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CONSTRAINED OPTIMIZATION PROBLEMS

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THE EXPANDED LAGRANGIAN SYSTEM

FOR CONSTRAINED OPTIMIZATION PROBLEMS

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ABSTRACT

Smooth penalty functions can be combined with numerical continuation/bifurcation techniques to produce a class of robust and fast algorithms for constrained optimization problems. The key to the development of these algorithms is the Expanded Lagrangian System which is derived and analyzed in this work. This parametrized system of nonlinear equations contains the penalty path as a solution, provides a smooth homotopy into the first-order necessary conditions, and yields a global optimization technique. Furthermore, the inevitable ill-conditioning present in a sequential optimization algorithm is removed for three penalty methods: the quadratic penalty function for equality constraints, and the logarithmic barrier function (an interior method) and the quadratic loss function (an exterior method) for inequality constraints. Although these techniques apply to optimization in general and to linear and nonlinear programming, calculus of variations, optimal control and parameter identification in particular, the development is primarily within the context of nonlinear programming.

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1. Introduction

The use of smooth penalty functions in a sequential optimization algorithm to solve constrained optimization problems has long been regarded as unfashionable and numerically defective, principally because of an inevitable ill-conditioning that occurs as the penalty parameter tends to the prescribed limit. This view, which is prevalent in most texts and review articles [5, 6, 9, 19, 20], is quite valid and certainly motivated development of other numerical optimization techniques such as augmented Lagrangians and exact penalty functions. Our objective herein is to re-examine the use of these smooth penalty functions, not in a sequential optimization algorithm, but in a continuation-based algorithm for following the penalty function path defined as a solution of a parametrized system of nonlinear equations. This methodology now becomes viable because of the extensive development of numerical continuation/bifurcation techniques during the last decade [1, 11, 16, 17, 25] and because we can remove the ill-conditioning for three fundamentally important smooth penalty functions. These continuation methods are capable of producing robust algorithms competitive with the fastest optimization techniques currently available and yield a method for global optimization.

Although the techniques discussed here apply to constrained optimization in general and to linear and nonlinear programming, calculus of variations, optimal control and parameter identification in particular, our main focus in this work is on the general nonlinear programming problem

$$\min\{f(\underset{\sim}{x}) \mid \underset{\sim}{h}(\underset{\sim}{x}) = \underset{\sim}{0},\ \underset{\sim}{g}(\underset{\sim}{x}) \geq \underset{\sim}{0}\}$$

where $f: \mathbb{R}^n \to \mathbb{R}^1$, $\underset{\sim}{h}: \mathbb{R}^n \to \mathbb{R}^q$ and $\underset{\sim}{g}: \mathbb{R}^n \to \mathbb{R}^p$ are assumed to be twice continuously differentiable. (Section 5 contains examples from linear programming and the calculus of variations.) Within this context, the strength of the combination of nonlinear equations and smooth penalty functions is perhaps best explained by first examining the attributes of these two methods for solving optimization problems.

The use of nonlinear equations to solve constrained opimization problems can be based on solving the first-order necessary conditions by Newton's method or one of its many variants [3; 5, p. 138]. An important attribute of Newton's method is its speed of convergence, but there are many deficiencies: a good initial approximation is needed, the derivatives must be supplied, and the linear algebra can be expensive. Two popular techniques for alleviating the first difficulty are continuation (embedding and homotopy) and damping while quasi-Newton methods and sequencing the matrix factorizations are useful for the latter two difficulties. For optimization problems there are additional difficulties. The inequality constraints and the sign of their corresponding multipliers must be satisfied and, most importantly, convergence should be to a local optimum.

In spite of the ill-conditioning problem, smooth penalty functions have been extensively investigated and are known to have exceptional theoretical strengths. A particularly relevant and generic result pertains to a penalized objective function $P(\underset{\sim}{x}, r)$ where the penalty parameter is arranged so that $r = 0$ is the desired limit. If $\{r_k\}$ is a decreasing sequence of penalty parameter values converging to zero and if $\{\underset{\sim}{x}_k\}$ is a corresponding sequence of global minimizers, then in the

presence of a constraint qualification any limit point of $\{\underset{\sim}{x}_k\}$ solves the original problem. If $\{\underset{\sim}{x}_k\}$ is relaxed to a sequence of local minimizers, then the limit point is only claimed to satisfy the first-order necessary conditions. In practice one normally follows a path of local minimizers, but in spite of this deficiency smooth penalty methods have been highly successful [13], modulo the ill-conditioning of the Hessian, in tracking these local minima to a solution of the original problem. From this result one naturally conjectures the existence of a parametrized system of equations which contains the penalty path and which reduces to the first-order necessary conditions at $r = 0$.

Such a system is the Expanded Lagrangian System (ELS) which arises in one variant of the method as follows. Let $P(\underset{\sim}{x}, r)$ denote the penalized objective function. Then the penalty path(s) is described as the solution set of min $P(\underset{\sim}{x}, r)$ as r varies and must, by the first-order necessary conditions, be a solution of $\nabla P = 0$. Then one formally identifies the gradient of the penalty function, $\bar{\nabla} P$, with that of the Lagrangian, $\bar{\nabla}\mathcal{L}$, by identifying the multipliers. Using the definition of these multipliers as additional equations, one obtains an Expanded Lagrangian System which essentially represents a perturbation of the first-order necessary conditions of Karush-Kuhn-Tucker. Furthermore, the inequality constraints and the sign of their corresponding multipliers are satisfied, and one has an opportunity to obtain a local optimum. Thus, three of the problems associated with solving the first-order necessary conditions are resolved.

Returning to the question of ill-conditioning, we shall show that there are only three smooth penalty functions that yield well-conditioned Expanded Lagrangian Systems and each is a method of order one (see

Section 4). The canonical examples of these three classes are the quadratic penalty function for equality constraints, logarithmic barrier function (an interior method) and the quadratic loss function (an exterior method) for inequality constraints. The remaining smooth penalty functions introduce artificial singularities and ill-conditioning into the ELS. In addition, one frequently leaves equality affine constraints out of the penalized objective function as is illustrated in Section 5. There is one additional difficulty that necessitates modification of the standard penalty functions. As r tends to zero, a multiplier may tend to infinity for two basic reasons: it may not be possible to satisfy a constraint or a constraint qualification may fail. This difficulty is resolved by using a Fritz John type ELS.

