

## Numerical Optimization at Big-Level



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### ABSTRACT:

Here we consider sequential quadratic programming methods (SQP methods) for the general optimization problem

$$\begin{array}{ll} \text{NCB} & \text{minimize } \phi(x) \\ & x \in \mathbb{R}^n \\ & \text{subject to } c(x) = 0, \quad \ell \leq x \leq u. \end{array}$$

As with the BCL and LCL approaches, SQP methods use a sequence of subproblems

to find estimates  $(x_k, y_k)$  that reduce certain augmented Lagrangians. An important function of the subproblems is to estimate which inequalities in  $\ell \leq x \leq u$  are active. Rather many iterations (called minor iterations) may be needed to solve each subproblem.

In BCL and LCL methods, the subproblem objective is the current augmented Lagrangian, which must be evaluated each minor iteration. In MINOS, for example, the Reduced-Gradient method that solves the LCL subproblems requires an average of 2 or 3 evaluations of the functions and gradients per minor iteration. This is acceptable if the function and gradient evaluations are cheap (as they are in the GAMS and AMPL environments) but may be prohibitive in other applications. For example, shape optimization in aerospace design requires the solution of a partial differential equation each time  $f(x)$  and  $c(x)$  are evaluated.

SQP methods economize by using quadratic programming (QP) subproblems to estimate the set of active constraints. Again, many minor iterations may be needed to solve the subproblems, but the functions and gradients are not being evaluated during that process.

## An NPSOL Application

NPSOL [9] is a successful "dense" SQP implementation. It has found wide use within the NAG Library and has proved remarkably robust and efficient on highly nonlinear optimization problems, particularly within the aerospace industry.

For interest, the largest application we know of was a trajectory optimization at McDonnell Douglas Space Systems involving about 2000 variables and constraints, computing controls for the last breath-taking seconds of flight of the DC-Y, a proposed SSTO (Single-Stage-To-Orbit) manned spacecraft. The aim was to minimize the fuel needed as the rocket, descending nose-first to Earth, rotated from an altitude of 2800 feet just in time to land on its tail. NPSOL's solution showed that the landing maneuver could be accomplished using half the fuel estimated by classical techniques.

A second optimization was used to determine when the rotation should begin. With an extra constraint limiting acceleration to 3g (since a human crew would be aboard), the optimal rotation altitude proved to be only 1400 feet|the height of the Empire State Building. Such touchdowns would be far more abrupt and astonishing than the Apollo moon landings. (More like the Lunar Excursion Module's take-off from the moon played in reverse!)

## Quadratic Approximations in a Subspace

Linearized constraints are a key component of SQP methods, just as they are for LCL methods. They define a subspace in which it is reasonable to form a quadratic approximation to the augmented Lagrangian. Let  $(x_k, y_k)$  be the current solution estimate and  $\rho_k$  be the current penalty parameter. Also define  $J_k \equiv J(x_k)$ . The following functions are needed:

Linear approximation to  $c(x)$ :  $\bar{c}_k(x) = c(x_k) + J_k(x - x_k)$ .

Departure from linearity:  $d_k(x) = c(x) - \bar{c}_k(x)$ .

Modified augmented Lagrangian:

$$\begin{aligned} M_k(x) &= \phi(x) - y_k^T d_k(x) + \rho_k \|d_k(x)\|^2, \\ \nabla M_k(x) &= g_0(x) - (J(x) - J_k)^T \tilde{y}_k(x), \\ \nabla^2 M_k(x) &= H_0(x) - \sum_i (\tilde{y}_k(x))_i H_i(x) + \rho_k (J(x) - J_k)^T (J(x) - J_k), \\ \tilde{y}_k(x) &\equiv y_k - \rho_k d_k(x). \end{aligned}$$

