Reduced Hessian Successive Quadratic Programming for Realtime Optimization

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REDUCED HESSIAN SUCCESSIVE QUADRATIC PROGRAMMING FOR REALTIME OPTIMIZATION

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Abstract. **Reduced Hessian Successive Quadratic Programming (SQP) is well suited for the solution of large-scale process optimization problems with many variables and constraints but few degrees of freedom. The reduced space method involves four major steps: an *initial preprocessing phase* followed by an iterative procedure which requires the *solution of a set of nonlinear equations,* a *QP subproblem* and a *line search.* The overall performance of the algorithm depends directly on the robustness and computational efficiency of the techniques used to handle each of these sub-tasks. Here, we discuss improvements to all of these steps in order to specialize this approach to real-time optimization. A numerical comparison of reduced Hessian SQP with MINOS (Murtagh and Saunders, 1982, 1987) is provided for the optimization of the Sunoco Hydrocracker Fractionation Plant (Bailey *et* al., 1992). The case study consists of about 3000 variables and constraints and includes several scenarios related to parameter estimation and on-line process-wide optimization. A study of the effect of optimizing the DIB distillation column which constitutes a subproblem of the Sunoco example is also included. The results indicate that our algorithm is at least as robust and *an order of magnitude faster* than MINOS for this set of problems.**

Key Words. **Optimization; Large-Scale systems; Nonlinear Programming; Quadratic Programming; Computer-aided design**

1. REDUCED HESSIAN SQP

Reduced Hessian Successive Quadratic Programming (SQP) has been shown to be well suited for large-scale process optimization problems with relatively few degrees of freedom (see Vasantharajan *et* al., 1990). These problems are described by a nonlinear programming problem of the form

$$\min_{z \in \mathbb{R}^n} \quad f(z) \qquad (1)$$
$$\text{s.t.} \quad h(z) = 0$$
$$z^L \leq z \leq z^U$$

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $h : \mathbb{R}^n \rightarrow \mathbb{R}^m$. This formulation is not restrictive since inequality constraints are easily converted to equalities through the addition of slack variables. At the kth iteration, SQP methods generate a search direction d_k by solving the quadratic programming (QP) subproblem

$$\min_{z \in \mathbb{R}^n} \quad \nabla f(z_k)^T d_k + \tfrac{1}{2} d_k^T B_k d_k \qquad (2)$$
$$\text{s.t.} \quad h(z_k) + \nabla h^T(z_k) d_k = 0$$
$$z^L \leq z_k + d_k \leq z^u$$

Here, B_k denotes the Hessian of the Lagrange function or its approximation at iteration k. The reduced space SQP method results from a suitable change of basis representation applied to (2). The new basis vectors are obtained by partitioning the search space into two subspaces:

$$Z \in \mathbb{R}^{n \times (n-m)} \quad s.t. \nabla h^T(z_k) Z_k = 0 \qquad (3)$$
$$Y \in \mathbb{R}^{n \times m} \quad s.t. \ [Y \ Z] \text{ nonsingular} \qquad (4)$$

Thus, Y and Z together span the entire search space and the search direction d_k can be expressed as the sum of its components in the two subspaces

$$d_k = Y p_Y + Z p_Z \qquad (5)$$

Several reduced Hessian SQP methods, using different definitions for Y and Z have been discussed in the literature; for a comparison see Schmid and Biegler (1993a). For the purpose of this study, we divide the variables z into dependent variables $y \in \mathbb{R}^m$ with $\nabla_y h^T$ nonsingular, and independent variables $x \in \mathbb{R}^{n-m}$ and then use coordinate bases (Gabay, 1982; Locke *et* al., 1983),

$$Z = \begin{bmatrix} I \\ -\nabla_y h^{-T} \nabla_x h^T \end{bmatrix} \qquad Y = \begin{bmatrix} 0 \\ I \end{bmatrix} \qquad (6)$$

