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A SQP BASED ON AN INTERIOR-POINT STRATEGY FOR NONLINEAR INEQUALITY CONSTRAINED OPTIMIZATION PROBLEMS

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ABSTRACT

This paper describes a sequential quadratic programming (SQP) algorithm for solving nonlinear inequality constrained optimization problems. The QP subproblems are solved by a primal-dual interior-point method that uses a variant of the Mehrotra's predictor-corrector algorithm. Preliminary numerical testing indicates that the method is effective.

Key words: SQP, interior-point method.

1. INTRODUCTION

For easy of presentation, we consider the formulation of the nonlinear problem with inequality constraints and simple bounds as follows:

where $h_k: \mathbb{R}^n \to \mathbb{R}$ for k=1,...,m and $F: \mathbb{R}^n \to \mathbb{R}$ are nonlinear and twice continuously differentiable functions. r is the vector of ranges on the constraints h(x), u and l are the vectors of upper and lower bounds on the variables respectively and b is assumed to be a finite real vector. Elements of the vectors r, l and u are real numbers subject to the following limitations: $0 \le r_k \le \infty, -\infty \le l_i, u_i \le \infty$ for k = 1, ..., m, i = 1, ..., n. Constraints of the form $b \le h(x) \le b + r$ are denoted by range constraints. The equality constraints are treated as range constraints with r = 0.

Let $\nabla F(x)$ denote the gradient of F(x) and $\nabla \overline{h}(x)$ denote the Jacobian matrix of the constraint vector $\overline{h}(x)^T = [h(x) - b, b + r - h(x), x - l, u - x]$. A solution of (1) will be denoted by x^* , and we assume that there are a finite number of solutions. We also assume that the second order Kuhn-Tucker conditions hold (with strict complementarity) at x^* . Thus, the constraints are verified and there exists a Lagrange multiplier vector $\lambda^* \geq 0$ such that

$$\nabla F(x^*) = \nabla \overline{h}(x^*)^T \lambda^*, \quad \overline{h}(x^*)^T \lambda^* = 0.$$
 (2)

Methods for solving (1) are iterative in the sense that the new approximation is given by $x_{k+1} = x_k + \overline{\alpha}_k \triangle_k$, where x_k is the current approximation, \triangle_k is the search direction and $\overline{\alpha}_k$ is a nonnegative step length $(0 < \overline{\alpha}_k \le 1)$. The central feature of a sequential quadratic programming (SQP) method is that the search direction \triangle is the solution of a

quadratic programming subproblem whose objective function approximates the Lagrangian function and whose constraints are linear approximations to the constraints in (1). The usual definition of the QP subproblem is the following:

minimize
$$\begin{array}{ll} \underset{\triangle \in \mathbb{R}^n}{\text{minimize}} & \frac{1}{2} \triangle^T H_k \triangle + \nabla F_k^T \triangle \\ \text{subject to} & b \leq \nabla h_k \triangle + h_k \leq b + r, \ l \leq \triangle + x_k \leq u \end{array}$$
 (3)

where $\nabla h(x)$ denotes the Jacobian matrix of the constraint vector h(x), and ∇F_k , h_k and ∇h_k denote the relevant quantities evaluated at x_k . The matrix H_k is a symmetric positive definite approximation to the Hessian of the Lagrangian function. This problem has a solution Δ_k and a Lagrange multiplier π_k that satisfy the constraints and

$$H_k \triangle_k + \nabla F_k = \nabla \overline{h}_k^T \pi_k, \quad \pi_k^T \left(\nabla \overline{h}_k \triangle_k + \overline{h}_k \right) = 0, \quad \pi_k \ge 0.$$

Solving QP problems with equality constraints is straightforward. However, problems that have inequality constraints are significantly more difficult to solve than problems in which all constraints are equations since it is not known in advance which inequality constraints are active at the solution. Active-set methods move sequentially from one choice of active constraints to another choice that produces at least as good a solution. Clearly the most common approach for solving (3) considers active-set methods (see, for example, Nocedal and Wright (2001)). In this paper, we describe a new SQP method that is based on the interior-point paradigm for solving the QP subproblems.

