Interior Point Methods on the Solution of Conditional Models

V. Rico-Ramírez and A. W. Westerberg[1]

Institute for Complex Engineered Systems
Carnegie Mellon University, Pittsburgh, PA 15213

Abstract: Interior point methods have recently become an interesting alternative in a number of numerical applications. In particular, their performance in the solution of problems involving complementarity equations has been the subject of extensive research and their efficacy is well documented. In this chapter, following a description of the fundamentals of interior point methods, we describe the globally convergent framework proposed by Wang *et al* (1996) for solving a constrained system of nonlinear equations by an interior point potential reduction method. Also, we show how we can apply the potential reduction algorithm and its convergence result to the complementarity formulation described in Rico-Ramirez and Westerberg (1998). Based on that observation, we then apply the algorithm proposed by Wang to solve the complementarity examples used as case studies throughout this work. Moreover, we also apply some high order strategies designed to improve convergence (Mehrotra, 1992; Gondzio, 1996), and compare the results obtained with each of the methods. All those techniques have been incorporated to the ASCEND modeling environment with the implementation of the solver IPSlv.

Keywords: Interior point methods, complementarity formulation, conditional models.

1. Author to whom all correspondence should be addressed

Table of Contents

List of Tables

1 MOTIVATION

As early as in the late 1940's, almost at the same time as when Dantzig presented the simplex method for linear programming, several researches including Von Neumann (1947) and Frisch (1955) proposed interior point algorithms which transverse across the interior of the feasible region to avoid the complexity of vertex-following algorithms (Andersen *et. al*, 1996). Since then, there is a huge body of literature on the interior point methods which includes surveys and numerous articles. See for example Wright (1997), Lusting *et al.* (1994), and Gondzio and Terlaky (1994). Even though the initial effort on interior point methods was focused on linear programming problems, most recent works have concentrated on the common theoretical foundations of linear and nonlinear programming. It is now widely accepted that interior point methods constitute a powerful tool for solving both very large linear and nonlinear programming problems (Gondzio, 1996).

In the field of chemical engineering, interior point methods have been applied to solve data reconciliation, optimal control, multiperiod design and process optimization problems (Ternet, 1998). Alburquerque *et al*. (1997) and Ternet (1998) employ primal dual interior algorithms and high-order corrections to solve the quadratic programming subproblem within a sequential quadratic programming technique.

In this paper, we propose the application of interior point techniques for the solution of the complementarity formulation representing a conditional model (Rico-Ramirez and Westerberg, 1998). This approach is based on the work of Wang *et al*. (1996) and was specially motivated by the works of Simantiraki and Shanno (1995) and Wright and Ralph (1996) which apply infeasible interior point algorithms for mixed complementarity problems. Also, recent results reported in the field of chemical engineering by Ternet (1998) encourage the use of Mehrotra's second order method (Mehrotra,1992) and Gondzio's centrality corrections (Gondzio, 1996) to improve the convergence results obtained by Wang's algorithm.

2 BASICS OF PRIMAL-DUAL INTERIOR POINT METHODS

The so called primal-dual interior point methods have been shown to outperform the simplex method on many larger problems and to perform better than other interior point methods (Wright,

1997). In this section, we describe the fundamentals of a primal-dual interior point method. Consider the linear programming problem in standard form:

$$min\{c^T x \,|\, Ax = b, x \geq 0\} \quad \textbf{(1)}$$

The optimally conditions of (1) are given by:

$$\begin{aligned} A^T\lambda + s &= c \\ Ax &= b \\ x_i s_i &= 0 \\ x, s &\geq 0 \end{aligned} \quad \textbf{(2)}$$

If we modify (1) by applying a logarithmic barrier to the variables x then we get:

$$min\left\{ c^T x - \tau \sum_i \ln(x_i) \,\middle|\, Ax = b \right\} \quad \textbf{(3)}$$

similarly, the optimally conditions of (3) are given by:

$$\begin{aligned} A^T\lambda + s &= c \\ Ax &= b \\ XSe &= \tau e \end{aligned} \quad \textbf{(4)}$$

where X and S are the diagonal matrices whose elements are the components of the vectors x and s correspondingly, and e is the vector of all ones.

The system of equations (2) can be solved by applying the Newton method and carrying out a linear search to enforce the nonnegativity constraints of x and s. Unfortunately, we can often take only a small step before the nonnegativity constraints are violated, and, therefore, the iterates make little progress towards the solution. Rather than solving the system of equations (2), primal-dual interior point methods focus on the solution of the system (4) and introduce the concept of the *central path*. The central path is the set of points which are a solution of (4) for $\tau > 0$. The role of the parameter τ is to enforce that all the complementarity products have the same values for all indices i. Hence, the central path keeps the iterates biased towards the interior of the nonnegative

orthant $(x,s)\geq 0$. Note also that as τ goes to zero, the complementarity products decrease to zero at the same rate. For implementation purposes, τ is defined as the product of the parameters σ and μ, resulting in

$$\begin{aligned} A^T\lambda + s &= c \\ Ax &= b \\ XSe &= \sigma\mu e \end{aligned} \qquad \textbf{(5)}$$

μ is generally defined as the complementarity gap (average value of the n complementarity products):

$$\mu = \frac{x^T s}{n} \qquad \textbf{(6)}$$

and σ is the centering parameter with value between zero and one, $0\leq\sigma\leq 1$, such that $\sigma=0$ corresponds to a Newton step and $\sigma=1$ corresponds to a centering direction in which all the products $x_i s_i$ are equal to μ. Various methods differ in the way that μ and σ are chosen (Wright, 1997).

3 HIGH ORDER STRATEGIES FOR INTERIOR POINT METHODS

The solution of a system of equations defined by (5) involves the solution of the linearized system

$$\begin{bmatrix} 0 & A^T & I \\ A & 0 & 0 \\ S^k & 0 & X^k \end{bmatrix} \begin{bmatrix} \Delta x^k \\ \Delta\lambda^k \\ \Delta s^k \end{bmatrix} = \begin{bmatrix} c - A^T\lambda^k - s^k \\ b - Ax^k \\ -X^k S^k e + \sigma^k \mu^k e \end{bmatrix} \qquad \textbf{(7)}$$

at each iteration. It is estimated that the required factorization of the matrices

$$\begin{bmatrix} 0 & A^T & I \\ A & 0 & 0 \\ S^k & 0 & X^k \end{bmatrix}$$

takes 60 to 90% of the total CPU time needed to solve a problem (Gondzio, 1994). The use of

high order information has been motivated by the idea of using the same factorization for several different solves in order to reduce the number of interior point iterations required. As a matter of fact, second-order methods have been shown to give evident savings over the basic first order methods, and, therefore, they have became the computational state of the art (Lustig *et al*., 1992). In this section, we will review two of the most extensively applied high order methods found in the interior point literature: Mehrotra's second order method (Mehrotra,1992) and Gondzio's centrality correction (Gondzio, 1994). The algorithmic steps of both of those approaches can be found in Wright (1997) and Ternet (1998).