It is easily seen that the linearized equality constraints in (2) are reduced and p_Y is fully determined through the solution of a set of linear equations:

$$p_Y = -\nabla_y h^{-T} h \qquad (7)$$

Once the Y space move has been calculated, terms involving p_Y can be treated as constant and the QP subproblem (2) reduces to

$$\min_{p_Z} \quad [Z^T \nabla f + Z^T B Y p_Y]^T p_Z + \tfrac{1}{2} p_Z^T Z^T B Z p_Z \qquad (8)$$
$$\text{s.t.} \quad z^L \leq z_k + Y p_Y + Z p_Z \leq z^u$$

This reduced QP subproblem is solved in the space of the independent variables and, for most process optimization applications, (8) will be considerably smaller than (2). The second order information required for the objective function of (8) is often not available analytically, and must therefore be obtained through other means. The reduced Hessian, $Z^T BZ$, is expected to be positive definite at the solution of the NLP (1). Consequently, this matrix can be approximated by a positive definite quasi-Newton update formula such as BFGS. The other second order term, $Z^T BYp_Y$, is neglected in most reduced space SQP implementations because it is assumed that p_Y (the "Newton step") converges to zero faster than p_Z. For cases in which $Z^T BYp_Y$ is not small, Biegler *et al.* (1993) propose the inclusion of a second order correction term calculated via finite differences or a Broyden update formula.

The first order Kuhn-Tucker conditions which yield the multiplier values are given by

$$Y^T (BYp_Y + BZp_Z + \nabla h \lambda) = -Y^T \nabla f \qquad (9)$$

Since exact values of the multipliers are only required at the solution of (1), once the method has converged and $p_Y = p_Z = 0$, these multipliers can be estimated using

$$\lambda = -(Y^T \nabla h)^{-1} Y^T \nabla f \qquad (10)$$

2. SOLUTION TECHNIQUES

Having presented the mathematical framework for reduced Hessian SQP, we will now focus more closely on the individual steps of the algorithm and, in particular, the solution strategies used to handle each of these tasks.

The first step in the solution procedure is the partitioning of the variables into independent and dependent ones. For most real-time process optimization applications, this choice is straightforward since the control variables constitute a suitable set of independent variables. If, on the other hand, this selection cannot be made a priori, a number of options are available. The sparse linear equation solver MA28 provides a "rectangular option" which can be used to automatically select a consistent snhsefc of linparlv inrtanpivtant. #»nnalitv constraints and basic variables. A preprocessing step based on the solution of a linear programming problem at the initial point has the additional advantage of ensuring that the quadratic programming subproblem will be feasible (see Schmid and Biegler, 1993b).

The Y space move requires the solution of a system of linear equations according to (7) and can be calculated efficiently using any sparse linear equation solver such as MA28. In addition, the Newton step for individual units or even the entire process can also be generated using specialized solution techniques which take advantage of the mathematical structure of the model equations (see Schmid and Biegler, 1993a).

The reduced quadratic programming problem, which must be solved at every SQP iteration to obtain the search direction in the Z subspace, has the dimensionality of the number of degrees of freedom of the problem. For most process optimization applications it will therefore be quite small, as compared to the size of the full problem. To solve this subproblem efficiently, we have developed a new QP solver QPKWIK (see Schmid and Biegler, 1993b), motivated by the work of Goldfarb and Idnani (1983). This algorithm incorporates a procedure which allows us to update the inverse Cholesky factor of the reduced Hessian matrix directly; as a result, QPKWIK is $O(n^2)$ with respect to the number of variables in the QP as opposed to most existing solution procedures which require $O(n^3)$ operations. In addition, we take advantage of the fact that the quadratic program is only a subproblem of the SQP algorithm by incorporating a warm start strategy in order to improve the selection of the correct, set of active constraints. We also account explicitly for the doubly bounded nature of the inequalities in the QP resulting from the original bounds on the process variables. Finally, we have developed a strategy which allows QPKWIK to handle infeasible quadratic programmingsubproblcms properly. These result when the constraint linearizations are inconsistent and care must be taken not to violate the bounds on the variables since this could result in numerical difficulties.

