Primal-Dual Nonlinear Rescaling Method for Convex Optimization¹

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Abstract. In this paper, we consider a general primal-dual nonlinear rescaling (PDNR) method for convex optimization with inequality constraints. We prove the global convergence of the PDNR method and estimate the error bounds for the primal and dual sequences. In particular, we prove that, under the standard second-order optimality conditions, the error bounds for the primal and dual sequences converge to zero with linear rate. Moreover, for any given ratio $0 < \gamma < 1$, there is a fixed scaling parameter $k_{\gamma} > 0$ such that each PDNR step shrinks the primal-dual error bound by at least a factor $0 < \gamma < 1$, for any $k \ge k_{\gamma}$. The PDNR solver was tested on a variety of NLP problems including the constrained optimization problems (COPS) set. The results obtained show that the PDNR solver is numerically stable and produces results with high accuracy. Moreover, for most of the problems solved, the number of Newton steps is practically independent of the problem size.

Key Words. Nonlinear rescaling, duality, Lagrangian, primal-dual methods, multipliers methods.

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1. Introduction

For LP calculations, interior-point methods (IPM) in general and primal-dual IPM in particular are a great success story, brilliantly written in Ref. 1; see also the references therein. The key idea of the primal-dual (PD) methods consists in replacing the unconstrained optimization of the log-barrier function by solving a particular PD system of equations. Then, instead of solving the PD system, one has to perform one or two Newton steps toward the solution followed by a barrier parameter update.

In LP calculations, the central path properties (see Refs. 2–4), structure of the PD system, and substantial advances in numerical linear algebra (see Ref. 1) produced spectacular numerical results (see Refs. 1, 5–7). Moreover, along with polynomial complexity, superlinear or even quadratic rate of convergence was proven for some IPM (Ref. 8).

The success in LP stimulated the extension of the PD-IPM approach for nonlinear programming (NLP, see Refs. 9–12 and references therein). But the situation in NLP is not as bright as in LP. Even the most advanced solvers based on the PD-IPM approach sometimes experience numerical difficulties. This motivated us to try an alternative to the IPM approach based on NR theory (Refs. 13–17). There are four basic reasons for using NR theory to develop a PD method.

- (i) NR methods do not require an unbounded increase of the scaling parameter and they have better rate of convergence under standard assumption on the input data than classical barrier methods.
- (ii) The area where the Newton method for unconstrained minimization is well defined does not shrink to a point when the PD approximation approaches the PD solution.
- (iii) The condition number for the Hessian of the Lagrangian for the equivalent problem remains stable up to the end of the computation process.
- (iv) It does not require any computational effort to find the initial approximation for either the primal or dual vector, because the NR methods are exterior in primal space and interior in dual space.

Although fixing the scaling parameter is not our recommendation, the ability to find a good approximation to the primal-dual solution with a fixed and often not very large scaling parameter and use it as a starting point in the NR methods allowed us to produce robust and very accurate results on a number of large-scale and difficult NLP problems including the COPS set (Ref. 18).

In this paper, we describe and analyze the primal-dual method for constrained optimization with inequality constraints, which is based on NR theory. Each step of the NR method is equivalent to solving a primal-dual (PD) system of nonlinear equations. The first set of equations is defined by optimality criteria for the primal minimizer. The second set is given by the formulas for the Lagrange multipliers update.

The primal-dual NR (PDNR) method consists of using the Newton method for solving the PD system. The Newton method for the PD system converges locally to the primal-dual solution very fast under a fixed scaling parameter. To guarantee global convergence, we combined the PDNR method with the primal-dual path-following (PDPF) method, which converges globally, but not as fast.

We introduce a general class of constraint tranformations and formulate the PDPF method, establish convergence and estimate the rate of convergence of the PDPF method under very mild assumptions on the input data. This is our first contribution.

Our second contribution is the globally convergent PDNR method. One can consider PDNR as three-phase method. In the first phase, we fix the Lagrange multipliers and increase the scaling parameter from step to step, so that the primal-dual approximations stay close to the PDPF trajectory. In the second phase, we fix the scaling parameter and update the Lagrange multipliers from step to step, so that the primal-dual approximations follow the NR trajectory. In the final phase, the NR method turns automatically into the Newton method for the primal-dual NR system.

To formulate the PDNR method, we introduce a merit function, which measures the distance between a primal-dual approximation and a primal-dual solution. We proved convergence and estimated the rate of convergence of the PDNR method. It was shown in particular that under the standard second-order optimality conditions, from some point on only one PDNR step is required to shrink the distance from a primal-dual approximation to the primal-dual solution by a chosen factor $0 < \gamma < 1$. This is our third contribution.

Our fourth contribution is the numerical realization of the PDNR method. The MATLAB code, which is based on NR theory, has been tested on a wide class of NLP including the COPS set (Ref. 18). The numerical results obtained corroborate the theory and provide strong evidence that the PDNR method is numerically robust and able to produce solutions with high accuracy. Moreover, in many instances, the number of Newton steps is independent of the size of a problem.

The paper is organized as follows. In Section 2, we consider a convex optimization problem with inequality constraints and discuss the basic assumptions. In Section 3, we describe a class of concave and smooth

enough scalar functions of a scalar argument, which are used to transform the inequality constraints of a given constrained optimization problem into an equivalent set of constraints. We describe the basic global and local properties of the Lagrangian for the equivalent problem in the neighborhood of the primal-dual solution. The extra features of the Lagrangian for the equivalent problem (as compared with to the Lagrangian for the original problem) lead to the most important properties of the NR multipliers method, which we describe at the end of Section 3. In Section 4, we describe the primal-dual system of equations. Solving the system is equivalent to one step of the NR method. Then, we consider the Newton method for the PD system and show that the primal Newton direction for the PD system coincides with the Newton direction for the primal minimization of the Lagrangian for the equivalent problem.

The PDNR method converges fast, but locally in the neighborhood of the solution. Therefore, in Section 5, we consider the globally convergent path-following (PF) method and the corresponding trajectory. We prove convergence and establish the rate of convergence of the PF method under very mild assumptions on the input data. The results of this section complement the convergence results of SUMT type methods (see Refs. 19–21).

In Section 6, we consider the PDPF method. In Section 7, we establish the rate of convergence of the PDNR method under the standard second-order optimality conditions. In Section 8, we describe the globally convergent PDNR method for convex optimization, which combines the best properties of the PF and NR methods and, at the same time, is free from their main drawbacks. Also in Section 8, we describe the numerical realization of the PDNR method and provide some details about the MATLAB code, which is based on the PDNR method. In Section 9, we discuss the numerical results obtained for the COPS set (Ref. 18). In Section 10, we discuss issues related to future research.

2. Statement of the Problem and Basic Assumptions

Let $f : \mathbb{R}^n \to \mathbb{R}^1$ be convex; let $c_i : \mathbb{R}^n \to \mathbb{R}^1, i = 1, ..., m$, be concave and smooth functions. We consider a convex set

 $\Omega = \{x \in \mathbb{R}^n : c_i(x) \ge 0, i = 1, \dots, m\}$

and the following convex optimization problem:

 $x^* \in X^* = \operatorname{Argmin}\{f(x) | x \in \Omega\}.$

We assume that:

- (A) The optimal set X^* is not empty and bounded.
- (B) The Slater condition holds; i.e., there exists $\hat{x} \in \mathbb{R}^n : c_i(\hat{x}) > 0$, i = 1, ..., m.

Due to the Assumption (B), the Karush-Kuhn-Tucker (KKT) conditions hold true; i.e., there exists a vector $\lambda^* = (\lambda_1^*, \dots, \lambda_m^*) \in \mathbb{R}^m_+$ such that

$$\nabla_{x}L(x^{*},\lambda^{*}) = \nabla f(x^{*}) - \sum_{i=1}^{m} \lambda_{i}^{*} \nabla c_{i}(x^{*}) = 0, \qquad (1)$$

where

$$L(x, \lambda) = f(x) - \sum_{i=1}^{m} \lambda_i c_i(x)$$

is the Lagrangian for the primal problem ${\cal P}$ and the complementary slackness conditions hold; i.e.,

$$c_i(x^*) \ge 0, \quad \lambda_i^* \ge 0, \quad \lambda_i^* c_i(x^*) = 0, i = 1, \dots, m.$$
 (2)

Also, due to (B), the dual optimal set

$$L^* = \left\{ \lambda \in \mathbb{R}^m_+ : \nabla f(x^*) - \sum_{i=1}^m \lambda_i \nabla c_i(x^*) = 0, \, x^* \in X^* \right\}$$
(3)

is bounded.

Along with the primal problem \mathcal{P} , we consider the dual problem \mathcal{D} ,

$$\lambda^* \in L^* = \operatorname{Argmax} \{ d(\lambda) | \lambda \in \mathbb{R}^m_+ \},\$$

where

$$d(\lambda) = \inf_{x \in \mathbb{R}} L(x, \lambda)$$

is the dual function.

3. Equivalent Problem and Nonlinear Rescaling Method

Let $-\infty < t_0 < 0 < t_1 < \infty$. We consider a class Ψ of twice continuously differential functions $\psi: (t_0, t_1) \to \mathbb{R}$ that satisfy the following properties:

(i) $\psi(0) = 0$, (ii) $\psi'(t) > 0$, (iii) $\psi'(0) = 1$, (iv) $\psi''(t) < 0$, (v) there is a > 0 that $\psi(t) \le -at^2$, $t \le 0$, (vi) $\psi'(t) \le bt^{-1}$, $-\psi''(t) \le ct^{-2}$, t > 0, b > 0, c > 0.

It follows from (vi) that

(vii) $\lim_{\tau \to 0_+} \tau \psi'(z/\tau) = 0, \forall z \ge 0.$

The functions $\psi \in \Psi$ are used to transform the constraints of a given constrained optimization problem into an equivalent set of constraints. Let us consider a few transformations $\psi \in \Psi$:

(a) exponential transformation (Ref. 22),

$$\psi_1(t) = 1 - e^{-t};$$

(b) logarithmic modified barrier function (Ref. 13),

 $\psi_2(t) = \log(t+1);$

(c) hyperbolic modified barrier function (Ref. 13),

 $\psi_3(t) = t/(1+t).$

Each of the above transformation can be modified in the following way. For a given $-1 < \tau < 0$, we define the quadratic extrapolation of the transformations (a)–(c) by the formulas

$$(d)\psi_{q_i}(t) = \begin{cases} \psi_i(t), & t \ge \tau, \\ q_i(t) = a_i t^2 + b_i t + c_i, & t \le \tau, \end{cases}$$

where a_i, b_i, c_i are found from the following equations:

$$\psi_i(\tau) = q_i(\tau), \quad \psi'_i(\tau) = q'_i(\tau), \quad \psi''_i(\tau) = q''_i(\tau).$$

We obtain

$$a = 0.5\psi''(\tau), b = \psi'(\tau) - \tau\psi''(\tau), c = \psi(\tau) - \tau\psi'(\tau) + \tau^2\psi''(\tau),$$

so that $\psi_{q_i}(t) \in C^2$. Such modification of the logarithmic modified barrier function (MBF) was introduced in Ref. 23 and was successfully used in Ref. 24 for solving large-scale NLP.

The modification leads to transformations, which are defined on $(-\infty, \infty)$ and, along with the penalty function properties, have some extra important features. Other examples of transformations with similar properties can be found in Refs. 14, 17, 19.

For any given transformation $\psi \in \Psi$ and any k > 0, due to properties (i)–(iii), we obtain

$$\Omega = \{x : k^{-1} \psi(kc_i(x)) \ge 0, i = 1, \dots, m\}.$$
(4)

Therefore, for any k > 0, the following problem:

$$x^* \in X^* = \operatorname{Argmin}\{f(x)|k^{-1}\psi(kc_i(x)) \ge 0, i = 1, \dots, m\}$$
(5)

is equivalent to the original problem \mathcal{P} . The classical Lagrangian $\mathcal{L}: \mathbb{R}^n \times \mathbb{R}^m_+ \times \mathbb{R}^1_+ \to \mathbb{R}^1$ for the equivalent problem (5), which is our main tool, is given by the formula

$$\mathcal{L}(x,\lambda,k) = f(x) - k^{-1} \sum_{i=1}^{m} \lambda_i \psi(kc_i(x)).$$
(6)

It follows from the convexity of f(x), concavity of $c_i(x)$, i = 1, ..., m, and concavity of ψ that $\mathcal{L}(x, \lambda, k)$ is convex in $x \in \mathbb{R}^n$ for any $\lambda \in \mathbb{R}^m_+$ and k > 0.

Due to property (vii), for any given $\lambda \in \mathbb{R}_{++}^{m}$ and k > 0, there exists

$$x(\lambda, k) = \operatorname{argmin}\{\mathcal{L}(x, \lambda, k) | x \in \mathbb{R}^n\}.$$

Therefore, the following NR method is well defined.

