ACKNOWLEDGMENTS

For financial support the authors are grateful to the National Science Foundation. Part of this research was conducted while Ellen Pawlikowski held a fellowship from the Fannie and John Hertz Foundation.

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Manuscript received January 4, 1982; revision received April 26, and accepted May 13, 1982.

Improved Successive Quadratic Programming Optimization Algorithm for Engineering Design Problems

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INTRODUCTION

We present an algorithm for optimizing structured engineering processes which is computationally more efficient and conceptually cleaner than an earlier one described in Berna et al. (Bern80, 1980). The algorithm is based on sequential quadratic programming. It is a special case of a broader a class of algorithms developed by Edahl (Edah82, 1982).

THEORY

The optimization problem can be stated as follows:

$$\begin{aligned} &\min \Phi(z) \\ &s.t.\ g(z) = 0 \\ &z_{\min} \leq z \leq z_{\max} \qquad \text{(P1)} \\ &z \in E^{n+r} \\ &g: E^{n+r} \to E^n \\ &\Phi: E^{n+r} \to E^1 \end{aligned}$$

The Lagrangian of this problem is:

$$L(z,\tau,\kappa_{\min},\kappa_{\max}) = \Phi(z) - \tau^T g(z) - \kappa_{\min}^T(z_{\min} - z) + \kappa_{\max}^T(z_{\max} - z),$$

with τ the Lagrange multipliers on the equality constraints and $\kappa_{\min}$ and $\kappa_{\max}$ the Kuhn-Tucker multipliers on the lower and upper bounds of z, respectively.

The Kuhn-Tucker conditions for this problem are:

$$\kappa_{\min}[z_{\min} - z] = 0$$

$$\kappa_{\max}[z_{\max} - z] = 0$$

$$\kappa_{\min},\kappa_{\max} \leq 0$$

For a typical flowsheet calculation of the type we are considering, n may be on the order of 10,000, with r on the order of 10. This formulation is quite general as general inequality constraints can be converted to equality constraints through the use of bounded slack variables.

Powell's (Powe77, 1977) approach to solving this problem is to linearize the equality constraints, assume a quadratic approximation to the objective function, and solve the resulting QPP. Variables are then updated by taking the step

$$\Delta z = \alpha d$$

where d is the step calculated by the QPP.

The disadvantage of using Powell's method is the size of the Hessian Matrix for the QPP. For a problem with 10,000 variables, the Hessian contains 100 million elements, far too many for even the most advanced machines to handle. By partitioning the variables into two sets, the independent or decision variables, u, and the dependent or pivoted variables, x, we now show how a QPP can be set up on the decision variables only.

Let x_k and u_k be the values of the dependent and independent variables respectively at the present iteration. Linearizing the equality constraints about this point gives:

$$g(x_{k+1},u_{k+1}) \sim g(x_k,u_k) + (\partial g/\partial x^T)_k \Delta x_k + (\partial g/\partial u^T)_k \Delta u_k$$

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Setting $g(x_{k+1},u_{k+1})$ equal to 0, and requiring that $(\partial g/\partial x^T)_k$ be nonsingular yields:

$$\Delta x_k = -(\partial g \partial x^T)_k^{-1}\{g(x_k,u_k) + (\partial g/\partial u^T)_k \Delta u_k\}$$

For any choice of Δu_k, a value for Δx_k can be calculated. The problem can then be stated as one to calculate Δu_k^*, the optimal change in the decision variables:

$$\min_{\Delta u_k} F(\Delta u_k)$$

$$s.t.\ u_{\min} - u_k \le \Delta u_k \le u_{\max} - u_k$$

$$x_{\min} - x_k \le -(\partial g/\partial x^T)_k^{-1}\{g(u_k,x_k) + (\partial g/\partial u^T)_k \Delta u_k\} \le x_{\max} - x_k \quad \text{(P2)}$$