Once the search direction has been determined, a line search is still required in order to guarantee sufficient progress towards the solution. Here, we use the line search method proposed by Biegler and Cuthrell (1985) which is based on an augmented line search function. It has been tested succesfully on a number of problems and exhibits global and local superlinear convergence properties.

3. PROCESS OPTIMIZATION

The first set of results provides a comparison of the reduced Hessian algorithm discussed above with MINOS 5.1, a nonlinear programming software package developed by Murtagh and Saunders (1982). The problem considered is that of determining the optimal operating conditions of the Sunoco Hydrocracker Fractionation Plant; we use the model presented by Bailey *et al.* (1992). This case study is based on an existing process and is typical of real-time optimization problems. The fractionation plant, shown in Fig. 1 is used to separate the effluent stream from a hydrocracking unit. The portion of the fractionation plant which is represented by the model is highlighted in Fig. 1; it includes the absorber, the stripper, debutanizer, C3/C4 splitter and deisobutanizer. Details on the individual units may be found in Bailey *et al.* (1992).

In addition to solving the optimization problem from the given initial point, a two-step procedure was also considered. As in Bailey *et al.* (1992), we first solve a single square parameter case in order to fit the model to an operating point. The optimization is then performed starting from the "good" initial point thus obtained. In an on-line system, the solution to the parameter case would be readily available, since it constitutes the current operating conditions. In addition to the equality constraints used to describe the process, a number of simple bounds are also included in the model. These bounds fall into three main categories:

1. Bounds representing actual physical limits (e.g. nonnegativity constraints on temperatures) are included to prevent numerical problems.
2. For the optimization cases, bounds placed on key variables prevent the solution from moving too far from the starting point. These bounds are specified so that the control system would be able to take the maximum step and bring the plant back to steady-state over a one to three hour span.
3. Upper and lower bounds which are used to fix certain variables:
   (a) Variables fixed in both the parameter and optimization case constitute variables that are not part of the optimization but are included for consistency. These include the composition and thermal conditions of the feed streams entering the absorber/stripper.
   (b) Certain variables are fixed only for the parameter case. In effect, enough variables must be fixed for each piece of equipment such that a square system results.
   (c) Finally, a number of variables are calculated during the parameter case and then fixed for the optimization. Typically, these include heat exchange coefficients, heat loss factors and catalyst activities.

The problem statistics are summarized in Table 1.

Table 1 Problem Statistics for the Hydrocracker Fractionation Plant.

		Parameter Case	Optimization Case
Variables		2891	2891
Equality constraints		2S36	2836
Jacobian elements		24123	24123
Fixed variables:	(a)	42	42
	(b)	13	0
	(c)	0	3
Independent variables		0	10

The objective function which drives the operating conditions of the plant must account for energy costs and provide a measure of the value added to the raw materials through processing. The form of the objective function used for this study is given by (11). Details on each of the four terms in this equation may be found in Bailey *et al.* (1992).

$$P = \sum_{i \in G} z_i C_i^G + \sum_{i \in E} z_i C_i^E + \sum_{m=1}^{N_P} \sum_{i \in P_m} z_i C_{P_m} - U \qquad \text{(ii)}$$

where

p	=	profit,
C^G	=	feed and product streams valued as gasoline,
C^E	=	feed and product streams valued as fuel,
C^{P_m}	=	pure component feed and products, and
u	=	utility costs.

Ill addition to the base optimization case (Case 1), the effect of heat exchanger fouling on the optimal solution was considered (Cases 2 and 3) as was the effect of changing market conditions (Cases 4 and 5). The effect of fouling is simulated by reducing the heat exchanger coefficients for the debutanizer and the splitter feed/bottoms exhangers. Changing market conditions are reflected by an increase in the price for propane (Case 4) or an increase in the base price for gasoline together with an increase in the octane credit (Case 5). The numerical values for the above parameters are included in Table 2.