The paper is organized as follows. Section 2 describes the interior-point method used to solve the QP subproblems. Section 3 reports on the used merit function to ensure convergence and Section 4 contains the numerical results and some concluding remarks.

2. THE INTERIOR-POINT PARADIGM FOR SOLVING QP

This section describes an infeasible primal-dual interior-point method for solving the quadratic subproblem (3). We refer to Vanderbei (1994) for details. Adding slack variables w, p, q and t, (3) becomes

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\triangle^T H_k\triangle + \nabla F_k^T\triangle \\ \text{subject to} & \nabla h_k\triangle - w = b - h_k, \ \nabla h_k\triangle + p = b + r - h_k, \ \triangle - g = l - x_k, \\ & \triangle + t = u - x_k, \ w, p, g, t \geq 0. \end{array}$$

The nonnegativity constraints are then eliminated by incorporating them in logarithmic barrier terms in the objective function transforming (4) into

minimize
$$\frac{1}{2}\triangle^T H_k \triangle + \nabla F_k^T \triangle - \mu \sum_{j=1}^m \ln(w_j) - \mu \sum_{j=1}^m \ln(p_j) - \mu \sum_{i=1}^n \ln(g_i) - \mu \sum_{i=1}^n \ln(t_i)$$

subject to the same equality constraints, with μ a positive barrier parameter. Optimality conditions for this subproblem produce the standard primal-dual system

$$H_{k}\triangle + \nabla F_{k} - \nabla h_{k}^{T}y - z + s = 0, \quad WVe_{1} = \mu e_{1}, \quad \nabla h_{k}\triangle + h_{k} - b - w = 0,$$

$$y + q - v = 0, \quad PQe_{1} = \mu e_{1}, \quad r - w - p = 0,$$

$$GZe_{2} = \mu e_{2}, \quad \triangle + x_{k} - l - g = 0,$$

$$TSe_{2} = \mu e_{2}, \quad u - \triangle - x_{k} - t = 0,$$

$$(5)$$

where $V = diag(v_1,...,v_m), \ Q = diag(q_1,...,q_m), \ Z = diag(z_1,...,z_n), \ S = diag(s_1,...,s_n), \ W = diag(w_1,...,w_m), \ P = diag(p_1,...,p_m), \ G = diag(g_1,...,g_n), \ T = diag(t_1,...,t_n), \ e_1 = diag(t_1,...,t_n), \ e_$

 $(1,1,...,1)^T$ and $e_2=(1,1,...,1)^T$ are m and n vectors respectively and y=v-q. The first two equations define the conditions of dual feasibility, the next four equations are the complementarity conditions and the last four equations define the primal feasibility. This is a nonlinear system of 5n+5m equations in 5n+5m unknowns. It has a unique solution in the strict interior of an appropriate orthant in primal-dual space $\{(\triangle,g,w,t,p,y,z,v,s,q):g,w,t,p,z,v,s,q\geq 0\}$.

The central path is an arc of strictly feasible points. It is parameterized by the scalar μ , and each point on the central path solves the primal-dual system (5). As μ tends to zero, the central path converges to an optimal solution to both primal and dual problems.

For a value of μ , let $(\triangle, g, w, ..., q)$ denote the current point in the orthant. Our aim is to find $(\triangle\triangle, \triangle g, \triangle w, ..., \triangle q)$ such that the new point $(\triangle + \triangle\triangle, g + \triangle g, w + \triangle w, ..., q + \triangle q)$ lies approximately on the primal-dual central path at the point $(\triangle_{\mu}, g_{\mu}, w_{\mu}, ..., q_{\mu})$. We see that the new point $(\triangle + \triangle\triangle, g + \triangle g, w + \triangle w, ..., q + \triangle q)$, if it were to lie exactly on the central path at μ , would be defined by

$$-H_{k}\triangle\triangle + \nabla h_{k}^{T}\triangle y + \triangle z - \triangle s = H_{k}\triangle + \nabla F_{k} - \nabla h_{k}^{T}y - z + s \equiv \sigma,$$