3.1 MEHROTRA'S PREDICTOR-CORRECTOR TECHNIQUE

Mehrotra's predictor-corrector technique (Mehrotra, 1990; Mehrotra, 1992; Lustig *et al*.,1992) has three main components (Wright, 1997; Ternet, 1998):

- A **predictor step**: a pure Newton (also known as affine-scaling) direction. For problem (5), this step is calculated by solving (7) with $\sigma=0$:

$$\begin{bmatrix} 0 & A^T & I \\ A & 0 & 0 \\ S^k & 0 & X^k \end{bmatrix} \begin{bmatrix} \Delta_p x^k \\ \Delta_p \lambda^k \\ \Delta_p s^k \end{bmatrix} = \begin{bmatrix} c - A^T \lambda^k - s^k \\ b - Ax^k \\ -X^k S^k e \end{bmatrix} \qquad \textbf{(8)}$$

- An adaptive approach to compute the centering parameter. This parameter is calculated in terms of the complementarity gap at the current point and the complementarity gap after a hypothetical step in the affine scaling direction is taken. In general, the centering parameter is small when good progress can be made in the affine direction and large when the affine direction produces little improvement. The actual calculation of the centering parameter is given by:

$$\begin{aligned} \mu^k &= (x^k)^T s^k / n \\ \mu_{aff} &= [(x^k + \alpha \Delta_p x^k)^T (s^k + \alpha \Delta_p x^k)] / n \\ \sigma^k &= (\mu^k / \mu_{aff})^3 \end{aligned} \qquad \textbf{(9)}$$

where the factor α defines the maximum stepsize in the affine-scaling direction that can be taken

while preserving the nonnegativity of the variables *(x,s)*.

- A **corrector step:** essentially a step based on Taylor series expansion of the complementarity equations. For problem (5), this step is calculated by:

$$\begin{bmatrix} 0 & A^T & I \\ A & 0 & 0 \\ S^k & 0 & X^k \end{bmatrix} \begin{bmatrix} \Delta_c x^k \\ \Delta_c \lambda^k \\ \Delta_c s^k \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \sigma^k \mu^k e - \Delta_p X^k \Delta_p S^k e \end{bmatrix} \quad \textbf{(10)}$$

where $\Delta_p X^k$ and $\Delta_p S^k$ are the diagonal matrices whose elements are the components of the vectors $\Delta_p x^k$ and $\Delta_p s^k$ calculated in the predictor step.

The corrector step is best understood by the following analysis. If a full step ($\alpha=1$) were achieved in the affine scaling direction, the new complementarity conditions would be given by:

$$(S^k + \Delta S_p^k)e \cdot (X^k + \Delta X_p^k)e = X^k S^k e + S^k \Delta S_p^k e + X^k \Delta X_p^k e + \Delta X_p^k \Delta S_p^k e \quad \textbf{(11)}$$

However, the last equation of the system of equations (8) is:

$$S^k \Delta S_p^k e + X^k \Delta X_p^k e = -X^k S^k e \quad \textbf{(12)}$$

and (11) reduces to:

$$(S^k + \Delta S_p^k)e \cdot (X^k + \Delta X_p^k)e = \Delta X_p^k \Delta S_p^k e \quad \textbf{(13)}$$

Hence, the second order correction $\Delta_p X^k \Delta_p S^k e$ corresponds to the violation of the complementarity conditions if a full step in the affine-scaling direction were taken. Moreover, the corrector direction is supposed to drive from a hypothetical point $(x^k + \Delta x_p^k,\ s^k + \Delta s_p^k, \lambda^k + \Delta \lambda_p^k)$ to a point in the central trajectory (note also the presence of the centering correction $\sigma^k \mu^k e$ in the corrector step).

Because the corrector step is a second order correction, the stepsize determination in Mehrotra's technique consists of finding an $\bar{\alpha}>0$ such that for all $\alpha \in (0,\bar{\alpha})$ (Wright, 1997):

$$(x, s, \lambda)^{k+1} = (x, s, \lambda)^{k} + \alpha \cdot \Delta_p^k + \alpha^2 \Delta_c^k$$
$$(x, s)^{k+1} \geq 0 \qquad \textbf{(14)}$$

where Δ_p^k and Δ_c^k are the predictor and the corrector steps in the variables correspondingly.

3.2 GONDZIO'S CENTRALITY CORRECTIONS

Gondzio (Gondzio,1994; Gondzio and Terlaky, 1994; Andersen *et al.*, 1996) argues that what reduces most the efficiency of an interior point method is a large discrepancy among the complementarity products. Complementarity products that are too small or too large (compared with the average) are undesirable, with the former being the more disastrous.

Gondzio assumes that a predictor step (a step calculated with Mehrotra's approach, for instance) has been calculated and evaluates the complementarity products for the current point (trial point) $(\tilde{x}, \tilde{s})$:

$$\tilde{\vartheta} = (\tilde{X}\tilde{S}e) \in R^n \qquad \textbf{(15)}$$

Then, the trial point is projected componentwise onto a hypercube:

$$Hyp = [\beta_{min}\mu^k, \beta_{max}\mu^k]^n \qquad \textbf{(16)}$$

to define the target

$$\vartheta_t = \pi(\tilde{\vartheta} \,|\, Hyp) \in R^n \qquad \textbf{(17)}$$

Gondzio believes that the effort should be concentrated on correcting only outlier complementarity products (the ones that do not belong to the interval $[\beta_{min}\mu^k, \beta_{max}\mu^k]$). The parameters β_{min} and β_{max} in (16) are the relative threshold values for outlier complementarity products and are assumed as given (in Gondzio's implementation $\beta_{min}=0.1$ and $\beta_{max}=10$).