Let $\lambda^0 \in \mathbb{R}^m_{++}$ be the initial Lagrange multipliers vector and let k > 0 be fixed. We assume that the primal-dual pair $(x^s, \lambda^s) \in \mathbb{R}^n \times \mathbb{R}^m_{++}$ has been found already. We find the next approximation (x^{s+1}, λ^{s+1}) by the following formulas:

$$x^{s+1} = \operatorname{argmin}\{\mathcal{L}(x,\lambda^s,k) | x \in \mathbb{R}^n\}$$
(7)

or

$$x^{s+1} : \nabla_{x} \mathcal{L}(x^{s+1}, \lambda^{s}, k) = \nabla f(x^{s+1}) - \sum_{i=1}^{m} \psi' \left(kc_{i} \left(x^{s+1} \right) \right) \lambda_{i}^{s} \nabla c_{i}(x^{s+1}) = 0,$$
(8)

and

$$\lambda_i^{s+1} = \psi'\left(kc_i\left(x^{s+1}\right)\right)\lambda_i^s, \quad i = 1, \dots, m,$$
(9)

or

$$\lambda^{s+1} = \Psi'\left(kc\left(x^{s+1}\right)\right)\lambda^s,\tag{10}$$

where

$$\Psi'\left(kc\left(x^{s+1}\right)\right) = \operatorname{diag}\left(\psi'\left(kc_i\left(x^{s+1}\right)\right)\right)_{i=1}^{m}$$

From (8) and (9), for any k > 0, we have

$$\nabla_x \mathcal{L}(x^{s+1}, \lambda^s, k) = \nabla_x L(x^{s+1}, \lambda^{s+1}) = 0$$

For the dual function $d: \mathbb{R}^m_+ \to \mathbb{R}$, we have

$$d(\lambda^s) = L(x^s, \lambda^s), \, \lambda^s \in \mathbb{R}^m_{++}, \quad s \ge 1.$$

Generally speaking, the NR method is an exterior-point method for the primal problem and interior-point method for the dual problem due to (ii) and the formula (9) for the Lagrange multipliers update.

4. Newton Method for the Primal-Dual System

For a given $x \in \mathbb{R}^n$, Lagrange multiplier vector $\lambda \in \mathbb{R}^m_{++}$, and k > 0, one step of the NR method (7)-(9) is equivalent to solving the following primal-dual system:

$$\nabla_{x}\mathcal{L}(\hat{x},\lambda,k) = \nabla f(\hat{x}) - \sum_{i=1}^{m} \psi'(kc_{i}(\hat{x}))\lambda_{i}\nabla c_{i}(\hat{x})$$
$$= \nabla_{x}L(\hat{x},\hat{\lambda}) = 0, \qquad (11)$$
$$\hat{\lambda} = \Psi'(kc_{i}(\hat{x}))\lambda, \qquad (12)$$

for \hat{x} and $\hat{\lambda}$. We consider the Newton step for solving the system

$$\nabla_{x}L(\hat{x},\hat{\lambda}) = \nabla f(\hat{x}) - \sum_{i=1}^{m} \hat{\lambda}_{i} \nabla c_{i}(\hat{x}) = 0, \qquad (13)$$

$$\hat{\lambda} = \Psi'(kc_i(\hat{x}))\lambda, \tag{14}$$

for \hat{x} and $\hat{\lambda}$ under a fixed k > 0, using (x, λ) as a starting point. Assuming that

$$\hat{x} = x + \Delta x, \quad \hat{\lambda} = \bar{\lambda} + \Delta \lambda,$$

where

$$\bar{\lambda} = \Psi'(kc(x))\lambda,$$

and by linearizing (13)–(14), we obtain the following system for finding the primal-dual (PD) Newton direction $(\Delta x, \Delta \lambda)$:

$$\nabla_{xx}^2 L(x,\bar{\lambda})\Delta x - \nabla c(x)^T \Delta \lambda = -\nabla_x L(x,\bar{\lambda}) = -\nabla_x L(\cdot),$$
(15)

$$-k\Psi''(kc(x))\Lambda\nabla c(x)\Delta x + \Delta\lambda = 0,$$
(16)

where

$$\Psi''(\cdot) = \Psi''(kc(x))$$

= diag($\psi''(kc_i(x))$)_{i=1}^m
 $\Lambda = \text{diag}(\lambda_i)_{i=1}^m$,

or

$$N(\cdot) \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = \begin{bmatrix} \Delta_{xx}^2 L(\cdot) & -\nabla c^T(\cdot) \\ -k \Psi''(\cdot) \Lambda \nabla c(\cdot) & I \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = \begin{bmatrix} -\nabla_x L(\cdot) \\ 0 \end{bmatrix},$$
(17)

where *I* is the identity matrix in \mathbb{R}^m and $\nabla c(\cdot) = \nabla c(x)$.

The matrix $N(\cdot)$ is often sparse; therefore, sparse numerical linear algebra techniques are usually very efficient (see Refs. 1,7,12,25). We can reduce also the system (17) by substituting the value of $\Delta\lambda$ from (16) into (15). Then, the primal Newton direction is found from the following system:

$$M(x,\bar{\lambda},\lambda,k)\Delta x = -\nabla_x L(x,\bar{\lambda}), \tag{18}$$

where

$$M(\cdot) = M(x, \bar{\lambda}, \lambda, k)$$

= $\nabla_{xx}^2 L(x, \bar{\lambda}) - k \nabla c^T(x) \Psi''(kc(x)) \Lambda \nabla c(x).$

The matrix $M(\cdot)$ is not only symmetric, but also positive definite under some standard assumptions on the input data, which we will discuss later.

The Newton direction for the dual vector is found by the formula

$$\Delta \lambda = k \Psi''(kc(x)) \Lambda \nabla c(x) \Delta x. \tag{19}$$

So, we obtain the new primal-dual vector as

$$\begin{aligned} x &:= x + \Delta x, \quad \lambda := \bar{\lambda} + \Delta \lambda \\ &= \bar{\lambda} + k \Psi''(kc(x)) \Lambda \nabla c(x) \Delta x. \end{aligned}$$
(20)

In other words, one step of the primal-dual method consists of the following operations:

Step 1. Find the dual predictor

 $\bar{\lambda} = \Psi'(kc(x))\lambda.$

- Step 2. Find the primal corrector Δx from (17) or (18).
- Step 3. Find the dual corrector

$$\Delta \lambda = k \Psi''(kc(x)) \Lambda \nabla c(x) \Delta x.$$
⁽²¹⁾

Step 4. Find the new primal-dual vector

$$x := x + \Delta x, \quad \lambda := \lambda + \Delta \lambda. \tag{22}$$

Before we discuss some numerical aspects of the Newton method for the PD system, we would like to show that the primal Newton direction is at the same time the Newton direction for the unconstrained minimization of $\mathcal{L}(x, \lambda, k)$ in x under fixed $\lambda \in \mathbb{R}^m_{++}$ and k > 0. Thus, the following lemma takes place.

Lemma 4.1. The primal Newton direction for the PD system (13)–(14) coincides with the Newton direction for unconstrained minimization of $\mathcal{L}(x, \lambda, k)$ in x under fixed $\lambda \in \mathbb{R}^m_{++}$ and k > 0.

The proof of the lemma is in Ref. 26.

The most costly part of the Newton method for the primal-dual system is solving the system (17) or (18). We would like to concentrate on (18) for the moment. In contrast to the classical log-barrier function, the matrix $\nabla_{xx} \mathcal{L}(x, \lambda, k)$ exists at (x^*, λ^*) ; i.e., the matrix

$$M_{k} = M(x^{*}, \lambda^{*}, \lambda^{*}, k)$$

= $\nabla_{xx}^{2} L(x^{*}, \lambda^{*}) - k \psi''(0) \nabla c_{(r)}^{T}(x^{*}) \Lambda^{*} \nabla c_{(r)}(x^{*})$ (23)

exists and has a bounded condition number for any fixed k > 0.

If \mathcal{P} is a convex optimization problem and if f(x) or one of the functions $-c_i(x), i = 1, ..., m$, is strictly convex and the correspondent $\lambda_i^* > 0$, then the matrix M_k is positive definite. It remains true for any

matrix $M(x, \overline{\lambda}, \lambda, k)$ in the neighborhood of the primal-dual solution (x^*, λ^*) , if f and c_i are smooth enough.

Moreover, if the standard second-order optimality conditions are satisfied and if k > 0 is large enough, then due to the Debreu theorem, the matrix M_k is positive definite even if none of f(x) or $-c_i(x), i = 1, ..., p$, is convex. It remains true also for any matrix $M(\cdot) = M(x, \overline{\lambda}, \lambda, k)$, when (x, λ) is in the neighborhood of the primal-dual solution.

The possibility of using $M(\cdot)$ with a fixed k > 0 in the PDNR method is one of the most important features of the method. It keeps stable the condition number of matrix $M(\cdot)$ as well as the area where the Newton method is well defined (see Ref. 27) when the primal-dual sequence approaches the primal-dual solution (x^*, λ^*) . At the same time, the NR method (8)–(9) has a linear rate of convergence. The ability to compute the Newton direction with high accuracy allows us to obtain robust and very accurate results on a number of NLP including the COPS set (see Ref. 18).

Being very efficient in the neighborhood of the primal-dual solution, the Newton method for the PD system might not converge globally. In Section 5, we describe a general primal-dual path following (PDPF) method, which converges globally but not very fast. Later, we will describe an algorithm which allows us to turn automatically the PDPF method into the PDNR method from some point on. As a result, we obtain a globally convergent method, which combines the best qualities of both the PDPF and PDNR methods and at the same time is free from their main drawbacks.

5. Path Following Method

For a given transformation $\psi \in \Psi$ and a fixed k > 0, we consider the penalty type function $P : \mathbb{R}^n \times \mathbb{R}_+ \to \mathbb{R}^1$ given by formula

$$P(x,k) = \mathcal{L}(x, e, k)$$

= $f(x) - k^{-1} \sum_{i=1}^{m} \psi(kc_i(x)).$ (24)

Due to (vii), the primal minimizer

 $x(k) = \operatorname{argmin}\{P(x,k)|x \in \mathbb{R}^n\}$ (25)

exists for any given k > 0. So, x(k) is the solution for the following system:

$$\nabla_{x} P(x,k) = \nabla f(x) - \sum_{i=1}^{m} \psi'(kc_{i}(x)) \nabla c_{i}(x)$$

= 0. (26)

Let

 $\lambda(k) = (\lambda_1(k), \ldots, \lambda_m(k))$

be a vector of the Lagrange multipliers, where

$$\lambda_i(k) = \psi'(kc_i(x(k))), \quad i = 1, \dots, m.$$
 (27)

Then,

$$\nabla_{x} P(x(k), k) = \nabla f(x(k)) - \sum_{i=1}^{m} \lambda_{i}(k) \nabla c_{i}(x(k))$$
$$= \nabla_{x} L(x(k), \lambda(k))$$
$$= 0$$
(28)

and

$$\lambda(k) = \Psi'(kc(x(k)))e, \tag{29}$$

where

$$e = (1, \ldots, 1) \in \mathbb{R}^m.$$

The primal trajectory $\{x(k)\}_{k=1}^{\infty}$ is generally speaking an exterior-point trajectory, while the dual $\{\lambda(k)\}_{k=1}^{\infty}$ is an interior-point trajectory due to (ii) and (27).

First, we will show the convergence of the path-following method (25)–(27) and estimate the rate of convergence. Let

$$c_{-}(x(k)) = \max\{0, -c_{i}(x(k)) | i = 1, ..., m\}$$

be the maximum constraint violation at x(k). Keeping in mind that x(k) is generally speaking a primal exterior point, while $\lambda(k)$ is the dual interior point, we cannot claim that

 $f(x(k)) \ge d(\lambda(k)).$

To measure the duality gap, we introduce

$$\Delta(k) = |f(x(k)) - d(\lambda(k))| \le \sum_{i=1}^{m} \lambda_i(k) |c_i(x(k))|.$$

Keeping in mind that

$$\nabla_{x} L(x(k), \lambda(k)) = 0,$$

we can view

$$\mu(x(k), \lambda(k)) = \max\{c_{-}(x(k)), \Delta(k)\} \ge 0$$

as a merit function, which in a sense measures the distance from $(x(k), \lambda(k))$ to the primal dual solution (x^*, λ^*) , because

$$\mu(x(k), \lambda(k)) = 0 \Longleftrightarrow x(k) = x^*, \ \lambda(k) = \lambda^*.$$
(30)

In the following theorem, we establish convergence and estimate the rate of convergence of the PF method (25)–(27), assuming that $||x|| = \sqrt{x^T x}$.