$$-\triangle y - \triangle q + \triangle v = y + q - v \equiv \beta,$$

$$V^{-1}W\triangle v + \triangle w = \mu V^{-1}e_{1} - w - V^{-1}\triangle V\triangle w \equiv \gamma_{w},$$

$$P^{-1}Q\triangle p + \triangle q = \mu P^{-1}e_{1} - q - P^{-1}\triangle P\triangle q \equiv \gamma_{q},$$

$$G^{-1}Z\triangle g + \triangle z = \mu G^{-1}e_{2} - z - G^{-1}\triangle G\triangle z \equiv \gamma_{z},$$

$$T^{-1}S\triangle t + \triangle s = \mu T^{-1}e_{2} - s - T^{-1}\triangle T\triangle s \equiv \gamma_{s},$$

$$\nabla h_{k}\triangle\triangle - \triangle w = w + b - \nabla h_{k}\triangle - h_{k} \equiv \rho,$$

$$\triangle w + \triangle p = r - w - p \equiv \alpha,$$

$$\triangle \Delta - \triangle g = l - \triangle - x_{k} + g \equiv v,$$

$$\triangle \triangle + \triangle t = u - \triangle - x_{k} - t \equiv \tau,$$

$$(6)$$

where we have introduced notations σ , β , ρ , α , v, τ , γ_w , γ_q , γ_z , γ_s as short-hands for the right-hand side expressions. This is almost a linear system for the direction vectors ($\triangle\triangle$, $\triangle g$, $\triangle w$, ..., $\triangle q$). The only nonlinearities appear on the right-hand sides of the complementarity equations (*i.e.*, in γ_w , γ_q , γ_z , γ_s).

The algorithm implements a predictor-corrector (Mehrotra (1992)) approach to finding a good approximate solution to equations (6). First, we calculate the predictor step ($\triangle \triangle^p$, $\triangle g^p$, $\triangle w^p$, ..., $\triangle q^p$) which consists of dropping both the μ terms and the "delta" terms that appear on the right-hand side in (6).

To measure the effectiveness of this direction, we find $\overline{\alpha}^p$ to be the longest step length that can be taken along this direction before violating the nonnegative conditions $(g, w, t, p, z, v, s, q) \geq 0$, with an upper bound of 1. An explicit formula for this value, considering only the negative "delta" variables, is as follows:

$$\overline{\alpha}^{\mathbf{p}} = \min \left\{ 1, 0.95 \min \left(-\frac{w_j}{\triangle w_j^{\mathbf{p}}}, \dots, -\frac{t_i}{\triangle t_i^{\mathbf{p}}}, -\frac{v_j}{\triangle v_j^{\mathbf{p}}}, \dots, -\frac{s_j}{\triangle s_j^{\mathbf{p}}} \right) \right\}$$
 (7)

with $i \in \{1,...,n\}$ and $j \in \{1,...,m\}$. Then an estimate of an appropriate target value for μ is made using $\mu = \delta \left(\overline{z}^T \overline{g} + \overline{s}^T \overline{t} + \overline{v}^T \overline{w} + \overline{p}^T \overline{q}\right) / (2m+2n)$ with $\overline{z} = z + \overline{\alpha}^p \triangle z^p$, $\overline{g} = g + \overline{\alpha}^p \triangle g^p$, ..., $\overline{q} = q + \overline{\alpha}^p \triangle q^p$ and $\delta = \left((\overline{\alpha}^p - 1)/(\overline{\alpha}^p - 10)\right)^2$.

Then, the corrector step $(\triangle \triangle, \triangle g, \triangle w, ..., \triangle q)$ is obtained by reinstalling the μ and "delta" terms on the right-hand side in (6). This step is used to move to a new point

in primal-dual space. We calculate the maximum step $\overline{\alpha}$ that can be taken along these directions before violating the nonnegativity conditions by using a formula similar to (7). The new point is given by $\Delta = \Delta + \overline{\alpha}\Delta\Delta$, $w = w + \overline{\alpha}\Delta w$, ..., $v = v + \overline{\alpha}\Delta v$.