All cases were solved on a DEC 5000/200 using a convergence tolerance of 10^{-8}. The results are reported in Table 2, where "infeasible initialization" indicates initialization at the original initial point while the "parameter initialization" results

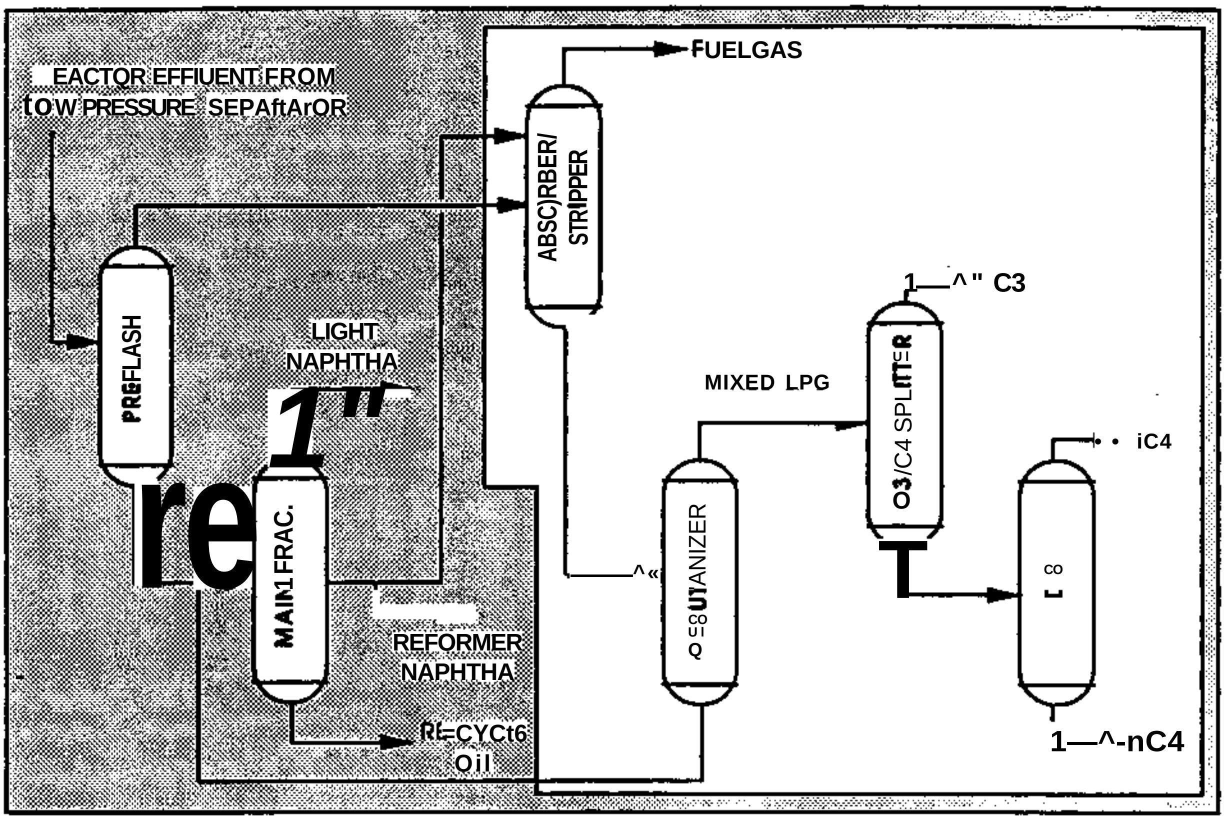

Fig. 1. Sunoco Hydrocracker Fractionation Plant.

were obtained using the solution to the parameter case as the initial point. For the optimization case, 10 of the 13 variables which are fixed only during the parameter case were used as independent variables. We also report the results obtained by Bailey *et al* (1992) using MINOS 5.1. In Table 2 their results for a VAX 6330 are converted to equivalent CPU seconds on a DEC 5000/200 using a conversion factor of 0.1518. In all cases, both our method and their MINOS cases terminated at the same optimal solution. For an interpretation of the objective function values, see Bailey *et al* (1992).