The salient features of this class of algorithms can now be described easily. One first uses an unconstrained optimization technique to get on the penalty path in a region where the problem is reasonably well conditioned, say $r \simeq 10^{-1}$. Then we switch to the ELS and use pseudo-arclength predictor-solver (corrector) continuation techniques [16, 17, 25] to follow the penalty path with one of two possible objectives. We may wish to get to optimality at $r = 0$ as quickly as possible, or continue in r past zero to obtain multiple optima. The global optimization technique arises in connection with the latter objective.

In this work we concentrate on the development and trajectory analysis of the Expanded Lagrangian System since it is the key link between the use of smooth penalty functions and continuation methods. The quadratic penalty-logarithmic barrier function and the quadratic penalty-quadratic loss function are examined in Sections 2 and 3,

respectively. In Section 4 we show that smooth penalty functions other than the aforementioned three introduce singularities into the penalty path at $r = 0$ and thus ill-conditioning near $r = 0$. To further illustrate the ELS, we present examples from linear programming and the calculus of variations in Section 5, and conclude with a brief discussion of the problems and issues not treated here in Section 6.

2. The Mixed Quadratic Penalty-Logarithmic Barrier Function

In this section we derive and analyze the Expanded Lagrangian System (ELS) for the general nonlinear programming problem when the quadratic penalty function is used for the equality constraints and the logarithmic barrier function, for the inequality constraints. This ELS represents a perturbation of the Karush-Kuhn-Tucker first-order necessary conditions and we modify it to obtain a perturbation of the Fritz John conditions. This modification is necessitated by the fact that a multiplier may become unbounded as r tends to zero. In Theorem 2.2 we analyze the trajectory through $r = 0$ by giving necessary and sufficient conditions for nonsingularity of the ELS at $r = 0$. These conditions are the same as those of the nonlinear programming problem, and thus the ELS is just as well conditioned, at least for small r.

The mixed quadratic penalty-logarithmic barrier function is

$$P(\underset{\sim}{x}, r) = f(\underset{\sim}{x}) + \frac{1}{2r}\, \underset{\sim}{h}^T(\underset{\sim}{x})\underset{\sim}{h}(\underset{\sim}{x}) - r \sum_{i=1}^{p} \ln(g_i(\underset{\sim}{x})). \tag{2.1}$$

Assuming $\{\underset{\sim}{x}: \underset{\sim}{g}(\underset{\sim}{x}) > \underset{\sim}{0}\}$ to be nonempty (in general it should be robust in the sense of Luenberger [20]), the first-order necessary conditions for a minimum of P is that $\nabla_{\underset{\sim}{x}} P = 0$, which is a parametrized system of nonlinear

equations. However, the numerical problem is that the Jacobian of ∇P, the Hessian of P, becomes increasingly ill conditioned as $r \to 0^+$. In fact, the ℓ_2 condition number $K_2(\nabla^2 P) = \mathcal{O}(\frac{1}{r})$ as $r \to 0^+$. A frequently used idea in bifurcation theory is that a singularity can sometimes be removed by expanding the system, and we use this idea here to remove the ill-conditioning. Because of its importance we state this as a theorem but forego its straightforward proof.

<u>THEOREM 2.1</u>. <u>Let</u> $f: \mathbb{R}^n \to \mathbb{R}^1$, $\underset{\sim}{h}: \mathbb{R}^n \to \mathbb{R}^q$ <u>and</u> $\underset{\sim}{g}: \mathbb{R}^n \to \mathbb{R}^p$ be C^1 <u>functions. Then when</u> $r \neq 0$ <u>and</u> $g_i(\underset{\sim}{x}) \neq 0$ $(i = 1, \ldots, p)$, $(\underset{\sim}{x}, r)$ <u>solves</u>

$$0 = \nabla P := \nabla f + (D\underset{\sim}{h})^T\left[\frac{\underset{\sim}{h}}{r}\right] - \sum_{i=1}^{p} \nabla g_i\left[\frac{r}{g_i}\right] \tag{2.2}$$

<u>if and only if</u> $(\underset{\sim}{x}, \underset{\sim}{\lambda}, \underset{\sim}{\mu}, r)$ <u>solves the Expanded Lagrangian System</u>

$$\begin{aligned} 0 &= \nabla f - (D\underset{\sim}{h})^T\underset{\sim}{\lambda} - (D\underset{\sim}{g})^T\underset{\sim}{\mu} \\ 0 &= \underset{\sim}{h} + r\underset{\sim}{\lambda} \\ 0 &= \Gamma\underset{\sim}{g} - r\underset{\sim}{e}, \quad \Gamma = \mathrm{diag}(\mu_1, \ldots, \mu_p) \end{aligned} \tag{2.3}$$

<u>where</u> $\underset{\sim}{e} = (1, 1, \ldots, 1)^T \in \mathbb{R}^p$ <u>and</u> D <u>is the transpose of the gradient operator</u> ∇.

The essence of this theorem is that we have identified the gradient of the penalized objective function P, ∇P, with the gradient of the Lagrangian $\mathcal{L}$, $\nabla\mathcal{L}$, by introducing the (perturbed) multipliers $\lambda_i = h_i/r$ and $\mu_j = r/g_j$ and then adding these as equations. The use of this ELS (2.3) in an algorithm starts with the use of an unconstrained optimization technique to solve min $P(\underset{\sim}{x}, r)$ for some value of r, say r_0. Let $\underset{\sim}{x}^0$ denote the solution, and define $\lambda_i^0 = h_i(\underset{\sim}{x}^0)/r_0$ and $\mu_j^0 = r_0/g_j(\underset{\sim}{x}^0)$. Then

$(\underset{\sim}{x}^0, \underset{\sim}{\lambda}^0, \underset{\sim}{\mu}^0, r^0)$ solves (2.3) and one can continue the solution from $r = r_0$ to $r = 0$ using numerical continuation techniques.

Since equation (2.3) is just a perturbation of the Karush-Kuhn-Tucker conditions, the system is just as well conditioned as the nonlinear programming problem itself, at least for small r. This expanded system is not new, for it has been in the literature for sometime and was used by Fiacco and McCormick [4] to investigate the behavior of the penalty path near $r = 0$. Numerically, the system (2.3) has a deficiency in that a multiplier may tend to infinity when either a constraint cannot be satisfied or a constraint qualification fails with the former probably occurring more often. The modification that we now introduce avoids this problem, allows continuation past $r = 0$, and provides a homotopy into the Fritz John first-order necessary conditions.