Theorem 5.1. If X^* and L^* are bounded, then:

(i)
$$\lim_{k \to \infty} f(x(k)) = f(x^*), \quad \lim_{k \to \infty} d(\lambda(k)) = d(\lambda^*).$$
 (31)

(ii) The following estimations hold

$$c_{-}(x(k)) = \mathcal{O}(k^{-1}),$$
 (32a)

$$\Delta(k) = \mathcal{O}(k^{-1}). \tag{32b}$$

Proof. Without restricting the generality, we can assume that Ω is bounded. If it is not so, then by adding one extra constraint $f(x) \le M$ for big enough M > 0, we obtain a bounded feasible set (see Ref. 21 Corollary 20 on p. 94) due to the boundedness of X^* . For M > 0 big enough, the extra constraint cannot affect the solution.

First, we prove that $\{x(k)\}_{k=1}^{\infty}$ is bounded. We consider the interior point $x^0: c_i(x^0) > 0$, which exists due to the Slater condition. Assuming that the sequence $\{x(k)\}_{k=1}^{\infty}$ is unbounded, we have

$$\lim_{k \to \infty} ||x(k) - x^0|| = \infty.$$
(33)

The sequence

$$\{z(k) = (x(k) - x^0) ||x(k) - x^0||^{-1}\}_{k=1}^{\infty}$$

is bounded. Without restricting generality, we can assume that

$$\bar{z} = \lim_{k \to \infty} z(k).$$

For

$$t(k) = ||x(k) - x^0||,$$

we have

 $x(k) = x^0 + t(k)z(k)$

and, due to (33), for any large enough t > 0, we can find k > 0 that $t(k) \ge t$. From boundedness of Ω , we obtain that, for any k > 0 large enough, $x(k) \notin \Omega$. Therefore, for such k > 0, there is an index $1 \le i < m$, such that

$$c_i(x^0) > 0$$
 and $c_i(x^0 + t(k)z(k)) < 0$.

Let i = 1; then, due to the continuity of $c_1(x)$, there is \bar{t}_k such that

$$c_1(x^0 + \bar{t}_k z(k)) = c_1(\bar{x}(k)) = 0$$

and we can assume that $\bar{x}(k) \in \partial \Omega$; i.e.,

 $c_i(\bar{x}(k)) \ge 0, \quad i = 1, \dots, m.$

If it is not so, we will continue this process up to the point when $\bar{x}(k) \in \partial \Omega$.

The sequence $\{\bar{t}_k\}$ is bounded. Without restricting generality, we can assume

$$\bar{t} = \lim_{k \to \infty} \bar{t}_k > 0.$$

Therefore,

$$\bar{x} = x^0 + \bar{t}\bar{z} \in \partial \Omega.$$

Let us assume that

$$c_1(x^0 + \bar{t}\bar{z}) = c_1(\bar{x}) = 0.$$

Then, from the concavity of $c_1(x)$, we obtain

$$c_1(x^0) = c_1(x^0) - c_1(x^0 + \bar{t}\bar{z}) \leq -\bar{t}(\nabla c_1(\bar{x}), \bar{z}),$$

i.e.,

$$(\nabla c_1(\bar{x}), \bar{z}) \leq -c_1(x^0)\bar{t}^{-1}$$

= $-\alpha, \quad \alpha > 0.$

Therefore, for $k_0 > 0$ large enough and any $k \ge k_0$, we obtain

$$(\nabla c_1(\bar{x}(k)), z(k)) \le -\alpha/2, \quad k \ge k_0.$$
 (34)

For a given vector $x \in \mathbb{R}^n$, we consider two sets of indices,

 $I_+(x) = \{i : c_i(x) > 0\}$

and

$$I_{-}(x) = \{i : c_i(x) < 0\}.$$

In view of

$$x(k) = \operatorname{argmin}\{P(x, k) | x \in \mathbb{R}^n\},\$$

we obtain that, for any k > 0,

$$f(x(k)) - k^{-1} \sum_{i=1}^{m} \psi(kc_i(x(k))) \le f(x^0) - k^{-1} \sum_{i=1}^{m} \psi(kc_i(x^0)) \le f(x^0).$$

Keeping in mind that

$$\psi(kc_i(x^0)) > 0, \quad i = 1, \dots, m,
\psi(kc_i(x(k))) < 0, \quad i \in I_-(x(k)),$$

the convexity of f(x), the concavity of $\psi(t)$, as well as properties (i)–(v) of the transformation ψ , we obtain

$$ka(c_{1}(x(k)))^{2} \leq -k^{-1}\psi(kc_{1}(x(k)))$$

$$\leq f(x^{0}) - f(\bar{x}(k)) + f(\bar{x}(k)) - f(x(k))$$

$$+k^{-1}\sum_{i\in I_{+}(x(k))}(\psi(kc_{i}(k))) - \psi(0))$$

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

$$+\sum_{i\in I_{+}(x(k))}c_{i}(x(k)) - (t(k) - \bar{t}_{k})(\nabla f(\bar{x}(k), z(k)))$$

$$+\sum_{i\in I_{+}(x(k))}(c_{i}(x(k)) - c_{i}(\bar{x}(k))))$$

$$+\sum_{i\in I_{+}(x(k))}c_{i}(\bar{x}(k)). \qquad (35)$$

Invoking the concavity of $c_1(x)$, we obtain

$$c_{1}(x(k)) = c_{1}(x(k)) - c_{1}(\bar{x}(k))$$

$$\leq (\nabla c_{1}(\bar{x}(k)), x(k) - \bar{x}(k))$$

$$\leq (t(k) - \bar{t}_{k})(\nabla c_{1}(\bar{x}(k)), z(k)).$$

Keeping in mind (34), we have

$$ka(c_1(x(k)))^2 \ge ka(\alpha^2/4)(t(k) - \bar{t}_k)^2.$$

Using concavity of $c_i(x)$, $i \in I_+(x(k))$, we obtain

$$c_i(x(k)) - c_i(\bar{x}(k)) \le (\nabla c_i(\bar{x}(k)), x(k) - \bar{x}(k))$$
$$= (t(k) - \bar{t}_k)(\nabla c_i(\bar{x}(k)), z(k)).$$

Let

$$|(\nabla f(\bar{x}), \bar{z})| = \beta_0, \quad |f(x^0) - f(\bar{x})| = \gamma_0, |(\nabla c_i(\bar{x}), \bar{z})| = \beta_i, \quad c_i(\bar{x}) = \gamma_i, i \in I_+(x(k)).$$

Then, for k > 0 large enough, we have

$$\begin{split} |(\nabla f(\bar{x}(k)), z(k))| &\leq 2\beta_0, \\ |(\nabla c_i(\bar{x}(k)), z(k))| &\leq 2\beta_i, \\ c_i(\bar{x}(k)) &\leq 2\gamma_i, i \in I_+(x(k)), \\ |f(x^0) - f(\bar{x}(k))| &\leq 2\gamma_0. \end{split}$$

Therefore, we can rewrite inequality (35) as follows:

$$ka(\alpha^{2}/4)[t(k) - \bar{t}_{k}]^{2} \leq 2 \bigg[\gamma_{0} + (t(k) - \bar{t}_{k})\beta_{0} + \sum_{i \in I_{+}(x(k))} \beta_{i}(t(k) - \bar{t}_{k}) + \sum_{i \in I_{+}(x(k))} \gamma_{i} \bigg].$$
(36)

By introducing

$$\bar{\alpha} = a\alpha^2/8, \quad \bar{\beta} = \beta_0 + \sum_{i \in I_+(x(k))} \beta_i,$$
$$\gamma = \gamma_0 + \sum_{i \in I_+(x(k))} \gamma_i, \quad \tau_k = t(k) - \bar{t}_k,$$

we can rewrite inequality (36) as follows:

$$k\bar{\alpha}\tau_k^2-\bar{\beta}\tau_k-\gamma\leq 0.$$

Therefore,

$$t(k) - \bar{t}_k = \tau_k \le (2k\bar{\alpha})^{-1} \left[\bar{\beta} + \sqrt{\bar{\beta}^2 + 4k\bar{\alpha}\gamma} \right] = \mathcal{O}(k^{-1/2})$$

and

$$||x(k) - \bar{x}(k)|| = (t(k) - \bar{t}(k))||z(k)|| = t(k) - \bar{t}_k = \mathcal{O}(k^{-1/2}),$$

where $\bar{x}(k) \in \Omega$.

Let us consider the distance from $x(k) \notin \Omega$ to Ω ,

$$d(x(k), \Omega) = \min\{||x(k) - x|||x \in \Omega\} \\= ||x(k) - y(k)||.$$

Then,

$$d(x(k), \Omega) = ||x(k) - y(k)|| \le ||x(k) - \bar{x}(k)|| = \mathcal{O}(k^{-1/2})$$

and

$$\lim_{k \to \infty} c_{-}(x(k)) = 0. \tag{37}$$

The sequence $\{x(k)\}_{k=1}^{\infty}$ is bounded due to the boundedness of Ω and (37). The dual sequence $\{\lambda(k)\}_{k=1}^{\infty}$ is also bounded. In fact, assuming the opposite, we can find such index i_0 that $\lim_{k\to\infty} \lambda_{i0}(k) = \infty$. We can assume

$$\lambda_{i_0}(k) = \max\{\lambda_i(k) | 1 \le i \le m\},\$$

for all $k \ge 1$. By dividing the left-hand side of (28) by $\lambda_{i_0}(k)$, we obtain

$$\lambda_{i_0}^{-1}(k)\nabla f(x(k)) - \sum_{i=1}^{m} \bar{\lambda}_i(k)\nabla c_i(x(k)) = 0,$$
(38)

where

$$\bar{\lambda}(k) = (\bar{\lambda}_i(k) = \lambda_i(k)\lambda_{i_0}^{-1}(k), \ i = 1, \dots, m).$$

The dual sequence $\{\bar{\lambda}(k)\}_{k=1}^{\infty}$ is bounded. Therefore, both $\{x(k)\}_{k=1}^{\infty}$ and $\{\bar{\lambda}(k)\}_{k=1}^{\infty}$ have converging subsequences. Without restricting the generality, we can assume that

$$\bar{x} = \lim_{k \to \infty} x(k)$$
 and $\bar{\lambda} = \lim_{k \to \infty} \bar{\lambda}(k)$.

Passing to the limit (38) and keeping in mind that, due to (vi),

$$\bar{\lambda} = \lim_{k \to \infty} \psi'(kc_i(x(k))) = 0, \quad i \in I_+(\bar{x}),$$

we obtain

$$\sum_{i\in\bar{I}}\bar{\lambda}_i\nabla c_i(\bar{x})=0,\tag{39}$$

where

$$\bar{I} = \{i : c_i(\bar{x}) = 0\}.$$

Due to (37), we have $\bar{x} \in \Omega$. In fact, $\bar{x} \in \partial \Omega$ and $\exists \bar{\lambda}_i > 0$, $i \in \bar{I}$. However, (39) is impossible due to the Slater condition. So, both the primal sequence $\{x(k)\}_{k=1}^{\infty}$ and the dual sequence $\{\lambda(k)\}_{k=1}^{\infty}$ are bounded.

We consider any converging primal-dual subsequence

 $\{x(k), \lambda(k)\}_{k \in K} \subset \{x(k), \lambda(k)\}_{k=1}^{\infty}$

and the primal-dual limit point

$$\bar{x} = \lim_{k \in K} x(k), \quad \bar{\lambda} = \lim_{k \in K} \lambda(k).$$

Keeping in mind that

$$\lim_{k\to\infty} d(x(k),\,\Omega) = 0,$$

we obtain

$$\lim_{k\to\infty}c_i(x(k))=c_i(\bar{x})\geq 0, \quad i=1,\ldots,m.$$

Passing (28) to the limit, we obtain

$$\lim_{k\to\infty} \nabla_x L(x(k),\lambda(k)) = \nabla_x L(\bar{x},\bar{\lambda}) = 0.$$

Also, for $I_{+}(\bar{x})$ we have $c_{i}(\bar{x}) > 0$ and, due to (vi), we have

$$\bar{\lambda}_i = \lim_{k \to \infty} \psi'(kc_i(x(k))) = 0, \quad i \in I_+(\bar{x}).$$

Therefore, the pair $(\bar{x}, \bar{\lambda})$ satisfies the KKT condition; hence, $\bar{x} = x^*$, $\bar{\lambda} = \lambda^*$. In other words, any limit point of the primal-dual sequence is the primal-dual solution. Therefore,

$$\lim_{k \to \infty} f(x(k)) = f(x^*), \qquad \lim_{k \to \infty} d(\lambda(k)) = d(\lambda^*).$$

Now, we will prove that

 $c_{-}(x(k)) = \mathcal{O}(k^{-1}).$

Let us consider the sets

$$\Omega_i = \{ x \in \mathbb{R}^n | c_i(x) \ge 0 \}, \quad i = 1, \dots, m.$$

Then,

$$\tilde{x}_i(k) = \operatorname{argmin}\{||x(k) - x|||x \in \Omega_i\}$$

is a projection of x(k) onto the set Ω_i . If $x(k) \notin \Omega$, then for k > 0 large enough, there exists at least one active constraint which is violated at x(k). In fact, due to

$$\lim_{k\to\infty} d(x(k), X^*) = 0,$$

none of the passive constraints can be violated for k > 0 large enough. We assume that $c_1(x)$ is violated and therefore

$$c_1(\tilde{x}_1(k)) = 0.$$

We can assume also that

$$\max_{1 \le i \le m} ||x(k) - \tilde{x}_i(k)|| = ||x(k) - \tilde{x}_1(k)||.$$

For any k > 0 and $\tilde{x} = \tilde{x}_1(k)$, we have

$$f(x(k)) - k^{-1} \sum_{i=1}^{m} \psi(kc_i(x(k))) \le f(\tilde{x}) - k^{-1} \sum_{i=1}^{m} \psi(kc_i(\tilde{x})).$$

Keeping in mind that $\psi(kc_1(\tilde{x})) = 0$, we have

$$\begin{aligned} -k^{-1}\psi(kc_1(x(k))) &\leq f(\tilde{x}) - f(x(k)) \\ &+ k^{-1}\sum_{i=2}^m \psi(kc_i(x(k))) - k^{-1}\sum_{i=2}^m \psi(kc_i(\tilde{x})) \end{aligned}$$

$$= f(\tilde{x}) - f(x(k)) + \sum_{i=2}^{m} \psi'(\cdot)_i (c_i(x(k)) - c_i(\tilde{x})),$$
(40)

where

$$\psi'(\cdot)_i = \psi'(c_i(\tilde{x}) + \theta_i^k(c_i(x(k)) - c_i(\tilde{x}))), \quad 0 < \theta_i^k < 1.$$

We can assume that

$$c_i(x(k)) - c_i(\tilde{x}) \ge 0, \quad i = 2, \dots, m;$$

indeed, if for a particular i = 2, ..., m it is not so, we can omit the correspondent term in (40) and strengthen the inequality.