From Table 2 it is apparent that, for this problem, our algorithm is at least as robust and considerably more efficient than MINOS 5.1. Let us now consider each of the sets of results in turn. Reduced Hessian SQP was 5 times faster than MINOS as far as the parameter case is concerned. This is to be expected since, for a square system, SQP simply reduces to Newton's method for solving a set of linear equations while MINOS is unable to take advantage of the fact that the problem solution is completely determined by the constraints. Bailey *et al* (1992) report only one result for an optimization case which was initialized at the original "infeasible initialization". When this MINOS result is compared to the SQP result, there is a difference of almost two orders of magnitude. It seems that, for this problem, SQP is less sensitive to a poor initial point than MINOS. However, as mentioned earlier, the solution to the parameter case would be available in an on-line system, so it is more important to compare the "parameter initialization" results. Here, the results in Table 2 indicate an order of magnitude improvement in CPU times when comparing our algorithm to MINOS.

The second set of numerical results deals with optimization of the deisobutanizer (DIB) column; a sub-unit of the Sunoco Hydrocracker Fractionation Plant. A mixture of butane and iso-butane containing small amounts of propane and iso-pentane enters the column. Iso-butane is retrieved at the top of the column while the bottoms product is rich in butane. The model developed by Bailey *et al* (1992) includes 361 variables and 351 equality constraints, with 2211 nonzero elements in the constraint Jacobian. As for the optimization of the full plant, we solve both the parameter and optimization cases. 10 variables are fixed for the parameter case to give a square system. Two of these are freed for the optimization case; these provide a natural choice of independent variables. For the optimization case, bounds on the variables of type (1) and (2), as discussed above, are also included. Bounds such as nonnegativity of the exit flow rates are not expected to be active at the solution but are required to prevent numerical difficulties during the course of the optimization. The

Table 2 Numerical results for the Sunoco Hydrocracker Fractionation Plant problem.

	Case 0 Base Parameter	Case 1 Base Optimization	Case* 2 Fouling 1	Case 3 Fouling 2	Case 4 Changing Market 1	Case 5 Changing Market 2
Heat Exchange Coefficient (GJ/d°C)						
Debutanizer Feed/Bottoms	0.6565	0.6565	0.5000	0.2000	0.6565	0.6565
Splitter Feed/Bottoms	1.030	1.030	0.500	0.200	1.030	1.030
Pricing						
Propane ($/m³)	180	180	ISO	180	300	ISO
Gasoline Base Price ($/m³)	300	300	300	300	300	350
Octane Credit ($/(RON m³))	2.5	2.5	2.5	2.5	2.5	10
Profit	230968.96	239277.37	239*207.57	236706.82	258913.2S	370053.98
Change from base case	-	8308.41	829S.G1	5737.86	27944.32	139085.02
(«/d, %)		(3.6%)	(:uvX)	(2.5%)	(12.1%)	(60.2%)
Infeasible Initialization						
MINOS						
Iterations (Major/Minor)	5/275	9/788	-	-	-	-
CPU Time (s)	1S2	5768	-	-	-	–
SQP						
Iterations	5	20	12	24	17	12
CPU Time (s)	23.3	80.1	54.0	93.9	69.8	54.2
Parameter Initialization						
MINOS						
Iterations (Major/Minor)	n/a	12/132	14/120	16/156	11/166	11/76
CPU Time (s)	n/a	462	408	1022	916	309
SQP						
Iterations	n/a	13	8	IS	11	10
CPU Time (s)	n/a	58.8	43.8	74.4	52.5	49.7
Time SQP/ Time MINOS (%)	12.S%	12.7%	10.7%	7.3%	5.7%	16.1%

second class of bounds defines the operating limits of the system; these constraints are frequently active at the solution. Here, upper bounds on the amount of butane and iso-butane in the top and bottom exit streams respi.r lively are included so as to ensure a minimum purity of the exit streams. In addition, bounds are placed on the reflux ratio as well as the heat duties of the reboiler and condenser. These bounds reflect the range of normal operating conditions of 1 he 1)113 column and characterize the boundaries of 1 lie region for which we are confident of the validity of the model.