To achieve the modification, we multiply the first equation in (2.3) through by α, rewrite $r\underset{\sim}{\lambda}$ in the second equation as $\left[\frac{r}{\alpha}\right]\alpha\underset{\sim}{\lambda}$, and multiply the third equation by α and rewrite $\alpha r\underset{\sim}{e}$ as $\alpha^2\left[\frac{r}{\alpha}\right]\underset{\sim}{e}$. Then redefine the variables $r := \frac{r}{\alpha}$, $\underset{\sim}{\lambda} := \alpha\underset{\sim}{\lambda}$, and $\underset{\sim}{\mu} := \alpha\underset{\sim}{\mu}$. The parameter α allows one to normalize the multipliers to 1, but rather than using the notation α we replace it with μ_{p+1}. With these modifications the Expanded Lagrangian System can be written as

$$
\begin{aligned}
0 &= \nabla_{\underset{\sim}{x}} \mathcal{L} \\
0 &= \underset{\sim}{h} + r\underset{\sim}{\lambda} \\
0 &= r\underset{\sim}{g} - \mu_{p+1}^2 r\underset{\sim}{e} \\
0 &= \|\underset{\sim}{\mu}\|_2^2 + \|\underset{\sim}{\lambda}\|_2^2 - 1
\end{aligned}
\tag{2.4}
$$

where $\mathcal{L} = \mu_{p+1} f - \sum_{j=1}^{q} h_j \lambda_j - \sum_{i=1}^{p} \mu_i g_i$ and $\underset{\sim}{\mu} = (\mu_1, \ldots, \mu_{p+1})^T$. Note that

if we drop the normalization and set $\mu_{p+1} = 1$, we are back to the system (2.3). Given this formulation we can now state necessary and sufficient conditions for the system (2.4) be regular at $r = 0$.

THEOREM 2.2. Let the system (2.4) be denoted by $\underset{\sim}{F}(\underset{\sim}{z}, r) = \underset{\sim}{0}$ with $\underset{\sim}{z} = (\underset{\sim}{x}^T, \underset{\sim}{\lambda}^T, \underset{\sim}{\mu}^T)^T$. Let $(\underset{\sim}{z}^0, 0)$ be a solution of $\underset{\sim}{F} = \underset{\sim}{0}$ and assume f, $\underset{\sim}{h}$ and $\underset{\sim}{g}$ are twice continuously differentiable in a neighborhood of $\underset{\sim}{x}^0$. Define two index sets $\bar{\mathcal{A}}$ and $\mathcal{A}$ and a corresponding tangent spaces $\bar{T}$ by

$$\bar{\mathcal{A}} = \{i: 1 \le i \le p,\ g_i(\underset{\sim}{x}^0) = 0\}$$

$$\mathcal{A} = \{i \in \bar{\mathcal{A}}: \mu_i^0 \ne 0\}$$

$$\bar{T} = \{\underset{\sim}{y} \in \mathbb{R}^n: D_{\underset{\sim}{x}} h_j(\underset{\sim}{x}^0)\underset{\sim}{y} = 0\ (j = 1, \ldots, q)$$

$$D_{\underset{\sim}{x}} g_i(\underset{\sim}{x}^0)\underset{\sim}{y} = 0\ (i \in \bar{\mathcal{A}})\}.$$

A necessary and sufficient condition that $D_{\underset{\sim}{z}}\underset{\sim}{F}(\underset{\sim}{z}^0, 0)$ be nonsingular is that each of the following three conditions hold:

a) $\bar{\mathcal{A}} = \mathcal{A}$;

b) $S := \left\{\{\nabla_{\underset{\sim}{x}} g_i(\underset{\sim}{x}^0)\}_{i\in\bar{\mathcal{A}}} \cup \{\nabla_{\underset{\sim}{x}} h_j(\underset{\sim}{x}^0)\}_{j=1}^q\right\}$ is a linearly independent collection of $q + |\bar{\mathcal{A}}|$ vectors where $|\bar{\mathcal{A}}|$ denotes the cardinaltiy of $\bar{\mathcal{A}}$;

c) The Hessian of the Lagrangian $\nabla^2_{\underset{\sim}{x}}\mathcal{L}$ is nonsingular on the tangent space $\bar{T}$ at $\underset{\sim}{z}^0$.

If $D_{\underset{\sim}{z}}\underset{\sim}{F}(\underset{\sim}{z}^0, 0)$ is nonsingular, there exist neighborhoods $\mathcal{B}_1$ of $r = 0$ and $\mathcal{B}_2$ of $(\underset{\sim}{z}^0, 0)$ and a function $\underset{\sim}{\phi} \in C^1(\mathcal{B}_1)$ such that $\underset{\sim}{F}(\underset{\sim}{\phi}(r), r) = 0$ for all $r \in \mathcal{B}_1$ and $\underset{\sim}{\phi}(0) = \underset{\sim}{z}^0$. This solution is locally unique in the sense that if $(\underset{\sim}{z}, r) \in \mathcal{B}_2$ and $\underset{\sim}{F}(\underset{\sim}{z}, r) = \underset{\sim}{0}$, then $\underset{\sim}{z}$ belongs to the manifold defined by $\underset{\sim}{\phi}$, i.e., $\underset{\sim}{z} = \underset{\sim}{\phi}(r)$. Furthermore, if f, $\underset{\sim}{g}$ and $\underset{\sim}{h}$ are C^k (C^∞ or real analytic) then $\underset{\sim}{\phi}$ is C^{k-1} (C^∞ or real analytic, respectively) on $\mathcal{B}_1$.

Since this theorem has been established previously [24] in a slightly different context, the proof will not be repeated here; however, several remarks are in order. If $\underset{\sim}{x}^0$ is a Fritz John or Karush-Kuhn-Tucker point, condition (a) is called strict complementarity ($g_i(\underset{\sim}{x}^0) = 0$ implies μ_i^0 is nonzero) while condition (b) is the Mangasarian-Fromowitz constraint qualification [21]. Furthermore, if conditions (a) and (b) are satisfied and condition (c) is strengthened to the Hessian of the Lagrangian being positive definite on the tangent space, then we have a second-order sufficient condition for $\underset{\sim}{x}^0$ to be a local minimum provided $\underset{\sim}{\mu}^0 \geq \underset{\sim}{0}$ and $\underset{\sim}{g} \geq \underset{\sim}{0}$.

If conditions (a), (b) and (c) are satisfied at $(\underset{\sim}{z}^0, 0)$, then $\mu_{p+1}^0 \neq 0$ and we might as well use system (2.3) computationally since it is simpler. To decide which of the two systems one should use we should start with (2.3) and if the Lagrange multipliers become large as $r \to 0^+$, then we would switch to system (2.4).