Hence, a corrector term of the current iterate solves the system:

$$\begin{bmatrix} 0 & A^T & I \\ A & 0 & 0 \\ S^k & 0 & X^k \end{bmatrix} \begin{bmatrix} \Delta_m x^k \\ \Delta_m \lambda^k \\ \Delta_m s^k \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vartheta_t - \tilde{\vartheta} \end{bmatrix} \quad \textbf{(18)}$$

where $\vartheta_t - \tilde{\vartheta}$ is given by (Wright, 1997;Ternet, 1998):

$$(\vartheta_t - \tilde{\vartheta})_i = \begin{cases} (\beta_{min}\mu^k - \tilde{\vartheta}_i) & if\ \tilde{\vartheta}_i < \beta_{min}\mu^k \\ (\beta_{max}\mu^k - \tilde{\vartheta}_i) & if\ \tilde{\vartheta}_i > \beta_{max}\mu^k \\ -\beta_{max}\mu^k & if\ \tilde{\vartheta}_i > 2\beta_{max}\mu^k \\ 0 & otherwise \end{cases} \quad \textbf{(19)}$$

$$\forall i \in 1 \ldots n$$

Note that system (18) is full of zeros since $\vartheta_t - \tilde{\vartheta}$ is nonzero only for components that refer to the complementarity products that do not belong to $[\beta_{min}\mu^k, \beta_{max}\mu^k]$. Also note that for large complementarity products, $\tilde{\vartheta}_i > 2\beta_{max}\mu^k$, a more conservative value for the target is used in order to prevent the undesirable effect of bad scaling (Wright, 1997).

4 AN INTERIOR POINT POTENTIAL REDUCTION METHOD FOR CONSTRAINED EQUATIONS

In this section we describe the globally convergent framework developed by Wang *et al*. (1996). They combined the classical damped Newton Method with interior point potential reduction methods for solving a constrained system of nonlinear equations. They show how their formulation provides a unified framework for many mathematical problems, including complementarity problems and nonlinear programs.

4.1 THE MODEL

Let Ω be a closed subset of the Euclidean space R^n, where n is a positive integer. Ω is assumed to have a nonempty interior, denoted by *int* Ω. Let $H{:}\Omega \to R^n$ be a continuous mapping defined on Ω. Consider the problem of finding a vector ω satisfying:

$$H(\omega) = 0 \tag{20}$$

The basic structure that Wang *et al*. impose is that there is a partition of the range space of the mapping H :

$$H(\omega) = \begin{bmatrix} F(\omega) \\ G(\omega) \end{bmatrix}, \omega \in \Omega \tag{21}$$

for some functions $F{:}\Omega \to R^{n_1}$ and $G{:}\Omega \to R^{n_2}$ with $n_1 + n_2 = n$. Now let

$$\Omega_\Sigma = \{\omega \in int\Omega \,|\, G(\omega) > 0\} \tag{22}$$

where the inequality $G(\omega) > 0$ is to be understood component wise. The assumptions made by Wang and coworkers are the following:

1. $\Omega_\Sigma \neq \varnothing$ and $\Omega_\Sigma = \{\omega \in \Omega \,|\, G(\omega) > 0\}$.
2. H is continuously differentiable on the set Ω_Σ.
3. The Jacobian matrix $H'(\omega)$ is nonsingular for all $\omega \in \Omega_\Sigma$.

A real-valued function $\psi(\omega)$: $\Omega_\Sigma \to R$ is also defined:

$$\psi(\omega) = \zeta \cdot \log(F(\omega)^T F(\omega) + e^T G(\omega)) - \sum_i^{n_2} \log G_i(\omega) \tag{23}$$

where ζ is a fixed but arbitrary scalar satisfying $\zeta > n_2$ and e is the vector of all ones. When $n_2 = 0$, (23) reduces (without the logarithm) to the standard merit function used in the Newton method for solving the system of equations $F(\omega) = 0$. If we decrease $\psi(\omega)$, the first term in (23) contributes to reduce some norm of the function $H(\omega)$. The second term is the logarithmic barrier function whose role is to prevent a point ω from reaching the boundary of Ω_Σ.

Hence, the goal of Wang's approach is to develop an iterative algorithm for solving (21) while (23) plays the role of a merit function which guides the generation of the iterates ω^k.

4.2 AN INTERIOR POINT APPROACH

Wang's approach originates from the extension of path-following interior point methods for their application to the nonlinear case. The algorithm proposes to calculate a perturbed Newton direction in order to keep the iterates close to the central path of Ω_Σ. For a given vector $\omega \in \Omega_\Sigma$, the perturbed Newton direction at ω is obtained by solving the following system of linear equations:

$$H'(\omega)d = \begin{bmatrix} F'(\omega)d \\ G'(\omega)d \end{bmatrix} = \begin{bmatrix} -F(\omega) \\ -G(\omega) + \sigma\mu(\omega)e \end{bmatrix} \quad \textbf{(24)}$$

where $\mu(\omega) = e^T G(\omega)/n_2$, and σ is the centering parameter. Based on the work of Kojima *et al.* (1994), Wang shows that a solution d of (24) is a descent direction for the function $\psi(\omega)$ defined by (23) such that:

$$\psi(\omega + \lambda d) - \psi(\omega) \leq -\alpha\lambda(1 - \sigma)(\zeta - n_2) \quad \textbf{(25)}$$

where $\alpha \in (0,1)$ and λ is a scalar such that for all $\lambda \in (0,\bar{\lambda})$, $\bar{\lambda}>0$, we get $\omega + \lambda d \in \Omega_\Sigma$ (*i.e.* $\bar{\lambda}$ is the factor in the linear search of the damped Newton method). Note that the right hand side of (25) is always negative.

Furthermore, in order to prove convergence, Wang and coworkers define a function $\nu(\omega)$ as a measure of the error of a given iterate ω^k:

$$\nu(\omega) = F(\omega)^T F(\omega) + e^T G(\omega) \quad \textbf{(26)}$$

and show that a sequence of iterates generated by their approach satisfies the following properties:

1. The sequence $\{\nu(\omega^k)\}$ is bounded.
2. If the sequence of iterates $\{\omega^k\}$ is bounded, then

$$\lim_{k \to \infty} \nu(\omega^k) = 0 \quad \textbf{(27)}$$

The derivation of equation (25) is shown in Appendix A. For the derivation of equation (27) and

the demonstration of the above properties, the reader is referred to the paper of Wang *et al.* (1996).