$$\Delta u_k \in E^r$$

$$x_k \in E^n$$

$$g{:}E^{n+r} \rightarrow E^n$$

where

$$F(\Delta u_k) = \Phi(x_k + \Delta x_k, u_k + \Delta u_k).$$

Expanding $F(\Delta u_k)$ in a Taylor series about the point $\Delta u_k = 0$ yields the following QPP associated with Eq. 2:

$$\min_{\Delta u_k} \{(Q(\Delta u_k)|Q(\Delta u_k) = a_k + b_k^T \Delta u_k + \tfrac{1}{2}\Delta u_k^T C_k \Delta u_k\}$$

$$s.t.\ u_{\min} - u_k \le \Delta u_k \le u_{\max} - u_k$$

$$-(\partial g/\partial x^T)_k^{-1}(\partial g/\partial u^T)_k \Delta u_k \le x_{\max} - x_k + (\partial g/\partial x^T)_k^{-1} g(x_k,u_k)\ (\partial g/\partial x^T)_k^{-1}(\partial g/\partial u^T)_k \Delta u_k \le x_k - x_{\min} - (\partial g/\partial x^T)_k^{-1} g(x_k,u_k) \quad \text{(P3)}$$

$$\Delta u_k \in E^r$$

$$x_k \in E^n$$

$$g{:}E^{n+r} \rightarrow E^n$$

The vector b is the reduced gradient $\delta\Phi/\delta u$, calculated by doing a Taylor series expansion on the objective function:

$$\Phi(x + \Delta x, u + \Delta u) = \Phi(x,u) + (\partial\Phi/\partial x^T)\Delta x + (\partial\Phi/\partial u^T)\Delta u$$

but

$$\Delta x = -(\partial g/\partial x^T)^{-1}\{g(x,u) + (\partial g/\partial u^T)\Delta u\}$$

then

$$\begin{aligned}\Delta\Phi = &-(\partial\Phi/\partial x^T)\{(\partial g/\partial x^T)^{-1}\{g(x,u) + (\partial g/\partial u^T)\Delta u\}\} + (\partial\Phi/\partial u^T)\Delta u \\ = &-(\partial\Phi/\partial x^T)((\partial g/\partial x^T)^{-1} g(x,u) + \{(\partial\Phi/\partial u^T) - (\partial\Phi/\partial x^T)((\partial g/\partial x^T)^{-1}(\partial g/\partial u^T)\}\Delta u\end{aligned}$$

The coefficient of Δu gives the constrained derivative of Φ with respect to u:

$$b_k = \delta\Phi/\delta u = (\partial\Phi/\partial u) - \{(\partial g/\partial x^T)^{-1}(\partial g/\partial u^T)\}^T(\partial\Phi/\partial x).$$

The fact that $g(x,u)$ is not 0 does not effect the term b_k. It simply adds something to the scalar a_k.
The matrix C is an approximation to the Hessian of the Lagrange Function formed from the problem:

$$\min \Phi(u,x(u))$$

$$s.t.\ u_{\min} \le u \le u_{\max}$$

$$x_{\min} \le x(u) \le x_{\max} \quad \text{(P4)}$$

$$x(u){:}g(x,u) = 0$$

$$u \in E^r$$

$$x \in E^n$$

The Lagrange of Eq. P4 is:

$$L = \Phi(u,x(u)) - \beta_{\min}^T[u_{\min} - u] + \beta_{\max}^T[u_{\max} - u] - \pi_{\min}^T[x_{\min} - x(u)] + \pi_{\max}^T[x_{\max} - x(u)].$$

C is initialized to the identity matrix and updated each iteration using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) updating formula, as suggested by Powell (Powe77, 1977).

