (1.1b)–(1.1c) is instead to minimize the non-differentiable ℓ_1-penalty function

$$\phi^{\mathrm{P}}(x;\nu) = f(x) + \nu \vartheta^{\mathrm{P}}(x), \tag{2.1}$$

where

$$\vartheta^{\mathrm{P}}(x) \stackrel{\text{def}}{=} \sum_{i \in \mathcal{E}} |c_i(x)| + \sum_{i \in \mathcal{I}} \max[-c_i(x), 0], \tag{2.2}$$

for some sufficiently large penalty parameter $\nu > 0$. It is well-known that the minimization of ϕ^{P} may be reformulated as a smooth problem (see, for example, Gill, Murray and Wright, 1981, §4.2.3).

To see this, consider first an equality constraint $c_i(x) = 0$. The penalty contribution from this constraint, $\nu|c_i(x)|$, may be expressed as

$$\nu[r_i + s_i], \ \text{ where } \ c_i(x) = r_i - s_i \ \text{ and } \ (r_i, s_i) \geq 0, \tag{2.3}$$

or alternatively as

$$\nu[c_i(x) + 2s_i], \ \text{ where } \ c_i(x) + s_i \geq 0 \ \text{ and } \ s_i \geq 0.$$

Now turning to an inequality constraint $c_i(x) \geq 0$. Its penalty contribution, $\nu \max(-c_i(x), 0)$, may be expressed as

$$\nu s_i, \ \text{ where } \ c_i(x) = r_i - s_i \ \text{ and } \ (r_i, s_i) \geq 0,$$

or alternatively as

$$\nu s_i, \ \text{ where } \ c_i(x) + s_i \geq 0 \ \text{ and } \ s_i \geq 0.$$

Thus the minimization of ϕ^{P} may be expressed as (1.3), i.e.,

$$\begin{array}{ll} \underset{x \in \mathbb{R}^n,\, s \in \mathbb{R}^{n_\mathcal{C}}}{\text{minimize}} & \phi^{\mathrm{S}}(x, s; \nu) \stackrel{\text{def}}{=} f(x) + \nu \sum_{i \in \mathcal{E}} [c_i(x) + 2s_i] + \nu \sum_{i \in \mathcal{I}} s_i \\ \text{subject to} & c_i(x) + s_i \geq 0 \ \text{ and } \ s_i \geq 0, \ \text{ for all } \ i \in \mathcal{C}. \end{array}$$

Notice that for given x, any set of values $s_i \geq \max(-c_i(x), 0)$ provides an initial feasible point for the "enlarged" feasible region involving (x, s), and that this point lies in the strict interior if $s_i > \max(-c_i(x), 0)$

for all $i \in \mathcal{C}$. The central idea of this paper will then be to apply a primal-dual interior-point method to solve (1.3).

This is not the only possible reformulation of (1.2). For example (2.3) might equally have been rewritten as

$$\nu[2r_i - c_i(x)], \quad \text{where } r_i - c_i(x) \geq 0 \text{ and } r_i \geq 0$$

for all $i \in \mathcal{E}$, leading to the equivalent

$$\begin{array}{cl} \underset{x\in\mathbb{R}^n,\, r\in\mathbb{R}^{n_\mathcal{E}},\, s\in\mathbb{R}^{n_\mathcal{I}}}{\text{minimize}} & f(x) + \nu\sum_{i\in\mathcal{E}}[2r_i - c_i(x)] + \nu\sum_{i\in\mathcal{I}} s_i \\ \text{subject to} & (r_i - c_i(x), r_i) \geq 0 \text{ for all } i \in \mathcal{E}, \\ \text{and} & (c_i(x) + s_i, s_i) \geq 0 \text{ for all } i \in \mathcal{I}. \end{array} \tag{2.4}$$

Which of (1.3) or (2.4) is preferable might depend on the initial value of $c_i(x)$; a positive initial value might favour (1.3) since then the added elastic s_i need not be (significantly) larger than zero, while a negative initial value might favour (2.4) for the same reason—of course, a mixture of the two reformulations on a constraint-by-constraint basis is also possible. Finally, it is possible to "average" (1.3) and (2.4) to obtain

$$\begin{array}{cl} \underset{x\in\mathbb{R}^n,\, s\in\mathbb{R}^{n_\mathcal{C}}}{\text{minimize}} & f(x) + \nu\sum_{i\in\mathcal{C}} s_i \\ \text{subject to} & -s_i \leq c_i(x) \leq s_i \text{ for all } i \in \mathcal{E}, \\ \text{and} & c_i(x) + s_i \geq 0 \text{ and } s_i \geq 0 \text{ for all } i \in \mathcal{I}. \end{array} \tag{2.5}$$

This "symmetric" formulation has the advantage that no *a priori* bias is introduced through the initial value of x. Notice also that the constraint functions do not occur in the objective function for (2.5), but that equality constraints have been replaced by a pair of inequalities. While, for simplicity, we shall concentrate on the formulation (1.3) in this paper, equivalent algorithms and theory can immediately be developed for the alternatives (2.4) and (2.5).

As we have already mentioned, one could go one stage further here and minimize (1.3) as a function of s to arrive at the equivalent problem

$$\text{minimize } f(x) + \nu\sum_{i\in\mathcal{E}} c_i(x) \text{ subject to } c_i(x) \geq 0 \text{ for all } i \in \mathcal{C}. \tag{2.6}$$

However, we choose not to since then it is unobvious how to find an initial feasible point for (2.6).

We now examine the consequences of our reformulation.

2.2 Notation and definitions

Some basic notation has already been introduced in the previous sections. We summarize it here and introduce further notational conventions.

2.2.1 Vectors and sequences

If $q \geq 0$ and $v \in \mathbb{R}^q$, we shall denote its i-th component by a subscript v_i. If $\mathcal{S} \subseteq \{1, \ldots, q\}$, we write $v_\mathcal{S}$ for the subvector of v whose components are the v_i, $i \in \mathcal{S}$. Likewise, if $M \in \mathbb{R}^{q\times p}$, $M_\mathcal{S}$ is the submatrix of M whose rows are indexed by $\mathcal{S}$. In an algorithmic context, the value taken by the vector v at iteration k will be denoted by a superscript v^k and its i-th component is v_i^k. A sequence indexed by the set $\mathbb{N}$ of nonnegative integers whose general term is v^k is denoted $\{v^k\}$ and a subsequence indexed by the infinite index set $\mathcal{K} \subseteq \mathbb{N}$ is denoted $\{v^k\}_\mathcal{K}$.

As exceptions to the above, if $e_\mathcal{E}$ and $e_\mathcal{I}$ are vectors of ones of dimension $n_\mathcal{E}$ and $n_\mathcal{I}$ respectively, we define two vectors

$$e_\mathcal{E}^0 = \begin{bmatrix} e_\mathcal{E} \\ 0 \end{bmatrix} \text{ and } e_\mathcal{I}^0 = \begin{bmatrix} 0 \\ e_\mathcal{I} \end{bmatrix},$$

in $\mathbb{R}^{n_\mathcal{C}}$, and let $e = e_\mathcal{E}^0 + e_\mathcal{I}^0$. Wherever appropriate, the notation e_p denotes the vector of all ones in $\mathbb{R}^p$ and similarly, 0_p denotes the zero vector of $\mathbb{R}^p$. In addition, $I_\mathcal{E}$ and $I_\mathcal{I}$ are identity matrices of dimensions $n_\mathcal{E}$ and $n_\mathcal{I}$ respectively.

2.2.2 The Lagrangian and dual variables for the original problem

We denote the full vector of constraints by $c : \mathbb{R}^n \to \mathbb{R}^{n_\mathcal{C}}$. The Lagrangian associated with problem (1.1) is

$$L(x, \lambda) = f(x) - \lambda_\mathcal{E}^T c_\mathcal{E}(x) - \lambda_\mathcal{I}^T c_\mathcal{I}(x), \tag{2.7}$$

where $\lambda_\mathcal{E} \in \mathbb{R}^{n_\mathcal{E}}$, $\lambda_\mathcal{I} \in \mathbb{R}_+^{n_\mathcal{I}}$ and $\lambda = (\lambda_\mathcal{E}, \lambda_\mathcal{I})$. A vector $z = (x, \lambda)$ is a *first-order critical point* for (1.1) if it satisfies the Karush-Kuhn-Tucker (KKT) conditions

$$\begin{aligned} \nabla f(x) - J_\mathcal{E}^T(x)\lambda_\mathcal{E} - J_\mathcal{I}^T(x)\lambda_\mathcal{I} &= 0, && (2.8a)\\ C_\mathcal{I}(x)\lambda_\mathcal{I} &= 0, && (2.8b)\\ c_\mathcal{E}(x) &= 0 && (2.8c)\\ \text{and } c_\mathcal{I}(x), \lambda_\mathcal{I} &\geq 0; && (2.8d) \end{aligned}$$

here and elsewhere $J_\mathcal{E}(x)$ and $J_\mathcal{I}(x)$ are the Jacobian matrices of $c_\mathcal{E}(x)$ and $c_\mathcal{I}(x)$ respectively, while a capitalised (e.g.) $C_\mathcal{I}(x)$ denotes the diagonal matrix whose entries are the components of the vector (e.g.) $c_\mathcal{I}(x)$.

2.2.3 The Lagrangian and dual variables for the reformulated problem

It will be convenient in what follows to express the objective function of (1.3) as

$$\phi^{\text{S}}(x, s; \nu) = f(x) + \nu\vartheta(x, s), \tag{2.9}$$

where

$$\vartheta(x, s) = \sum_{i\in\mathcal{E}}[c_i(x) + 2s_i] + \sum_{i\in\mathcal{I}} s_i \tag{2.10}$$

is the *measure of infeasibility*. The Lagrangian for problem (1.3) is

$$\mathcal{L}(x, s, y, u; \nu) = \phi^{\text{S}}(x, s; \nu) - y^T(c(x) + s) - u^T s, \tag{2.11}$$

where the Lagrange multipliers $y = (y_\mathcal{E}, y_\mathcal{I}) \in \mathbb{R}_+^{n_\mathcal{C}}$ and $u = (u_\mathcal{E}, u_\mathcal{I}) \in \mathbb{R}_+^{n_\mathcal{C}}$ are associated with the constraints $c(x) + s \geq 0$ and $s \geq 0$ of (1.3) respectively. The vectors

$$v_\text{P} = (x, s) \text{ and } v_\text{D} = (y, u)$$

contain primal and dual variables/Lagrange multipliers for (1.3) respectively.

The gradient of (2.9) may be expressed as

$$\nabla\phi^{\text{S}}(x, s; \nu) = \begin{bmatrix} \nabla f(x) \\ 0 \end{bmatrix} + \nu\nabla\vartheta(x, s) = \begin{bmatrix} \nabla f(x) \\ 0 \end{bmatrix} + \nu \begin{bmatrix} J_\mathcal{E}^T(x)e_\mathcal{E} \\ e + e_\mathcal{E}^0 \end{bmatrix}, \tag{2.12}$$

while the $2n_\mathcal{C} \times (n + n_\mathcal{C})$ Jacobian of the constraints of (1.3) with respect to v_P can be written as

$$J^{\text{S}}(v_\text{P}) = \begin{bmatrix} J_\mathcal{E}(x) & I_\mathcal{E} & 0 \\ J_\mathcal{I}(x) & 0 & I_\mathcal{I} \\ 0 & I_\mathcal{E} & 0 \\ 0 & 0 & I_\mathcal{I} \end{bmatrix} = \begin{bmatrix} J(x) & I_\mathcal{C} \\ 0 & I_\mathcal{C} \end{bmatrix}, \tag{2.13}$$

where we have denoted the $n_\mathcal{C} \times n$ Jacobian matrix of the full vector of constraint functions $c(x)$ by

$$J(x) = \begin{bmatrix} J_\mathcal{E}(x) \\ J_\mathcal{I}(x) \end{bmatrix}. \tag{2.14}$$

This derivative structure enables us to express the KKT conditions for (1.3) as

$$\begin{aligned}
\nabla f(x) - J_{\mathcal{E}}^T(x)(y_{\mathcal{E}} - \nu e_{\mathcal{E}}) - J_{\mathcal{I}}^T(x) y_{\mathcal{I}} &= 0, && \text{(2.15a)}\\
\nu e_{\mathcal{E}} - (y_{\mathcal{E}} - \nu e_{\mathcal{E}}) - u_{\mathcal{E}} &= 0, && \text{(2.15b)}\\
\nu e_{\mathcal{I}} - y_{\mathcal{I}} - u_{\mathcal{I}} &= 0, && \text{(2.15c)}\\
(C(x) + S)y &= 0, && \text{(2.15d)}\\
Su &= 0, && \text{(2.15e)}\\
\text{and } c(x) + s, s, y, u &\geq 0. && \text{(2.15f)}
\end{aligned}$$

It should now be apparent from (2.8) and (2.15) that there is an intimate connection between the Lagrange multipliers λ for (1.1) and the multipliers y for (1.3). To keep later results concise, we formalise this as follows.