Solving the indefinite system: Clearly the main computational burden is to solve system (6) twice in each iteration. It is important to note that this is a large, sparse, indefinite, nonsymmetric linear system, that can be symmetrized. The symmetry of the resulting system suggests a systematic process of elimination which brings us to the so-called reduced KKT system:

$$\begin{bmatrix}
-(H_k + D) & \nabla h_k^T \\
\hline
\nabla h_k & E
\end{bmatrix}
\begin{bmatrix}
\triangle \triangle \\
\hline
\Delta y
\end{bmatrix} = \begin{bmatrix}
\sigma - ZG^{-1}\widehat{v} - ST^{-1}\widehat{\tau} \\
\rho - E(\widehat{\beta} - QP^{-1}\widehat{\alpha})
\end{bmatrix},$$

where
$$E = (VW^{-1} + QP^{-1})^{-1}$$
, $D = ZG^{-1} + ST^{-1}$, $\widehat{\beta} = \beta - VW^{-1}\gamma_w$, $\widehat{\alpha} = \alpha - PQ^{-1}\gamma_q$, $\widehat{v} = v + GZ^{-1}\gamma_z$ and $\widehat{\tau} = \tau - TS^{-1}\gamma_s$.

Once the reduced system has been solved for $\triangle \triangle$ and $\triangle y$, the other "delta" variables that were eliminated are recuperated by

$$\begin{split} \triangle w &= -E \left(\widehat{\beta} - Q P^{-1} \widehat{\alpha} + \triangle y \right), \quad \triangle t = T S^{-1} \left(\gamma_s - \triangle s \right), \\ \triangle q &= Q P^{-1} \left(\triangle w - \widehat{\alpha} \right), \qquad \qquad \triangle g = G Z^{-1} \left(\gamma_z - \triangle z \right), \\ \triangle z &= Z G^{-1} \left(\widehat{v} - \triangle \triangle \right), \qquad \qquad \triangle p = P Q^{-1} \left(\gamma_q - \triangle q \right), \\ \triangle s &= S T^{-1} \left(\triangle \triangle - \widehat{\tau} \right), \qquad \qquad \triangle v = V W^{-1} \left(\gamma_w - \triangle w \right) \end{split}$$

Implementation details: At each iteration k, to start the interior-point algorithm we need to provide initial values for all the variables. First, \triangle and y are found as solutions to the following system:

$$\left[\begin{array}{c|c} -(H_k+I) & \nabla h_k^T \\ \hline \nabla h_k & I \end{array}\right] \left[\begin{array}{c|c} \triangle_0 \\ \hline y_0 \end{array}\right] = \left[\begin{array}{c|c} \nabla F_k \\ \hline b-h_k \end{array}\right].$$

(For k = 0, we used $H_0 = \nabla^2 F(x_0)$ with guaranteed positive definiteness through a modified Cholesky decomposition.) The other variables are set as follows:

$$\begin{split} g_0 &= \max \left(abs(\triangle_0 + x_k - l), \overline{\theta} \right), \quad w_0 = \max \left(abs\left(\nabla h_k \triangle_0 + h_k - b \right), \overline{\theta} \right), \\ z_0 &= \max \left(abs(\triangle_0), \overline{\theta} \right), \qquad p_0 = \max \left(abs(r - w_0), \overline{\theta} \right), \\ t_0 &= \max \left(abs(u - \triangle_0 - x_k), \overline{\theta} \right), \qquad q_0 = \max \left(abs(y_0), \overline{\theta} \right), \\ s_0 &= \max \left(abs(\triangle_0), \overline{\theta} \right), \qquad v_0 = \max \left(abs(y_0 + q_0), \overline{\theta} \right), \end{split}$$

where max() and abs() denote componentwise maximum and absolute value, respectively. The parameter $\overline{\theta}$ is used to guarantee that all the variables constrained to be nonnegative are at least as large as $\overline{\theta}$. A solution of the quadratic subproblem is declared primal/dual feasible if the relative measures of primal and dual infeasibility are less than 10^{-4} . So, the QP subproblem has a solution (\triangle_k, π_k) with $\triangle_k = \triangle$ and $\pi_k^T = (v, q, z, s)$.