We also follow Powell's suggestion in calculating the step-size parameter, a:

Define $\Psi(a)$ as:

$$\Psi(a) = \Phi(u^*,x^*) + \sum \mu_i |g_i(u^*,x^*)| + \sum \zeta_{i,\max}|u_{i,\max} - u_i| + \sum \zeta_{i,\min}|u_i - u_{i,\min}| + \sum \nu_{i,\max}|x_{i,\max} - x_i| + \sum \nu_{i,\min}|x_i - x_{i,\min}|$$

where

$$u^* = u_k + ad_k,$$

$$x^* = x - a(\partial g/\partial x^T)^{-1}\{g(u_k,x_k) + (\partial g/\partial u^T)_k d_k\}$$

and μ_i, $\zeta_{i,\max}$, $\zeta_{i,\min}$, $\nu_{i,\max}$, and $\nu_{i,\min}$ are defined as

$$\mu_i = \max\{|\lambda_i|, \tfrac{1}{2}(\mu_i^\bullet + |\lambda_i|)\}$$

$$\zeta_{i,\max} = \max\{|\beta_{i,\max}|, \tfrac{1}{2}(\zeta_{i,\max}^\bullet + |\beta_{i,\max}|)\}$$

$$\zeta_{i,\min} = \max\{|\beta_{i,\min}|, \tfrac{1}{2}(\zeta_{i,\min}^\bullet + |\beta_{i,\min}|)\}$$

$$\nu_{i,\max} = \max\{|\pi_{i,\max}|, \tfrac{1}{2}(\nu_{i,\max}^\bullet + |\pi_{i,\max}|)\}$$

$$\nu_{i,\min} = \max\{|\pi_{i,\min}|, \tfrac{1}{2}(\nu_{i,\min}^\bullet + |\pi_{i,\min}|)\}$$

Note that values with a • indicate the value of that parameter at the previous iteration. λ_i is the current value of the Lagrangian multiplier for the equality constraints of the original problem (Eq. P1). λ is calculated by:

$$\lambda = (\partial g/\partial x^T)^{-1}\{\pi_{\max} - \pi_{\min} - (\partial\Phi/\partial x)\}.$$

$\pi_{\max}$ and $\pi_{\min}$ are the Kuhn-Tucker multipliers associated with the inequality constraints derived from upper and lower bounds on the pivoted variables x and are calculated by the QPP associated with problem (Eq. P2). $\beta_{\max}$ and $\beta_{\min}$ are Kuhn-Tucker multipliers associated with the upper and lower bounds of the decision variables, and are also calculated by the QPP. At each iteration the value of a used is the first one found which satisfies $\Psi(a) < \Psi(0)$. Usually a is 1, except perhaps for the first iterations.

ALGORITHM

Step 0: Initialization
i) Set $k = 0$, $C_1 = I$, $\mu_o = 0$ (with $C_1 = I$, the first direction predicted is the steepest descent direction).
ii) Initialize all variables $z_1 = [x_1,u_1]$
Step 1: Compute the Jacobian and Reduced Gradient
i) Increment k
ii) Evaluate $(\partial\Phi/\partial z)$, $g(z)$ and $(\partial g/\partial z^T)$ at z_k
iii) Perform forward Gaussian elimination to partition the Jacobian and find the L/U factors for $(\partial g/\partial x^T)_k$.
iv) Perform backward substitution to solve

$$(\partial g/\partial x^T)[v_k,A_k] = [g,(\partial g/\partial u^T)]_k$$

for $[v_k,A_k]$
and solve $(\partial g^T/\partial x)\lambda_k^* = (\partial\Phi/\partial x)_k$ for λ_k^*
v) Compute the reduced gradient

$$(\delta\Phi/\delta u)_k = (\partial\Phi/\partial u)_k - A_k^T(\partial\Phi/\partial x)_k$$

vi) If $k < 2$, go to Step 3; otherwise go to Step 2.
Step 2: Update C (*a la* Powell's Suggestions)
i) $\gamma_k = (\delta\Phi/\delta u)_k - A_k[\pi_{\min} - \pi_{\max}]_{k-1} - \omega_{k-1}$
ii) Let $\eta_k = \theta\gamma_k + (1 - \theta)C_{k-1}\delta_{k-1}$
where