4.3 THE ALGORITHM

The steps of the potential reduction algorithm for solving (21) are:

Step 1. Initialization. Let $\varsigma > n_2$, $\alpha \in (0,1)$, $\bar{\sigma} \in [0, 1)$, $\xi > 0$ and $\rho \in (0,1)$ be given. Choose a $\sigma^0 \in [0,\bar{\sigma}]$ and an initial point $\omega^0 \in \Omega_\Sigma$.

Step 2. Direction Generation. Solve the system of linear equations (24) at $\omega=\omega^k$:

$$H'(\omega^k)d = \begin{bmatrix} F'(\omega^k)d \\ G'(\omega^k)d \end{bmatrix} = \begin{bmatrix} -F(\omega^k) \\ -G(\omega^k) + \sigma^k \mu(\omega^k)e \end{bmatrix}$$

where $\mu(\omega^k) = e^T G(\omega^k)/n_2$, to obtain the search direction d^k.

Step 3. Stepsize determination. Let m_k be the smallest nonnegative integer m such that the following conditions hold:

$$\omega^k + \xi\rho^m d^k \in \Omega_\Sigma \qquad \textbf{(28)}$$

$$\psi(\omega^k + \xi\rho^m d^k) - \psi(\omega^k) \le -\alpha\xi\rho^m(1 - \sigma^k)(\zeta - n_2) \qquad \textbf{(29)}$$

and set $\omega^{k+1} = \omega^k + \xi\rho^{m_k} d^k$.

Step 4. Termination check. Terminate if ω^{k+1} satisfies a prescribed stopping rule. Otherwise, pick a $\sigma^{k+1} \in [0,\bar{\sigma}]$ and return to **Step 2**.

The values suggested by Wang for each of the parameters defined in **Step 1** are: $\varsigma = n_2 \cdot \sqrt{n_2}$, $\alpha = 0.5$, $\sigma = 0.5$, $\xi = 2$ and $\rho = 0.5$.

5 THE COMPLEMENTARITY REPRESENTATION OF A CONDITIONAL MODEL AND ITS RELATION TO WANG'S

FRAMEWORK

Consider the complementarity formulation described by Rico-Ramirez (1998) for a system of equations containing a disjunction with two disjunctive terms:

$$h(x) = 0$$

$$\begin{pmatrix} r_{1_j}(x) - p_{1_j} \\ r_{2_j}(x) - p_{2_j} \\ g_{l-\beta}(x) - p_{1_l} + p_{2_l} \end{pmatrix} = 0 \qquad \forall j \in [1 \ldots \beta],\ l \in [\beta + 1 \ldots \beta + \gamma]$$

$$\sum_{t=1}^{\beta+\gamma-s} p_{1_t} \cdot p_{2_{t+s}} + \sum_{t=\beta+\gamma-s+1}^{\beta+\gamma} p_{1_t} \cdot p_{2_{t+s-\beta-\gamma}} = 0 \qquad \forall s \in [0 \ldots \beta + \gamma - 1]$$

$$p_{i_q} \geq 0 \qquad \forall i \in [1 \ldots 2],\ q \in [1 \ldots \beta + \gamma]$$

and let n_x be the dimensionality of the vector of variables of the original conditional model, *i.e.* $x \in R^{n_x}$. The resulting complementarity problem is one of $n_x + 2(\beta+\gamma)$. variables and equations. Recall also that the positiveness in the variables p_{i_q} is imposed, that is $p_{i_q} \in R_+^{2(\beta+\gamma)}$. If we define:

- $\Omega = R_+^{2(\beta+\gamma)} \times R^{n_x}$
- $\omega \in \Omega$, that is $\omega = (p_{i_q}, x) \in R_+^{2(\beta+\gamma)} \times R^{n_x}$
- the partition $H(\omega)$ given by:

$$F(\omega) = \begin{pmatrix} \underline{h}(x) \\ r_{1_j}(x) - p_{1_j} \\ r_{2_j}(x) - p_{2_j} \\ g_{l-\beta}(x) - p_{1_l} + p_{2_l} \end{pmatrix} = 0 \qquad \forall j \in [1 \ldots \beta],\ l \in [\beta + 1 \ldots \beta + \gamma] \qquad \textbf{(30)}$$

$$G(\omega) = \left(\sum_{t=1}^{\beta+\gamma-s} p_{1_t} \cdot p_{2_{t+s}} + \sum_{t=\beta+\gamma-s+1}^{\beta+\gamma} p_{1_t} \cdot p_{2_{t+s-\beta-\gamma}} \right) = 0 \qquad \forall s \in [0 \ldots \beta + \gamma - 1]$$

and assume:

- the continuous differentiability of the function $F(\omega): R_+^{2(\beta+\gamma)} \times R^{n_x}$ at every point $\omega=(p_{i_q}, x) \in R_{++}^{2(\beta+\gamma)} \times R^{n_x}$.
- and the nonsingularity of Jacobian matrix $H'(\omega)$ (this also implies that we assume the nondegeneracy of the complementarity equations $G(\omega)$ in order to avoid numerical singularities caused by such equations)

then we can apply the potential reduction algorithm and its convergence result to the complementarity formulation described earlier in this work.

6 IMPLEMENTATION OF WANG'S ALGORITHM AND HIGH ORDER TECHNIQUES FOR SOLVING A CONDITIONAL MODEL

The algorithm proposed by Wang and the second order corrections developed by Mehrotra and Gondzio have been implemented in a computer program called IPSlv for their application to the solution of conditional models formulated as a complementarity problem of the type represented by (30). The solver IPSlv has been incorporated into the ASCEND environment. Some details of the implementation of Wang's algorithm and both of the second order techniques are given in this section.