3. THE MERIT FUNCTION IN SQP

To ensure that the SQP method converges from any starting point we use a line search strategy. The chosen merit function is the augmented Lagrangian (Gill et al. (1986)), which has the form

$$\mathbb{L}\left(x,\lambda,ss;\overline{\beta}\right) = F\left(x\right) - \lambda^{T} \overline{h}(x) + \frac{\overline{\beta}}{2} \left(\overline{h}(x) - ss\right)^{T} \left(\overline{h}(x) - ss\right), \tag{8}$$

where $\overline{\beta} \geq 0$ is the penalty parameter, $\overline{h}(x)$ is the constraint vector, λ is the Lagrange multiplier vector associated to (1) and ss is a vector of slack variables that are used only in the line search procedure. The vector ss at the beginning of iteration k is taken as

$$ss_i = \left\{ \begin{array}{ll} \max(0,\,\overline{h}_i) & \text{if } \overline{\beta} = 0 \\ \max(0,\,\overline{h}_i - \lambda_i\,\big/\overline{\beta}\,) & \text{otherwise.} \end{array} \right.$$

As in Gill et al. (1986) we treat the elements of λ as additional variables so that π is used to define a "search direction", ξ , for the multiplier estimate λ , and the line search is performed with respect to both x and λ . At iteration k, a vector triple $d_k^T = (\triangle_k, \xi_k, \zeta_k)$ is computed to serve as direction of search for the variables (x_k, λ_k, ss_k) . The new values are defined by $x_{k+1} = x_k + \overline{\alpha}_k \triangle_k$, $\lambda_{k+1} = \lambda_k + \overline{\alpha}_k \xi_k$, $ss_{k+1} = ss_k + \overline{\alpha}_k \zeta_k$, and the vectors Δ_k , ξ_k and ζ_k are found from the QP subproblem (3) as described below. Thus ξ_k is defined as $\xi_k = \pi_k - \lambda_k$, so that if $\overline{\alpha}_k = 1$, $\lambda_{k+1} = \pi_k$. The vector ζ_k is then defined by $\nabla \overline{h}_k \triangle_k + \overline{h}_k = \zeta_k + ss_k$, from which we can see that $\zeta_k + ss_k$ is simply the residual of the inequality constraints from problem (3). Lemma 4.3 in Gill et al. (1986) establishes the existence of a nonnegative penalty parameter such that the direction d_k is a descent direction for the merit function (8). So, at iteration k, the penalty parameter $\overline{\beta}_k$ is defined as follows

$$\overline{\beta}_k = \begin{cases} \overline{\beta}_{k-1} & \text{if } \nabla \mathbb{L} \left(x_k, \lambda_k, s s_k; \overline{\beta}_{k-1} \right)^T d_k \leq -\frac{1}{2} \triangle_k^T H_k \triangle_k \\ \max(\widehat{\overline{\beta}}, \ 2\overline{\beta}_{k-1}) & \text{otherwise} \end{cases}$$

where $\overline{\beta}_0 = 0$ and $\widehat{\overline{\beta}}_k = 2 \|\xi_k\|_2 / (\|\overline{h}_k - ss_k\|)$ (see Lemma 4.3 in Gill et al. (1986)). Then, an Armijo type rule is used to guarantee a sufficient decrease of the merit function along the iterative process.

4. RESULTS AND CONCLUDING REMARKS

To test this SQP framework based on the primal-dual interior-point strategy we selected 32 constrained problems from Hock and Schittkowski collection (HS). The tests were done in double precision arithmetic with a Pentium 4 and Fortran 90. For a successful termination of the algorithm, the iterative sequence of x-values must converge and the final point must satisfy the first-order Kuhn-Tucker conditions (see (2)) with a 10^{-4} tolerance.