It follows from the boundedness of the sequence $\{x(k)\}_{k=1}^{\infty}$ that its projection $\{\tilde{x}_1(k)\}_{k=1}^{\infty}$ on a convex set Ω_1 is also bounded. Therefore, taking into account properties (iii)–(iv) of the transformation ψ , we can find such B > 0 that $0 < \psi'(\cdot)_i < B$. Keeping in mind property (v), from (40) we obtain

$$akc_{1}^{2}(x(k)) \leq f(\tilde{x}) - f(x(k)) + \sum_{i=2}^{m} B(c_{i}(x(k)) - c_{i}(\tilde{x})).$$
(41)

Recall that

$$\tilde{x} = \operatorname{argmin}\{||x(k) - x|| | x \in \Omega_1\}, \quad x(k) \notin \Omega_1.$$

Then, $c_1(\tilde{x}) = 0$ and

$$(\nabla c_1(\tilde{x}), x(k) - \tilde{x}) = -||\nabla c_1(\tilde{x})||||x(k) - \tilde{x}|| < 0.$$

Using the concavity of $c_1(x)$ and $c_1(\tilde{x}) = 0$, we have

$$c_1(x(k)) = c_1(x(k)) - c_1(\tilde{x})$$

$$\leq (\nabla c_1(\tilde{x}), x(k) - \tilde{x})$$

$$< 0,$$

i.e.,

$$-c_1(x(k)) \ge -(\nabla c_1(\tilde{x}), x(k) - \tilde{x})$$

> 0,

or

$$|c_1(x(k))| \ge |(\nabla c_1(\tilde{x}), x(k) - \tilde{x})|$$

= ||\nabla c_1(\tilde{x})||||x(k) - \tilde{x}||.

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Note that there is a $\mu > 0$ such that

$$||\nabla c_1(\tilde{x})|| \ge \mu > 0, \quad \forall \tilde{x} : c_1(\tilde{x}) = 0;$$

otherwise,

$$\nabla c_1(\tilde{x}) = 0, \quad c_1(\tilde{x}) = \max_{x \in \mathbb{R}^n} c_1(x) = 0,$$

which contradict the Slater condition. Then,

$$||x(k) - \tilde{x}|| = |(\nabla c_1(\tilde{x}), x(k) - \tilde{x})|/||\nabla c_1(\tilde{x})||$$

$$\leq |c_1(x(k))|/||\nabla c_1(\tilde{x})||$$

$$\leq |c_1(x(k))|/\mu,$$

or

$$c_1^2(x(k)) \ge \mu^2 ||x(k) - \tilde{x}||^2,$$

i.e.,

$$akc_1^2(x(k)) \ge ak\mu^2 ||x(k) - \tilde{x}||^2.$$

For the convex function f(x), we have

$$f(x(k)) - f(\tilde{x}) \ge (\nabla f(\tilde{x}), x(k) - \tilde{x}),$$

or

$$f(\tilde{x}) - f(x(k)) \le (\nabla f(\tilde{x}), \tilde{x} - x(k))$$
$$\le ||\nabla f(\tilde{x})|| ||x(k) - \tilde{x}||.$$

Using the concavity of $c_i(x)$, we obtain

$$c_i(x(k)) - c_i(\tilde{x}) \le (\nabla c_i(\tilde{x}), x(k) - \tilde{x})$$

$$\le ||\nabla c_i(\tilde{x})||||x(k) - \tilde{x}||, \quad i = 2, \dots, m.$$

Therefore, we can rewrite (41) as follows:

$$ak\mu^{2}||x(k) - \tilde{x}||^{2} \leq \left[||\nabla f(\tilde{x})|| + B\sum_{i=2}^{m} ||\nabla c_{i}(\tilde{x})||\right]||x(k) - \tilde{x}||,$$

or

$$||x(k) - \tilde{x}|| \le (a\mu^2)^{-1}k^{-1} \bigg[||\nabla f(\tilde{x})|| + B\sum_{i=2}^m ||\nabla c_i(\tilde{x})|| \bigg].$$

Since the sequence of projections $\{\tilde{x}(k)\}_{k=k_0}^{\infty}$ is bounded, we can find such C > 0 that

$$||\nabla f(\tilde{x})|| + B \sum_{i=2}^{m} ||\nabla c_i(\tilde{x})|| \le C.$$

Therefore,

$$||x(k) - \tilde{x}|| = \mathcal{O}(k^{-1}).$$

The concave functions $c_i(x), i = 1, ..., m$, are continuous in \mathbb{R}^n . On the other hand, there is a bounded and closed set $\tilde{X} \subset \mathbb{R}^n$ that $\{x(k)\}_{k=1}^{\infty}$ and $\{\tilde{x}(k)\}_{k=1}^{\infty} \subset \tilde{X}$. Therefore, the functions $c_i(x), i = 1, ..., m$, satisfy the Lipschitz conditions on \tilde{X} ; i.e.,

$$|c_i(\tilde{x}(k)) - c_i(x(k))| \le L ||\tilde{x}(k) - x(k)||, \quad i = 1, ..., m.$$

Without restricting generality, we can assume that

$$c_{-}(x(k)) = \max\{0, -c_{i}(x(k)) | i = 1, ..., m\}$$

= $-c_{1}(x(k))$
= $|c_{1}(\tilde{x}) - c_{1}(x(k))|$
 $\leq L||\tilde{x} - x(k)||$
= $\mathcal{O}(k^{-1}).$

Finally, let us estimate the duality gap

$$\Delta(k) \le \sum_{i=1}^m \lambda_i(k) |c_i(x(k))|.$$

For any $i = 1, \ldots, m$, we have

either
$$c_i(x(k)) < 0$$
 or $c_i(x(k)) \ge 0$.

If $c_i(x(k)) < 0$, then we have proven already that $|c_i(x(k))| = O(k^{-1})$. Due to the boundedness of $\{\lambda(k)\}_{k=1}^{\infty}$, we have

$$\lambda_i(k)|c_i(x(k))| = \mathcal{O}(k^{-1}).$$

If $c_i(x(k)) > 0$, then due to property (vi) of the transformation $\psi(t)$, we have

$$\lambda_i(k)c_i(x(k)) = \psi'(kc_i(x(k)))c_i(x(k))$$

$$\leq b(kc_i(x(k)))^{-1}c_i(x(k))$$

= bk^{-1} .

Therefore, the duality gap is

$$\Delta(k) = |f(x(k)) - d(\lambda(k))|$$

$$\leq \sum_{i=1}^{m} \lambda_i(k) |c_i(x(k))|$$

$$= \mathcal{O}(k^{-1}).$$

We have completed the proof of Theorem 5.1.

Theorem 5.1 complements the results regarding the convergence property of the SUMT type methods (see Refs. 19–21) for the class of constraint transformation Ψ . To find

$$x(k) = \operatorname{argmin}\{P(x, k) | x \in \mathbb{R}^n\},\$$

we will use the Newton method. The following lemma establishes the conditions under which the function P(x, k) is strongly convex.

Lemma 5.1. If the standard second-order optimality conditions are satisfied, then for $k_0 > 0$ large enough and any $k \ge k_0$, the function P(x, k) is strongly convex in the neighborhood of x(k).

The lemma is proven in Ref. 26.

The penalty function P(x,k) is strongly convex along the path $\{x(k), \lambda(k)\}_{k \ge k_0}^{\infty}$. Also, the penalty function P(x,k) is strongly convex in \mathbb{R}^n for any k > 0, if f(x) or one of the functions $-c_i(x)$ is strongly convex.

If f and all the functions $-c_i$ are just convex, but none of them is strongly convex, then to guarantee the correspondent property for the penalty function P(x, k) in \mathbb{R}^n and any k > 0, one can regularize the function f(x); (see Ref. 28). Let us consider instead of f(x) the regularized function

 $f_{\varepsilon}(x) := f(x) + \varepsilon ||x||^2,$

with $\varepsilon > 0$ small enough. Then, the following function:

$$P(x,k) = f(x) + \varepsilon ||x||^2 - k^{-1} \sum_{i=1}^{m} \psi(kc_i(x))$$

is strongly convex in $x \in \mathbb{R}^n$ for any k > 0. Let us assume that

$$x_{\varepsilon}^* = \operatorname{argmin} \{ f_{\varepsilon}(x) | x \in \Omega \}$$

is the solution of the regularized problem. Then,

$$f(x_{\varepsilon}^*) + \varepsilon ||x_{\varepsilon}^*||^2 \le f(x^*) + \varepsilon ||x^*||^2.$$

Keeping in mind that $x_{\varepsilon}^* \in \Omega$, we obtain

$$0 \le f(x_{\varepsilon}^*) - f(x^*)$$

$$\le \varepsilon((x^*, x^*) - (x_{\varepsilon}^*, x_{\varepsilon}^*))$$

and from the boundedness of Ω , we have

$$\lim_{\varepsilon \to 0} (f(x_{\varepsilon}^*) - f(x^*)) = 0.$$

So, for any a priori given accuracy $\gamma > 0$, one can find such small $\varepsilon > 0$ that an approximation to the solution of the regularized problem will be a solution to the original problem with a given accuracy.

In Section 6, we describe the primal-dual path following method, where the strong convexity property of P(x, k) plays an important role.

6. Primal-Dual Path Following Method

The PDPF method alternates one or few steps of the Newton method for solving the primal-dual system

$$\nabla_{x} P(\hat{x}, k) = \nabla f(\hat{x}) - \sum_{i=1}^{m} \hat{\lambda}_{i} \nabla c_{i}(\hat{x})$$

= $\nabla_{x} L(\hat{x}, \hat{\lambda})$
= 0, (42)

$$\hat{\lambda}_i = \psi'(kc_i(\hat{x})), \quad i = 1, \dots, m,$$
(43)

for \hat{x} and $\hat{\lambda}$ with the scaling parameter k > 0 update.

By linearizing the system (42)–(43) at (x, λ) , where

$$\lambda = (\lambda_1, \dots, \lambda_m)$$
 and $\lambda_i = \psi'(kc_i(x)), \quad i = 1, \dots, m,$

we obtain the following system for the primal-dual PF directions $(\Delta x, \Delta \lambda)$:

$$\nabla_{xx}^2 L(x,\lambda)\Delta x - \nabla c(x)^T \Delta \lambda = -\nabla_x L(x,\lambda),$$
(44)

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$$-k\Psi''(kc(x))\nabla c(x)\Delta x + \Delta\lambda = 0, \tag{45}$$

where

$$\Psi''(kc(x)) = \operatorname{diag}(\psi''(kc_i(x)))_{i=1}^m.$$

Let

$$L(\cdot) = L(x, \lambda), \quad \nabla c(\cdot) = \nabla c(x), \quad \Psi''(\cdot) = \Psi''(kc(x)).$$

We can rewrite the system (44)-(45) as follows

$$N(\cdot) \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = \begin{bmatrix} \Delta_{xx}^2 L(\cdot) & -\nabla c^T(\cdot) \\ -k\Psi''(\cdot)\nabla c(\cdot) & I \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix}$$
$$= \begin{bmatrix} -\nabla_x L(\cdot) \\ 0 \end{bmatrix},$$
(46a)

Then, the next primal-dual approximation is obtained by the formulas

$$\hat{x} := x + \Delta x, \quad \hat{\lambda} := \lambda + \Delta \lambda,$$
(46b)

where t > 0 is a steplength.