6.1 PRACTICAL IMPLEMENTATION OF WANG'S ALGORITHM

For purposes of implementation, we made some minor modifications to the algorithm described in 4.3:

1. First, the value for the centering parameter σ in Wang's algorithm is rather arbitrary. Wang's proposes using a value of 0.5 and dividing that value by 10 every time that a full Newton step in the variables can be taken. In our implementation we provide the option of defining an initial value of the centering parameter and modifying it under Wang's heuristic. However, we also support an evaluation of the centering parameter *a la* Mehrotra. For the later case, we need to substitute **Step 2** (direction generation) in algorithm 4.3 by the following steps:

- Calculate the affine direction d_p^k by solving (24) with $\sigma=0$.

$$H'(\omega^k)d_p^k = \begin{bmatrix} F'(\omega^k)d_p^k \\ G'(\omega^k)d_p^k \end{bmatrix} = \begin{bmatrix} -F(\omega^k) \\ -G(\omega^k) \end{bmatrix} \quad \textbf{(31)}$$

- Calculate the centering parameter (similarly to (9)):

$$\begin{aligned} \mu^k(\omega^k) &= e^T G(\omega^k)/n_2 \\ \mu_{aff}(\omega^k) &= e^T G(\omega^k + \lambda d_p^k)/n_2 \\ \sigma^k &= [\mu^k(\omega^k)/\mu_{aff}(\omega^k)]^3 \end{aligned} \quad \textbf{(32)}$$

where is λ is a scalar such that for all $\lambda \in (0,\bar{\lambda})$, $\bar{\lambda}>0$, we get $\omega^k + \lambda d_p^k \in R_+^{2(\beta+\gamma)} \times R^{n_x}$ (*i.e.* $\bar{\lambda}$ is the factor in the linear search of the damped Newton method).

- Solve equation (24) with the centering parameter calculated in the previous step.

$$H'(\omega^k)d_c^k = \begin{bmatrix} F'(\omega^k)d_c^k \\ G'(\omega^k)d_c^k \end{bmatrix} = \begin{bmatrix} -F(\omega^k) \\ -G(\omega^k) + \sigma^k \mu(\omega^k)e \end{bmatrix} \quad \textbf{(33)}$$

Here, the direction d_c^k is then used in **Step 3** (stepsize determination) of the algorithm 4.3.

Note that, even though two solves are required, the factorization of the Jacobian matrix *H'(ω)* is being done only once (as in second order methods). In other words, this option requires an extra backsolve to compute the affine direction but leaves us with a more reliable value for the centering parameter σ^k.

2. The second modification arises from the fact that, while solving a conditional model as a complementarity problem, the equations of the partition *G(ω)* may contain the summation of complementarity products rather than individual complementarity products. For that reason, we modified the second term in the right hand side (the logarithmic barrier term) of the merit function $\psi(\omega)$, Equation (23), to include the summation of the logarithm of each individual

complementarity product instead of the logarithm of each function $G_i(\omega)$. That modification is motivated solely by the observation that we need to prevent each individual complementarity product from going prematurely to zero (a $G_i(\omega)$ could be greater than zero but still an individual complementarity product in it could reach zero), but there is presently no theoretical basis to support it. As a matter of fact, Wang's proof of convergence does not strictly apply anymore after this modification is made.

6.2 IMPLEMENTATION OF SECOND ORDER CORRECTIONS

The linearization of the functions $F(\omega)$ in (24) may lead to infeasibilities in the solution to the problem (21). Hence, in order to strictly apply second order corrections to the problem (24), we should also consider a correction for the linearization of the equations $F(\omega)$. Still, here we are mainly concerned with the numerical problems associated with the complementarity equations $G(\omega)$, and, for those equations, an analogy to Mehrotra's second order correction and Gondzio's centrality correction can be derived. In our implementation of second order techniques, the main difference with respect to the original approaches is that, in the problem we are solving, the equations of the partition $G(\omega)$ may contain the summation of complementarity products.

6.2.1 Applying Mehrotra's corrector step

As in our implementation of Wang's algorithm, the implementation of Mehrotra's predictor corrector technique implies a modification of the direction generation step (**Step 2**) of algorithm 4.3. The three elements of Mehrotra's technique applied to the framework used in this work are:

- **Predictor** step. Calculation of the affine direction as in (31).
- Computation of the centering parameter σ^k as in (32).
- **Corrector** step. A second order corrector step for the system defined by (24) is given by the solution to the linear system:

$$H'(\omega^k)d_c^k = \begin{bmatrix} F'(\omega^k)d_c^k \\ G'(\omega^k)d_c^k \end{bmatrix} = \begin{bmatrix} 0 \\ \sigma\mu(\omega^k)e - C(d_p^k) \end{bmatrix} \quad \textbf{(34)}$$

where the vector $C(d_p^k)$ is a function of the affine direction and represents the second order

correction for the partition $G(\omega)$ (similar to the second order correction $\Delta X_p^k \Delta S_p^k e$ used in (10)). Specifically for the complementarity formulation used in this work (Equation (30)), the elements of the vector $C(d_p^k)$ are given by:

$$C_{s+1}(d_p^k) = \sum_{t=1}^{\beta+\gamma-s} \Delta p_{1_t} \cdot \Delta p_{2_{t+s}} + \sum_{t=\beta+\gamma-s+1}^{\beta+\gamma} \Delta p_{1_t} \cdot \Delta p_{2_{t+s-\beta-\gamma}} \qquad \forall s \in [0 \ldots \beta+\gamma-1] \tag{35}$$

For simplicity in the representation, note that we have omitted the index k (iteration) for the complementary variables p_{i_q}. Also, note that the corrector term for the partition $F(\omega)$ in (34) is zero. As stated before, a value of zero is strictly correct only in a case in which the equations of $F(\omega)$ are linear.

As an analogy to the discussion about the meaning of Mehrotra's second order correction given before for the linear programming case, the following simple example illustrates the meaning of the second order correction defined by (35):

Consider the complementarity equation (including two complementarity products) given by:

$$G_1(\omega) = 0 \qquad \Longrightarrow \qquad p_{1_1} \cdot p_{2_1} + p_{1_2} \cdot p_{2_2} = 0$$

The linearization of that complementarity equation in a Newton scheme is given by:

$$G_1'(\omega) d = -G(\omega) \qquad \Longrightarrow$$

$$p_{1_1} \cdot \Delta p_{2_1} + \Delta p_{1_1} \cdot p_{2_1} + p_{1_2} \cdot \Delta p_{2_2} + \Delta p_{1_2} \cdot p_{2_2} = -(p_{1_1} \cdot p_{2_1} + p_{1_2} \cdot p_{2_2}) \tag{36}$$