$$\theta = 1.\ \text{if}\ \delta_{k-1}^T C_{k-1} \delta k\text{–}1$$

Otherwise, set

$$\theta = [0.8\delta_{k-1}^T C_{k-1}\delta_{k-1}]/[\delta_{k-1}^T C_{k-1}\delta_{k-1} - \delta_{k-1}^T\gamma_k]$$

iii) Set $C_k = C_{k-1} - [C_{k-1}\delta_{k-1}\delta_{k-1}^T C_{k-1}]/[\delta_{k-1}^T C_{k-1}\delta_{k-1}] + [\eta_k\eta_k^T]/[\delta_{k-1}^T\eta_k]$

Step 3: Solve Associated *QPP*

i) Define $Q(\Delta u_k) = Q(x_k,u_k) + (\delta\Phi/\delta u^T)\Delta u_k + \frac{1}{2}\Delta u_k^T C_k \Delta u_k$

ii) Let d_k be the solution to the following *QPP:*

$$\min_{\Delta u_k} Q(\Delta u_k)$$

$$s.t. -A_k\Delta u_k \le x_{\max} - x_k + v_k$$

$$A_k\Delta u_k \le x_k - x_{\min} - v_k$$

$$u_{\min} - u_k \le \Delta u_k \le u_{\max} - u_k$$

Step 4: Compute Step Size Parameter, a_k

i) Calculate $\lambda_k = (\partial g^T/\partial x)^{-1}[\pi_{\max} - \pi_{\min}] - \lambda^*$

ii) Set $p_k = A_k d_k + v_k$

iii) Set $\mu_{ik} = \max\{|\lambda_{ik}|, \frac{1}{2}(\mu_{i(k-1)} + |\lambda_{ik}|)\}$

$$\zeta_{ik,\max} = \max\{|\beta_{ik,\max}|, \tfrac{1}{2}(\zeta_{i(k-1),\max} + |\beta_{ik,\max}|)\}$$

$$\zeta_{ik,\min} = \max\{|\beta_{ik,\min}|, \tfrac{1}{2}(\zeta_{i(k-1),\min} + |\beta_{ik,\min}|)\}$$

$$\nu_{ik,\max} = \max\{|\pi_{ik,\max}|, \tfrac{1}{2}(\nu_{i(k-1),\max} + |\pi_{ik,\max}|)\}$$

$$\nu_{ik,\min} = \max\{|\pi_{ik,\min}|, \tfrac{1}{2}(\nu_{i(k-1),\min} + |\pi_{ik,\min}|)\}$$

iv) Select $a_k \in [0,1]$ such that $\Psi(x^*,u^*,\mu_k) < \Psi(x_k,u_k,\mu_k)$ where $\Psi(x,u,\mu) = \Phi(x,u) + \mu^T|g(x,u)|$

$$+ \zeta_{\max}^T|u_{\max} - u_i| + \zeta_{\min}^T|u_i - u_{\min}|$$

$$+ \nu_{\max}^T|x_{\max} - x_i| + \nu_{\min}^T|x_i - x_{\min}|$$

$$x = x_k - aP_k$$

$$u^* = u_k + ad_k$$

v) Set $x_k = x^*$; $u_k = u^*$; $\delta_k = a_k d_k$

vi) Let $\omega_k = (\delta\Phi/\delta u)_k - A_k[\pi_{\min} - \pi_{\max}]_k$

Step 5: Check for Convergence

If $(d_k^T d_k + g_k^T g_k) < \epsilon$ then go to step 6; otherwise go to Step 1

Step 6: Stop

DISCUSSION

This algorithm differs from the Berna et al. (Bern80, 1980, algorithm and the one used is MINOS/AUGMENTED [Murtagh and Saunders (Murt80, 1980), Murtagh (Murt82, 1982)] in the way the Hessian matrix is created and used. In Berna et al. the Hessian is first created in the space of all variables, x and u, and then projected into the subspace of the decision variables, u. Actual storage of the full Hessian is avoided by storing and using the update vectors only. Storage requirements thus grow with the number of iterations of the optimization algorithm.