Usually, $N(\cdot)$ is sparse. Therefore, the system (46) can be solved efficiently when k > 0 is bounded. The system (46) can be reduced by substituting

 $\Delta \lambda = k \Psi''(\cdot) \nabla c(\cdot) \Delta x$

into (44). Then, one can find the primal Newton direction by solving the following system:

$$M(x,\lambda,k)\Delta x = -\nabla_x L(x,\lambda), \tag{47}$$

where

$$M(x, \lambda, k) = M(\cdot) = \nabla_{xx}^2 L(\cdot) - k \nabla c^T(\cdot) \Psi''(kc(\cdot)) \nabla c(\cdot).$$

It follows from property (vi) of the function ψ that, for $k_0 > 0$ large enough and for any $k \ge k_0$, we have

$$\psi''(kc_i(\cdot)) = \mathcal{O}(k^{-2}), \quad i \notin I^*.$$

Therefore,

$$M(\cdot) \approx \nabla_{xx}^2 L(x^*, \lambda^*) - k \psi''(0) \nabla c_{(r)}^T(x^*) \nabla c_{(r)}(x^*).$$
(48)

Under the standard second-order optimality condition for k > 0 large enough, and due to property (iv) and the Debreu theorem (Ref. 29), the matrix $M(\cdot)$ is positive definite even if none of the functions $f(x), -c_i(x)$ is convex.

Solving the system (46) is often much easier than solving (47) because usually the matrix $N(\cdot)$ is sparse, while $M(\cdot)$ might be dense. Also, the unbounded increase of k > 0 has a negative effect on the accuracy of the primal Newton direction Δx because the elements of the first term of matrix $M(x, \lambda, k)$ become negligibly smaller as compared to the elements of the second term, which eliminates the impact of the Hessian $\nabla_{xx}^2 L(\cdot)$ on the Newton direction Δx .

We would like to emphasize that, in LP calculations, the first term in (48) is just the zero matrix. Therefore, the ill-conditioning effect in LP is substantially different than in NLP. It is much easier to handle using the means of modern numerical linear algebra and the structure of the correspondent matrix $N(\cdot)$ in LP calculations (see Refs. 1,5–7,25). However, it is fortunate that, in NLP calculations, for not very large k the system (46) or (47) can be solved with high accuracy.

The following lemma is similar to Lemma 4.1.

Lemma 6.1. The primal Newton direction obtained from the system (44)–(45) coincides with the Newton direction for the minimization of P(x, k) in x.

The lemma is proven in Ref. 26.

Finding

 $x(k) = \operatorname{argmin}\{P(x, k) | x \in \mathbb{R}^n\}$

by the Newton method is generally speaking an infinite procedure. Also, the Newton method converges to x(k) from a neighborhood of x(k) where the Newton method is well defined (see Refs. 28, 30). To make the Newton method globally converging, one can use the stepsize Newton method with the Goldstein-Armijo rule by checking the inequality.

$$P(x + t\Delta x, k) - P(x) \le \varepsilon t(\nabla_x P(x, k), \Delta x), \quad 0 < \varepsilon \le 1/2.$$

Lemma 6.2. If P(x, k) is strongly convex, then for any k > 0 large enough, the following estimations hold:

$$|c_{-}(\hat{x}(k)) - c_{-}(x(k))| = \mathcal{O}(k^{-1}),$$

 $\Delta(\hat{x}(k)) = \mathcal{O}(k^{-1}).$

The lemma is proven in Ref. 26.

By using the logarithmic modified barrier function $\psi_2(t) = log(t+1)$ in the formulation of the PF method, we end up with the path-following method for the shifted barrier function. For a wide enough class of functions $c_i(x), i = 1, ..., m$, the corresponding function

$$P(x,k) = f(x) - k^{-1} \sum_{i=1}^{m} \log(kc_i(x) + 1)$$
(49)

possesses the self-concordance properties (see Ref. 31), so that the corresponding PF method under appropriate change of the scaling parameter k > 0 from step to step has polynomial complexity for LP and for some classes of NLP including important class of quadratic programming problems with quadratic constraints (see Ref. 31). The self concordance of P(x,k) can be used in the first phase of the PDNR method. Starting with a warm start for a given k > 0 and alternating the Newton step for the minimization of P(x,k) in x with appropriate scaling parameter update (see Ref. 31), one obtains an approximation for the primal minimizer with accuracy $\varepsilon > 0$ in $O(\sqrt{n}\log\varepsilon^{-1})$ steps.

At the point when the scaling parameter gets large enough, the PDPF becomes less efficient. At this point, the PDPF procedure turns into the PDNR method. It allows to speed up the process substantially without increasing the scaling parameter. At the same time, it keeps stable the area where the Newton's method is well defined (Refs. 28,30) as well as the condition number of the Hessian $\nabla_{xx} \mathcal{L}(\cdot)$. It allows us to compute the Newton direction with high accuracy and stabilize the computational process at the final stage. We describe the correspondent procedure in Section 8.

7. Rate of Convergence of the PDNR Method

In this section, we discuss the rate of convergence of the NR method (8)–(9). It turns out that, under the standard second-order optimality conditions, the NR method converges with Q-linear rate for any $\psi \in \Psi$. Moreover, the ratio $0 < \gamma < 1$, can be made as small as one wants by choosing a fixed but large enough $k \ge k_0$.

To keep the Q-linear convergence, there is no need to find the exact solution to problem (7). It is enough to find an approximation to x^{s+1} . We point out the accuracy for the approximation to x^{s+1} , which is enough to keep the Q-linear rate of convergence.

The main result of this section is Theorem 7.3, which establishes that, from some point on, only one Newton step for the primal-dual NR system

is enough to guarantee a linear rate of convergence with a priori given ratio $0 < \gamma < 1$.

To formulate the first result, we have to characterize the extended dual domain, where the main facts of the theorem takes place.

Let

 $0 < \delta < \min_{1 \le i \le r} \lambda_i^*$

be small enough and let $k_0 > 0$ be large enough. We split the extended dual domain in the active and passive parts, i.e.,

$$D(\cdot) = D(\lambda, k, \delta)$$

= $D_{(r)}(\cdot) \cup D_{(m-r)}(\cdot),$

where

$$D_{(r)}(\cdot) \equiv D(\lambda_{(r)}, k, \delta) = \{(\lambda_{(r)}, k) : \lambda_i \ge \delta, |\lambda_i - \lambda_i^*| \le \delta k, \\ i = 1, \dots, r, k \ge k_0\},$$
$$D_{(m-r)}(\cdot) \equiv D(\lambda_{(m-r)}, k, \delta) = \{(\lambda_{(m-r)}, k) : 0 \le \lambda_i \le \delta k, \\ i = r+1, \dots, m, k \ge k_0\}.$$

In the following, we assume that

$$||x|| = \max_{1 \le i \le n} |x_i|.$$

The following theorem establishes the rate of convergence of the NR method for any $\psi \in \Psi$. It generalizes results of Refs. 13, 16 on the class Ψ and explains the role of properties (i)–(vii) of the function ψ in the convergence analysis.

Theorem 7.1. If f(x) and all $c_i(x) \in C^2$ and if the standard second-order optimality conditions are satisfied, then:

- (i) For any $(\lambda, k) \in D(\lambda, k, \delta)$, there exists $\hat{x} = \hat{x}(\lambda, k) = \arg\min\{\mathcal{L}(x, \lambda, k) | x \in \mathbb{R}^n\}$; i.e., $\nabla_x \mathcal{L}(\hat{x}, \lambda, k) = 0$.
- (ii) For the pair $(\hat{x}, \hat{\lambda}): \hat{\lambda} = \hat{\lambda}(\lambda, k) = \Psi'(kc(\hat{x}))\lambda$, the following estimation holds:

$$||\hat{x} - x^*|| \le (c/k)||\lambda - \lambda^*||, \quad ||\hat{\lambda} - \lambda^*|| \le (c/k)||\lambda - \lambda^*||$$
(50)

and c > 0 is independent on $k \ge k_0$. Also, for any $k \ge k_0$, we have

$$\hat{x}(\lambda^*, k) = x^*$$
 and $\hat{\lambda}(\lambda^*, k) = \lambda^*;$

i.e. λ^* is a fixed point of map $\lambda \rightarrow \hat{\lambda}(\lambda, k)$ for any $k \ge k_0$.

(iii) The Lagrangian for the equivalent problem $\mathcal{L}(x, \lambda, k)$ is strongly convex in the neighborhood of $\hat{x} = \hat{x}(\lambda, k)$.

The proof of Theorem 7.1 is similar to correspondent proof of Theorem 6.2 in Ref. 16 and is given in Ref. 26.

It follows directly from Theorem 7.1 that the primal-dual sequence generated by the method (8)–(10) converges with Q-linear rate,

$$||x^{s+1} - x^*|| \le ck^{-1} ||\lambda^s - \lambda^*||, \quad ||\lambda^{s+1} - \lambda^*|| \le ck^{-1} ||\lambda^s - \lambda^*||.$$
(51)

It follows also from Theorem 7.1 and the estimation (50) that, if $(\lambda^s, k) \in D(\cdot)$, then

$$(\lambda^{s+1}, k) \in D(\cdot), \text{ for any } s \ge 1.$$

Therefore, for a given $0 < \gamma = ck^{-1} < 1$, one can find $k_{\gamma} \ge k_0$ such that, for any fixed $k \ge k_{\gamma}$, the following estimation holds:

$$||x^{s+1} - x^*|| \le \gamma ||\lambda^s - \lambda^*||, \quad ||\lambda^{s+1} - \lambda^*|| \le \gamma ||\lambda^s - \lambda^*||.$$
(52)

In other words, for any given $0 < \gamma < 1$, there is $k \ge k_{\gamma}$ such that

$$\max\{||x^{s} - x^{*}||, ||\lambda^{s} - \lambda^{*}||\} \le \gamma^{s}.$$
(53)

The ratio $0 < \gamma < 1$, can be made as small as one wants by choosing a fixed but large enough k > 0.

Finding x^{s+1} requires solving an unconstrained minimization problem (7), which is generally speaking an infinite procedure. So, to make the multiplier method (8)–(10) practical, one has to replace the infinite procedure of finding x^{s+1} by a finite one. As it turns out, x^{s+1} can be replaced by an approximation \bar{x}^{s+1} , which can be found in a finite number of Newton steps. If \bar{x}^{s+1} is used in the formula (10) for the Lagrange multiplier update, then an estimate similar to (50) remains true.

We assume that the pair $(\lambda, k) \in D(\cdot)$ and that the vector \bar{x} satisfies the inequality

$$\bar{x} : ||\nabla_{x} \mathcal{L}(\bar{x}, \lambda, k)|| \le \sigma k^{-1} ||\Psi'(kc(\bar{x}))\lambda - \lambda||$$

= $\sigma k^{-1} ||\bar{\lambda} - \lambda||,$ (54)

where $\bar{\lambda} = \Psi'(kc(\bar{x}))\lambda$. Then, the following theorem takes place.

Theorem 7.2. If the standard second-order optimality conditions hold and the Hessians $\nabla^2 f$ and $\nabla^2 c_i, i = 1, ..., m$, satisfy the Lipschitz conditions,

$$||\nabla^{2} f(x) - \nabla^{2} f(y)|| \le L_{0}||x - y||,$$
(55a)

$$||\nabla^2 c_i(x) - \nabla^2 c_i(y)|| \le L_i ||x - y||, \quad i = 1, \dots, m,$$
(55b)

then there is a $k_0 > 0$ large enough such that, for the pair $(\bar{x}, \bar{\lambda})$, the following estimations hold true:

$$||\bar{x} - x^*|| \le c(1 + \sigma)k^{-1} ||\lambda - \lambda^*||,$$
(56a)

$$||\bar{\lambda} - \lambda^*|| \le c(1+\sigma)k^{-1}||\lambda - \lambda^*||, \tag{56b}$$

and c > 0 is independent of $k \ge k_0$.

The bound (56) can be established for any $\psi \in \Psi$ using considerations similar to those which we used in Ref. 16 to prove Theorem 7.1. The bounds (56) can be used as stopping criteria, which makes the multiplier method (7)–(10) executable.