Definition 1. *For a given, fixed, value $\nu \geq 0$ of the penalty parameter, and given vectors x, y and λ, we define* shifted *vectors*

$$\begin{aligned}
y(\lambda, \nu) &\stackrel{\text{def}}{=} (\lambda_{\mathcal{E}} + \nu e_{\mathcal{E}}, \lambda_{\mathcal{I}}) = \lambda + \nu e_{\mathcal{E}}^0 && \text{(2.16a)}\\
\textit{and } \lambda(y, \nu) &\stackrel{\text{def}}{=} (y_{\mathcal{E}} - \nu e_{\mathcal{E}}, y_{\mathcal{I}}) = y - \nu e_{\mathcal{E}}^0 && \text{(2.16b)}
\end{aligned}$$

i.e., the vectors where the multipliers corresponding to the nonlinear equality constraints of (1.1) and (1.3) have been shifted by $\pm \nu e_{\mathcal{E}}$.

2.2.4 Infeasibility measures

A first-order locally smallest value of the ℓ_1-norm infeasibility measure (2.10), $\vartheta(x, s)$, under the constraints $c(x) + s \geq 0$ and $s \geq 0$ is attained at a (first-order) critical point (x, s) for which

$$\begin{aligned}
J^T(x)(\overline{y} - e_{\mathcal{E}}^0) &= 0,\\
e - (\overline{y} - e_{\mathcal{E}}^0) - \overline{u} &= 0,\\
(C(x) + S)\overline{y} &= 0,\\
S\overline{u} &= 0\\
\text{and } c(x) + s, s, \overline{y}, \overline{u} &\geq 0,
\end{aligned} \qquad \text{(2.17)}$$

where $\overline{y}$ and $\overline{u}$ are Lagrange multipliers associated with the inequality constraints $c(x) + s \geq 0$ and $s \geq 0$ respectively. It is important to recognize that such an x is also a critical point for the infeasibility measure (2.2), $\vartheta^{\mathrm{P}}(x)$, for the true constraints.

Theorem 2.1. *Suppose that (x, s) satisfies (2.17). Then x is a first-order critical point of (2.2).*

Proof. A first-order critical point for (2.2) satisfies

$$J^T(x)\lambda = 0, \qquad \text{(2.18)}$$

where the generalized gradient λ satisfies

$$\lambda_i \begin{cases}
= -1 & \text{if } c_i > 0 \text{ and } i \in \mathcal{E},\\
= 0 & \text{if } c_i > 0 \text{ and } i \in \mathcal{I},\\
= 1 & \text{if } c_i < 0,\\
\in [-1, 1] & \text{if } c_i = 0 \text{ and } i \in \mathcal{E},\\
\in [0, 1] & \text{if } c_i = 0 \text{ and } i \in \mathcal{I}.
\end{cases} \qquad \text{(2.19)}$$

(see, for example, Conn, Gould and Toint, 2000*a*, Example 11.4.1). Let $(\overline{y}, \overline{u})$ satify (2.17), and define $(\lambda, u) = (\overline{y} - e^0_{\mathcal{E}}, \overline{u})$ so that (2.17) becomes

$$\begin{aligned} J^T(x)\lambda &= 0, & (2.20a)\\ \lambda + u &= e, & (2.20b)\\ (C(x)+S)(\lambda + e^0_{\mathcal{E}}) &= 0, & (2.20c)\\ Su &= 0 & (2.20d)\\ \text{and } c(x)+s, s, \lambda + e^0_{\mathcal{E}}, u &\geq 0, & (2.20e)\end{aligned}$$

The requirement (2.18) follows directly from (2.20a), so it remains to show that the given λ satisfies (2.19).

Firstly, then, consider an index i for which $c_i(x) + s_i > 0$. In this case (2.20c) shows that $\lambda_i = -1$ if $i \in \mathcal{E}$ or or $\lambda_i = 0$ if $i \in \mathcal{I}$. In either case, (2.20b) then ensures that $u_i > 0$, and hence $c_i(x) > 0$ since necessarily (2.20d) shows that $s_i = 0$. These are the first two possibilites in (2.19). Since $c_i(x)+s_i \geq 0$, it remains to consider indices for which $c_i(x)+s_i = 0$. In this case $c_i(x) = -s_i$ and thus (2.20d) implies that $c_i(x)u_i = 0$. If $s_i \neq 0$, $c_i(x) < 0$ so that $u_i = 0$, and hence $\lambda_i = 1$ from (2.20b). This is the third possibility in (2.19). By contrast, if $s_i = 0$ then immediately $c_i = 0$. But (2.20b) and (2.20e) ensure that $\lambda_i \in [-1, 1]$ if $i \in \mathcal{E}$ and $\lambda_i \in [0, 1]$ if $i \in \mathcal{E}$ for any i, giving the final two possibilites in (2.19). □

2.2.5 Regularity

A nonlinear problem of the form (1.1) is said to satisfy the Mangasarian–Fromovitz (1967) constraint qualification (MFCQ) at a feasible point x^* if the vectors $\{\nabla c_i(x^*)\}_{i\in\mathcal{E}}$, are linearly independent and if there exists a direction $d \neq 0$ such that

$$d^T\nabla c_i(x^*) = 0 \quad \text{for } i \in \mathcal{E} \quad \text{and} \quad d^T\nabla c_i(x^*) < 0 \quad \text{for } i \in \mathcal{A},$$

where $\mathcal{A} = \{i \in \mathcal{I} \mid c_i(x^*) = 0\}$ is the set of active indices at x^*. If x^* is a first-order critical point for (1.1), let Λ^* be the set of all associated Lagrange multipliers, i.e, the set of all vectors $(\lambda_{\mathcal{E}}, \lambda_{\mathcal{I}})$ satisfying (2.8). Gauvin (1977) has shown that MFCQ being satisfied at x^* is equivalent to the boundedness of Λ^*.

The reformulated problem (1.3) is surprisingly regular, for we have

Theorem 2.2. *Suppose that (x, s) is a feasible point for (1.3) and that c is continuously differentiable in an open neighbourhood of x. Then* MFCQ *is satisfied at (x, s).*

Proof. Let $d = (0_n, -e)$. There are no equality constraints, and checking the remaining requirement that $J_{\mathcal{A}}(x, s)d < 0$ for active constraints is trivial given the form (2.13) of $J^{\mathrm{S}}(v_{\mathrm{P}})$. □

As a consequence, all sets of Lagrange multipliers associated with first-order critical points are bounded.

Note that this MFCQ condition is satisfied at *every* feasible (x, s) and not only at local solutions of (1.3), regardless of any constraint qualification being satisfied for (1.1). Of course Theorem 2.2 may have been anticipated, since the same is true for (1.2)—for this problem, the set of corresponding sub-gradients of the non-differentiable constraint norms is automatically bounded (see, for example, Fletcher, 1987, §14.3).

Some of the results we will establish later require a far stronger assumption, namely the linear independence constraint qualification (LICQ)—that the rows of (2.13) corresponding to active indices are independent—be satisfied for (1.3), To obtain LICQ on (1.3), one may unfortunately need to have as strong an assumption as the active constraint gradients being linearly independent over the whole feasible set.

We wish to stress that in the following, we are taking advantage of MFCQ being satisfied for (1.3) but for generality, are not tacitly assuming that MFCQ is satisfied for (1.1). We will however emphasize the stronger results which one obtains under this additional assumption.

2.3 Assumptions and basic results

We start with the following fundamental assumptions.

A1 The feasible set $\mathcal{F} \stackrel{\text{def}}{=} \{x \mid c_{\mathcal{E}}(x) = 0 \text{ and } c_{\mathcal{I}}(x) \geq 0\}$ for (1.1) is nonempty; and

A2 The functions f, $c_{\mathcal{E}}$ and $c_{\mathcal{I}}$ are twice-continuously differentiable over an open set covering all iterates encountered.

We now examine the relationships between stationary points of (1.1) and (1.3). The following results are adaptations or variations of results in Mayne and Polak (1976). Our first result gives an important property of solutions to (1.3).

Theorem 2.3. *If Assumptions A1–A2 are satisfied, if the vector (v_P, v_D) is a first-order critical point for (1.3) with fixed penalty parameter $\nu > 0$ and if $c_{\mathcal{E}}(x) = 0$ and $c_{\mathcal{I}}(x) \geq 0$ then $s = 0$.*

Proof. If $i \in \mathcal{E}$, $c_i(x) = 0$ and from (2.15d), we have $s_i y_i = 0$. It cannot be that $s_i > 0$ since then $y_i = 0$ and (2.15b) would imply $u_i = 2\nu$ and consequently (2.15e) gives that $s_i = 0$, which is a contradiction. Therefore $s_{\mathcal{E}} = 0$. For $i \in \mathcal{I}$, if $c_i(x) = 0$, as before (2.15c) and (2.15e) guarantee that $s_i = 0$. Otherwise, $c_i(x) > 0$ and (2.15f), (2.15d), (2.15c) and (2.15e) successively imply that $c_i(x) + s_i > 0$, that $y_i = 0$, that $u_i = \nu$ and finally that $s_i = 0$. Hence we also have $s_{\mathcal{I}} = 0$, which completes the proof. □

This first result confirms intuition about the reformulation that led to (1.3), namely that all the elastic variables should eventually vanish if a critical point which is also feasible for (1.1) has been found.

The following result establishes a correspondence between systems (2.8) and (2.15) and parallels Mayne and Polak (1976) and Proposition 3 of Tits et al. (2002).

Theorem 2.4. *If Assumptions A1–A2 are satisfied, if the vector (v_P, v_D) is a first-order critical point for (1.3) with fixed penalty parameter $\nu > 0$ and if $c_{\mathcal{E}}(x) = 0$ and $c_{\mathcal{I}}(x) \geq 0$, then the shifted vector $(x, \lambda(y, \nu))$ from (2.16b) is a first-order critical point for (1.1).*

Proof. Primal feasibility with respect to the linear constraints and non-negativity of x follows directly from the assumption. The dual feasibility condition (2.15a) readily implies that (2.8a) is satisfied with the given multipliers. The feasibility conditions (2.8c)–(2.8d) are satisfied by (2.15f) and our assumptions. Moreover, Theorem 2.3 gives that $s = 0$, and hence (2.15d) implies (2.8b) as $\lambda_{\mathcal{I}}(y, \nu) = y_{\mathcal{I}}$ by definition. □

Conversely, we now show that under a constraint qualification which guarantees finiteness of the Lagrange multipliers for (1.1) and for sufficiently large values of the penalty parameter, every stationary point of (1.1) is a stationary point of (1.3).

Theorem 2.5. *If Assumptions A1–A2 are satisfied, suppose x^* is a first-order critical point for (1.1) for which the Lagrange multipliers λ^* are finite. Then for all $\nu \geq \|\lambda^*\|_\infty$, the shifted primal-dual vector (v_P, v_D), where $v_P = (x^*, 0)$ and $v_D = (y(\lambda^*), \nu), \nu e - \lambda^*)$ from (2.16a), is a first-order critical point for (1.3).*

Proof. Because $\lambda^* \geq 0$, the smallest value of ν for which $\lambda^*_{\mathcal{E}} + \nu e_{\mathcal{E}} \geq 0$, $\nu e_{\mathcal{E}} - \lambda^*_{\mathcal{E}} \geq 0$ and $\nu e_{\mathcal{I}} - \lambda^*_{\mathcal{I}} \geq 0$ is given by $\|\lambda^*\|_\infty$. For any $\nu \geq \|\lambda^*\|_\infty$, the proof is completed by a straightforward verification that the given primal-dual vector satisfies (2.15) using the assumed conditions (2.8). □

Note that Theorem 2.5 deals with one particular critical point and one particular, possibly out of many, vector of Lagrange multipliers associated to it. A standard, but stronger, assumption to ensure boundedness of the multipliers in Theorem 2.5 is to impose MFCQ on (1.1) (Gauvin 1977).

3 The full algorithm

3.1 An interior-point method for the smooth reformulated penalty problem

As we have already suggested, an appealing way to solve the reformulated problem (1.3) is to (approximately) minimize a sequence of *logarithmic barrier* functions

$$\phi^{\mathrm{B}}(x,s;\mu,\nu) \stackrel{\mathrm{def}}{=} \phi^{\mathrm{S}}(x,s;\nu) - \mu \sum_{i\in\mathcal{C}} \log(c_i(x)+s_i) - \mu \sum_{i\in\mathcal{C}} \log s_i, \tag{3.1}$$

for a decreasing sequence $\{\mu^k\}$ of positive barrier parameters whose limit is zero and, in this case, a possibly increasing sequence $\{\nu^k\}$ of positive penalty parameters. Following the standard practice for mixed interior-exterior penalty methods (see, for instance, Fiacco and McCormick, 1968), a typical iteration involves the approximate minimization of the mixed-penalty function (3.1), a possible increase in the penalty parameter ν to compensate for insufficient progress towards feasibility, and a decrease in the barrier parameter μ. Hence we might outline our algorithm as Algorithm 3.1.

Algorithm 3.1: Prototype Algorithm—Outer Iteration (preliminary version)

Step 0. Choose initial points $s>0$ and x, for which $c(x)+s>0$, and initial values ν, $\mu>0$.