We first solve the param<.i« ·r case (Case 0), and the base optimization case (Case 1). We then resolve the problem with a dillerent objective function. Instead of maximizing profit, we wish to determine the maximum purity of iso-butane in the overhead product (Case 2) or of butane in the bottoms product (Case 3). given the above operating bounds. Finally, we remove the bounds on the reflux ratio and on ihe heat duties (Case 4). The results are given in Table 3 below. We indicate the profit at IIK solution as well as the mole fraction of iso-butane in the bottoms stream. In addition, we also report the value of the variables which are constrain*\\ by operating bounds and indicate which bounds become active at the solution.

Comparing the results for Case 0 and Case 1, we observe an increase of almost 50% in the profit as a results of optimizing t he operating conditions of the DM3 column. The solution is constrained by the lower bounds on the reflux ratio and the upper bound on the mole fraction of butane in the overhead stream. The results for Case 2 and Case 3 give us an upper bound on the maximum purity we can achieve, given the operating bounds on the variables. The maximum mole fraction of iso-butaue in the overhead stream is 0.927, as opposed 10 0.806 for Case 1. The maximum purity of butane is 0.849, only slightly higher than 0.84-1, 1I1.* mole fraction obtained for Case 1. In both cases, the profit is reduced. However, we have noi accounted for the possibility that the increase in purity may increase the sales price of the product. The point here was simply to determine 1 he achievable limits on purity. Finally, the results for Case 4 indicate that by removing the bounds on the reflux ratio and heat duties we are able \o almost double the profits as compared to Ca.se 1. This suggests that it may be worthwhile 10 investigate the physical effect of relaxing these bounds. In particular, the validity of the model ai these new operating conditions must be verified and certain parameters may have to be readjusted.

·1 CONCLUSION

This paper briefly presents the key steps of a reduced Hessian SQP algorithm. In addition, we summarize the solution techniques which we apply to each of the sub-tasks in order to achieve

Table 3 Numerical results for the. DIB column.

	Case 0	Case 1	Cas<; 2	Case 3	Case 4
Hclliix |{;iiio	9.05	8.00 **(LB)**	10.00 (UB)	9.66	5.40
Top Ural Duly	0.716	**0.670**	O.TIM)	0.70 (UB)	0.444
Bottom ll«\it Duty	0.734	**0.692**	U.S08	0.S12	0.465
Overhead Butane	0.019	0.05 **(UB)**	0.UIG	0.039	0.05 **(UB)**
Bottom is<>-Butane	0.053	**0.012**	0.05 **(UB)**	0.012	**0.05 (UB)**
Overlic.it 1 is.•-! kit.aue	0.924	**0.896**	0.927	0.906	0.895
Bottom 1iiiilaiic	0.820	**0.844**	O.SJ.i	0.849	0.S12
Profit (S/..I)	443.336	**663.373**	264.476	350.725	1167.011
Change in profit from	n/a	**220.037**	-178.800	-92.611	723.675
base case (*/«l, %)	n/a	**(49.63%)**	(-4O.:il(/t)	(-20.80%)	(163.23%)
SQP itoral i<»ns	5	**8**	')	12	9
CPU seconds on a DRO !'OMu/JOO	3.3	4.1	3.G	4.7	4.3

ficient for large-scale optimization. The numerical results indicate i !.ai i he algorithm is able to solve large problems wSii.ii are typical of process models. By consider; nv; <!i!!- rent initial points, we demonstrate the al i !ity of <>iir algorithm to determine the optima! solniion, oven when it is initialized relatively far from i ho solution at a point where the constraint linearizations may be inconsistent. Moreover, i !ie comparison with MINOS 5.1 for the optimi/a lion of the Sunoco Hydrocracker Fractionalio-: !Man! is very encouraging. The results indicate i i:ai I he reduced Hessian SQP algorithm is at lea-! as r.'hnst and an order of magnitude faster t! ··· M ! \<)S for this sot of problems.

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