In MINOS/AUGMENTED the reduced Hessian is obtained by projecting a quadratic approximation to the Lagangian onto the subspace of the decision variables, u. In this algorithm we estimate the reduced Hessian directly in the subspace of the decision variables, u, accounting for the curvature of x(u) as a consequence. The algorithm differs from MINOS/AUGMENTED in other ways which are beyond the scope of this discussion.

SAMPLE PROBLEMS

In this section we present the results of two test problems solved using the algorithm described in the previous section. The algorithm has been imbedded into the ASCEND-II flowsheet system (Lock81, 1981). Modules describing these test problems were written and added to the system.

Detailed Solution of a Small Problem

We wish to solve the problem:

$$\min\{\Phi\}$$

$$s.t.\ ab + bc - 1 = 0 = g_1$$

$$\Phi - a^2 - b^2 + c = 0 = g_2$$

$$0 \le a,b,c \le 1$$

Throughout the calculations variables Φ and a were the pivoted variables, while b and c were the independent (decision) variables. Initial values were: $a = 0, b = 1, c = 1, \Phi = 0$. Also, at the start we set $\mu_0 = 0$, and $C_1 = 1$.

The starting point gives an initial Jacobian Matrix of:

	a	b	c	Φ
g_1	1	1	1	0
g_2	0	−2	1	1

With Φ and a as pivoted variables the matrix $(\partial g/\partial x^T)$ is the identity matrix.

The initial righthand-side vector (g) is [0,0], so the vector v is also [0,0], while the matrix A is calculated to be:

$$\begin{matrix} 1 & 1 \\ -2 & 1 \end{matrix}$$

The initial *QPP* is:

$$\min[2 - 1]\,\begin{matrix}\Delta b \\ \Delta c\end{matrix} + \tfrac{1}{2}[\Delta b \Delta c]\begin{matrix} 1 & 0 \\ 0 & 1\end{matrix}\,\begin{matrix}\Delta b \\ \Delta c\end{matrix}$$

$$s.t. -1 \leqslant \Delta b \leqslant 0$$

$$-1 \leqslant \Delta c \leqslant 0$$

$$\begin{matrix} -1 \leqslant \\ -\infty \end{matrix} \begin{matrix} 1 & 1 \\ -2 & 1 \end{matrix} \begin{matrix}\Delta b \\ \Delta c\end{matrix} \begin{matrix} \leqslant 0 \\ \infty \end{matrix}$$

The solution to this *QPP* is [−1,0]. The Lagrange multipliers on the original equality constraints are [0,−1]. Table 1 summarizes the search for a such that $\Psi(a) < \Psi(0)$. Using a step size of 0.25, the variable values after the first iteration are: $a = 0.25$, $b = 0.75$, $c = 1.0$, $\Phi = -0.5$.

Throughout the remaining iterations, $c = 1$ and $a = 1$. The constrained derivative for iteration 2 is: $\delta\Phi/\delta u = [-0.6667, -1.5]$ and the Hessian Matrix after the first update is:

$$\begin{matrix} 5.33 & 2. \\ 2.0 & 1.891 \end{matrix}$$

Table 2 shows the progress of the calculations to the solution.