Step 1. Inner iteration: Find an approximate unconstrained minimizer of (3.1) with the current values of ν and μ fixed.

Step 2. Decrease the barrier parameter μ and possibly update the penalty parameter ν. Go back to Step 1 until (1.3) has been solved to a satisfactory tolerance.

Although both linesearch and trust-region methods might be used in the crucial Step 1 in this algorithm, we shall concentrate on the latter here.

A number of important details not mentioned in Algorithm 3.1 must be carefully described and analyzed. These include a description of the trust-region approach we wish to use in Step 1, the mechanism used to promote global convergence, the conditions under which the penalty parameter is updated and the assumptions necessary to guarantee that a critical point identified by this algorithm corresponds to a critical point of the original problem (1.1). We examine them in turn in the remainder of this section.

3.2 Gradients, Lagrange multipliers and optimality conditions

For convenience, we define (primal) first-order Lagrange multiplier estimates

$$y(x,s) \stackrel{\mathrm{def}}{=} \mu(C(x)+S)^{-1}e \tag{3.2a}$$

$$\text{and } u(s) \stackrel{\mathrm{def}}{=} \mu S^{-1}e, \tag{3.2b}$$

where, as before, a capital letter denotes the diagonal matrix whose diagonal is the vector denoted by the corresponding lowercase letter. Using these multiplier estimates, the gradient of the barrier function with respect to $v_{\mathrm{P}} = (x,s)$ is

$$\nabla\phi^{\mathrm{B}}(v_{\mathrm{P}};\mu,\nu) = \begin{bmatrix} \nabla f(x) - J^T(x)(y(x,s)-\nu e^0_{\mathcal{E}}) \\ \nu e - (y(x,s)-\nu e^0_{\mathcal{E}}) - u(s) \end{bmatrix}. \tag{3.3}$$

Given fixed values of the barrier and penalty parameters $\mu,\nu \geq 0$, primal and dual vectors $v_{\mathrm{P}} = (x,s)$ and $v_{\mathrm{D}} = (y,u)$ and primal-dual vector $v = (v_{\mathrm{P}}, v_{\mathrm{D}})$, we also define the primal-dual function $\Phi : \mathbb{R}^{n+3n_\mathcal{C}} \rightarrow$

$\mathbb{R}^{n+3nc}$ as

$$\Phi(v;\mu,\nu) \stackrel{\text{def}}{=} \begin{bmatrix} \nabla f(x) - J^T(x)(y - \nu e_{\mathcal{E}}^0) \\ \nu e - (y - \nu e_{\mathcal{E}}^0) - u \\ (C(x) + S)y - \mu e \\ Su - \mu e \end{bmatrix}. \tag{3.4}$$

As is well known, the first-order criticality conditions for (1.4) are equivalently described by the *primal-dual* system

$$\begin{aligned} \Phi(v;\mu,\nu) &= 0 && (3.5\text{a}) \\ \text{and } (c(x)+s, s, y, u) &\geq 0 && (3.5\text{b}) \end{aligned}$$

in the *primal* case, where $(y,u) = (y(x,s), u(s))$ as given by (3.2). In addition, observe that the KKT conditions (2.15) for (1.3) are simply (3.5) with (3.5a) replaced by

$$\Phi(v;0,\nu) = 0. \tag{3.6}$$

3.3 The outer iteration, revisited

We now present the algorithm we plan to use, before turning to global and local convergence analyses in §4.

We call $\epsilon(\cdot)$ a *forcing function* if $\epsilon(\mu) > 0$ for all $\mu > 0$ and $\epsilon(\mu) \downarrow 0$ as $\mu \downarrow 0$ (see, Ortega and Rheinboldt, 1970). Since the Hessian of the logarithmic barrier function (3.1) can be highly ill-conditioned, it is vital that we dynamically (and implicitly) scale the variables to mitigate this effect. We shall measure variables using an (iteration-dependent) norm, say $\|\cdot\|_P$, designed to achive this, and gradients in the dual, $\|\cdot\|_{[P]}$, of the norm. We shall return to this shortly. We summarize our algorithm as Algorithm 3.2.

Algorithm 3.2: Prototype Algorithm—Outer Iteration (refined version)

Step 0. Let the forcing functions $\epsilon^{\text{D}}(\cdot)$, $\epsilon^{\text{C}}(\cdot)$ and $\epsilon^{\text{U}}(\cdot)$ be given, and let $\kappa_\nu > 0$. Choose $x^0 \in \mathbb{R}^n$, $s^0 \in \mathbb{R}^{nc}_+$ such that $c(x^0) + s^0 > 0$, initial dual estimates $y^0, u^0 \in \mathbb{R}^{nc}_+$, and penalty and barrier parameters ν^0 and $\mu^0 > 0$, and set $k = 0$.

Step 1. Inner Iteration: find a new primal-dual iterate $v^{k+1} = (x^{k+1}, s^{k+1}, y^{k+1}, u^{k+1})$ satisfying

$$\begin{aligned} \left\| \begin{bmatrix} \nabla f(x^{k+1}) - J^T(x^{k+1})(y^{k+1} - \nu^k e_{\mathcal{E}}^0) \\ \nu^k e - (y^{k+1} - \nu^k e_{\mathcal{E}}^0) - u^{k+1} \end{bmatrix} \right\|_{[P^{k+1}]} &\leq \epsilon^{\text{D}}(\mu^k) && (3.7\text{a}) \\ \|(C(x^{k+1}) + S^{k+1})y^{k+1} - \mu^k e\| &\leq \epsilon^{\text{C}}(\mu^k). && (3.7\text{b}) \\ \|S^{k+1}u^{k+1} - \mu^k e\| &\leq \epsilon^{\text{U}}(\mu^k) && (3.7\text{c}) \\ \left(c(x^{k+1}) + s^{k+1}, s^{k+1}\right) &> 0 && (3.7\text{d}) \\ \text{and } \left(\nu^k[e + e_{\mathcal{E}}^0] + \kappa_\nu e, \nu^k[e + e_{\mathcal{E}}^0] + \kappa_\nu e\right) \geq \left(y^{k+1}, u^{k+1}\right) &> 0 && (3.7\text{e}) \end{aligned}$$

for some suitable scaling norm $\|.\|_{P^{k+1}}$ by (for example) approximately minimizing (3.1).

Step 2. Select a new barrier parameter, $\mu^{k+1} \in (0, \mu^k]$ such that $\lim_{k\to\infty} \mu^k = 0$. If necessary, adjust the penalty parameter, ν^k. Increment k by one, and return to Step 1.

A few comments on Algorithm 3.2 are in order. Firstly note that the forcing functions in (3.7a)–(3.7c) allow for early termination of the inner iteration which may prove particularly beneficial in the early iterations, when remote from a solution of (1.1). Step 1 leaves the details of the inner iteration unspecified, emphasizing only the stopping conditions which should be satisfied by any approximate solution it produces. Some details are given in §3.5 but are not crucial to the analysis of the algorithm. The stopping conditions (3.7a)–(3.7c) are directly based on (scalings of) the definition (3.5a). The required upper bounds on the dual variables (y^{k+1}, u^{k+1}) in (3.7e) are simply those ultimately implied by (2.15b), (2.15c) and (2.15f), with a little "elbow room" provided by $\kappa_\nu > 0$ to allow for finite termination of the inner iteration. Crucially, although the primal multiplier estimates $y^{k+1} = y(x^{k+1}, s^{k+1})$ and $u^{k+1} = u(s^{k+1})$ might be used in (3.7), there is no necessity that this be so.

The update of the barrier parameter in Step 2 may follow traditional rules but should ultimately allow for a superlinear decrease if fast asymptotic convergence is sought. For instance it may be made to decrease linearly in the early iterations but superlinearly once close to a suspected solution. This is essential if an asymptotic superlinear convergence rate of the iterates, such as the local subquadratic componentwise asymptotic convergence discussed by Gould, Orban, Sartenaer and Toint (2001), is required—this issue is addressed in §4.3.

In the next sections, we examine issues concerning Algorithm 3.2 which deserve further attention, namely the choice of the (possibly iteration-dependent) scaling norm $\|\cdot\|_{P^k}$, the update of the penalty parameter ν^k and the choice of dual variables (y^k, u^k). The choice of $\|\cdot\|_{P^k}$ will follow the guidelines given in Conn, Gould, Orban and Toint (2000*b*) and Gould, Orban and Toint (2003*b*). We return to this in Section 3.5. Values of the dual variables suggested by the primal-dual system (3.5a) might not be sufficiently accurate in the early stages of the iteration and should be properly controlled when convergence occurs to ensure fast asymptotic convergence while preventing desperately ill-conditioned systems on problem with large, or infinite, multipliers. A particular choice towards these goals is discussed in Section 3.6. The penalty parameter update appears in Step 2 of the algorithm for clarity, but a practical implementation might make provision for updates of ν^k *inside* the inner iteration and possibly to allow occasional decreases of ν. A suitable update for the penalty parameter is less obvious, but we shall discuss alternatives in Section 3.7.

3.4 The trust-region inner iteration

Given a strictly feasible point $v_{\rm P}$, a typical primal interior-point trust-region method for solving (1.4) attempts to find an improved point $v_{\rm P} + d = (x + d_x, s + d_s)$, where $d = (d_x, d_s)$ is constrained to lie within a *trust region*

$$\mathcal{B}(\Delta) = \left\{ d \in \mathbb{R}^{n+n_c} \mid \|d\|_P \le \Delta \right\}, \tag{3.8}$$

where $\|\cdot\|_P$ is an appropriate scaling norm, and d approximately solves the primal model-subproblem

$$\underset{d \in \mathcal{B}(\Delta)}{\text{minimize}} \;\; d^T \nabla_{v_{\rm P}} \phi^{\rm B}(v_{\rm P}; \mu, \nu) + \tfrac{1}{2} d^T \nabla_{v_{\rm P} v_{\rm P}} \phi^{\rm B}(v_{\rm P}; \mu, \nu) d$$

for some appropriate trust-region radius $\Delta > 0$ and preconditioning matrix P. This model simply gives a Newton approximation to a minimizer of $\phi^{\rm B}$. However considerable experience with interior-point methods (see for example, Andersen, Christiansen, Conn and Overton, 2001, Conn et al., 2000*a*, Conn et al., 2000*b*, and Wright, 1997) has suggested that a far superior model may be provided by considering the dual variables u and y as *independent* variables, rather than dependent ones defined by (3.2). This results in the *primal-dual* model subproblem

$$\underset{d \in \mathcal{B}(\Delta)}{\text{minimize}} \;\; d^T \nabla_{v_{\rm P}} \phi^{\rm B}(v_{\rm P}; \mu, \nu) + \tfrac{1}{2} d^T H^{\rm PD}(v) d, \tag{3.9}$$

where the primal-dual Hessian is defined by

$$H^{\rm PD}(v) = \begin{bmatrix} H(x, \lambda(y, \nu)) + J^T(x)\Theta(v)J(x) & J^T(x)\Theta(v) \\ \Theta(v)J(x) & \Theta(v) + US^{-1} \end{bmatrix}, \tag{3.10}$$

with

$$\Theta(v) = Y(C(x) + S)^{-1}, \tag{3.11}$$

for some suitable strictly positive primal-dual multiplier estimates u and y, where

$$H(x, \lambda) = \nabla_{xx} f(x) - \sum_{i \in \mathcal{C}} \lambda_i \nabla_{xx} c_i(x) = \nabla_{xx} L(x, \lambda) \tag{3.12}$$

is the Hessian of the Lagrangian (2.7), and $\lambda(y, \nu)$ is defined by (2.16b). Under standard assumptions on these estimates and as convergence occurs, the difference between the primal and primal-dual Hessians is insignificant (see, for example, Conn et al., 2000*a*, Theorem 13.9.1).

Besides the step-computing procedure, our trust-region algorithm is quite standard. The step d is accepted or rejected based on how much of the reduction in (3.1) predicted by (3.9) is actually achieved—a poor prediction results in a reduction in the trust-region radius, Δ, while an accurate one may be rewarded by an increase in Δ. Since the logarithmic barrier function is undefined outside (or on the boundary) of the shifted feasible region $\{(x, s) \mid c(x) + s \geq 0 \text{ and } s \geq 0\}$, any step $v_{\mathrm{P}} + d_{\mathrm{P}}$ outside this region is automatically rejected, and the trust-region radius reduced. See Conn et al. (2000*a*, Chapter 13) for more details. Unlike other trust-region interior-point methods such as KNITRO (Byrd, Gilbert and Nocedal, 2000), no direct attempt is made to enforce feasibility by imposing extra constraints on the trust-region subproblem.

3.5 The trust-region subproblem, preconditioning and the scaling norm

It is not necessary to solve the trust-region subproblem (3.9) exactly, and it suffices to find an approximate solution d which gives as least as much reduction as the Cauchy point for the subproblem (see, for example, Conn et al., 2000*a*). Significantly, suitably preconditioned conjugate-gradient/Lanczos methods automatically generate "Cauchy-improving" iterates, and thus are ideal for approximate subproblem solution.