If a full step were achieved in the affine-scaling (Newton) direction, the new complementarity conditions would be given by:

$$(p_{1_1} + \Delta p_{1_1}) \cdot (p_{2_1} + \Delta p_{2_1}) + (p_{1_2} + \Delta p_{1_2}) \cdot (p_{2_2} + \Delta p_{2_2}) = p_{1_1} \cdot p_{2_1} + p_{1_2} \cdot p_{2_2} +$$
$$p_{1_1} \cdot \Delta p_{2_1} + \Delta p_{1_1} \cdot p_{2_1} + p_{1_2} \cdot \Delta p_{2_2} + \Delta p_{1_2} \cdot p_{2_2} +$$
$$\Delta p_{1_1} \cdot \Delta p_{2_1} + \Delta p_{1_2} \cdot \Delta p_{2_2}$$

which, after substituting (36), reduces to

$$(p_1^1 + \Delta p_1^1) \cdot (p_1^2 + \Delta p_1^2) + (p_2^1 + \Delta p_2^1) \cdot (p_2^2 + \Delta p_2^2) = \Delta p_{1_1} \cdot \Delta p_{2_1} + \Delta p_{1_2} \cdot \Delta p_{2_2} \qquad \textbf{(37)}$$

The right hand side of (37) is the second order corrector term defined by (35). Similar to the linear case, the second order correction (35) corresponds to the violation of the complementarity conditions *G(ω)* if a full step in the affine-scaling direction were taken. Hence, the corrector direction is supposed to drive from a hypothetical point $(\omega^k + d_p^k)$ to a point in the central trajectory.

When applying a second order correction, we also have to modify **Step 3** of algorithm 4.3 (stepsize determination). Since the corrector step is a second order term, equation (28) has to be substituted by

$$\omega^k + \xi\rho^m d_p^k + (\xi\rho^m)^2 d_c^k \in \Omega_\Sigma \qquad \textbf{(38)}$$

where d_p^k is the affine direction (predictor step) and d_c^k is the second order corrector direction. Recall that, specifically for our problem, $\Omega = R_+^{2(\beta+\gamma)} \times R^{n_x}$ and $\Omega_\Sigma = R_{++}^{2(\beta+\gamma)} \times R^{n_x}$.

6.2.2 Applying Gondzio's centrality corrections

As in Gondzio's original method, in this implementation we assume that a predictor direction (a Mehrotra's step or a step generated by Step 2 in Wang's algorithm, for instance) has been calculated, and, therefore, the complementarity equations for the resulting point can be evaluated:

$$\tilde{\Upsilon} = G(\tilde{\omega}) \in R^{n_2} \qquad \textbf{(39)}$$

If we would strictly follow Gondzio's method, the next step would be to define a hypercube

$$Hyp = [\beta_{min}\mu^k, \beta_{max}\mu^k]^{n_2} \quad \textbf{(40)}$$

and project the complementarity equations componentwise to define the target:

$$\Upsilon_t = \pi(\tilde{\Upsilon}|Hyp) \in R^{n_2} \quad \textbf{(41)}$$

In Gondzio's original approach, each complementarity equation contains only one complementarity product. In that way, a correction term can be evaluated for each complementarity product. On the contrary, here we recall once again the fact that, for the complementarity representation of a conditional models, the complementarity equations $G(\omega)$ may consist of the summation of complementarity products rather than individual complementarity products. Hence, the value of a corrector term for each complementarity product cannot be explicitly estimated.

In this implementation of Gondzio's centrality correction, equations(40) and (41) are not used directly. In order to best describe our implementation of Gondzio's centrality correction, let n_g be the number of complementarity products in each complementarity equation, and for purposes of illustration, consider that n_g is the same for each complementarity equation.

Hence, the complementarity equations evaluated at the trial point can be represented in terms of the individual complementarity products as:

$$G_i(\tilde{\omega}) = \sum_{j=1}^{j=n_g} g_{ij}(\tilde{\omega}) \qquad \forall i \in 1 \ldots n_2 \quad \textbf{(42)}$$

where $g_{ij}(\tilde{\omega})$ is the *j-th* complementarity product in the *i-th* complementarity equation. Furthermore, the components of a vector $\tilde{\gamma} \in R^{n_2 \times n_g}$ including all the individual complementarity products are given by:

$$\tilde{\gamma}_{(i-1)\cdot n_g + j} = g_{ij}(\tilde{\omega}) \qquad \forall i \in 1 \ldots n_2, \forall j \in 1 \ldots n_g \quad \textbf{(43)}$$

Once the vector of individual complementarity products for the trial point $\tilde{\gamma}$ has been evaluated, we can use a procedure analogous to the one suggested by Gondzio. The vector $\tilde{\gamma}$ is projected on a hypercube

$$Hyp_g = [\beta_{min}(\mu^k / n_g), \beta_{max}(\mu^k / n_g)]^{n_2 \times n_g} \quad \textbf{(44)}$$

to define the target

$$\gamma = \pi(\tilde{\gamma}|Hyp_g) \in R^{n_2 \times n_g} \tag{45}$$

which results in the difference vector $\gamma - \tilde{\gamma}$ being:

$$(\gamma - \tilde{\gamma})_k = \begin{cases} (\beta_{min}(\mu^k / n_g) - \tilde{\gamma}_k) & if \tilde{\gamma}_k < \beta_{min}(\mu^k / n_g) \\ (\beta_{max}(\mu^k / n_g) - \tilde{\gamma}_k) & if \tilde{\gamma}_k > \beta_{max}(\mu^k / n_g) \\ -\beta_{max}(\mu^k / n_g) & if \tilde{\gamma}_k > 2\beta_{max}(\mu^k / n_g) \\ 0 & otherwise \end{cases} \tag{46}$$
$$\forall k \in 1 \ldots n_2 \times n_g$$

Thus, we define the corrector term for each complementarity equation as the summation of the corrector terms for each of the complementarity products:

$$C_i(\tilde{\omega}) = \sum_{k = (i-1) \cdot n_g + 1}^{k = i \cdot n_g} (\gamma - \tilde{\gamma})_k \tag{47}$$
$$\forall i \in 1 \ldots n_2$$

Finally, an analogy to Gondzio's centrality correction for the complementarity representation of a conditional model will be given by:

$$H'(\omega^k) d_g^k = \begin{bmatrix} F'(\omega^k) d_g^k \\ G'(\omega^k) d_g^k \end{bmatrix} = \begin{bmatrix} 0 \\ C(\tilde{\omega}) \end{bmatrix} \tag{48}$$

To summarize, in our implementation of Gondzio's method,

- the complementarity equations are decomposed in terms of their individual complementarity products,
- a correction term for each outlier complementarity product is evaluated,
- the corrector term for a complementarity equation is obtained as the summation of the corrections of each of its individual complementarity products and, finally,
- Gondzio's corrector step is evaluated by solving the linear system defined by (48).