This brings us to the case in which the Jacobian $D_{\underset{\sim}{z}}\underset{\sim}{F}(\underset{\sim}{z}^0, 0)$ is singular at $r = 0$. This situation can be analyzed effectively using bifurcation and singularity theory as in, for example, the book of Golubitsky and Schaefer [11]. Note that the singularities can be classified into seven classes depending on which of the three conditions (a), (b) and (c) in Theorem 2.2 are violated. One of these cases, namely the situation in which strict complementarity is violated but the other two conditions are valid, has been examined by K. Jittorntrum and M. R. Osborne [14], under the assumption that the Hessian of the Lagrangian is positive definite on the tangent space $\bar{T}$. This problem under weaker

assumptions and the remaining cases will be treated in forthcoming work. Such an analysis is important for the determination of the expected behavior and for sensitivity analysis.

Before closing this section, we should address a major weakness of interior penalty methods: the requirement that the interior of $\{\underset{\sim}{x}: g(\underset{\sim}{x}) \geq \underset{\sim}{0}\}$ be robust and the requirement of the existence of an interior feasible point $\underset{\sim}{x}^0$ such that $g(\underset{\sim}{x}^0) > \underset{\sim}{0}$. Clearly this is not always possible. Although we investigate an exterior method in the next section as one possible solution, another is to perturb the inequality constraints by the parameter r and still use the logarithmic barrier function. As an example, suppose $g_i(\underset{\sim}{x}^0) \leq 0$ instead of $g_i(\underset{\sim}{x}^0) > 0$. Then we could modify the constraint $g_i(\underset{\sim}{x}) \geq 0$ to $g_i(\underset{\sim}{x}) - \frac{r}{r_0}(g_i(\underset{\sim}{x}^0) - 1) \geq 0$ where r_0 is an initial value of the penalty parameter r. Then we modify the corresponding penalty function from $-r \ln(g_i(\underset{\sim}{x}))$ to $-r \ln(g_i(\underset{\sim}{x}) - \frac{r}{r_0}(g_i(\underset{\sim}{x}^0)-1))$ since $g_i(\underset{\sim}{x}^0) - \frac{r_0}{r_0}(g_i(\underset{\sim}{x}^0)-1) = 1 > 0$. An unconstrained optimization technique can still be used to get on the perturbed penalty path.

3. The Quadratic Penalty-Quadratic Loss Function

In this section we will use the quadratic loss function, an exterior method, to handle the inequality constraints. Since the virtues of exterior methods have been discussed previously [4], we forego an extensive comparison of interior and exterior methods. The essence of their advantage is that an initial strictly feasible point is not required and that when many inactive inequality constraints are present, the resulting problem size is much smaller than that for an interior method.

The price to be paid for these advantages is a lack of higher-order differentiability; however, when the three conditions of Theorem 2.2 hold, the lack of second-order differentiability is only apparent as will be shown in Theorem 3.2.

The quadratic penalty-quadratic loss function used in this section is

$$P(\underset{\sim}{x}, r) = f(\underset{\sim}{x}) + \frac{1}{2r}\underset{\sim}{h}^T(\underset{\sim}{x})\underset{\sim}{h}(\underset{\sim}{x}) + \frac{1}{2r}(\underset{\sim}{g}^-(\underset{\sim}{x}))^T(\underset{\sim}{g}^-(\underset{\sim}{x})) \tag{3.1}$$

where $\underset{\sim}{g}^- = (g_1^-, \ldots, g_p^-)^T$ and $g_i^-(\underset{\sim}{x}) = \min(g_i(\underset{\sim}{x}), 0)$. A difficulty with this penalty function is that the Hessian becomes discontinuous across an inequality constraint boundary $g_i = 0$. Although this discontinuity is a simple finite jump discontinuity, the jump in $\nabla^2 P$ tends to infinity as r tends to zero, and the additional and inevitable ill-conditioning is still present in $\bar{\nabla}^2 P$. In the Expanded Lagrangian System the jump discontinuity tends to zero as r tends to zero and the ill-conditioning is removed! In the presence of a second-order sufficient condition Fiacco and McCormick [4] have shown that there is no jump for sufficiently small r. We extend this result in Theorem 3.2, but first we derive the Expanded Lagrangian System.

<u>THEOREM 3.1</u>. <u>Let the hypotheses of Theorem 2.1 be satisfied and let</u> P <u>be the penalized objective function defined by equation (3.1). Then</u> $\underset{\sim}{x}$ <u>is a minimizer of</u> P <u>provided</u>

$$0 = \nabla P := \nabla f + (D\underset{\sim}{h})^T\left[\frac{\underset{\sim}{h}}{r}\right] + (D\underset{\sim}{g})^T\left[\frac{\underset{\sim}{g}^-}{r}\right] \tag{3.2}$$

<u>where</u> $\underset{\sim}{g}^-$ <u>is defined following equation (3.1). Also,</u> $(\underset{\sim}{x}, r)$ <u>solves (3.2) for</u> $r \neq 0$ <u>if and only if</u> $(\underset{\sim}{x}, \underset{\sim}{\lambda}, \underset{\sim}{\mu}, r)$ <u>solves the Expanded Lagrangian System</u>

$$
(3.3) \qquad \begin{aligned}
0 &= \nabla \mathcal{L} \\
0 &= \underset{\sim}{h} + r\underset{\sim}{\lambda} \\
0 &= g_i + \mu_i r, \quad i \in V(\underset{\sim}{x}) \\
0 &= \mu_i, \quad i \notin V(\underset{\sim}{x})
\end{aligned}
$$

<u>where</u> $\mathcal{L} = f - \underset{\sim}{h}^T\underset{\sim}{\lambda} - \underset{\sim}{g}^T\underset{\sim}{\mu}$ <u>and</u> $V(\underset{\sim}{x}) = \{i: 1 \le i \le p,\ g_i(\underset{\sim}{x}) \le 0\}$.

We again omit the straightforward proof. The only difficulty is in the manipulation of $\underset{\sim}{g}^-$ and its derivative, but this is explained in Luenberger [20].

Since multipliers may tend to infinity we use instead the equivalent normalized problem

$$
(3.4) \qquad \underset{\sim}{G}(\underset{\sim}{x}, \underset{\sim}{\lambda}, \underset{\sim}{\mu}, r) := \begin{Bmatrix} \nabla \mathcal{L} \\ \underset{\sim}{h} + \underset{\sim}{\lambda} r \\ g_i + \mu_i r \quad (i \in V(\underset{\sim}{x})) \\ \mu_i \quad (i \notin V(\underset{\sim}{x})) \\ \sum_{j=1}^{q} \lambda_j^2 + \sum_{i=1}^{p+1} \mu_i^2 - 1 \end{Bmatrix} = 0
$$

where the Lagrangian $\mathcal{L} = \mu_{p+1} f - \sum_{j=1}^{q} h_i \lambda_j - \sum_{i=1}^{p} g_i \mu_i$. This system is derived in a fashion similar to the derivation of $\underset{\sim}{F} = \underset{\sim}{0}$ in equation (2.4), and the corresponding trajectory analysis is given as follows.