TABLE 1. SEARCH FOR a

$\bar{a}$	Φ	$\mu^T g$	Ψ
0.0	0.0	0.0	0.0
0.25	−0.375	0.125	−0.25
0.5	−0.5	0.5	0.0
0.75	−0.375	1.125	0.75
1.0	0.0	2.0	2.0

TABLE 2. PROGRESS OF THE CALCULATIONS

Iteration	a	b	RHS	Φ
0	0.0	1.0	0.0	0.0
1	0.25	0.75	0.0988	−0.5
2	0.5417	0.6250	0.0757	−0.4170
3	0.3910	0.7101	0.0232	−0.3738
4	0.3947	0.7170	5.4E-5	−0.3301
5	0.3308	0.7498	3.9E-3	−0.3345
6	0.3780	0.7248	2.2E-3	−0.3346
7	0.3815	0.7238	9.6E-6	−0.330514
8	0.3807	0.7242	5.7E-7	−0.330501
9	0.3803	0.7245	2.1E-7	−0.330501
10	0.380278	0.724492	7.6E-13	−0.330500

Other Computational Experience

The algorithm has been applied to several flowsheeting problems. The largest contained 156 generally nonlinear equations with 161 calculated variables, leaving 5 degrees of freedom. The algorithm was able to find the optimal solution to this problem without difficulty. Typical convergence was in 10 to 20 iterations for all problems.

ACKNOWLEDGMENT

This work was partially funded by NSF Grant ECS-8026777 (Edahl) and by a grant from the Exxon Corp. (Locke and Westerberg).

NOTATION

a	= scalar term in quadratic approximation to objective function
A	= matrix $\left(\frac{\partial g}{\partial x^T}\right)^{-1}\left(\frac{\partial g}{\partial u^T}\right)$
b	= vector of coefficients for linear terms in quadratic approximation to objective function
C	= approximation to Hessian matrix in space of decision variables
d	= step calculated in QPP
$F(\Delta u_k)$	= approximation to objective function after linearizing equality constraints and eliminating pivoted variables
$g(z)$	= nonlinear equality constraints
H	= approximation to Hessian in space of all the problem variables
I	= identity matrix
k	= subscript designating interaction number
$L(\ )$	= scalar value of Lagrange function
n	= number of equality constraints and pivoted (x) variables
p	= direction of step taken when updating pivoted variables
$Q(\Delta u_k)$	= quadratic approximation to objective function in terms of decision variables
r	= number of decision variables
u	= decision variables
u^*	= updated values of decision variables
u_{MIN}, u_{MAX}	= lower and upper bounds on decision variables
v	= Newton step, $\left(\frac{\partial g}{\partial x^T}\right)^{-1} g$
x	= values of pivoted variables
x_{MIN}, x_{MAX}	= lower and upper bounds on pivoted variables
z	= problem variables
$z_{MIN} z_{MAX}$	= lower and upper bounds on problem variables

Greek Letters

α	= step size parameter
β_{MIN}, β_{MAX}	= Kuhn-Tucker multipliers on upper and lower bounds of decision variables
γ_k	= change in constraint derivative of Lagrange function associated with Eq. P4
δ	= step taken in decision variables
ϵ	= convergence tolerance
ζ_{MIN}, ζ_{MAX}	= vector quantity used in calculation of Ψ function
η	= vector used in Hessian update
θ	= scalar used in Hessian update
$\kappa_{MIN}, \kappa_{MAX}$	= Kuhn-Tucker multipliers for lower and upper bounds on z variables of Eq. P1
λ	= Lagrange multipliers on equality constraints of Eq. P1
λ^*	= contribution to λ
μ	= vector quantity used in calculation of Ψ function
ν_{MIN}, ν_{MAX}	= vector quantities used in calculation of Ψ function
π_{MIN}, π_{MAX}	= Kuhn-Tucker multipliers associated with inequality constraints of problem (Eq. P3)
τ	= vector of Lagrange multipliers on equality constraints of Eq. P1
$\Phi(z)$	= objective function
Ψ	= function used to determine step size
ω	= intermediate used in calculation of γ

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Manuscript received October 5, 1982; revision received January 31, and accepted February 9, 1983.