This implementation was motivated by Gondzio's original goal of correcting (if necessary) each complementarity product of each complementarity equation. However, we recognize here a fundamental incorrectness of the approach presented in this section: there is no guarantee that the corrector term $C_i(\tilde{\omega})$ indeed provides a correction for each complementarity product. Hence, this implementation is not theoretically sound, and it should only be considered as an initial study to discover the difficulties and the benefits of the implementation on the solution of our complementarity formulation. Future work should be aimed for obtaining a theoretically sound implementation.

6.3 THE SOLVER IPSLV

The numerical techniques described in this section have been implemented in a computer code called IPSlv and incorporated to the ASCEND modeling environment. As such, the selection of the specific technique as well as the values of the various parameters can be specified interactively through the ASCEND solver interface. This implementation can be applied not only to the complementarity representation of a conditional model but also to any kind of complementarity problems described by (21). Also, it can be used for any system like (5), generated by the optimality conditions of a linear programming problem. The main options offered by this solver are:

1. Numerical technique:
   - Wang's potential reduction method.
   - Mehrotra's second order method.

   Gondzio's centrality corrections can be applied to the point generated by any of those techniques at each iteration.
2. Calculation of the centering parameter σ:

- Given initial value modified heuristically as proposed by Wang.
- Calculated *a la* Mehrotra by using the affine scaling direction.

If Mehrotra's technique is being used, only the second alternative is available. Calculation *a la* Mehrotra is the default option.

3. Calculation of the potential function $\psi(\omega)$:

- Include the summation of residuals of the complementarity equations in the logarithmic barrier term.
- Include the summation of the values of the individual complementarity products in the logarithmic barrier term. This is the default option as described earlier.

7 NUMERICAL RESULTS

The numerical methods described in this paper were used to solve the complementarity problems described in Rico-Ramirez and Westerberg (1998). The number of iterations that we used to obtain the solution of each of these problems is shown in Table 1.

Table 1: Numerical results by using interior point methods.

Example	Reference	Wang	Wang + Mehrotra	Wang + Gondzio	Wang + Mehrotra + Gondzio
Flow Transition (sonic-subsonic)	Zaher (1995)	7	7	7	7
Phase Equilibria	Zaher (1995)	11	8	11	8
Heat exchanger	Zaher (1995)	9	8	9	8
Pipeline network	Bullard and Biegler (1992)	34	33	36	33
Simple L-V flash	King (1980)	26	23	32	23
Linear mass balance	Grossmann and Turkay (1996)	15	14	15	14

8 DISCUSSION

Regarding the numerical results obtained for this set of examples, we can make the following

observations:

- A sequence of steps generated by Wang's algorithm successively converged to a the solution in all of the complementarity problems.
- Also, in all the cases, the use of Mehrotra's second order correction resulted in a reduction in the number of iterations required for convergence by Wang's algorithm.
- Finally, the application of Gondzio's corrector step did not provide a significant improvement with respect to a step calculated solely by Wang's algorithm or a step including Mehrotra's correction.

However, we are aware that this reduced set of examples may not be enough to draw a meaningful conclusion regarding the numerical performance of each of the techniques. So, for instance, we still consider that a corrector step a la Gondzio might reduce the problems associated with scaling in some other complementarity problems.

Rather than a formal comparison among the performance of these methods, we consider that a major result obtained from the experiments shown in the previous section is that we could establish the viability of the use of interior point methods in the solution of conditional models represented as complementarity problems. That is what we believe is one the contributions of this work.

The use of interior point methods in the solution of conditional models represented as complementarity problems provides some theoretical and numerical advantages with respect to both of the approaches discussed in Rico-Ramirez and Westerberg (1998):

1. First, a theoretical proof of convergence exists for the interior point algorithm used in this work (Wang *et al.*, 1996).
2. The use of interior point methods will prevent the complementarity products of the complementarity equations from prematurely reaching zero. In practice, this feature benefits the numerical performance by *i)* avoiding numerical singularities during the iterative solution process and *ii)* allowing to take larger steps in a Newton-based technique before the nonnegativity constraints of the complementarity variables are violated.
3. The use of second order corrections in interior point methods, specially Gondzio's centrality

correction, can help prevent numerical problems associated to bad scaling.

Finally, the implementation of second order techniques for the complementarity formulation developed in this work must only be considered as an initial study which discovers the complications and potential benefits of such an implementation. Hence, we want to emphasize that a conceptual gap still exists between the application of second order methods for the linear programming problem case and their application for our complementarity formulation; future research should be aimed at bridging this gap as far as possible.

9 ACKNOWLEDGMENTS

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APPENDIX A PROOF OF THE DESCENT OF THE POTENTIAL FUNCTION IN WANG'S ALGORITHM

This appendix presents the demonstration developed by Wang *et al.* (1996). Based on the work of Kojima *et al.* (1994), Wang shows that perturbed Newton direction d is a descent direction of the function potential function $\psi(\omega)$ such that:

$$\psi(\omega + \lambda d) - \psi(\omega) \leq -\alpha\lambda(1 - \sigma)(\zeta - n_2)$$

where $\alpha \in (0,1)$, λ is a scalar and there exists a $\bar{\lambda}>0$ such that, for all $\lambda \in (0,\bar{\lambda})$, we get $\omega + \lambda d \in \Omega_\Sigma$.

A.1 Demonstration

Wang *et al*. (1996) establish some important properties about the perturbed Newton direction calculated within the potential reduction algorithm. These properties are established in Lemma 1 below.

Lemma 1. Let $\zeta > n_2$ be given. Under the assumptions

- $\Omega_\Sigma \neq 0$ and $\Omega_\Sigma = \{\omega \in \Omega | G(\omega) > 0\}$ and
- H is continuously differentiable on the set Ω_Σ,

the following properties are valid for an arbitrary vector $\omega \in \Omega_\Sigma$ and any scalar $\alpha \in (0, 1)$:

(i) $\Psi(\omega) \geq (\zeta - n_2) \cdot \log(\nu(\omega)) + n_2 \log(n_2)$

(ii) ψ is continuously differentiable at ω and has a gradient:

$$\nabla\psi(\omega) = \frac{\zeta}{\nu(\omega)} \cdot (2\nabla F(\omega)F(\omega) + \nabla G(\omega)e) - \nabla G(\omega)G(\omega)^{-1}$$