<u>THEOREM 3.2</u>. <u>Let the hypotheses of Theorem 2.2 be satisfied. Then</u> $(\underset{\sim}{z}^0, 0)$ <u>is a solution of</u> $\underset{\sim}{F} = \underset{\sim}{0}$ <u>if and only if it is a solution of</u> $\underset{\sim}{G} = 0$ <u>where</u> $\underset{\sim}{F}$ <u>is defined by equation (2.4) and</u> $\underset{\sim}{G}$ <u>by (3.4). Furthermore, given this</u> $(\underset{\sim}{z}^0, 0)$, $D_{\underset{\sim}{z}}\underset{\sim}{F}(\underset{\sim}{z}^0, 0)$ <u>is nonsingular if and only if</u> $D_{\underset{\sim}{z}}\underset{\sim}{G}(\underset{\sim}{z}^0, 0)$ <u>is</u>

nonsingular. Thus the three conditions (a), (b) and (c) in Theorem (2.2) guarantee the nonsingularity of $D_{\underset{\sim}{z}}\underset{\sim}{G}(\underset{\sim}{z}^0, 0)$.

Let $(\underset{\sim}{z}^0, 0)$ be a solution of $\underset{\sim}{G} = 0$, suppose $D_{\underset{\sim}{z}}\underset{\sim}{G}(\underset{\sim}{z}^0, 0)$ is nonsingular, and modify (3.4) by replacing $V(\underset{\sim}{x})$ by $V(\underset{\sim}{x}^0)$. The resulting modified equations, denoted by $\underset{\sim}{G}^0(\underset{\sim}{z}, r) = \underset{\sim}{0}$, have a solution $(\underset{\sim}{z}, r) = (\underset{\sim}{\Phi}(r), r)$ with the following properties: There exist neighborhoods, $\mathcal{B}_1$ of $r = 0$ and $\mathcal{B}_2$ of $(\underset{\sim}{z}^0, 0)$ such that $\underset{\sim}{\Phi} \in C^1(\mathcal{B}_1)$, $\underset{\sim}{G}^0(\underset{\sim}{\Phi}(r), r) = 0$ for all $r \in \mathcal{B}_1$ and $\underset{\sim}{\Phi}(0) = z_0$. This solution is locally unique in the sense that $(\underset{\sim}{z}, r) \in \mathcal{B}_2$ and $\underset{\sim}{G}^0(\underset{\sim}{z}, r) = 0$ implies $\underset{\sim}{z} = \underset{\sim}{\Phi}(r)$. Furthermore, if f, g and h are in C^k (C^∞ or real analytic) then $\underset{\sim}{\Phi}$ is C^{k-1} (C^∞ or real analytic).

The proof follows directly from the implicit function theorem [2] and our previous work [24] and is thus omitted. This theorem gives a smooth path through the given solution $(\underset{\sim}{z}^0, 0)$ only by fixing $V(\underset{\sim}{x}^0)$ and thus modifying $\underset{\sim}{G}$. In practice we start with a positive r so that equation (3.4) implies $\mu_i \geq 0$. If in addition $D_{\underset{\sim}{z}}\underset{\sim}{G}(\underset{\sim}{z}^0, 0)$ is nonsingular, then $\mu_i^0 > 0$ for $i \in V(\underset{\sim}{x}^0)$ and $\mu_i^0 = 0$ otherwise. Thus the eventual active inequality constraints approach from the exterior of the feasible region, which implies that the solution $(\underset{\sim}{z}, r) = (\underset{\sim}{\Phi}(r), r)$ has the stated smoothness only for $r \in (0, \infty) \cap \mathcal{B}_1$. Although the change in $V(\underset{\sim}{x})$ as r passes through zero produces a discontinuity in the path direction, the real problem is that removing one index from $V(\underset{\sim}{x}^0)$ may cause another index that ordinarily would have been removed to stay in V. Thus, it is unclear how the equations become modified as r crosses zero. If this problem could be easily resolved, continuation past $r = 0$ could be undertaken. On the other hand, one can still continue in the positive r direction in

hopes of hitting a turning point and return to $r = 0$. In this sense this method still maintains a "global-like" capability.

4. Other Penalty Functions

In this section we show that the three penalty methods described in the previous section are essentially the only smooth penalty methods that do not introduce artificial singularities and thus ill-conditioning into the penalty path for nonsingular nonlinear programming problems. Our classification of interior and exterior methods for inequality constraints and of equality penalty methods is based on the work of Lootsma [19].

We shall use the customary term barrier function instead of interior penalty function. These functions generally have the following properties [23]:

$$\text{(4.1)} \qquad \begin{aligned} &\text{(i)} \quad \phi: \mathbb{R}^+ \to \mathbb{R}, \ \lim_{u \to 0^+} \phi = +\infty, \\ &\text{(ii)} \quad \phi' < 0 \text{ and } \phi'' > 0 \text{ on } \mathbb{R}^+, \end{aligned}$$

where $\mathbb{R}^+ = (0, \infty)$. For our purposes we need a refinement of these properties and use a classification given by F. A. Lootsma [19].

<u>Definition 4.1</u>. A barrier function $\phi: \bar{\mathbb{R}}^+ \to \bar{\mathbb{R}}$ satisfying properties (i) and (ii) in equation (4.1) is said to be a barrier function of order α if ϕ' is real analytic on $\mathbb{R}^+$ and has a pole of order α at the origin.

The three most popular barrier functions are $\phi = -\ln u$ ($\alpha = 1$) due to Frisch (1955), $\phi = u^{-1}$ ($\alpha = 2$) due to Carroll (1961), and $\phi = u^{-2}$ ($\alpha = 3$) due to Kowalik (1966), Box (1969) and Fletcher and McCann (1969) [19]. The principal result is contained in

THEOREM 4.1. Let ϕ be a barrier function of order α and let f, $\underset{\sim}{g}$ and $\underset{\sim}{h}$ be C^2 functions. Then $\alpha \geq 1$ and if $\alpha > 1$, the Expanded Lagrangian System is singular at the penalty parameter value $r = 0$.