Let us consider the PD approximation (x^s, λ^s) as a starting point. Then, using the stopping criteria (54), we can generate a PD approximation $(\bar{x}^{s+1}, \bar{\lambda}^{s+1})$ by the following formulas:

$$\bar{x}^{s+1} : ||\nabla_{x} \mathcal{L}(\bar{x}^{s+1}, \lambda^{s}, k)|| \le \sigma k^{-1} ||\Psi'(kc(\bar{x}^{s+1}))\lambda^{s} - \lambda^{s}|| = \sigma k^{-1} ||\bar{\lambda}^{s+1} - \lambda^{s}||,$$
(57)

$$\bar{\lambda}^{s+1} = \Psi'(kc(\bar{x}^{s+1}))\lambda^s.$$
(58)

It follows from Theorem 7.2 that if, f and $c_i, i = 1, ..., m$, are smooth enough, and if the standard second-order optimality conditions are satisfied, then the following estimation holds for any $s \ge 1$:

$$||\bar{x}^{s+1} - x^*|| \le c(1+\sigma)k^{-1}||\lambda^s - \lambda^*||,$$
(59a)

$$||\bar{\lambda}^{s+1} - \lambda^*|| \le c(1+\sigma)k^{-1}||\lambda^s - \lambda^*||.$$
(59b)

In other words, for any given $0 < \gamma < 1$, we can find $k_{\gamma} \ge k_0$ that, for any $k \ge k_{\gamma}$, we have

$$(1+\sigma)ck^{-1} < \gamma < 1 \tag{59c}$$

and

$$\max\{||\bar{x}^{s} - x^{*}||, ||\bar{\lambda}^{s+1} - \lambda^{*}||\} \le \gamma ||\lambda^{s} - \lambda^{*}||.$$
(60)

Finding \bar{x}^{s+1} by using the stopping criteria (57) may require several Newton steps (20). We conclude this section by establishing that from some point on only one Newton step for solving the primal-dual system (11)–(12) is enough to shrink the distance from the current approximation to the solution by a given factor $0 < \gamma < 1$. We call such point the hot start (see Ref. 13).

For a given $\varepsilon > 0$ small enough, we consider an ε -neighborhood

$$\Omega_{\varepsilon} = \{ z = (x, \lambda) \in \mathbb{R}^n \times \mathbb{R}^m_+ : ||z - z^*|| \le \varepsilon \}$$

of the primal-dual solution $z^* = (x^*, \lambda^*)$. The following theorem establishes the existence of the hot start.

Theorem 7.3. If the standard second-order optimality conditions are satisfied and if the Lipschitz conditions (55) hold, then for a given $0 < \gamma < 1$, there exists $k_{\gamma} \ge k_0$ and $\varepsilon > 0$ small enough such that, for any fixed $k \ge k_{\gamma}$ and for any PD pair $(x^s, \lambda^s) \in \Omega_{\varepsilon}$ as a starting point, it requires only one primal-dual NR step (18)–(22) to obtain the new PD approximation (x^{s+1}, λ^{s+1}) such that the following bound holds:

$$\max\{||x^{s+1} - x^*||, \, ||\lambda^{s+1} - \lambda^*||\} \le \varepsilon \gamma.$$
(61)

Proof. We start by establishing the bound (61) for the PD pair $(\bar{x}^{s+1}, \bar{\lambda}^{s+1})$ given by (57)–(58). Then, we prove it for (x^{s+1}, λ^{s+1}) . Recall that, due to the standard second-order optimality conditions, for a given fixed $k \ge k_0$, there exists $0 < m_k^* < M_k^*$, such that

$$m_k^*(y, y) \le (\nabla_{xx}^2 \mathcal{L}(x^*, \lambda^*, k)y, y)$$

$$\le M_k^*(y, y), \forall y \in \mathbb{R}^n.$$

If the Lipschitz conditions (55) hold, then corresponding bounds remain true in the neighborhood Ω_{ε} of the primal-dual solution; i.e., there are 0 < m < M, such that the following inequalities hold:

$$m(y, y) \le (\nabla_{xx}^2 \mathcal{L}(x, \lambda, k)y, y)$$

$$\le M(y, y), \quad \forall y \in \mathbb{R}^n \text{ and } \forall (x, \lambda) \in \Omega_{\mathcal{E}}.$$
 (62)

Again due to the Lipschitz condition (55), there exists L > 0 such that, for a fixed $k \ge k_0$, we have

$$||\nabla_{xx}^{2}\mathcal{L}(x_{1},\lambda,k) - \nabla_{xx}^{2}\mathcal{L}(x_{2},\lambda,k)|| \le L||x_{1} - x_{2}||,$$
(63)

if $(x_1, \lambda) \in \Omega_{\varepsilon}, (x_2, \lambda) \in \Omega_{\varepsilon}$.

Together, conditions (62) and (63) guarantee that the Newton method for the minimization of $\mathcal{L}(x, \lambda^s, k)$ in x converges with quadratic rate from any starting point x^s such that $(x^s, \lambda^s) \in \Omega_{\varepsilon}$; (see Ref. 32, page 28).

This means that, for $\bar{x}^{s+1} = x^s + \Delta x$, we can find R > 0, which is independent of (x^s, λ^s) and $k \ge k_0$, such that

$$||\bar{x}^{s+1} - x(\lambda^s, k)|| \le R||x^s - x(\lambda^s, k)||^2$$
,

where

 $x(\lambda^s, k) = \operatorname{argmin}\{\mathcal{L}(x, \lambda^s, k) | x \in \mathbb{R}^n\}.$

We recall also (see Lemma 4.1) that each primal-dual NR step produces the primal Newton direction Δx for the minimization of $\mathcal{L}(x, \lambda^s, k)$ in x.

First, we show that, for $\varepsilon > 0$ small enough and a given γ , $0 < \gamma < 1$, there is $k_{\gamma} > k_0$ that, for any $k > k_{\gamma}$, one Newton step in the primal space followed by the Lagrange multiplier update produces a primal-dual pair $(\bar{x}^{s+1}, \bar{\lambda}^{s+1})$ such that

$$||\bar{x}^{s+1} - x^*|| \le \gamma \varepsilon, \quad ||\bar{\lambda}^{s+1} - \lambda^*|| \le \gamma \varepsilon, \quad \forall (x^s, \lambda^s) \in \Omega_{\varepsilon}.$$
(64)

In other words, we assume that Δx is found from the primal-dual system (17) with $x = x^s$ and $\lambda = \lambda^s$ as a PD starting point. Then, Δx is the Newton direction for finding $\min_{x \in \mathbb{R}^n} \mathcal{L}(x, \lambda^s, k)$ and

$$\bar{x}^{s+1} = x^s + \Delta x, \quad \bar{\lambda}^{s+1} = \Psi'(kc(\bar{x}^{s+1}))\lambda^s)$$

We will prove that, for the PD pair $(\bar{x}^{s+1}, \bar{\lambda}^{s+1})$, the bound (64) holds. We consider two cases.

Case 1. The approximation \bar{x}^{s+1} satisfies the inequality

$$||\nabla_{x}\mathcal{L}(\bar{x}^{s+1},\lambda^{s},k)|| \leq \sigma k^{-1} ||\Psi'(kc(\bar{x}^{s+1}))\lambda^{s}-\lambda^{s}||,$$

for some $\sigma > 0$.

Case 2. The approximation \bar{x}^{s+1} satisfies the inequality

$$||\nabla_{x}\mathcal{L}(\bar{x}^{s+1},\lambda^{s},k)|| > \sigma k^{-1}||\Psi'(kc(\bar{x}^{s+1}))\lambda^{s}-\lambda^{s}||.$$
(65)

In Case 1. the bound (64) follows from Theorem 7.2; i.e.,

$$\max\{||\bar{x}^{s+1} - x^*||, ||\bar{\lambda}^{s+1} - \lambda^*||\}$$

$$\leq c(1+\sigma)k^{-1}||\lambda^s - \lambda^*|| \leq \gamma\varepsilon$$
(66)

Now, we consider Case 2. Let us estimate $||\nabla_x \mathcal{L}(\bar{x}^{s+1}, \lambda^s, k)||$. We recall that $\nabla^2 f(x)$ and $\nabla^2 c_i(x)$ satisfy the Lipschitz conditions (55) and

so it is true for the gradients $\nabla f(x)$ and $\nabla c_i(x)$; i.e., there is such L > 0 that

$$||\nabla f(x) - \nabla f(y)|| \le L||x - y||,$$
 (67)

$$||\nabla c_i(x) - \nabla c_i(y)|| \le L||x - y||, \quad i = 1, \dots, m.$$
(68)

It follows from (62)-(63) that the Newton method applied to finding

 $x(\lambda^s, k) = \operatorname{argmin} \{ \mathcal{L}(x, \lambda^s, k) | x \in \mathbb{R}^n \}$

converges with quadratic rate; i.e., there is R > 0 such that

$$||\bar{x}^{s+1} - x(\lambda^s, k)|| \le R ||x^s - x(\lambda^s, k)||^2.$$
(69)

Keeping in mind that k > 0 is fixed and $||\lambda^s - \lambda^*|| \le \varepsilon$, it follows from (67)–(69) the existence of $L_1 > 0$ such that

$$\begin{aligned} ||\nabla_{x}\mathcal{L}(\bar{x}^{s+1},\lambda^{s},k)|| &= ||\nabla_{x}\mathcal{L}(\bar{x}^{s+1},\lambda^{s},k) - \nabla_{x}\mathcal{L}(x(\lambda^{s},k),\lambda^{s},k)|| \\ &\leq L_{1}||\bar{x}^{s+1} - x(\lambda^{s},k)|| \\ &\leq L_{1}R||x^{s} - x(\lambda^{s},k)||^{2} \\ &= C_{1}||x^{s} - x(\lambda^{s},k)||^{2}, \quad C_{1} = L_{1}R. \end{aligned}$$

Since

$$||x^s - x^*|| \le \varepsilon,$$

from Theorem 7.1 we obtain

 $||x(\lambda^s, k) - x^*|| \le c\varepsilon/k$

and c > 0 is independent of $k_{\gamma}, k \ge k_{\gamma} \ge k_0$. Therefore, for $k_0 > 0$ large enough, we have

$$||x^{s} - x(\lambda^{s}, k)|| \leq ||x^{s} - x^{*}|| + ||x(\lambda^{s}, k) - x^{*}||$$

$$\leq (1 + c/k)\varepsilon$$

$$\leq 2\varepsilon.$$
(70)

Hence, we have

$$\begin{aligned} ||\nabla_{x}\mathcal{L}(\bar{x}^{s+1},\lambda^{s},k)|| &= ||\nabla_{x}L(\bar{x}^{s+1},\bar{\lambda}^{s+1})|| \\ &\leq C_{2}\varepsilon^{2}, \quad C_{2} = 4C_{1}. \end{aligned}$$

Therefore, from inequality (65), we have

$$k^{-1}||\Psi'(kc(\bar{x}^{s+1})\lambda^s - \lambda^s)|| < C_3\varepsilon^2, \quad C_3 = \sigma^{-1}C_2.$$
(71)

Let us consider separately the active and the passive constraints sets I^* and $I_0 = \{r + 1, ..., m\}$. For $i \in I^*$, we have

$$c_i(x^*) = 0, \quad \psi'(c_i(x^*)) = 1.$$

Therefore,

$$\begin{split} \psi'(kc_{i}(\bar{x}^{s+1}))\lambda_{i}^{s} - \lambda_{i}^{s} &= \psi'(kc_{i}(\bar{x}^{s+1}))\lambda_{i}^{s} - \psi'(kc_{i}(x^{*}))\lambda_{i}^{s} \\ &= k\psi''(\theta_{i}^{s}c_{i}(\bar{x}^{s+1}))(c_{i}(\bar{x}^{s+1}) - c_{i}(x^{*}))\lambda_{i}^{s} \\ &= k\psi''(\theta_{i}^{s}c_{i}(\bar{x}^{s+1}))c_{i}(\bar{x}^{s+1})\lambda_{i}^{s}, \\ &\quad 0 < \theta_{i}^{s} < 1, \quad i \in I^{*}. \end{split}$$

From (71), we obtain

$$|\psi''(\theta_i^s c_i(\bar{x}^{s+1}))c_i(\bar{x}^{s+1})\lambda_i^s| \le c_3\varepsilon^2, \quad i \in I^*.$$

Moreover for $\varepsilon > 0$ small enough, there is $\delta > 0$ such that

$$|\psi''(\theta_i^s c_i(\bar{x}^{s+1}))| \ge \delta.$$

Due to the standard second-order optimality conditions and $||\lambda^s - \lambda^*|| \le \varepsilon$, there is a $\overline{\delta} > 0$ such that

$$\lambda_i^s \ge \bar{\delta} > 0, \quad i \in I^*.$$

So, there is a $C_4 > 0$ such that

$$|c_i(\bar{x}^{s+1})| \le C_4 \varepsilon^2, \quad C_4 = C_3(\delta \bar{\delta})^{-1}, \quad i \in I^*.$$

Now, let us consider the passive set I_0 . We recall that the transformation $\psi(t)$ satisfies the following property (vi):

$$\psi'(t) \le bt^{-1}, \quad t \ge 0, \quad b > 0.$$

Due to the standard second-order optimality conditions, there exists $\eta_1 > 0$, such that

$$\eta_1 < c_i(\bar{x}^{s+1}), \quad i \in I_0, \text{ if } (x^s, \lambda^s) \in \Omega_{\varepsilon}.$$

Therefore, for the Lagrange multipliers which correspond to the passive constraints, we have

$$\bar{\lambda}_i^{s+1} = \lambda_i^s \psi'(kc_i(\bar{x}^{s+1}))$$
$$\leq b\lambda_i^s/kc_i(\bar{x}^{s+1})$$

$$\leq b\lambda_i^s/k\eta_1$$

= $(C_5/k)\lambda_i^s$, $C_5 = b/v_1$.