We may find an approximation to the solution to (3.9) using the Generalized Lanczos Trust-Region (GLTR) method of Gould, Lucidi, Roma and Toint (1999). This method requires that, at each iteration, we solve "preconditioning" systems of the form (now dropping suffices $^{\mathrm{PD}}$)

$$K(v)d \equiv \begin{bmatrix} P + J^T(x)\Theta(v)J(x) & J^T(x)\Theta(v) \\ \Theta(v)J(x) & \Theta(v) + US^{-1} \end{bmatrix} \begin{bmatrix} d_x \\ d_s \end{bmatrix} = \begin{bmatrix} r_x \\ r_s \end{bmatrix} \equiv r \tag{3.13}$$

for appropriate right-hand sides r and where $\Theta(v)$ is defined in (3.11). Here P is a suitable "preconditioning" approximation to H, and can range from the naive ($P = I$) to the sophisticated ($P = H$), but must be chosen so that the coefficient matrix, $K(v)$, of (3.13) is positive definite. As we explained in Conn et al. (2000*b*), the preconditioner used defines the scaling norm appropriate for the trust-region in (3.9) and the dual norm appropriate to measure progress towards dual feasibility. In particular the dual norm satisfies $\|r\|_{[P]} = d^T r$, where d is the solution to (3.13).

Of particular concern, however, is that the matrix $J^T(x)\Theta(v)J(x)$ in (3.13) might be rather dense, making a direct factorization of $K(v)$ unviable. Fortunately, we may be able to avoid this difficulty. To see this, define new variables

$$\xi = \Theta(v)(J(x)d_x + d_s).$$

Then (3.13) may be rewritten as the larger but potentially sparser

$$\begin{bmatrix} P & 0 & J^T(x) \\ 0 & US^{-1} & I \\ J(x) & I & -\Theta^{-1}(v) \end{bmatrix} \begin{bmatrix} d_x \\ d_s \\ \xi \end{bmatrix} = \begin{bmatrix} r_x \\ r_s \\ 0 \end{bmatrix}. \tag{3.14}$$

A further simplification occurs if we eliminate d_s to obtain

$$\begin{bmatrix} P & J^T(x) \\ J(x) & -\Theta^{-1}(v) - U^{-1}S \end{bmatrix} \begin{bmatrix} d_x \\ \xi \end{bmatrix} = \begin{bmatrix} r_x \\ -U^{-1}Sr_s \end{bmatrix} \tag{3.15}$$

and then recover d_s from

$$d_s = -U^{-1}S\xi + U^{-1}Sr_s.$$

Thus we might solve (3.13) by instead factorizing either of the coefficient matrices M of (3.14) or N of (3.15).

Significantly $K(v)$ is positive definite if and only if M (or equivalently N) has precisely $n_{\mathcal{C}}$ negative eigenvalues, so we can ensure that P is appropriate whenever an inertia-calculating factorization (such as those given by the HSL, 2002, codes `MA27` and `MA57`) is used.

3.6 Updating the dual variables

There is a wide choice of suitable dual variables. Given newly computed primal values v_{P}^+, we follow Conn et al. (2000*b*) and project candidate dual variables v_{D}^+ componentwise into the interval

$$\left[\begin{bmatrix} y^{\mathrm{L}} \\ u^{\mathrm{L}} \end{bmatrix}, \begin{bmatrix} y^{\mathrm{U}} \\ u^{\mathrm{U}} \end{bmatrix}\right], \tag{3.16}$$

where

$$\begin{aligned}
y^{\mathrm{L}} &= \kappa_l \min\left[e, y, \mu^k (C(x^+) + S^+)^{-1} e\right], \\
y^{\mathrm{U}} &= \max\left[\kappa_u e, y, \kappa_u (\mu^k)^{-1} e, \kappa_u \mu^k (C(x^+) + S^+)^{-1} e\right], \\
u^{\mathrm{L}} &= \kappa_l \min\left[e, u, \mu^k (S^+)^{-1} e\right] \quad \text{and} \\
u^{\mathrm{U}} &= \max\left[\kappa_u e, u, \kappa_u (\mu^k)^{-1} e, \kappa_u \mu^k (S^+)^{-1} e\right],
\end{aligned}$$

in order to ensure that the multipliers remain (sufficiently) positive and (suitably) bounded. Here $0 < \kappa_l < 1 < \kappa_u$, and values $\kappa_l = \frac{1}{2}$ and $\kappa_u = 10^{20}$ have proved to be satisfactory. Notice that the primal estimates (3.2), $v_{\mathrm{D}}^+ = v_{\mathrm{D}}(v_{\mathrm{P}}^+)$, naturally lie in the interval. However, as we have just mentioned, we usually prefer to use primal-dual estimates $v_{\mathrm{D}}^+ = v_{\mathrm{D}} + s_{\mathrm{D}}$ of the dual variables, where s_{D} are dual variable estimates obtained from the trust-region subproblem (3.9). Our convergence analysis is actually independent of how this is done, so long as the resulting estimates lie in (3.16).

There may be some virtue in further projecting v_{D}^+ so that the optimal upper bounds $\nu^k\left(e + e_{\mathcal{E}}^0, e + e_{\mathcal{E}}^0\right)$ implied by (2.15b), (2.15c) and (2.15f), or perhaps the relaxed requirement in (3.7e), remain satisfied.

3.7 Updating the penalty parameter

The purpose of the penalty parameter is to force satisfaction of the equality and inequality constraints for (1.1) rather than simply having $c(x) \geq -s$ with $s \geq 0$ for (1.3). Thus, a possible update strategy is to increase ν^k whenever violation of the constraints for (1.1) has not decreased sufficiently.

Introducing decreasing sequences $\{\eta_{\mathcal{E}}^k\}$ and $\{\eta_{\mathcal{I}}^k\}$ converging to zero, this condition might be stated as

$$\|c_{\mathcal{E}}(x^k)\| > \eta_{\mathcal{E}}^k \qquad \text{or} \qquad \|c_{\mathcal{I}}^-(x^k)\| > \eta_{\mathcal{I}}^k, \tag{3.17}$$

where $c_{\mathcal{I}}^-(x) = \min[0, c_{\mathcal{I}}(x)]$. Then one possibility is to update ν^k using

$$\nu^{k+1} = \begin{cases} \max[\tau_1 \nu^k, \nu^k + \tau_2] & \text{if (3.17) is satisfied,} \\ \nu^k & \text{otherwise,} \end{cases} \tag{3.18}$$

for some preset constants $\tau_1 > 1$ and $\tau_2 > 0$, following rules suggested by Mayne and Polak (1976) and Conn et al. (2000*a*).

Quite remarkably, the convergence results of Section 4.2 are independent of the particular form of the sequences $\{\eta_{\mathcal{E}}^k\}$ and $\{\eta_{\mathcal{I}}^k\}$ besides the fact that they are sequences of positive numbers converging to zero. In practice, any such sequences might not be equally efficient and sequences converging to zero at a reasonable rate should be chosen.

4 Convergence analysis

In this section, we discuss the convergence properties of Algorithm 3.2 for the solution of (1.1). We consider, in turn, the global convergence of the inner iteration, of the outer iteration, and fast local convergence issues.

In order to derive suitable convergence results for the convergence of our interior-point method, we make the following additional assumptions.

A3 The logarithmic barrier function $\phi^{\mathrm{B}}(x, s; \mu, \nu)$ for problem (1.3), defined in (3.1), is bounded below over the set $\{(x, s) \mid c(x) + s \geq 0,\ s \geq 0\}$ for all values of $\mu > 0$; and

A4 The iterates remain in a region Ω over which the first and second derivatives $\nabla f(x)$, $\nabla_{xx} f(x)$, $\nabla c_i(x)$ and $\nabla_{xx} c_i(x)$ for all $i \in \mathcal{C}$ remain uniformly bounded.

4.1 Convergence of the inner iteration

Each inner iteration—Step 2 of Algorithm 3.2—proceeds by computing a vector of primal $v_{\mathrm{P}}^k = (x^k, s^k)$ and dual variables $v_{\mathrm{D}}^k = (y^k, u^k)$ satisfying (3.7) by means of the method described in Conn et al. (2000*b*). We thus devote this section to verifying that the assumptions required by this method are satisfied in the present case, and to recalling the main convergence properties of the resulting inner iteration. We shall only be concerned with the exact gradients and derivatives of the quantities involved here, but wish to stress that the aforementioned inner iteration makes provision for inexact Hessian matrices provided they satisfy appropriate regularity and asymptotic properties.

As we already mentioned, we must require the following condition on the preconditioning matrices P^k chosen during Step 3 of Algorithm 3.2.

A5 Each preconditioning matrix P^k is both bounded from above in norm, and such that the smallest eigenvalue of the matrix K from the system (3.13) is uniformly positive for all iterates encountered.

For simplicity, we consider the matrix P^k fixed during an inner iteration, although this need not be the case (see Conn et al., 2000*b*). Let an outer iteration index be denoted by k and the successive values taken by a generic vector v during the inner iterations corresponding to this outer iteration be denoted by $v^{k,j}$, $j = 1, 2, \ldots$. The following assumption introduces upper bounds on the sequences of multipliers.

A6 For all $k \geq 0$, there exists a constant $\kappa^{\mathrm{D}}(k)$ depending only on k such that

$$\begin{aligned} y_i^{k,j} &\leq \kappa^{\mathrm{D}}(k) \max\left[\frac{1}{c_i(x^{k,j}) + s_i^{k,j}}, 1\right] & i \in \mathcal{I} \cup \mathcal{E}, \text{ and} \\ u_i^{k,j} &\leq \kappa^{\mathrm{D}}(k) \max\left[\frac{1}{s_i^{k,j}}, 1\right] & i \in \mathcal{I} \cup \mathcal{E}. \end{aligned}$$

In view of MFCQ, requiring that the Lagrange multipliers remain bounded is very reasonable for fixed (μ^k, ν^k). Indeed, if (3.7e) were to be imposed for every inner iteration, A6 would automatically be satisfied.

Armed with the above assumptions, the next result corresponds to Theorem 2 of Conn et al. (2000*b*).

Theorem 4.1. *Under Assumptions A1–A6, the inner iteration procedure corresponding to outer iteration k of Algorithm 3.2 generates a sequence $\{(x^{k,j}, s^{k,j})\}$ satisfying*

$$\lim_{j\to\infty} \|\nabla \phi^{B}(v_{P}^{k,j}; \mu^k, \nu^k)\|_{[P^k]} = \lim_{j\to\infty} \|\nabla \phi^{B}(v_{P}^{k,j}; \mu^k, \nu^k)\| = 0.$$

Proof. It is readily verified that Assumptions A1–A6 imply Assumptions A1–A8 of Conn et al. (2000*b*) and thus global convergence of the inner iteration. Theorem 2 of Conn et al. (2000*b*) concludes the proof. □

Thus Theorem 4.1 shows that the inner-iteration termination test will be satisfied after a finite number of iterations if primal multiplier estimates $y^{k+1} = y(x^{k+1}, s^{k+1})$ and $u^{k+1} = u(s^{k+1})$ are used.

If we plan to use other dual variables, we require an extra assumption, namely that the primal-dual estimates converge to their ideal, primal, values when convergence takes place.

A7 The inner iteration produces dual sequences $\{u^{k,j}\}$ and $\{y^{k,j}\}$ satisfying

$$\begin{aligned}\lim_{j\to\infty} \|u^{k,j} - \mu^k (S^{k,j})^{-1} e\| &= 0\\ \lim_{j\to\infty} \|y^{k,j} - \mu^k (C(x^{k,j}) + S^{k,j})^{-1} e\| &= 0,\end{aligned}$$

whenever

$$\lim_{j\to\infty} \|\nabla \phi^{\mathrm{B}}(v_{\mathrm{P}}^{k,j}; \mu^k, \nu^k)\|_{[P^k]} = 0.$$

With this additional assumption, we obtain the following result.

Theorem 4.2. *Under Assumptions A1–A7, the inner iteration procedure corresponding to outer iteration k of Algorithm 3.2 generates a sequence $\{(v_P^k, v_D^k)\}$ satisfying the stopping conditions (3.7) after finitely many steps.*

Proof. The stated assumptions allow us to use Theorem 4 of Conn et al. (2000*b*) to deduce that the sequence $\{(v_{\mathrm{P}}^{k,j}, v_{\mathrm{D}}^{k,j})\}$ generated by Algorithm 3.2 ultimately satisfies

$$\lim_{j\to\infty} \Phi(v^{k,j}; \mu^k, \nu^k) = 0 \;\text{ and }\; \lim_{j\to\infty} (c(x^{k,j}) + s^{k,j}, s^{k,j}, y^{k,j}, u^{k,j}) \geq 0$$

and thus indirectly that

$$\lim_{j\to\infty} \left(y^{k,j} + \nu^k e_{\mathcal{E}}^0, u^{k+1}\right) \leq \nu^k \left(e + e_{\mathcal{E}}^0, e + e_{\mathcal{E}}^0\right).$$

Thus (3.7) is satisfied after finitely many steps, since Lemma 2 of Conn et al. (2000*b*) shows that the $\|.\|_{[P^{k+1}]}$ and Euclidean norms are equivalent for fixed k. □

The numerical method suggested in Sections 3.4–3.6 to tackle the inner iteration satisfies the assumptions stated here, and thus guarantees global convergence of the each iteration.