Proof: We first note that $\alpha < 1$ implies that $\lim_{u \to 0^+} \phi(u) = +\infty$ is violated. Thus we restrict ourselves to the case $\alpha \geq 1$. We consider, without loss of generality, the nonlinear programming problem $\min\{f(\underset{\sim}{x}): \underset{\sim}{g}(\underset{\sim}{x}) \geq \underset{\sim}{0}\}$, which has the penalized objective function

$$P(\underset{\sim}{x}, r) = f(\underset{\sim}{x}) + r^{\alpha} \sum_{i=1}^{p} \phi(g_i(\underset{\sim}{x}))$$

where the power of r is included so that the minimizer $\underset{\sim}{x}(r)$ will be smooth in r (Lootsma [19]). A minimizer $\underset{\sim}{x}(r)$ must satisfy

$$0 = \nabla P := \nabla f + r^{\alpha} \sum_{i=1}^{p} \phi'(g_i) \nabla g_i \tag{4.2}$$

for which the expanded system is

$$\begin{aligned} 0 &= \nabla_x \mathcal{L} \\ 0 &= \Gamma \underset{\sim}{G} + r^{\alpha} \underset{\sim}{e} \end{aligned} \tag{4.3}$$

where $\Gamma = \mathrm{diag}(\mu_1, \ldots, \mu_p)$, $\underset{\sim}{G} = \left[\frac{-1}{\phi'(g_1)}, \ldots, \frac{-1}{\phi'(g_p)}\right]^T$ and $\mathcal{L} = f - \underset{\sim}{g}^T \underset{\sim}{\mu}$. Now since ϕ has a pole of order α at the origin, $\frac{\phi''(u)}{[\phi'(u)]^2} = \sigma(u^{\alpha-1})$ as $u \to 0$. Thus $\alpha > 1$ implies $\frac{\phi''(u)}{[\phi'(u)]^2} \to 0$ as $u \to 0^+$. To complete the proof for $\alpha > 1$, it suffices to consider the case $g_i(x) \to 0$ as $r \to 0$ either smoothly or as a sequence. Now the $(n + i)^{th}$ row of the Jacobian of the expanded system (4.3) has as the only potential nonzero entries $\frac{1}{\phi'(g_i)}$ and

$\frac{-\mu_i \phi''(g_i)}{[g'(g_i)]^2} Dg_i$, both of which tend to zero as $g_i \to 0^+$. Thus, the $(n + i)^{th}$ row of the Jacobian approaches zero at $r \to 0^+$. (Notice that we could have arrived at this same conclusion by extending the definition of $\frac{\phi''}{[\phi']^2}$ to $u = 0$ by continuity.)

Q.E.D.

In case $\alpha = 1$, the quotient $\frac{\phi''(u)}{[\phi'(u)]^2}$ tends to a finite nonzero limit as $u \to 0^+$ and one can establish the nonsingularity of the Expanded Lagrangian System just as in Theorem 2.2. Of course, the canonical example from the class of barrier functions of order one is the logarithmic barrier function which was examined in Section 2.

The next class of penalty methods to be considered is the class of exterior penalty functions which we call loss functions [4]. We generally require that a loss function satisfy the properties

(iii) $\Psi(u) = 0$ for $u \geq 0$, $\Psi(u) > 0$ for $u < 0$,

(4.4) (iv) $\Psi'(u) < 0$ and $\Psi''(u) > 0$ for $u < 0$,

(v) Ψ is continuous across $u = 0$.

Following Lootsma [19], we further restrict this class of exterior methods:

<u>Definition 4.3</u>. A loss function Ψ satisfying (4.4) is said to be of order $\gamma > 0$ provided $\Psi'(u)$ is real analytic for $u < 0$ with a zero of order γ at $u = 0$, i.e., $\Psi'(u) = \sigma((-u)^\gamma)$ as $u \to 0^-$.

Given this definition we can state the principal results for exterior methods.

THEOREM 4.2. *Let* f, $\underset{\sim}{g}$, $\underset{\sim}{h}$ *be* C^2 *functions and suppose* $\Psi(u)$ *is a loss function of order* γ. *If either* $0 < \gamma < 1$ *or* $\gamma > 1$, *the corresponding Expanded Lagrangian System is singular at* $r = 0$.

Proof: It suffices again to consider the problem $\min\{f(\underset{\sim}{x}): g(\underset{\sim}{x}) \geq \underset{\sim}{0}\}$ with the corresponding penalized objective function

$$P(\underset{\sim}{x}, r) = f(\underset{\sim}{x}) + r^{-\gamma} \sum_{i=1}^{p} \Psi(g_i(\underset{\sim}{x}))$$

where Ψ is a loss function of order γ and the power γ of r is included to ensure a smooth dependence of $\underset{\sim}{x}$ on r [19]. Then a minimizer of P satisfies

$$\underset{\sim}{0} = \nabla P := \nabla f + r^{-\gamma}(D\underset{\sim}{g})^T(\Psi'(g_1), \ldots, \Psi'(g_p))^T$$

which has the Expanded Lagrangian System

$$\begin{aligned} 0 &= \nabla_x \mathcal{L} \\ 0 &= (\Psi'(g_1), \ldots, \Psi'(g_p))^T - r^{\gamma}\underset{\sim}{\mu} \end{aligned} \tag{4.5}$$

where the Lagrangian $\mathcal{L} = f - g^T\underset{\sim}{\mu}$. If $\gamma < 1$, then $\Psi'(u)$ becomes unbounded as $u \to 0^-$. Thus (4.5) is singular in that $\Psi'(u)$ becomes unbounded as $u \to 0^-$. If $\gamma > 1$, then $g_i \to 0$ as $r \to 0^+$ implies that the $(n + i)^{th}$ row of the Jacobian tends to zero so that the system (4.5) becomes singular.

Q.E.D.

For the case $\gamma = 1$, one can again prove a result similar to that obtained in Section 3 for the canonical quadratic loss function. Finally

we come to the penalty functions for equality constraints. In analogy with our two previous definitions we define penalty functions for equality constraints as follows.

<u>Definition 4.4</u>. Let $\theta: \mathbb{R} \to \mathbb{R}^+ \cup \{0\}$. We say that θ is a penalty function of order β, provided $\theta'' > 0$, $\theta' < 0$ for $u < 0$ and $\theta' > 0$ for $u > 0$, θ is analytic on $\mathbb{R} - \{0\}$ and θ' has a zero of order β at $u = 0$, i.e. $\theta = \sigma(|u|^{\beta})$ as $u \to 0$.

For this class of penalty methods, the corresponding result is contained in

<u>THEOREM 4.3</u>. <u>Let θ be a penalty function for equality constraints of order β. Then the use of θ to incorporate equality constraints into the penalized objective function yields a corresponding singular Expanded Lagrangian System if $\beta < 1$ or $\beta > 1$.</u>

We omit the proof of this theorem since it closely parallels the previous proof. If $\beta = 1$, one can prove a theorem corresponding to those in the previous two sections. The canonical order-one method is the quadratic penalty function $\theta(u) = u^2$.