Let us summarize the results obtained. If $(x^s, \lambda^s) \in \Omega_{\varepsilon}$, then for the next primal-dual approximation $(\bar{x}^{s+1}, \bar{\lambda}^{s+1})$, the following bounds hold true:

$$||\nabla_x L(\bar{x}^{s+1}, \bar{\lambda}^{s+1})|| \le C_3 \varepsilon^2, \tag{72}$$

$$|c_i(\bar{x}^{s+1})| \le C_4 \varepsilon^2, \quad i \in I^*, \tag{73}$$

$$\bar{\lambda}_i^{s+1} | \le (C_5/k)\varepsilon, \quad i \in I_0.$$
(74)

Let us estimate $||\bar{x}^{s+1} - x^*||$. Due to (50) and (69), we have

$$\begin{aligned} ||\bar{x}^{s+1} - x^*|| &\leq ||\bar{x}^{s+1} - x(\lambda^s, k)|| + ||x(\lambda^s, k) - x^*|| \\ &\leq R||x^s - x(\lambda^s, k)||^2 + ||x(\lambda^s, k) - x^*|| \\ &\leq 4R\varepsilon^2 + (c/k)\varepsilon \\ &\leq (C_6/k)\varepsilon, \end{aligned}$$

where

$$C_6 = 4Rk\varepsilon + c.$$

Notice that k > 0 is fixed; therefore, for $\varepsilon > 0$ small enough, $C_6 > 0$ is independent of k.

Using (72) and (73), we obtain the following bound for the gradient of the reduced Lagrangian which corresponds to the active constraints:

$$\begin{aligned} ||\nabla_{x}L(\bar{x}^{s+1},\bar{\lambda}_{(r)}^{s+1})|| &= ||\nabla f\bar{x}^{s+1} - \nabla c_{(r)}(\bar{x}^{s+1})^{T}\bar{\lambda}_{(r)}^{s+1} \\ &-\nabla c_{(m-r)}(\bar{x}^{s+1})^{T}\bar{\lambda}_{(m-r)}^{s+1} \\ &+\nabla c_{(m-r)}(\bar{x}^{s+1})^{T}\bar{\lambda}_{(m-r)}^{s+1}|| \\ &\leq ||\nabla_{x}L(\bar{x}^{s+1},\bar{\lambda}^{s+1})|| \\ &+||\nabla c_{(m-r)}(\bar{x}^{s+1})|||\bar{\lambda}_{(m-r)}^{s+1}|| \\ &\leq C_{3}\varepsilon^{2} + (C_{5}\eta_{2}/k)\varepsilon \leq (C_{7}/k)\varepsilon, \end{aligned}$$
(75)

where

 $||\nabla c_{(m-r)}(\bar{x}^{s+1})|| \le \eta_2$

and

$$C_7 = C_3 k \varepsilon + C_5 \eta_2$$

is independent of k > 0.

Using the smoothness of $f(x), c_i(x), i = 1, ..., m$, and $\nabla_x L(x^*, \lambda_{(r)}^*) = 0$, we obtain

$$\begin{aligned} \nabla_{x}L(\bar{x}^{s+1},\bar{\lambda}^{s+1}_{(r)}) &= \nabla_{x}L(x^{*},\bar{\lambda}^{s+1}_{(r)}) + \nabla^{2}_{xx}L(x^{*},\bar{\lambda}^{s+1}_{(r)})(\bar{x}^{s+1}-x^{*}) \\ &+ \mathcal{O}||\bar{x}^{s+1}-x^{*}||^{2} \\ &= \nabla_{x}L(x^{*},\bar{\lambda}^{s+1}_{(r)}) - \nabla_{x}L(x^{*},\lambda^{*}_{(r)}) \\ &+ \nabla^{2}_{xx}L(x^{*},\bar{\lambda}^{s+1}_{(r)})(\bar{x}^{s+1}-x^{*}) + \mathcal{O}||\bar{x}^{s+1}-x^{*}||^{2} \\ &= \nabla^{2}_{xx}L(x^{*},\bar{\lambda}^{s+1}_{(r)})(\bar{x}^{s+1}-x^{*}) \\ &- \nabla c_{(r)}(x^{*})^{T}(\bar{\lambda}^{s+1}_{(r)}-\lambda^{*}_{(r)}) + \mathcal{O}||\bar{x}^{s+1}-x^{*}||^{2}. \end{aligned}$$

Also,

$$c_{(r)}(\bar{x}^{s+1}) = c_{(r)}(x^*) + \nabla c_{(r)}(x^*)(\bar{x}^{s+1} - x^*) + \mathcal{O}||\bar{x}^{s+1} - x^*||^2$$

= $\nabla c_{(r)}(x^*)(\bar{x}^{s+1} - x^*) + \mathcal{O}||\bar{x}^{s+1} - x^*||^2.$

Let us rewrite the expressions above in the matrix form

$$\begin{bmatrix} \nabla_{xx}^{2} L(x^{*}, \bar{\lambda}_{(r)}^{s+1}) & -\nabla c_{(r)}(x^{*})^{T} \\ \nabla c_{(r)}(x^{*}) & 0 \end{bmatrix} \begin{bmatrix} \bar{x}^{s+1} - x^{*} \\ \bar{\lambda}_{(r)}^{s+1} - \lambda_{(r)}^{*} \end{bmatrix}$$
$$= \begin{bmatrix} \nabla_{x} L(\bar{x}^{s+1}, \bar{\lambda}_{(r)}^{s+1}) + \mathcal{O} || \bar{x}^{s+1} - x^{*} ||^{2} \\ c_{(r)}(\bar{x}^{s+1}) + \mathcal{O} || \bar{x}^{s+1} - x^{*} ||^{2} \end{bmatrix}$$
$$= \begin{bmatrix} \alpha(\bar{x}^{s+1}, \bar{\lambda}_{(r)}^{s+1}, x^{*}) \\ \beta(\bar{x}^{s+1}, x^{*}) \end{bmatrix}.$$
(76)

Keeping in mind that

$$||\bar{x}^{s+1} - x^*|| \le (C_6/k)\varepsilon$$

and the inequalities (73) and (74), we can find $C_8 > 0$ independent of k > 0 such that

$$\left| \left| \begin{array}{c} \alpha(\bar{x}^{s+1}, \bar{\lambda}^{s+1}_{(r)}, x^*) \\ \beta(\bar{x}^{s+1}, x^*) \end{array} \right| \right| \leq (C_8/k)\varepsilon.$$

Let us show that the matrix

$$M = \begin{bmatrix} \nabla_{xx}^2 L(x^*, \bar{\lambda}_{(r)}^{s+1}) & -\nabla c_{(r)}(x^*)^T \\ \nabla c_{(r)}(x^*) & 0 \end{bmatrix}$$

is nonsingular, which is equivalent to showing that

$$MW = 0 \Longrightarrow W = 0.$$

Using standard considerations (see for example Ref. 32), from MW = 0 we obtain

$$(\nabla_{xx}^2 L(x^*, \bar{\lambda}_{(r)}^{s+1})u, u) = 0.$$
(77)

On the other hand, from the standard second-order optimality conditions, we obtain

$$\nabla c_{(r)}(x^*)u = 0 \Rightarrow (\nabla_{xx}^2 L(x^*, \lambda_{(r)}^*)u, u) \ge \rho(u, u), \quad \rho > 0.$$

$$(78)$$

Now, we show that, for the Hessian $\nabla^2_{xx} L(x^*, \bar{\lambda}^{s+1}_{(r)})$, we can obtain a similar estimation. First of all, we have

$$||\nabla_{xx}^{2}L(x^{*},\bar{\lambda}_{(r)}^{s+1})-\nabla_{xx}^{2}L(x^{*},\lambda_{(r)}^{*})|| \leq \sum_{i=1}^{r}|\bar{\lambda}_{i}^{s+1}-\lambda_{i}^{*}|||\nabla^{2}c_{i}(x^{*})||.$$

From (71), we have

 $||\bar{\lambda}^{s+1} - \lambda^s|| \le kC_3\varepsilon^2.$

Hence, for a fixed $k \ge k_0$ and small enough $\varepsilon > 0$, we have

$$||\bar{\lambda}^{s+1} - \lambda^s|| \leq C_9 \varepsilon$$

with

$$C_9 = kC_3\varepsilon > 0$$

independent of k. Therefore,

$$\begin{aligned} ||\bar{\lambda}^{s+1} - \lambda^*|| &\leq ||\bar{\lambda}^{s+1} - \lambda^s|| + ||\lambda^s - \lambda^*|| \\ &\leq C_9 \varepsilon + \varepsilon \\ &= (C_9 + 1)\varepsilon. \end{aligned}$$

So, for small enough $\varepsilon > 0$, it follows from (78) that

$$(\nabla_{xx}^{2} L(x^{*}, \bar{\lambda}_{(r)}^{s+1})u, u) \ge \rho_{1}(u, u), \ \forall u : \nabla c_{(r)}(x^{*})u = 0, 0 < \rho_{1} < \rho.$$
(79)

It follows from (77) and (79) that u = 0. Keeping in mind that

$$\operatorname{rank} c_{(r)}(x^*) = r,$$

we conclude that $\nu = 0$. Therefore, the matrix M is nonsingular and $||M^{-1}|| \le m_0$. Then, from the system (76), we obtain

$$\left\| \begin{vmatrix} \bar{x}^{s+1} - x^* \\ \bar{\lambda}^{s+1}_{(r)} - \lambda^*_{(r)} \end{vmatrix} \right\| = \left\| M^{-1} \begin{bmatrix} \alpha(\bar{x}^{s+1}, \bar{\lambda}^{s+1}_{(r)}, x^*) \\ \beta(\bar{x}^{s+1}, x^*) \end{bmatrix} \right\|$$
$$\leq m_0(C_8/k)\varepsilon$$
$$= (C_{10}/k)\varepsilon,$$

and $C_{10} = m_0 C_8$ is independent of $k \ge k_0$ and $\varepsilon > 0$.

In other words, in Case 2, we have also local linear convergence. Therefore, combining Cases 1 and 2, we establish the following estimation:

$$\max\{||\bar{x}^{s+1} - x^*||, ||\bar{\lambda}^{s+1} - \lambda^*||\} \le (C_{11}/k)\varepsilon,$$
(80)

where

 $C_{11} = \max\{c(1+\sigma), C_5, C_6, C_{10}\}$

is independent of a fixed $k \ge k_0$ for $\varepsilon > 0$ small enough.

We complete the proof of Theorem 7.3 by establishing the bound (61). For

 $x^{s+1} = \bar{x}^{s+1} = x^s + \Delta x,$

we have already proved that

$$||x^{s+1} - x^*|| \le (C_{11}/k)\varepsilon.$$

Let us estimate $||\lambda^{s+1} - \lambda^*||$. We have

$$\begin{split} \bar{\lambda}^{s+1} &= \Psi'(kc(\bar{x}^{s+1}))\lambda^s \\ &= \Psi'(kc(x^s + \Delta x))\lambda^s \\ &= \Psi'(kc(x^s))\lambda^s + k\Psi''(kc(x^s))\Lambda^s \nabla c(x^s)\Delta x \\ &+ \mathcal{O}||\bar{x}^{s+1} - x^s||^2 \\ &= \lambda^{s+1} + \mathcal{O}||\bar{x}^{s+1} - x^s||^2, \end{split}$$

i.e.,

$$||\bar{\lambda}^{s+1} - \lambda^{s+1}|| = \mathcal{O}(||\bar{x}^{s+1} - x^s||^2).$$

Keeping in mind that

$$||\bar{x}^{s+1} - x^s|| \le ||\bar{x}^{s+1} - x^*|| + ||x^s - x^*|| \le (c_{11}/k + 1)\varepsilon$$

and the bound

$$||\bar{\lambda}^{s+1} - \lambda^*|| \le (c_{11}/k)\varepsilon,$$

we obtain

$$||\lambda^{s+1} - \lambda^*|| \le ||\bar{\lambda}^{s+1} - \lambda^*|| + ||\lambda^{s+1} - \bar{\lambda}^{s+1}|| \le (C_{11}/k)\varepsilon + \mathcal{O}(\varepsilon^2)$$
$$= (C/k)\varepsilon.$$

So, for $\varepsilon > 0$ small enough, there exists C > 0 independent of $k \ge k_0$ such that, for the pair (x^{s+1}, λ^{s+1}) , taking $k \ge \max\{k_0, Cr^{-1}\}$, we obtain

$$\max\{||x^{s+1} - x^*||, ||\lambda^{s+1} - \lambda^*||\} \le (C/k)\varepsilon \le \gamma\varepsilon.$$

The proof of Theorem 7.3 is complete.