4.2 Convergence of the outer iteration

We now study the convergence of the outer iteration algorithm. We shall concentrate on the case where the penalty parameter is updated as suggested in Section 3.7. For convenience, we state this as

Algorithm 4.1: Prototype Algorithm—Outer Iteration (final version)

Algorithm 3.2, in which the penalty parameter ν^k is updated in Step 2 according to the rule (3.18).

Our first task is to show that although we are measuring the violation of dual feasibility in (3.7a) in the $\|\cdot\|_{[P^{k+1}]}$ norm, this actually allows us to make deductions in the Euclidean norm. To do this, we need to be slightly more restrictive in the choice of our forcing functions ϵ^{D}, ϵ^{C} and ϵ^{U}, and we make the following assumption.

A8 The forcing functions ϵ^{D}, ϵ^{C} and ϵ^{U} satisfy the bounds

$$\epsilon^{\mathrm{C}}(\mu) \leq \kappa_c \mu, \tag{4.1a}$$
$$\epsilon^{\mathrm{U}}(\mu) \leq \kappa_c \mu \text{ and} \tag{4.1b}$$
$$\epsilon^{\mathrm{D}}(\mu) \leq \kappa_d \mu^{\frac{1}{2}+\gamma^k} \tag{4.1c}$$

for some constants $\kappa_c \in (0,1)$ and $\kappa_d > 0$ and sequence $\{\gamma^k\} > 0$.

We then have the following result.

Lemma 4.3. *Suppose that the iterates $v^{k+1} = (x^{k+1}, s^{k+1}, y^{k+1}, u^{k+1})$ are generated by Algorithm 3.2, and that Assumptions A4, A5 and A8 hold. Then there exist constants $\mu_{\max}$ and $\kappa > 0$ for which*

$$\|v\| \leq \kappa \frac{\nu^k + \kappa_\nu}{\sqrt{\mu^k}} \|v\|_{[P^{k+1}]} \tag{4.2}$$

for all $\mu^k \leq \mu_{\max}$ and all vectors v, and, additionally,

$$\|v\| \leq \kappa(\nu^k + \kappa_\nu)(\mu^k)^{\gamma^k} \tag{4.3}$$

whenever $\|v\|_{[P^{k+1}]} \leq \epsilon^{D}(\mu^k)$.

Proof. The requirements (3.7b) and (4.1a) imply that

$$(c_i(x^{k+1}) + s_i^{k+1}) y_i^{k+1} \geq (1-\kappa_c)\mu^k.$$

Combining this bound with the required upper bound from (3.7e) reveals

$$c_i(x^{k+1}) + s_i^{k+1} \geq \frac{(1-\kappa_c)\mu^k}{y_i^{k+1}} \geq \frac{(1-\kappa_c)\mu^k}{2\nu^k + \kappa_\nu} > \frac{(1-\kappa_c)\mu^k}{2(\nu^k + \kappa_\nu)}. \tag{4.4}$$

Similarly, (3.7c) and (3.7e) and (4.1b) give that

$$s_i^{k+1} \geq \frac{(1-\kappa_c)\mu^k}{2\nu^k + \kappa_\nu} > \frac{(1-\kappa_c)\mu^k}{2(\nu^k + \kappa_\nu)}. \tag{4.5}$$

But the form of the Jacobian in (2.13) together with Assumptions A4, A5 and A8 are sufficient to allow us to invoke Conn et al. (2000*b*, Lemma 4.1) to deduce that

$$\|v\|_{[P^{k+1}]} \geq \kappa_2 \min\left(\min_{i\in\mathcal{C}} \frac{c_i(x^{k+1}) + s_i^{k+1}}{\sqrt{\mu^k}}, \min_{i\in\mathcal{C}} \frac{s_i^{k+1}}{\sqrt{\mu^k}}, 1 \right) \|v\| \tag{4.6}$$

for some $\kappa_2 > 0$ and all v. Combining (4.4)–(4.6), we see that

$$\|v\|_{[P^{k+1}]} \geq \kappa_2 \min\left(\frac{(1-\kappa_c)\sqrt{\mu^k}}{2(\nu^k + \kappa_\nu)}, 1 \right) \|v\| \geq \frac{\kappa_2(1-\kappa_c)\sqrt{\mu^k}}{2(\nu^k + \kappa_\nu)} \|v\|$$

for all $\mu^k \leq \mu_{\max} \stackrel{\text{def}}{=} (2\kappa_\nu/(1-\kappa_c))^2$, which is the required result (4.2) when $\kappa \stackrel{\text{def}}{=} 2/(\kappa_2(1-\kappa_c))$. The remaining bound (4.3) follows directly from (4.1c) and (4.2). $\square$

We derive some properties of the sequences generated by the final Algorithm 4.1. In the following results, we shall be concerned with limit points $v_{\mathrm{P}}^* = (x^*, s^*)$ and $v_{\mathrm{D}}^* = (y^*, u^*)$, of the primal and dual sequences respectively, generated by Algorithm 4.1. As mentioned earlier and in order to easily make connections with Theorem 2.4, we shall be using the *shifted* limit point $(x, \lambda(y*, \nu^*))$ as defined in (2.16b).

We first consider the case where the penalty parameter remains bounded.

Lemma 4.4. *Suppose that Assumptions A1–A2 and A4–A8 hold. Assume Algorithm 4.1 generates infinite sequences $\{v_{\text{P}}^k\}$ and $\{v_{\text{D}}^k\}$ and the penalty parameter ν^k is updated only finitely many times to eventually reach its final value ν^*. Then the sequence $\{(s^k, y^k, u^k)\}$ is bounded. Moreover, if $\{x^k\}$ has a limit point and if $(v_{\text{P}}^*, v_{\text{D}}^*)$ is any limit point of $\{v^k\}$, then $s^* = 0$ and the shifted limit point $(x, \lambda(y^*, \nu^*))$ is a first-order critical point for (1.1).*

Proof. By assumption, there exists a positive integer N such that $\nu^k = \nu^*$ for all $k \geq N$. The updating rule (3.18) then implies that

$$\|c_{\mathcal{E}}(x^k)\| \leq \eta_{\mathcal{E}}^k \text{ and } \|c_{\mathcal{I}}^-(x^k)\| \leq \eta_{\mathcal{I}}^k. \tag{4.7}$$

Consequently, $\lim c_{\mathcal{E}}(x^k) = 0$ and $\lim c_{\mathcal{I}}(x^k) \geq 0$.

We first show that $\{s^k\}$ is bounded. Assume by contradiction that $s_i^k \to \infty$ for some $i \in \mathcal{C}$. By using the forcing property of the functions $\epsilon^{\text{D}}(\cdot)$, $\epsilon^{\text{U}}(\cdot)$ and $\epsilon^{\text{C}}(\cdot)$, Lemma 4.3 and the fact that $\mu^k \downarrow 0$, from (3.7c), we must have $u_i^k \to 0$ and from (3.7a), $\{y_i^k\}$ must be bounded. Hence, (3.7b) imposes $c_i(x^k) \to -\infty$, which is a contradiction. Thus $\{s^k\}$ must be bounded. Moreover, for all $k \geq N$, (3.7e) implies that $\{(y^k, u^k)\}$ satisfies the bounds $(y_i^k, u_i^k) \in [0, \kappa_\nu + 2\nu^*]$ for $i \in \mathcal{E}$ and $(y_i^k, u_i^k) \in [0, \kappa_\nu + \nu^*]$ for $i \in \mathcal{I}$.

Suppose that $\lim_{k \in \mathcal{K}} v^k = (v_{\text{P}}^*, v_{\text{D}}^*)$. Along the subsequence defined by $\mathcal{K}$, (3.7b)–(3.7d), the forcing property of the function $\epsilon^{\text{D}}(\cdot)$, Lemma 4.3 and the fact that $\mu^k \downarrow 0$ together guarantee that

$$\lim_{k \in \mathcal{K}} \left\| \begin{bmatrix} \nabla f(x^{k+1}) - J^T(x^{k+1})(y^{k+1} - \nu^k e_{\mathcal{E}}^0) \\ \nu^k e - (y^{k+1} - \nu^k e_{\mathcal{E}}^0) - u^{k+1} \end{bmatrix} \right\| = \left\| \begin{bmatrix} \nabla f(x^*) - J^T(x^{k+1})(y^* - \nu^* e_{\mathcal{E}}^0) \\ \nu^k e - (y^* - \nu^* e_{\mathcal{E}}^0) - u^* \end{bmatrix} \right\| = 0$$

as well as $(C(x^*) + S^*)y^* = 0$ and $S^* u^* = 0$. Thus $(v_{\text{P}}^*, v_{\text{D}}^*)$ satisfies (3.5b) and (3.6) and the assumptions of Theorem 2.3 and Theorem 2.4. $\square$

Finally, we consider the consequences of an unbounded penalty parameter.

Lemma 4.5. *Suppose that Assumptions A1–A2 and A4–A8 hold. Let $\{v_{\text{P}}^k\}$ and $\{v_{\text{D}}^k\}$ be sequences generated by Algorithm 4.1. Assume the penalty parameter ν^k is updated infinitely many times at iterations $k \in \mathcal{K}$. Then the subsequence $\{(y^k, u^k)\}_{\mathcal{K}}$ is unbounded. If, in addition the sequence $\{v_{\text{P}}^k\}$ has a limit point v_{P}^*, v_{P}^* is a first-order critical point of (2.17) subject to $c(s) + s \geq 0$ and $s \geq 0$, and x^* is a first-order critical point of (2.2).*

Proof. Along $\mathcal{K}$, (3.18) implies $\nu^{k+1} \geq \nu^k + \tau_2$ with $\tau_2 > 0$ and thus $\{\nu^k\}_{\mathcal{K}} \to \infty$. Since ν^k is nondecreasing, the whole sequence $\{\nu^k\} \to \infty$. Consequently, for all $k \in \mathcal{K}$, the condition (3.17) is satisfied.

Now suppose that $\{v_{\text{D}}^k\}_{\mathcal{K}}$ is bounded and thus has a limit point v_{D}^*. In particular, there are vectors y^* and u^* such that $\{y_{\mathcal{E}}^k\}_{\mathcal{K}'} \to y^*$ and $\{u^k\}_{\mathcal{K}'} \to u^*$ for some $\mathcal{K}' \subseteq \mathcal{K}$, and thus both $\|y^k\| \leq 2\|y^*\|$ and $\|u^k\| \leq 2\|u^*\|$ for all sufficiently large $k \in \mathcal{K}'$. But then the triangle inequality, the stopping condition (3.7a) and Lemma 4.3 give that

$$\sqrt{n_{\mathcal{C}}}\nu^{k-1} - (\|y^k\| + \|u^k\|) \leq \|\nu^{k-1}e - y_{\mathcal{E}}^k - u_{\mathcal{E}}^k\| \leq \kappa(\nu^{k-1} + \kappa_\nu)(\mu^{k-1})^{\gamma^k}$$

and this combines with the bounds on $\|y^k\|$ and $\|u^k\|$ to give

$$(\sqrt{n_{\mathcal{C}}} - \kappa(\mu^{k-1})^{\gamma^k})\nu^{k-1} \leq (\|y^k\| + \|u^k\|) + \kappa\kappa_\nu(\mu^{k-1})^{\gamma^k} \leq 2(\|y^*\| + \|u^*\|) + \kappa\kappa_\nu(\mu^{k-1})^{\gamma^k} \tag{4.8}$$

for all sufficiently large $k \in \mathcal{K}'$. Taking the limit of (4.8) as $k \to \infty$ then contradicts the unboundedness of $\{\nu^{k-1}\}$. Thus $\{v_{\text{D}}^k\}_{\mathcal{K}}$ is unbounded.