In conclusion, any of the order-one methods lead to well-conditioned Expanded Lagrangian Systems, and the canonical examples of these order-one penalty functions are the quadratic penalty function for equality constraints, the logarithmic barrier function, an interior method, and the quadratic-loss function, an exterior method, for inequality constraints.

5. Application to Other Optimization Examples

The three penalty functions described in the previous sections form the basis for the derivation of the Expanded Lagrangian System (ELS). There is, however, one important variant. When equality affine constraints are present, one frequently leaves them out of the penalized objective function. In this case the first-order necessary conditions are used to derive the ELS. Although these techniques apply equally well to constrained optimization problems in the calculus of variations including variational formulations of partial differential equations, optimal control, and parameter identification, we present only two additional examples -- one from linear programming and one from the calculus of variations. The former is chosen because of the current interest in the Karmarkar algorithm [15] and the latter, because it is an infinite-dimensional problem.

In linear programming many researchers [8] have observed the apparent unsatisfactory feature that the simplex method traverses the boundary of the feasible region. From the outset attempts were made to cross the interior of the feasible region in hopes of producing a faster algorithm, but none of these attempts have succeeded, except possibly for the recently (1984) published Karmarkar algorithm [15]. This algorithm is claimed to be faster than the simplex method, and although these claims have been controversial at times, the idea of following a smooth path to optimality has always been an appealing one. A similar class of algorithms can be based on the use of the three penalty methods of the last three sections. As an example we next derive the Expanded Lagrangian

Systems for an LP problem in standard form using the logarithmic barrier function.

A standard form of the LP problem with corresponding first-order necessary conditions is

	LP Problem	Karush-Kuhn-Tucker Conditions
(5.1)	Min $\underset{\sim}{c}^T\underset{\sim}{x}$	$\underset{\sim}{c} - A^T\underset{\sim}{\lambda} - \underset{\sim}{\mu} = 0$
	s.t. $A\underset{\sim}{x} - \underset{\sim}{b} = 0$	$A\underset{\sim}{x} - \underset{\sim}{b} = 0,\ \underset{\sim}{x} \geq 0,\ \underset{\sim}{\mu} \geq 0$
	$\underset{\sim}{x} \geq \underset{\sim}{0}$	$\Gamma\underset{\sim}{x} = 0,\ \Gamma = \mathrm{diag}(\mu_1, \ldots, \mu_n)$.

If the logarithmic barrier function is used for the inequality constraints and the affine equality constraints are left out of the penalized objective function, then we have the following problem formulation and corresponding first-order necessary conditions:

	Log Barrier Formulation	Karush-Kuhn-Tucker Conditions
(5.2)	Min $c^T\underset{\sim}{x} - r\sum \ln(x_i)$	$\underset{\sim}{c} - A^T\underset{\sim}{\lambda} - \left[\frac{r}{x_1}, \ldots, \frac{r}{x_n}\right]^T = 0$
	s.t. $A\underset{\sim}{x} - \underset{\sim}{b} = \underset{\sim}{0}$	$A\underset{\sim}{x} - \underset{\sim}{b} = 0$.

From the KKT conditions we identify $\mu_i = \frac{r}{x_i}$ $(i = 1, \ldots, n)$ and expand the system to obtain the

Expanded Lagrangian System

$$\underset{\sim}{c} = A^T\underset{\sim}{\lambda} - \underset{\sim}{\mu} = 0$$

$$(5.3) \qquad A\underset{\sim}{x} - \underset{\sim}{b} = 0$$

$$\Gamma\underset{\sim}{x} - r\underset{\sim}{e} = 0,\ \Gamma = \mathrm{diag}(\mu_1, \ldots, \mu_n)$$

where $\underset{\sim}{e}$ is a vector in $\mathbb{R}^n$ containing a one (1) in each entry. We observe again that the ELS is a simple perturbation of the KKT conditions for the original problem. The normalization used for equation (2.4) is not needed here since we start the algorithm with an $\underset{\sim}{x}^0$ satisfying $A\underset{\sim}{x}^0 = \underset{\sim}{b}$ and $\underset{\sim}{x}^0 > \underset{\sim}{0}$ and a constraint qualification is not required for an LP problem.

The problem formulation 5.2 is the same as that used by Gill, Murray, Saunders, Tomlin and Wright [8] to show a formal equivalence between their projected Newton barrier method and the Karmarkar algorithm [15]. One of the deficiencies of this particular formulation is the requirement that one must first obtain an $\underset{\sim}{x}^0 > 0$ satisfying $A\underset{\sim}{x}^0 - \underset{\sim}{b} = \underset{\sim}{0}$. In some cases this requires half of the total computational effort [8], but there are techniques that can be used to alleviate this problem. One could consider using a quadratic penalty function for the equality affine constraints, the quadratic loss function for the inequality constraints, or a perturbation technique similar to that discussed at the end of Section 2. In any event, the same least squares technique used in the Karmarkar algorithm [15] and the projected Newton barrier method [8] can be used to solve the linear algebra problem that arises in the solve phase of the predictor-solver numerical continuation techniques [16, 25]. Furthermore, the use of higher-order predictors adds significantly to the speed of the method.

Finally, we consider an isoperimetric problem from the calculus of variations [7 , p. 42]. The problem is

$$(5.4) \qquad \mathrm{Min}\{J[y] := \int_a^b F(x, y, y')dx \,|\, K[y] := \int_a^b G(x, y, y')dx = \ell\}$$

where the class of admissible functions is $\{y \in C^2[a, b]: y(a) = A$ and $y(b) = B\}$. Assuming that F and G are smooth, the first-order necessary condition for the existence of a solution y is that if y is not an extremal of K[y] (a constraint qualification), then there exists a constant λ such that y is an extremal of $\int_a^b (F + \lambda G)dx$ satisfying $K[y] = \ell$, i.e.,

$$(5.5)\qquad \begin{cases} F_y - \frac{d}{dx}F_{y'} + \lambda(G_y - \frac{d}{dx}G_{y'}) = 0 \\ K[y] - \ell = 0 \\ y(a) = A,\ y(b) = B. \end{cases}$$

To derive the Expanded Lagrangian System for (5.4) we incorporate the equality constraint into a quadratic penalty function and define

$$(5.6)\qquad L[y] = J[y] + \frac{1}{2r}(K[y] - \ell)^2$$

and minimize this functional over $\{y \in \mathcal{C}^2[a, b]: y(a) = A,\ y(b) = B\}$. The first variation of L along with the definition $\lambda = (K[y] - \ell)/r$ leads to the Expanded Lagrangian System

$$(5.7)\qquad \begin{cases} F_y - \frac{d}{dx}F_{y'} + \lambda(G_y - \frac{d}{dx}G_{y'}) = 0 \\ K[y] - \ell - r\lambda = 0 \\ y(a) = A,\ y(b) = B. \end{cases}$$

Again we observe that these equations are a perturbation of the first-order necessary conditions given in (5.5).