Our numerical results are reported in parts 5 and 6 of Table 1. Each of these parts contains the number of QP subproblems solved (N_{QP}) , the total number of iterations (TN_{it}) and the number of function evaluations (N_{fe}) . We exercised the algorithm using a symmetric positive definite quasi-Newton BFGS approximation to the Hessian of the Lagrangian $(H_0 = \nabla^2 F(x_0))$, with guaranteed positive definiteness) (part 6), and the modified Cholesky factorization of the Lagrangian Hessian (part 5), as H_k . Clearly, the use of the BFGS approximation to the Lagrangian Hessian gives better results than the version with the Lagrangian Hessian. The table also contains the number of iterations (N_{it}) and the number of function evaluations required by a primal-dual interior-point method (IP) to solve problem (1), in parts 3 and 4. As in our SQP framework we tested two versions. One uses the modified Lagrangian Hessian (part 3) and the other implements a quasi-Newton BFGS approximation to the Hessian (part 4). Except for 11 problems, our quasi-Newton SQP framework requires less function evaluations than the corresponding IP method. Column 2 reports the number of iterations needed by the solver SNOPT (a specific implementation of an active-set method) to solve the chosen problems as published in http://www.princeton.edu/~rvdb/cute_table.pdf.

Table 1: Results of SNOPT, IP method and our SQP(IP) method

Prob.	SNOPT	IP		IP/BFGS		SQP(IP)			SQP(IP)/BFGS		
	N_{it}	N_{it}	N_{fe}	N_{it}	N_{fe}	N_{QP}	TN_{it}	N_{fe}	N_{QP}	TN_{it}	N_{fe}
HS1	33	28	59	24	52	48	102	97	44	95	103
HS2	30	33	79	42	87	19	45	39	13	28	29
HS3	5	1	4	1	4	1	2	3	1	2	3
HS4	2	5	12	5	12	2	10	11	2	10	12
HS5	10	4	10	9	36	5	23	12	9	29	40
HS15	2	27	60	-	-	7	90	199	10	78	71
HS16	1	26	54	24	55	12	81	25	5	46	11
HS17	12	15	48	7	18	18	108	38	12	73	27
HS18	15	26	126	12	89	11	67	164	6	38	73
HS19	4	74	398	31	80	9	103	77	7	61	15
HS20	1	25	53	34	70	-	-	-	7	52	16
HS21	3	5	12	5	12	2	12	15	2	12	15
HS23	2	-	-	31	110	6	40	19	6	39	13
HS24	6	14	31	16	36	10	69	73	6	29	13
HS30	5	16	34	8	18	24	81	49	11	37	23
HS31	15	16	34	13	28	-	-	-	7	28	75
HS32	4	22	71	8	43	9	38	23	5	26	11
HS33	1	12	26	10	22	5	25	11	5	22	11
HS34	5	10	26	10	23	7	31	25	8	28	39
HS35	16	2	6	2	6	2	6	5	2	6	5
HS36	3	11	27	17	39	-	-	-	6	25	35
HS37	7	7	16	18	38	-	-	-	9	37	19
HS38	123	33	159	25	64	38	92	90	13	18	27
HS41	11	16	47	39	85	4	20	10	12	51	25
HS44	7	10	22	19	40	2	16	5	6	36	22
HS45	0	1	4	4	10	20	121	255	5	24	11
HS53	8	18	41	9	24	14	70	29	3	15	7
HS55	3	6	14	11	24	1	4	3	1	4	3
HS60	12	22	169	11	30	14	43	154	12	36	64
HS63	30	10	22	11	24	12	120	27	9	47	21
HS64	37	38	169	50	118	19	120	192	-	-	-
HS65	22	16	34	9	20	16	40	33	10	31	64

The numerical results show that our SQP framework based on a quasi-Newton primaldual interior-point method for solving the QP subproblems is effective on small dimensional problems. Future work will include testing with larger problems and possibly the implementation of limited-memory quasi-Newton approximations to H_k .

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