To prove the second part of the lemma, we now suppose that $\{v_{\text{P}}^k\}$ has a limit point v_{P}^*. Define

$$\overline{y}^{k+1} = \frac{y^{k+1}}{\nu^k} \text{ and } \overline{u}^{k+1} = \frac{u^{k+1}}{\nu^k}.$$

Then the stopping rules (3.7) and Lemma 4.3 give that

$$\begin{aligned}
\left\| \begin{bmatrix} \frac{1}{\nu^k}\nabla f(x^{k+1}) - J^T(x^{k+1})(\overline{y}^{k+1} - e^0_{\mathcal{E}}) \\ e - (\overline{y}^{k+1} - e^0_{\mathcal{E}}) - \overline{u}^{k+1} \end{bmatrix} \right\| &\leq \kappa_p (\mu^k)^{\gamma^k} && (4.9a)\\
\left\| (C(x^{k+1}) + S^{k+1})\overline{y}^{k+1} - \frac{\mu^k}{\nu^k} e \right\| &\leq \frac{\epsilon^{\mathrm{C}}(\mu^k)}{\nu^k}. && (4.9b)\\
\left\| S^{k+1}\overline{u}^{k+1} - \frac{\mu^k}{\nu^k} e \right\| &\leq \frac{\epsilon^{\mathrm{U}}(\mu^k)}{\nu^k} && (4.9c)\\
(c(x^{k+1}) + s^{k+1}, s^{k+1}) &> 0 && (4.9d)\\
\text{and} \quad \left(\left[1 + \frac{\kappa_\nu}{\nu^0}\right] e + e^0_{\mathcal{E}}, \left[1 + \frac{\kappa_\nu}{\nu^0}\right] e + e^0_{\mathcal{E}} \right) \geq (\overline{y}^{k+1}, \overline{u}^{k+1}) &> 0 && (4.9e)
\end{aligned}$$

where $\kappa_p \overset{\text{def}}{=} \kappa(1 + \kappa_\nu/\nu^0)$. Since (4.9e) implies that $(\overline{y}^{k+1}, \overline{u}^{k+1})$ is bounded, there is a subsequence $\mathcal{K}' \subseteq \mathcal{K}$ for which $\lim_{k \in \mathcal{K}' \to \infty} (\overline{y}^{k+1}, \overline{u}^{k+1}) = (y^*, u^*)$. Taking limits of (4.9) as $k \in \mathcal{K}' \to \infty$ (and thus $\mu^k \to 0$ and $\nu^k \to \infty$) shows that (x^*, s^*, y^*, u^*) satisfies (2.17), and hence (x^*, s^*) is a first-order critical point of (2.10) subject to $c(s) + s \geq 0$ and $s \geq 0$. The remaining result then follows directly from Theorem 2.1. □

To summarize, Lemmas 4.4–4.5 lead to the following global convergence result

Theorem 4.6. *Suppose that Assumptions A1–A2 and A4–A8 hold. Let $\{v^k_{\mathrm{P}}\}$ and $\{v^k_{\mathrm{D}}\}$ be sequences generated by Algorithm 4.1, and that x^* is a limit point of $\{x^k\}$. Then either $\{\nu^k\}$ remains bounded, and x^* is a first-order critical point for the nonlinear programming problem (1.1), or $\{\nu^k\}$ diverges, and x^* is a first-order critical point of the infeasibility (2.2).*

4.3 Fast asymptotic convergence

We examine in this section the superlinear convergence properties of iterates generated by Algorithm 4.1 in the regular case where LICQ is satisfied for simplicity, although past research suggests that similar convergence properties could be derived under MFCQ (Wright and Orban 2002). Fast convergence properties of Algorithm 6.1 may be derived in a similar manner.

The framework is that of Gould et al. (2001) and Gould, Orban, Sartenaer and Toint (2002*b*). From Theorem 4.6, we assume that Algorithm 4.1 generates a sequence $\{v^k\}$ from which a convergent subsequence $\{v^k\}_{\mathcal{K}}$ may be extracted, where $\mathcal{K}$ is an infinite index set, whose limit point $v^* = (v^*_{\mathrm{P}}, v^*_{\mathrm{D}})$ is feasible, and hence for which the penalty parameter ν^k is only updated finitely many times. We denote its final value by $\nu^* > 0$, and let $\lambda^* = \lambda(y^*, \nu^*)$ We consider indices $k \in \mathcal{K}$ sufficiently large that $\nu^k = \nu^*$ and for related positive quantities α and β, we write $\alpha = O(\beta)$ if there is a constant $\kappa > 0$ such that $\alpha \leq \kappa\beta$ for all β sufficiently small. We write $\alpha = o(\beta)$ if $\alpha/\beta \to 0$ as $\beta \to 0$. We also write $\alpha = \Theta(\beta)$ if $\alpha = O(\beta)$ and $\beta = O(\alpha)$.

¿From Lemma 4.4, we have that $s^* = 0$, which enables us to conveniently formulate our assumptions in term of (1.1) instead of (1.3). In particular, all the bound constraints on s in (1.3) are active and we may thus define the set of active indices in the nonlinear constraints of (1.3) as $\mathcal{A} \cup \mathcal{E}$ where

$$\mathcal{A} = \{i \in \mathcal{I} \mid c_i(x^*) = 0\}. \tag{4.10}$$

Note that $\mathcal{A}$ is also the set of active inequality constraints for (1.1). We make the following standard assumptions on (1.1).

$\boxed{\textbf{A9}}$ The gradients $\{\nabla c_i(x^*),\ i \in \mathcal{A} \cup \mathcal{E}\}$ form a linearly independent set of vectors;

$\boxed{\textbf{A10}}$ The strong second-order sufficiency conditions for (1.1) are satisfied at (x^*, λ^*), i.e., $d^T \nabla_{xx} L(x^*, \lambda^*) d > 0$ for all nonzero vector d such that $d^T \nabla c_i(x^*) = 0$ for all $i \in \mathcal{A} \cup \mathcal{E}$;

A11 $\|\lambda^*\|_\infty < \nu^*$ and $\lambda_i^* > 0$ for all $i \in \mathcal{A}$;

A12 The functions f, $c_\mathcal{E}(x)$ and $c_\mathcal{I}(x)$ are three times continuously differentiable over the intersection of an open neighbourhood of x^* with the feasible set of (1.1).

Lemma 4.7. *The penalty problem (1.3) satisfies* LICQ*, the strong second-order sufficient condition and strict complementarity at v^* with a value of the penalty parameter equal to ν^* if and only if A9–A11 are satisfied. Moreover, if A12 holds, the objective and constraint functions for (1.3) are three times continuously differentiable in an open neighbourhood of v_P^*.*

Proof. Upon defining the $|\mathcal{A}| \times n$ matrices $J_\mathcal{A}(x^*)$ and $E_\mathcal{A}$ as the rows of the matrices $J_\mathcal{I}(x^*)$ and $I_\mathcal{I}$ corresponding to indices in $\mathcal{A}$ respectively, the active part of the Jacobian $J^\text{S}(v^*)$ defined in (2.13) is

$$J^\text{S}_\mathcal{A}(x^*, 0) = \begin{bmatrix} J_\mathcal{E}(x^*) & I_\mathcal{E} & 0 \\ J_\mathcal{A}(x^*) & 0 & E_\mathcal{A} \\ 0 & I_\mathcal{E} & 0 \\ 0 & 0 & I_\mathcal{I} \end{bmatrix}. \tag{4.11}$$

The matrix (4.11) has full row rank if and only if the matrix

$$\begin{bmatrix} J_\mathcal{E}(x^*) \\ J_\mathcal{A}(x^*) \end{bmatrix}, \tag{4.12}$$

has full row rank. This latter condition is equivalent to A9.

Because the variables s appear linearly in the Lagrangian (2.11), its Hessian with respect to primal variables $v_\text{P} = (x, s)$ is

$$\nabla_{v_\text{P} v_\text{P}} \mathcal{L}(v;\nu) = \begin{bmatrix} \nabla_{xx}\mathcal{L}(v;\nu) & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} \nabla_{xx}L(x, \lambda(y,\nu)) & 0 \\ 0 & 0 \end{bmatrix},$$

where $L(x,\lambda)$ is the Lagrangian (2.7) and $\lambda(y,\nu)$ is defined by (2.16b), hence imposing the strong second-order sufficient condition on (1.3) at v^* amounts to A10. The requirement on d follows from (4.11).

Since $c_\mathcal{E}(x^*) = 0$ and $s^* = 0$, strict complementarity on (1.3) imposes $y_i^* > 0$ for all $i \in \mathcal{A} \cup \mathcal{E}$ and $u_i^* > 0$ for all $i \in \mathcal{C}$. Eliminating u_i^* using the identities (2.15b)–(2.15c) gives $y^* < \nu^*(e + e_\mathcal{E})$, which is in turn equivalent to the bound $\|\lambda^*\|_\infty < \nu^*$ on the multipliers $\lambda^* \equiv \lambda(y^*, \nu^*) = y^* - \nu^* e_\mathcal{E}^0$ associated to (1.1). The final part of the proof is immediate. □

Under A11, the central trajectory approaches its end point non-tangentially to active constraints (Wright 1992). Differentiating the primal-dual system with respect to μ yields an explicit expression of the *tangent vector* $\dot{v}(\mu)$

$$\nabla_v \Phi(v;\mu,\nu)\dot{v}(\mu) = \begin{bmatrix} 0 \\ 0 \\ -e_{2n_\mathcal{C}} \end{bmatrix}. \tag{4.13}$$

As $\mu \downarrow 0$, this tangent vector converges to a nonzero limit vector $\dot{v}(0)$. As will appear in Theorem 4.9, the individual components of $\dot{v}(0)$ are relevant to fast local convergence issues.

Slightly strengthening (4.1), we assume in this section that the forcing functions in Algorithm 4.1 have the following asymptotic form

A13 $\epsilon^\text{D}(\mu^k) = \Theta((\mu^k)^{\gamma^k+1})$ and $\epsilon^\text{C,U}(\mu^k) = \Theta(\mu^k)$, where $0 < \gamma^k < 1$ for all sufficiently large $k \in \mathcal{K}$.

For the purpose of demonstrating the fast local convergence properties of Algorithm 4.1, we first rephrase it as Algorithm 4.2.

Algorithm 4.2: Prototype Algorithm—Outer Iteration (local version)

Step 0. Let the forcing functions $\epsilon^{\mathrm{D}}(\cdot)$, $\epsilon^{\mathrm{C}}(\cdot)$ and $\epsilon^{\mathrm{U}}(\cdot)$ satisfy A13, and let $0 < \epsilon_\tau < 1/2$. Choose $x^0 \in \mathbb{R}^n$, $s^0 \in \mathbb{R}^{n_{\mathcal{C}}}_+$ such that $c(x^0) + s^0 > 0$, initial dual estimates $y^0, u^0 \in \mathbb{R}^{n_{\mathcal{C}}}_+$, and penalty and barrier parameters ν^0 and $\mu^0 > 0$, and set $k = 0$.

Step 1. Inner Iteration: Obtain the primal-dual Newton step d^{N}_k as a solution to the linear system

$$\nabla_v \Phi(v^k; \mu^k, \nu^*) d^{\mathrm{N}} = -\Phi(v^k; \mu^k, \nu^*), \tag{4.14}$$

where the function $\Phi(v; \mu, \nu)$ is defined in (3.4), and set $v^{k+1} = v^k + d^{\mathrm{N}}_k$.

Step 2. Select a new barrier parameter according to

$$\mu^{k+1} = \Theta\left((\mu^k)^{\tau^k}\right) \qquad \text{where} \qquad 1 + \epsilon_\tau \le \tau^k \le \frac{2}{1+\gamma^{k+1}} - \epsilon_\tau. \tag{4.15}$$

Increment k by one, and return to Step 1.

Note that from Assumptions A9–A11, the Jacobian matrix on the left-hand side of (4.14) remains uniformly nonsingular.

Upon defining the set of nonzero components of the tangent vector (4.13) to the primal-dual central path at v^*,

$$\mathcal{J} = \{i = 1, \ldots, n + 2n_{\mathcal{C}} \mid \dot{v}(0)_i \ne 0\}, \tag{4.16}$$

and under the above assumptions, Algorithm 4.2 fits in the framework of Gould et al. (2001) and Gould et al. (2002*b*) and we obtain the following results, simple modifications of the main results of the aforementioned papers, which we state without proof.

The first result states that the Newton step d^{N} defined in (4.14) is strictly feasible and $v^k + d^{\mathrm{N}}$ satisfies the stopping conditions (3.7) with barrier parameter μ^k.

Theorem 4.8. *(Gould et al., 2001, Theorem 6.2). Under Assumptions A9–A13 for $k \in \mathcal{K}$ sufficiently large, the stopping conditions (3.7) are satisfied at v^{k+1} with $\mu = \mu^k$, and*

$$\|\Phi(v^{k+1}; \mu^k, \nu^*)\| = o(\mu^k). \tag{4.17}$$

The next result states the precise rate of convergence, not only in the error in norm, but in some individual components, defined by (4.16), of the error. It states that the same rate takes place in individual components of the *residuals in complementarity.* More precisely, let

$$\Phi^{\mathrm{C}}(v; \mu, \nu) = \begin{bmatrix} (C(x) + S)y - \mu e \\ Su - \mu e \end{bmatrix}, \tag{4.18}$$

represent the $2n_{\mathcal{C}}$-dimensional subsystem of (3.4) containing only the perturbed complementarity components. If $\dot{\Phi}$ denotes the vector on the right-hand side of (4.13), we have the following nonsingular relationship

$$\nabla_v \Phi(v^*; 0, \nu^*) \dot{v}(0) = \dot{\Phi}.$$

Note that the components of $\Phi^{\mathrm{C}}(v; \mu, \nu)$ correspond precisely to the nonzero components of $\dot{\Phi}$. Following Gould et al. (2002*b*), an interpretation of $\dot{\Phi}$ is as a tangent vector at the end point of a trajectory approximately tracked by the sequence $\{\Phi(v^{k+1}; \mu^k, \nu^k)\}$.