8. Primal-Dual Nonlinear Rescaling Method

We combine the primal-dual path-following method (46) with the NR multiplier method (57)–(58), which from some point turns into the PDNR method (20).

To guarantee global convergence, the path-following method is used at the first stage. When the scaling parameter becomes big enough, the PF method turns into the NR method. At this stage finding an approximation for the primal minimizer followed by the Lagrange multiplier update while the scaling parameter is fixed. At the final stage, the NR method automatically turns into the PDNR method.

Although we are using potentially different tools at different stages of the computational process, the core of our computation at each step is solving the primal-dual system of equations, which arise out of either the PF or NR method.

The turning points where the PF method turns into NR method and the latter turns into the PDNR method can be characterized through the parameters of the problem at the solution, which are not available a priori. Therefore, we introduce a merit function

$$\nu(x,\lambda) = \max\left\{ ||\nabla_x L(x,\lambda)||, -\min_{1 \le i \le m} c_i(x), -\min_{1 \le i \le m} \lambda_i, \sum_{i=1}^m |\lambda_i c_i(x)| \right\}.$$

which, together with the stopping criteria (57), controls the convergence and allows eventually to turn the process into PDNR method. Due to

(27), we have $\lambda(k) \in \mathbb{R}^{m}_{++}$ and, due to (28),we have $\nabla_{x}L(x(k), \lambda(k)) = 0$; therefore, the merit function $\nu(x, \lambda)$ for x = x(k) and $\lambda = \lambda(k)$ coincides with the merit function $\mu(x(k), \lambda(k))$, which has been used in the PF method; see Section 5.

The method is designed in such a way that, from the very beginning, it performs a step of PDNR algorithm. If it does not reduce the value of the merit function ν by a given factor $0 < \gamma < 1$, then it switches into the NR method by using the Newton direction Δx for primal minimization. If again the algorithm does not reduce the merit function $\nu(x, \lambda)$ by the given factor $0 < \gamma < 1$, the algorithm increases the scaling parameter following the PF trajectory. Since the PF algorithm is globally convergent, the global convergence of whole method can be guaranteed. On the other hand, since each step of the algorithm starts with the Newton step for primal-dual NR system the method turns to PDNR automatically when the primal-dual approximation (x^s, λ^s) is in the Newton area for the primal-dual NR system and the Lagrange multipliers $\lambda^s \in D(\cdot)$.

The situation here is similiar to the Newton method with steplength for unconstrained minimization. The difference is that, instead of finding a Newton direction for minimization, in fact we perform from some point on only one Newton step for solving the Lagrange system of equations which corresponds to the active constraints.

The PDNR method is implemented according to the following algorithm.

- Step 1. Initialization. An initial primal approximation $x^0 \in \mathbb{R}^n$ is given. An accuracy parameter ε and an initial scaling parameter k are given. Parameters $\alpha > 1, 0 < \gamma < 1, \sigma > 0, \theta > 0, 0 < \eta < 0.5$ are also given. Set $x := x^0, \lambda := (1, ..., 1) \in \mathbb{R}^m, r := \nu(x, \lambda), x_p := x^0$.
- Step 2. If $r \leq \varepsilon$, stop; output x, λ .
- Step 3. Find the dual predictor $\overline{\lambda}$ and the primal-dual direction $(\Delta x, \Delta \lambda)$.

Set $\hat{x} := x + \Delta x$, $\hat{\lambda} := \bar{\lambda} + \Delta \lambda$

- Step 4. If $\nu(\hat{x}, \hat{\lambda}) \leq \gamma r$, set $x := \hat{x}, \lambda := \hat{\lambda}, r := \nu(x, \lambda)$. Go to Step 2.
- Step 5. Find t such that

$$\mathcal{L}(x + t\Delta x, \lambda, k) - \mathcal{L}(x, \lambda, k) \le \eta t \left(\nabla \mathcal{L}((x, \lambda, k), \Delta x)\right)$$

Step 6. Set $\hat{x} := x + t\Delta x$, $\hat{\lambda} := \lambda \psi'(kc(\hat{x}))$. Step 7. If $\|\nabla_x \mathcal{L}(\hat{x}, \lambda, k)\| \le (\alpha/k^{1+\theta}) \|\hat{\lambda} - \lambda\|$, go to Step 9. Step 8. Find the primal direction Δx . Step 9. If $\lambda = e$, set $x_p := \hat{x}$. Step 10. If $\nu(\hat{x}, \hat{\lambda}) > \gamma r$, set $k := k\alpha, x := x_p, \lambda := e$, go to Step 2. Step 11. Set $x := \hat{x}, \lambda := \hat{\lambda}, r := \nu(x, \lambda)$; go to Step 2.

The most costly computational part is finding the primal-dual Newton direction from the system (17) or (46). Sometimes the system (17) or (46) can be reduced to (18) or (47). The matrices $M(x, \overline{\lambda}, \lambda, k)$ and $M(x, \lambda, k)$ are positive semidefinite and symmetric. For such systems, modern linear algebra techniques (see e.g. Refs. 1,6,12,25) usually are very efficient. If $M(x, \overline{\lambda}, \lambda, k)$ or $M(x, \lambda, k)$ are dense, then to find the primal-dual direction one has to use the PD system (17) or (46), for which the correspondent matrices are usually sparse. The sparcity of (17) or (46) is one of the motivations for developing the PDNR method. Also, it can be efficient to fix matrix $M(\cdot)$ for a number of Newton steps to avoid the factorization of $M(\cdot)$ at each Newton step.

We conclude this section with a few comments in regard of the complexity of the PDNR method. A slight modification of the PDNR method allows us to turn directly the PF method into the PDNR method.

As we mentioned in Section 6, the penalty function (49) with the logarithmic MBF transformation

$$\psi_2(t) = \log(t+1)$$

possesses the self-concordance properties (Ref. 31) for a wide enough class of constraints $c_i(x) \ge 0, i = 1, ..., m$. So, if only the PF method is used, then under appropriate change of the scaling parameter the complexity is $\mathcal{O}(\sqrt{n}\log\varepsilon^{-1})$, where $\varepsilon > 0$ is the required accuracy, $0 < \varepsilon \ll 1$. In such case, we move from one warm start to another warm start. Therefore, if the NR phase never occurs, then it requires $\mathcal{O}(\sqrt{n}\log\varepsilon^{-1})$ Newton steps to find an approximation $(x, \lambda) : \mu(x, \lambda) \le \varepsilon$. Any attempt to switch from the PF method to the PDNR method i.e., from warm start to hot start has the risk of extra computational work, which eventually will never be used.

So, if we consider each new primal-dual approximation in the PF method as a potential hot start, but the hot start never occurs, then instead of $\mathcal{O}(\sqrt{n}\log\varepsilon^{-1})$ Newton steps in PF we have to compute in the worst case

$$N_0 = \mathcal{O}(\sqrt{n}\log^2 \varepsilon^{-1}) \tag{81}$$

Newton steps.

On the other hand, if the triplet (x_0, λ_0, k_0) is a hot start, then to get the primal-dual solution $(x, \lambda) : \mu(x, \lambda) \le \varepsilon$ from the starting point $(x_0, \lambda_0) : \mu(x_0, \lambda_0) \le \varepsilon_0$, $(0 < \varepsilon_0 < 1)$, will take due to Theorem 7.3 only $\mathcal{O}(\log \varepsilon^{-1} + \log \varepsilon_0)$ PDNR steps.

So, if the hot start (x_0, λ_0, k_0) is correctly identified, then the total number of Newton steps is

$$N_1 = \mathcal{O}(\sqrt{n}\log\varepsilon_0^{-1}) + \mathcal{O}(\log\varepsilon^{-1} + \log\varepsilon_0).$$
(82)

The first term corresponds to the PF part of the trajectory, which we followed from a starting point to the triple (x_0, λ_0, k_0) . The second term is the number of PDNR steps from the triple (x_0, λ_0, k_0) to the point $(x, \lambda): \mu(x, \lambda) \le \varepsilon$. If $\varepsilon \ll \varepsilon_0$, then the estimation (82) represents a substantial improvement as compared to the PF estimation $\mathcal{O}(\sqrt{n}\log^2 \varepsilon^{-1})$.

9. Numerical Results

The PDNR method has been implemented in MATLAB and tested extensively on a variety of large scale NLP including the COPS set(Ref. 18), which is a selection of difficult nonlinear constrained optimization problems from applications in optimal design, fluid dynamics, population dynamics, trajectory optimization, and optimal control.

One of the main purposes of testing the PDNR solver is to observe the hot start phenomenon (see Theorem 7.3). The other goal was to obtain results with high accuracy in order to check the numerical stability of the PDNR. We tried also to understand the robustness of the PDNR. Therefore, it was tested on a wide class of NLP.

For the numerical results obtained, we refer the reader to Ref. 26. In most cases, we used the transformation

 $\psi(t) = \log(t+1).$

We concentrated in particular on the COPS set (Ref. 18). The description of the problems and basic parameters such as number of variables, constraints, etc can be found in Ref. 18.

In Tables 1–12 of Ref 26, we show the results of testing the COPS set. The tables describe whether or not the PDNR solved the problem, the constraint violation at the solution, the duality gap, and the number of PDNR iterations, which is in fact the number of Newton steps. Tables 13–18 of Ref. 26 show the number of Newton steps required to reduce the infeasibility and the primal-dual gap by an order of magnitude. We show the number of variables n and constraints m.

The results obtained corroborate the theory: the primal-dual method converges very fast in the neigborhood of the solution (see Theorem 7.3). In most cases, the path-following phase of calculations never occurs. So, the algorithm performs as the combination of the NR multiplier method with the PDNR method. Practically, the scaling parameter never exceeds $k = 10^4$ (in most cases, $k = 10^2 - 10^3$), which contributes to the numerical stability. On the other hand, it is enough to guarantee fast convergence and to optain solutions with high accuracy. In particular, for all problems solved, the duality gap and primal infeasibility are of order 10^{-10} at least.

In all problems solved, we observed the hot start phenomenon, which was predicted in Ref. 13 (see also Ref. 16 and Theorem 7.3) where few steps and from some point on only one PDNR step are required to improve the primal-dual approximation by an order of magnitude. Moreover, for each set of problems, the total number of Newton steps is independent of the problem size.

The PDNR method is an exterior-points method. Therefore, the value of the infeasibility is a very important parameter. As it turns out, the constraint violation and the duality gap occurs simultaneously. They both converge to zero with practically the same rate. The dynamics of the primal-dual gap and constraint violation reduction is given in Tables 13–18 of Ref. 26.

The PDNR solver turned out to be robust. It failed in very few cases and produced results with high accuracy. In most cases, the number of Newton steps corresponds to the estimation (82) rather than (81). Overall, the numerical results obtained show that the PDNR solver has a good potential to become competitive in the NLP arena.

10. Concluding Remarks

The NR approach for constrained optimization produced results which are in full compliance with the outline theory. In particular, we observed systematically the so called hot start phenomenon, justified by Theorem 7.3. Due to the hot start, it is possible to reduce substantially the number of Newton steps required for the reduction of the primal-dual gap and the infeasibility value by a given factor. Moreover, from some point on, only one Newton step is enough for such reduction.

Both the theoretical and numerical results obtained show that there is a fundamental difference between the PF and methods. The PF methods not only converge globally, they allow also to establish the rate of convergence and estimate the complexity under very mild assumptions on the input data. However, the rate of convergence for the PF methods is rather slow. Moreover, to guarantee the convergence of the PF method, one has to increase the penalty parameter unboundedly, which might compromise the numerical stability and in many cases makes difficult to obtain solutions with high accuracy.

On the other hand the NR method may not be effcient far from the solution because it requires the minimization of the Lagrangian $\mathcal{L}(x, \lambda, k)$ in x at each step. But it is very efficient in the neighborhood of the solution, because it does not require the unbounded increase of the scaling parameter and keeps stable the area where the Newton method is well defined. The PDNR methods provides a unified approach combining the advantages of both the PF and NR methods and eliminating their basic drawbacks.

A few issues remain for future research. First, the linear rate of convergence for the PDNR method can be improved by increasing the scaling parameter from step to step without sacrificing the numerical stability, because at the final phase the PDNR method does not require primal minimization. The numerical results show that it can be done; it seems important to understand better this phenomenon. Second, in the NR method with dynamic scaling parameters update (see Ref. 17), the Lagrange multipliers which correspond to the passive constraints converge to zero quadratically. Therefore, at the final stage of the computational process, the PDNR methods turns into the Newton method for the Lagrange system of equations which correspond to the active constraints. Thus, under the standard second-order optimality conditions one can expect a quadratic convergence (see Theorem 9, p. in Ref. 32).

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