The numerical procedure to be used starts with a discretization of (5.6) possibly using a coarse grid. Then an unconstrained code is used to minimize this discrete problem. Using the discrete version of $\lambda=(K[y]-\ell)/r$, we switch to (5.7) and use numerical continuation techniques to trace the solution to r=0. Of course, one of the advantages is that we could refine the discretization as $r \to 0^+$, say by interpolation. Furthermore, we could continue past r=0 and investigate the possibility of multiple minima by hitting limit points and returning to r = 0 on different branches of the solution curves. In practice, we again stress that λ could tend to infinity because either y is an extremal of K[y] or the constraint $K[y] = \ell$ cannot be satisfied. In this case the Fritz John

type formulation similar to that developed in Sections 2 and 3 could be used.

6. Discussion and Conclusions

One of the objectives in this work has been to re-examine the use of smooth penalty functions as an effective computational technique in light of recent developments in numerical continuation techniques. The Expanded Lagrangian System, which has been a focal point of this work, is the key link between these methods as well as the key to the removal of the ill-conditioning traditionally associated with smooth penalty methods. This parametrized system of nonlinear equations with the penalty parameter being the parameter is well conditioned only for three smooth penalty methods, each of order one as defined in Section 4. The canonical examples are the quadratic penalty function for equality constraints, logarithmic barrier function, an interior method, and the quadratic loss function, an exterior method, for inequality constraints.

Although the algorithm that makes use of the ELS has many variants, the essential features can easily be described. In the first phase one uses a linearly constrained or unconstrained optimization technique to get on the penalty path for a value of the penalty parameter where the Hessian of the penalty function is well conditioned. Rather than following the penalty path using sequential unconstrained optimization techniques, which leads to ill-conditioning, we switch to the Expanded Lagrangian System and use numerical continuation techniques. There are at least two strategies for continuing in r. The first is to continue to $r = 0$, and hopefully optimality, as quickly as possible. A second strategy is to investigate

the solution set for r varying over some range [A, B] where A < 0 < B in hopes of reaching multiple optima. This latter strategy yields a global optimization technique and is a significant additional advantage of the method.

The speed of this algorithm is highly dependent upon the unconstrained optimization techniques, the efficiency of the predictors and the linear algebra in the corrector or solve phase. To get on the penalty path initially, a quasi-Newton method using a BFGS update and an inexact line search is usually recommended for medium-size problems [3]; however, the preconditioned conjugate gradients are also popular for large-scale problems arising in optimal control, calculus of variations and parameter identification [10, 12]. Once on the penalty path the efficiency of the predictor-solve/corrector continuation technique to traverse the curve is of primary importance.

A currently popular and acceptable predictor technique is Euler's method with error and stepsize control [25]. The philosophy is to use the predictor to get within the domain of contraction of Newton's method and then iterate to convergence. This domain is reached by specifying an error in the predicted value and then choosing a stepsize to achieve this error. Generally, one can use a higher-order predictor such as an Adams-Bashforth predictor [26, 27] and obtain the same accuracy with a much larger stepsize. This efficient stepping along the curve can add significantly to the speed of the algorithm and will be investigated in a forthcoming work.

The linear algebra involved in the correction back to the curve is essentially that of Newton's method or one of its many variants [3, 10].

The use of highly accurate predictors and relatively large stepsizes considerably reduces the number of matrix decompositions. To be sure, this aspect of the problem needs extensive investigation since the most efficient methods are yet to be determined. However, for the linear programming problem of Section 5, the same least squares used by Karmarkar [15] and Gill, Murray, Saunders, Tomlin and Wright [8] can be used in the solve phase.

Once on the penalty path one continues to track a minimum unless an eigenvalue changes its sign. Such a change generically corresponds to a bifurcation of the penalty path, and the minimum may be lost or it may persist locally. Although bifurcation techniques for branch switching [16, 25] can also be used, the frequency of this bifurcation in the continuation of the penalty path from $r = 0.1$ or 0.01 to 0.0 is unclear. However, it most assuredly occurs when the continuation is over a large interval $[A, B]$.

Since in the continuation of the penalty path from $r = 10^{-1}$ to $r = 0$ the parameter r is small, a practical approach to the bifurcation problem as well as the intimately related sensitivity problem is to investigate the bifurcation behavior of the Expanded Lagrangian System for the nonlinear parametric programming problem

$$\min\{f(\underset{\sim}{x}, \underset{\sim}{\alpha}) : \underset{\sim}{h}(\underset{\sim}{x}, \underset{\sim}{\alpha}) = \underset{\sim}{0},\ \underset{\sim}{g}(\underset{\sim}{x}, \underset{\sim}{\alpha}) \geq \underset{\sim}{0}\}$$

where $\underset{\sim}{\alpha} \in \mathbb{R}^m$ is a vector of parameters in the case that the Jacobian $\underset{\sim}{D}_{\underset{\sim}{z}}\underset{\sim}{F}(\underset{\sim}{z}^0, \underset{\sim}{\alpha}^0, \underset{\sim}{0})$ is singular. Perturbed bifurcation theory [11] is a possible tool for answering this question. The behavior is important from a computational viewpoint since one would like to know the expected behavior and difficulties.

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16. Abstract

Smooth penalty functions can be combined with numerical continuation/bifurcation techniques to produce a class of robust and fast algorithms for constrained optimization problems. The key to the development of these algorithms is the Expanded Lagrangian System which is derived and analyzed in this work. This parameterized system of nonlinear equations contains the penalty path as a solution, provides a smooth homotopy into the first-order necessary conditions, and yields a global optimization technique. Furthermore, the inevitable ill-conditioning present in a sequential optimization algorithm is removed for three penalty methods: the quadratic penalty function for equality constraints, and the logarithmic barrier function (an interior method) and the quadratic loss function (an exterior method) for inequality constraints. Although these techniques apply to optimization in general and to linear and nonlinear programming, calculus of variations, optimal control and parameter identification in particular, the development is primarily within the context of nonlinear programming.

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