Theorem 4.9. *(Gould et al., 2001, Theorem 6.5, and Gould et al., 2002b, Theorem 3.2). Under Assumptions A9–A13, the complete sequence* $\{v^k\}$ *converges to* v^**, the sequence* $\{\Phi(v^{k+1};\mu^k,\nu^k)\}$ *converges to zero and we have the asymptotic expansions*

$$v^{k+1} = v^* + \mu^k \dot{v}(0) + o(\mu^k) \qquad \textit{and} \qquad \Phi^{C}(v^{k+1};\mu^k,\nu^*) = -\mu^k e + o(\mu^k). \tag{4.19}$$

As a consequence, the asymptotic convergence rate is described by

$$\frac{|v_i^{k+2} - v_i^*|}{|v_i^{k+1} - v_i^*|^{\tau^k}} = \Theta(1) \quad i \in \mathcal{J} \qquad \textit{and} \qquad \frac{|\Phi_i^{C}(v^{k+2};\mu^{k+1},\nu^*)|}{|\Phi_i^{C}(v^{k+1};\mu^k,\nu^*)|^{\tau^k}} = \Theta(1) \quad i = 1,\ldots,2n_{\mathcal{C}}, \tag{4.20}$$

for k *sufficiently large, where* τ^k *is as in (4.15), which implies that the iterates* v^{k+1} *and the residuals in complementarity converge componentwise Q-superlinearly to their limit, along the given components. The remaining components satisfy*

$$|v_i^{k+1} - v_i^*| = o(\mu^k) \quad i \notin \mathcal{J} \qquad \textit{and} \qquad \Phi_i(v^{k+1};\mu^k,\nu^*) = o(\mu^k).$$

As a consequence of Theorem 4.9, a Q-rate of convergence which is as close to quadratic as desired, and which takes place not only in norm but in all the indicated components, is achievable by constructing the sequence $\{\gamma^k\}$ so it converges to zero, by choosing $\epsilon_\tau \simeq 0$ in Algorithm 4.2 and by selecting τ^k equal to its upper bound in (4.15).

Note that in the asymptotics, Algorithm 4.2 branches into Algorithm 6.1 with little modification.

5 Treatment of linear constraints

We briefly digress in this section on the possibility of treating linear constraints explicitly, if any are present, rather than penalizing them. We might distinguish linear equations from the remaining constraints by including the constraints

$$A_E x = b_E, \tag{5.1}$$

where A_E has full row rank, in the general statement (1.1). We consider this case since in practice we may aim to find and maintain feasible points for simple constraints such as (5.1) before treating the nonlinear ones, and also to reflect the generality which must be addressed by a practical implementation.

The reformulation given in §2.1 results in a *linearly-constrained* mixed interior-exterior penalty problem. The Jacobian of the constraints of this problem now takes the form

$$J^{\rm S}(v_{\rm P}) = \begin{bmatrix} J_{\mathcal{E}}(x) & I_{\mathcal{E}} & 0 \\ J_{\mathcal{I}}(x) & 0 & I_{\mathcal{I}} \\ A_E & 0 & 0 \\ 0 & I_{\mathcal{E}} & 0 \\ 0 & 0 & I_{\mathcal{I}} \end{bmatrix}. \tag{5.2}$$

Note that explicit treatment of the linear equations (5.1) preserves the Magansarian–Fromovitz constraint qualification.

Explicit linear *inequality* constraints

$$A_I x \geq b_I, \tag{5.3}$$

including the special case of simple bounds such as

$$x \geq 0, \tag{5.4}$$

might also be treated directly instead of being penalized. In this case, the objective function of the barrier problem will incorporates logarithmic terms to treat the linear inequalities (5.3). The Jacobian of the constraints including both (5.1) and (5.3) is then given by

$$J^{\mathrm{S}}(v_{\mathrm{P}}) = \begin{bmatrix} J_{\mathcal{E}}(x) & I_{\mathcal{E}} & 0 \\ J_{\mathcal{I}}(x) & 0 & I_{\mathcal{I}} \\ A_E & 0 & 0 \\ A_I & 0 & 0 \\ 0 & I_{\mathcal{E}} & 0 \\ 0 & 0 & I_{\mathcal{I}} \end{bmatrix}. \tag{5.5}$$

Unfortunately, MFCQ is no longer automatically satisfied even in the special case of simple bounds (5.4), as it requires that there is a vector d in the nullspace of A_E such that $a_i^T d_i < 0$ for each active inequality $a_i^T x \geq b_i$. A condition such as LICQ on (1.1) is sufficient for this, and provides a consistent context with §4.3.

The convergence theory remains essentially unaltered upon adding the linear constraints (5.1) and (5.3). However, the preconditioning matrices P^k used in (3.7a) and in the trust region (3.8) must this time be uniformly second-order sufficient, which essentially amounts to uniform positive definiteness on the nullspace of the matrix A_E (Conn et al. 2000*b*), on which they define uniformly equivalent norms. Again, the seminorms used in (3.7a) and (3.8) are dual of each other and allow for efficient treatment of the linear constraints.

¿From the practical point of view, the GALAHAD code LSQP (see Gould et al., 2003*b*) may be used to find an approximation to the analytic center for the constraints (5.1) and (5.3). The constraints are preprocessed using the GALAHAD package PRESOLVE (see Gould and Toint, 2002) to remove fixed variables and (some) redundant constraints, and to simplify the remaining constraints if possible. Provided that the linear constraints have a feasible (interior) point, we use the resulting point x^0, for which

$$A_E x^0 = b_E \;\text{ and }\; A_I x^0 > b_I,$$

as a starting point for the remainder of our calculation. We may safely assume that A_E is of full rank, since any rank-deficiency will have been identified and removed by PRESOLVE.

A practical implementation might offer the choice to penalize all constraints altogether or to keep non-redundant linear constraints explicit. Extensive numerical tests are required before we can can we can make firm recommendations.

6 Enhanced and alternative inner iterations

Whilst the inner-iteration algorithm outlined in Section 3.4–3.6 is certainly suitable for our purposes, it is by no means the only possibility. In this section we consider both a simple enhancement to the basic method and a complete alternative based on this enhancement.

6.1 Magical steps

Suppose that our inner-iteration trust-region algorithm has produced a new approximation $(x^{k,j}, s^{k,j})$ to the minimizer of the barrier function $\phi^{\rm B}(x, s; \mu^k, \nu^k)$. Since $\phi^{\rm B}(x, s; \mu, \nu)$ is a *separable* function of s, we might then aim to improve on $(x^{k,j}, s^{k,j})$ by finding the (global) minimizer $s(x)$ of $\phi^{\rm B}(x, s; \mu, \nu)$ for the given $x = x^{k,j}$. Replacing $(x^{k,j}, s^{k,j})$ by the improvement $(x^{k,j}, s(x^{k,j}))$ is an example of what is known as a *magical step*, and fortunately the use of such steps does not interfere with global convergence of the underlying algorithm (see, for example, Conn et al., 2000*a*, Section 10.4.1).

To compute the elastics $s(x)$, note that $s(x)$ necessarily satisfies (componentwise) the equations

$$r(s(x)) \equiv \nabla_s \phi^{\rm B}(x, s(x); \mu, \nu) = \nu(e + e^0_{\mathcal{E}}) - y(x, s(x); \mu) - u(s(x); \mu) = 0, \tag{6.1}$$

for a given x. We may summarize the properties of (6.1) as follows.

Lemma 6.1. *Let Assumptions A1 and A2 be satisfied, the function $r(s(x))$ be defined by (6.1) where x is fixed and the multiplier estimates be given by (3.2). We then have the following properties:*

(i) $r(s)$ is a separable function of s,

(ii) $r(s(x))$ has a unique root, $s(x)$, for which $(x, s(x))$ lies in the interior of the feasible set of (1.3),

(iii) $s(x)$ is twice continuously differentiable for $\max(0, -c_i(x)) < s(x) < \infty$.

Proof. The first and last points are straightforward, given (6.1) and the implicit function theorem. For the second point, notice that $r(s)$ has poles at $s = -c(x)$ and $s = 0$, that $\nabla_s s(x) e > 0$, and that $\lim_{s\to+\infty} r(s) = \nu(e + e^0_{\mathcal{E}}) > 0$. □

In our case, a simple calculation reveals that the magical correction for s is given (componentwise) by

$$s_i^{k,j} = \begin{cases} \dfrac{\mu^k}{2\nu^k} - \dfrac{c_i(x^{k,j})}{2} + \sqrt{\left(\dfrac{c_i(x^{k,j})}{2}\right)^2 + \left(\dfrac{\mu^k}{2\nu^k}\right)^2} & \text{for } i \in \mathcal{E} \\[2ex] \dfrac{\mu^k}{\nu^k} - \dfrac{c_i(x^{k,j})}{2} + \sqrt{\left(\dfrac{c_i(x^{k,j})}{2}\right)^2 + \left(\dfrac{\mu^k}{\nu^k}\right)^2} & \text{for } i \in \mathcal{I}. \end{cases}$$

6.2 An alternative algorithm using implicit elastics

As we have just suggested, we may improve upon a given (x, s) by replacing it by the "magical" $(x, s(x))$. However, this is somewhat inefficient as x is chosen without regard to what $s(x)$ might result. This suggests a better approach might be to treat the elastic variables as implicitly dependent on x *throughout* the inner iteration.

With this in mind, in this section we present an *implicit elastics* alternative to Algorithm 3.2. Since we know from Lemma 6.1 that $s(x)$ is (at least) twice continuously differentiable, we might instead minimize

$$\psi(x) \equiv \phi^{\rm B}(x, s(x); \mu, \nu) \tag{6.2}$$

solely as a function of the variables x. Here $\phi^{\rm B}(\cdot)$ is as defined by (1.4), and we have hidden the dependency of $\psi(\cdot)$ on μ and ν for brevity. In practice, in addition to the reduction in dimension this suggests, the definition of $s(x)$ should help to keep the constraints a comfortable distance from their boundaries, preventing steps from being repeatedly cut back. We now show that a classical trust-region algorithm for the minimization of $\psi(x)$ is well defined.

For future reference, we now give the derivatives of (6.2) in the following result.

Lemma 6.2. *Under Assumption A4, the first and second derivatives of (6.2) are given by*

$$\begin{aligned} \nabla_x \psi(x) &= \nabla f(x) - J^T(x)\sigma(x) \text{ and} && (6.3a)\\ \nabla_{xx}\psi(x) &= H(x,\sigma(x)) + \mu J^T(x)\left[(C(x)+S(x))^2 + S(x)^2\right]^{-1} J(x), && (6.3b)\\ &\equiv H(x,\sigma(x)) + J^T(x)\left[(C(x)+S(x))Y^{-1}(x) + S(x)Y^{-1}(x)\right]^{-1} J(x) && (6.3c)\end{aligned}$$

where we have defined the Lagrange multiplier estimates

$$\begin{aligned} y(x) &\equiv y(x,s(x)) = \mu(C(x)+S(x))^{-1}e, && (6.4a)\\ u(x) &\equiv u(s(x)) = \mu S^{-1}(x)e \text{ and} && (6.4b)\\ \sigma(x) &= y(x) - \nu e^0_{\mathcal{E}}, && (6.4c)\end{aligned}$$

and $H(x,\sigma)$ is given by (3.12).

Proof. Elementary calculations with (6.1) prove (6.3a). We note from (6.1) that $\nabla_x r(s(x)) = 0$, implying $(C(x)+S(x))^{-2}(J(x)+\nabla_x s(x)) = -S^{-2}(x)\nabla_x s(x)$. Extracting $\nabla_x s(x)$ from this identity gives

$$\nabla_x s(x) = -\left[I + (C(x)+S(x))^2 S^{-2}(x)\right]^{-1} J(x),$$

which combines with (6.4c) to yield

$$\nabla_x \sigma(x) = -\mu(C(x)+S(x))^{-2}(J(x)+\nabla_x s(x)) = \mu S^{-2}(x)\nabla_x s(x)$$

and finally, (6.3b). The alternative (6.3c) follows by simple manipulation. □

Note that the second term in the right-hand side of (6.3b) is positive semi-definite.

A typical primal-dual trust-region method for minimizing $\psi(x)$ computes a correction d to the current solution estimate x so as to (approximately)

$$\underset{d}{\text{minimize}} \;\; d^T\nabla\psi(x) + \tfrac{1}{2} d^T B(x,\sigma) d \;\text{ subject to }\; \|d\|_M \le \Delta, \qquad (6.5)$$

where the trust-region radius $\Delta > 0$. The approximation $B(x,\sigma)$ might be the primal Hessian $\nabla_{xx}\psi(x)$ but, as in Section 3.4, there are advantages in instead using the primal-dual approximation

$$B^{\text{PD}}(x,\sigma) = H(x,\sigma) + J^T(x)\left[\Theta^{-1}(x) + U^{-1}S(x)\right]^{-1} J(x), \qquad (6.6)$$

where

$$\begin{aligned} \Theta(x) &= Y(C(x)+S(x))^{-1}, && (6.7a)\\ u &\approx u(x) > 0, && (6.7b)\\ y &\approx y(x) > 0 \text{ and} && (6.7c)\\ \sigma &\approx \sigma(x) && (6.7d)\end{aligned}$$

(c.f. (3.11) and (6.7a)).