(iii) If d is a solution of

$$H'(\omega)d = \begin{bmatrix} F'(\omega)d \\ G'(\omega)d \end{bmatrix} = \begin{bmatrix} -F(\omega) \\ -G(\omega) + \sigma\mu(\omega)e \end{bmatrix}$$

then

$$\nabla\psi(\omega)^T d \leq -(1-\sigma) + (\zeta - n_2);$$

hence there exists a scalar $\bar{\lambda}>0$ such that for all $\lambda \in (0,\bar{\lambda})$

$$\omega + \lambda d \in \Omega_\Sigma,$$

$$\psi(\omega + \lambda d) - \psi(\omega) \leq -\alpha\lambda(1-\sigma)(\zeta - n_2) < 0$$

Proof. The inequality *(i)* is frequently used in the study of interior point methods. This proof is taken from Kojima *et al.* (1994):

Starting with the definitions of the potential function $\psi(\omega)$:

$$\psi(\omega) = \zeta \cdot \log(F(\omega)^T F(\omega) + e^T G(\omega)) - \sum_i^{n_2} \log G_i(\omega)$$

and the measure of the error $\nu(\omega)$:

$$\nu(\omega) = F(\omega)^T F(\omega) + e^T G(\omega)$$

Then, we get

$$\psi(\omega) = \zeta \cdot \log(\nu(\omega)) - \sum_i^{n_2} \log G_i(\omega) \qquad \textbf{(A.1)}$$

$$\psi(\omega) = (\zeta - n_2) \cdot \log(\nu(\omega)) + n_2 \cdot \log(\nu(\omega)) - \sum_i^{n_2} \log G_i(\omega) \qquad \textbf{(A.2)}$$

$$\psi(\omega) \geq (\zeta - n_2) \cdot \log(\nu(\omega)) + n_2 \cdot \log(e^T G(\omega)) - \sum_i^{n_2} \log G_i(\omega) \qquad \textbf{(A.3)}$$

$$\psi(\omega) \geq (\zeta - n_2) \cdot \log(\nu(\omega)) + n_2 \cdot \log\left(\frac{(e^T G(\omega))/n_2}{\left(\prod_{i=1}^{n_2} G_i(\omega)\right)^{1/n_2}}\right) + n_2 \log(n_2) \qquad \textbf{(A.4)}$$

$$\Psi(\omega) \geq (\zeta - n_2) \cdot \log(\nu(\omega)) + n_2 \log(n_2) \qquad \textbf{(A.5)}$$

Here the last inequality follows from

$$n_2 \cdot \log\left(\frac{(e^T G(\omega))/n_2}{\left(\prod_{i=1}^{n_2} G_i(\omega) \right)^{1/n_2}} \right) \geq 0 \qquad \textbf{(A.6)}$$

The identity in (ii) follows from the following computation. Consider the definition of $\psi(\omega)$ given in (A.1). For each $j = 1,2,...n_1+n_2$,

$$\frac{\partial \psi(\omega)}{\partial \omega_j} = \frac{\zeta}{\nu(\omega)} \cdot \left(\sum_{i=1}^{n_1} 2F_i(\omega) \cdot \frac{\partial F_i(\omega)}{\partial \omega_j} + \sum_{i=1}^{n_2} \frac{\partial G_i(\omega)}{\partial \omega_j} \right) - \sum_{i=1}^{n_2} G_i(\omega)^{-1} \cdot \frac{\partial G_i(\omega)}{\partial \omega_j} \qquad \textbf{(A.7)}$$

and, therefore,

$$\nabla \psi(\omega) = \frac{\zeta}{\nu(\omega)} \cdot (2\nabla F(\omega) F(\omega) + \nabla G(\omega) e) - \nabla G(\omega) G(\omega)^{-1} \qquad \textbf{(A.8)}$$

To prove the first inequality in *(iii)*, we use *(ii)* and the definition of $\mu(\omega) = e^T G(\omega)/n_2$ to get

$$\nabla \psi(\omega)^T d = \frac{\zeta}{\nu(\omega)} \cdot (2F(\omega)^T F'(\omega) d + e^T G'(\omega) d) - (G(\omega)^{-1})^T G'(\omega) d \qquad \textbf{(A.9)}$$

(A.10)

$$\nabla \psi(\omega)^T d = \frac{\zeta}{\nu(\omega)} \cdot (2F(\omega)^T (-F(\omega)) + e^T (-G(\omega)) + \sigma\mu(\omega) n_2) + n_2 - \sigma\mu(\omega) e^T G(\omega)^{-1}$$

(A.11)

$$\nabla\psi(\omega)^T d \;=\; -\frac{\zeta}{\nu(\omega)} \cdot (2F(\omega)^T F(\omega) + (1-\sigma)e^T G(\omega)) + n_2 - \sigma n_2 \frac{e^T G(\omega)}{n_2} \cdot \frac{e^T G(\omega)^{-1}}{n_2}$$

$$\nabla\psi(\omega)^T d \le -\zeta(1-\sigma) + n_2 - \sigma n_2 \left[\prod_{i=1}^{n_2} G_i(\omega)\right]^{1/n_2} \left[\prod_{i=1}^{n_2} G_i(\omega)^{-1}\right]^{1/n_2} \qquad \textbf{(A.12)}$$

$$\nabla\psi(\omega)^T d \le -\zeta(1-\sigma) + n_2(1-\sigma) \qquad \textbf{(A.13)}$$

$$\nabla\psi(\omega)^T d \le -(1-\sigma) + (\zeta - n_2) \qquad \textbf{(A.14)}$$

where the inequality in (A.12) follows from the arithmetic-geometric mean inequality applied to the terms $e^T G(\omega)/n_2$ and $e^T G(\omega)^{-1}/n_2$ and the fact that $2 > (1-\sigma)$.

Finally, Wang establishes the last assertion in *(iii)*. Using the second assumption and the fact that Ω_Σ is an open set, it is concluded that there exists a scalar $\bar{\lambda}>0$ such that, for all $\lambda \in (0,\bar{\lambda})$, $\omega + \lambda d \in \Omega_\Sigma$ and

$$\psi(\omega + \lambda d) - \psi(\omega) \le \lambda(\nabla\psi(\omega)^T d + (1-\alpha)(1-\rho)(\zeta - n_2)) \qquad \textbf{(A.15)}$$

$$\psi(\omega + \lambda d) - \psi(\omega) \le -\alpha\lambda(1-\sigma)(\zeta - n_2) \qquad \textbf{(A.16)}$$

Q.E.D.