As in Section 3.4, lengths of steps and gradients should be measured in norms that reflect curvature. The trust-region norm $\|\cdot\|_M$ ($\equiv \sqrt{\langle\cdot, M\cdot\rangle}$) depends on a suitable symmetric, positive-definite approximation M to $B(x,\sigma)$, and we shall use

$$M = P + J^T(x)\left[U^{-1}S(x) + \Theta^{-1}(x)\right]^{-1} J(x),$$

where as before, P can range from simple-minded ($P = I$) to sophisticated ($P = H(x, \sigma)$). To be specific, we shall assume that, at the termination of the k-th inner-iteration,

A14 each matrix M_k is defined by (6.8), where $P = P^k$ satisfies A5.

The counterpart of the preconditioning system (3.13) is here that

$$M d_x = r_x \tag{6.8}$$

for some given r_x. Significantly, upon introducing auxiliary $d_s = -\left[\Theta(x) + US^{-1}(x)\right]^{-1} J(x)\Theta(x)d_x$, we see that (6.8) is equivalent to (3.13) in the case that $r_s = 0$. In particular, since

$$\nabla_{v_{\mathrm{P}}} \phi^{\mathrm{B}}(x, s(x); \mu, \nu) = \begin{bmatrix} \nabla_x \psi(x) \\ 0 \end{bmatrix}.$$

when $s = s(x)$, we may replace condition (3.7a) with

$$\|\nabla\psi(x^{k+1})\|_{M_{k+1}^{-1}} \le \epsilon^{\mathrm{D}}(\mu^k).$$

The resulting trust-region method is entirely standard, except that any trial value x for which $s(x)$ is undefined or infeasible will be rejected and the trust-region radius retracted.

In order to show that the resulting method is globally convergent, we must make sure that the Hessian matrix of the model, $B^{\mathrm{PD}}(x, \sigma)$, is bounded. To this end, let $\delta_i = 1$ if $i \in \mathcal{E}$ and 0 otherwise.

Lemma 6.3. *The Lagrange multiplier estimates satisfy the bounds*

$$0 < y(x) < \nu(e + e^0_{\mathcal{E}}) \;\; \textit{and} \;\; 0 < u(x) < \nu(e + e^0_{\mathcal{E}}), \tag{6.9}$$

and

$$-\nu e^0_{\mathcal{E}} < \sigma(x) < \nu e. \tag{6.10}$$

Proof. Identities (6.1) and (6.7) combine to give the bounds (6.9). In turn, these bounds an (6.4c) together imply (6.10). □

In view of the required approximations (6.7b)–(6.7d) and Lemma 6.3, we make the further reasonable assumption.

A15 For given ν, the Lagrange multiplier estimates y, u and σ are bounded.

Given this assumption, we now show that our model Hessian remains bounded.

Lemma 6.4. *Under Assumptions A4 and A15, the primal-dual Hessian approximation (6.6) remains bounded for fixed values of $\mu > 0$ and $\nu > 0$.*

Proof. Since (6.6) implies that

$$\|B^{\mathrm{PD}}(x, \sigma)\| \le \|H(x, \sigma)\| + \|J(x)\|\|J^T(x)\|\|\left[Y^{-1}(C(x) + S(x)) + U^{-1}S(x)\right]^{-1}\|,$$

and as Assumptions A4 and A15 ensure that $\|H(x, \sigma)\|$, $\|J(x)\|$ and $\|J^T(x)\|$ are bounded, it remains to show that the (diagonal) entries

$$s_i(x)/u_i + (c_i(x) + s_i(x))/y_i \tag{6.11}$$

of the diagonal matrix $Y^{-1}(C(x) + S(x)) + U^{-1}S(x)$ are bounded away from zero. But combining (6.4a) and (6.4b) with (6.9) shows that

$$c_i(x) + s_i(x) > \frac{\mu}{\nu(1 + \delta_i)} \;\; \text{and} \;\; s_i(x) > \frac{\mu}{\nu(1 + \delta_i)} \;\; \text{and}$$

and this together with A15 gives the required lower bound on (6.11). □

Algorithm 6.1: Prototype Algorithm—Outer Iteration (Implicit Elastics)

Step 0. Let the forcing functions $\epsilon^{\mathrm{D}}(\cdot)$, $\epsilon^{\mathrm{C}}(\cdot)$ and $\epsilon^{\mathrm{U}}(\cdot)$ be given, and let $\kappa_\nu > 0$. Choose $x^0 \in \mathbb{R}^n$, $s^0 \in \mathbb{R}^{nc}_+$ such that $c(x^0) + s^0 > 0$, initial dual estimates $y^0, u^0 \in \mathbb{R}^{nc}_+$, and penalty and barrier parameters ν^0 and $\mu^0 > 0$, and set $k = 0$.

Step 1. Inner Iteration: find a new primal-dual iterate $(x^{k+1}, s(x^{k+1}), y^{k+1}, u^{k+1})$ satisfying

$$\begin{aligned}
\left\|\nabla f(x^{k+1}) - J^T(x^{k+1})(y^{k+1} - \nu^k e^0_{\mathcal{E}})\right\|_{M^{-1}_{k+1}} &\leq \epsilon^{\mathrm{D}}(\mu^k) && (6.12a)\\
\|(C(x^{k+1}) + S(x^{k+1}))y^{k+1} - \mu^k e\| &\leq \epsilon^{\mathrm{C}}(\mu^k). && (6.12b)\\
\|S(x^{k+1})u^{k+1} - \mu^k e\| &\leq \epsilon^{\mathrm{U}}(\mu^k) && (6.12c)\\
\big(c(x^{k+1}) + s(x^{k+1}), s(x^{k+1})\big) &> 0 && (6.12d)\\
\text{and}\quad \big(\nu^k[e + e^0_{\mathcal{E}}] + \kappa_\nu e, \nu^k[e + e^0_{\mathcal{E}}] + \kappa_\nu e\big) \geq \big(y^{k+1}, u^{k+1}\big) &> 0 && (6.12e)
\end{aligned}$$

for some suitable scaling norm $\|.\|_{P^{k+1}}$ by (for example) approximately minimizing (6.2).

Step 2. Select a new barrier parameter, $\mu^{k+1} \in (0, \mu^k]$ such that $\lim_{k\to\infty} \mu^k = 0$. Update the penalty parameter ν^k according to the rule (3.18). Increment k by one, and return to Step 1.

We summarize the results of this section by stating Algorithm 6.1. The convergence properties of Algorithm 6.1 are summarized Theorem 6.5, which we state without proof. This result is a direct parallel of Theorem 4.6.

Theorem 6.5. *Suppose that Assumptions A1–A2, A4, A6–A8 and A14 hold. Suppose that x^* is a limit point of the sequence $\{x^k\}$ generated by Algorithm 6.1. Then either $\{\nu^k\}$ remains bounded, and x^* is a first-order critical point for the nonlinear programming problem (1.1), or $\{\nu^k\}$ diverges, and x^* is a first-order critical point of the infeasibility (2.2). In the first case, the multipliers $\{\sigma(x^k)\}$ generated converge to $\lambda(y^*, \nu^*)$ defined in (2.16).*

In addition to the reasons mentioned earlier in this section, this alternative is attractive in that it empirically stabilizes the algorithm. In contrast with Algorithm 3.2, it also helps prevent infeasible steps from being generated and repeatedly cut. Indeed, it is easy to see from (6.7) and (6.9) that

$$c_i(x) + s_i(x) > \frac{\mu}{\nu(1+\delta_i)} \geq \frac{\mu}{2\nu}, \quad \text{and} \quad s_i(x) > \frac{\mu}{\nu(1+\delta_i)} \geq \frac{\mu}{2\nu}.$$

so long as $s(x)$ exists.

For completeness, in view of Lemma 6.4 and Theorem 4 of Conn et al. (2000*b*), it is straightforward to show the following result, which again we state without proof.

Theorem 6.6. *Under Assumptions A1–A2, A4, A6–A8 and A14, the implicit-elastic inner iteration procedure outlined in this section generates a sequence $\{(x^{k+1}, s(x^{k+1}), y^{k+1}, u^{k+1})\}$ satisfying the inner-iteration stopping conditions (6.12) for iteration k of Algorithm 6.1. after finitely many steps.*

7 Practical considerations, enhancements and refinements

Here we mention a number of other important practical considerations.

7.1 Initial elastics

As mentioned earlier, finding an initial strictly feasible estimate (x^0, s^0) for (1.3) is trivial. Any value $s^0 > \max[0, -c(x^0)]$ is acceptable. In practice, only those s_i (or r_i, depending on the formulation chosen) that are required to be positive because of the initial x need be retained, although it is actually prudent to keep those for which s_i (or r_i) needs to be larger than some "small" positive value (say, 0.1). More generally, it may be beneficial to track each $s_i^{k,j}$ as the iteration progresses and to remove it as soon as the corresponding $c_i(x^{k,j})$ is sufficiently positive. Doing so does not effect the convergence results described in this paper, as there can only be a finite number of these removals.

7.2 Two-sided inequalities

In the presence of two-sided inequality constraints

$$c_i^{\mathrm{L}} \leq c_i(x) \leq c_i^{\mathrm{U}}$$

the obvious penalty term $\nu \max(c_i^{\mathrm{L}} - c_i(x), c_i(x) - c_i^{\mathrm{U}}, 0)$ may be replaced by νs_i, where s_i is required to satisfy

$$s_i + c_i^{\mathrm{U}} - c_i(x) \geq 0, \quad s_i + c_i(x) - c_i^{\mathrm{L}} \geq 0 \text{ and } s_i \geq 0.$$

Thus a single elastic variable suffices, rather than the pair that might have been anticipated if $c_i(x) \geq c_i^{\mathrm{L}}$ and $c_i(x) \leq c_i^{\mathrm{U}}$ had been considered separately.

If we wish to improve the value of $\phi^{\mathrm{B}}(v_{\mathrm{P}}; \mu, \nu)$ using a magical step as described in Section 6.1 or to use the implicit-elastic approach of Section 6.2, the defining equation

$$r(x) \equiv \nu(e + e^0_{\mathcal{E}}) - \mu[C(x) - C^{\mathrm{L}} + S(x)]^{-1}e - \mu[C^{\mathrm{U}} - C(x) + S(x)]^{-1}e - \mu S^{-1}(x)e = 0$$

for the $s(x)$ for a two-sided inequality may be reduced to a cubic equation. While it is possible to give an explicit formula for the required root, in practice it is just as easy to use a safeguarded univariate Newton method to find it.

7.3 Imposing upper bounds on the elastics

There may be some virtue in adding an upper bound s^{U} on the elastic variables in order to prevent $c(x)$ and s simultaneously diverging to infinity. Of course it is far from obvious what globally a good value for s^{U} might be, but the a simple choice of $\max(10, 2s^0)$ has proved to be sufficient in early experiments. The resulting two-sided bound

$$0 \leq s \leq s^{\mathrm{U}}$$

may then be handled exactly as in Section 7.2.

8 Conclusions and alternatives

In this paper we have presented a mixed interior-exterior penalty method for the general nonlinear programming problem (1.1). The problem undergoes a change of variables whose benefit is to yield a continuously differentiable, exact, merit function as well as to ensure that the new feasible set has a nonempty strict interior. Noticeably, the problem turns out to also be surprisingly regular in that it satisfies MFCQ without any regularity assumption on (1.1). Additionally, there is much freedom and ease in choosing a starting point.

The reformulated problem turns out to be well suited for a primal-dual interior-point method, and global and local convergence results from Conn et al. (2000*b*), Gould et al. (2001) and Mayne and Polak (1976) combine to ensure general and robust properties for the method, under mild assumptions. While the inner-iteration subproblem may be solved in terms of both the original and added elastic variables, an alternative in which the elastics depend implicitly on the original ones has also been considered.

The whole approach is currently being implemented as a new solver for general nonlinear programs as part of the GALAHAD library (Gould et al., 2003*b*). We feel that it is premature to report numerical results at this stage as we wish our conclusions to be based on a careful rather than prototype implementation of our algorithm, especially one suited to solving large-scale problems. We will report on the effectiveness of our approach in due course.

Clearly, we recognize that the particular approach adopted in this paper is not the only possible one. Another possibility is to use the ℓ_∞ penalty function

$$\phi(x,\nu) = f(x) + \nu \max_{i\in\mathcal{E}} |c_i(x)| + \nu \max_{i\in\mathcal{I}} (-c_i(x), 0) \tag{8.1}$$

instead of (2.1). As before, it is easy to show that this may be reformulated as

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n,\, s\in\mathbb{R}}{\text{minimize}} & f(x) + \nu s \ \text{ subject to } \ c_i(x) + s \geq 0 \ \ (i \in \mathcal{E}\cup\mathcal{I}) \\ & s - c_i(x) \geq 0 \ \ (i\in\mathcal{E}) \ \text{ and } \ s \geq 0 \end{array}$$

involving a single "elastic" variable s. Once again one might apply an interior-point algorithm to such a problem, and again it is trivial to find an initial interior point. The advantage now is clearly this formulation involves significantly fewer surplus variables. The ℓ_∞ approach is also examined in the framework of so-called *elastic mode* in Boman (1999).

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