The last four expressions simplify greatly when  $x = x_k$ . In particular,  $d_k(x_k) = 0$ ,  $\tilde{y}_k(x_k) = y_k$ , and terms involving  $J(x)$  and  $\rho_k$  vanish:

$$\begin{aligned} M_k(x_k) &= \phi(x_k), \\ \nabla M_k(x_k) &= g_0(x_k), \\ \nabla^2 M_k(x_k) &= H_0(x_k) - \sum_i (y_k)_i H_i(x_k). \end{aligned}$$

With  $\Delta x \equiv x - x_k$ , the quadratic approximation to  $M_k(x)$  at  $x_k$  on the subspace  $\bar{c}_k(x) = 0$  is therefore

$$Q_k(x) = \phi(x_k) + g_0(x_k)^T \Delta x + \frac{1}{2} \Delta x^T \nabla^2 M_k(x_k) \Delta x,$$

where the quadratic term may or may not be available.

## NPSOL

Recall that the MINOS subproblem takes the form

$$\begin{array}{ll} \text{LC}_k & \text{minimize}_{x \in \mathbb{R}^n} \quad M_k(x) = \phi(x) - y_k^T d_k(x) + \frac{1}{2} \rho_k \|d_k(x)\|^2 \\ & \text{subject to} \quad \bar{c}_k(x) = 0, \quad \ell \leq x \leq u. \end{array}$$

The stabilized LCL method adapts early subproblems judiciously to ensure global convergence, but ultimately the subproblems become  $\text{LC}_k$  and their solutions  $(x_k^*, y_k^*)$  converge rapidly, as predicted by Robinson (1972).

The SQP methods in NPSOL and SNOPT are based on the same subproblem, but with the objective  $M_k(x)$  replaced by a quadratic approximation  $Q_k(x)$ :

$$\begin{array}{ll} \text{QP}_k & \text{minimize}_{x \in \mathbb{R}^n} \quad Q_k(x) = \phi(x_k) + g_0(x_k)^T \Delta x + \frac{1}{2} \Delta x^T H_k \Delta x \\ & \text{subject to} \quad \bar{c}_k(x) = 0, \quad \ell \leq x \leq u, \end{array}$$

where  $H_k$  is a quasi-Newton approximation to  $\nabla^2 M_k(x)$ . To achieve global convergence,  $\text{QP}_k$  is regarded as providing a search direction  $(\Delta x, \Delta y)$  along which the augmented Lagrangian may be reduced (as a function of both primal and dual variables).

Note that the true Hessian of  $M_k(x)$  is zero in rows and columns associated with linear variables. In NPSOL, slack variables are therefore excluded from  $H_k$ , and in SNOPT both slacks and other linear variables in  $x$  are excluded. The quasi-Newton Hessian approximations are therefore of the form,

$$H_k = \begin{pmatrix} \bar{H}_k & \\ & 0 \end{pmatrix},$$

where  $\bar{H}_k$  is positive definite. The positive-definiteness provides an intrinsic bound on the relevant parts of  $\Delta x$ , improving the validity of the quadratic model.

### NPSOL's Merit Function

Let  $(x_k^*, y_k^*)$  be the primal and dual solution to  $QP_k$ . NPSOL forms the search direction

$$\begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \begin{pmatrix} x_k^* - x_k \\ y_k^* - y_k \end{pmatrix}$$

and seeks a steplength  $\alpha$  such that moving to the point  $(x_k + \alpha\Delta x, y_k + \alpha\Delta y)$  (where  $0 < \alpha \leq 1$ ) produces a sufficient decrease in the augmented Lagrangian

$$L(x, y, \rho_k) = \phi(x) - y^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2.$$

Initially  $\rho_k = 0$ . Later,  $\rho_k$  is increased if necessary to ensure descent for the merit function. It may also be decreased a limited number of times, because a finite (unknown) value is always adequate for well defined problems, and because  $\rho_k = 0$  becomes acceptable within some neighborhood of a solution to NCB.

The global convergence properties of NPSOL's linesearch strategy are described in [11]. The QP subproblems are assumed to be feasible (and to be solved accurately).

## Hessian Updates

A dense triangular factorization  $H_k = R_k^T R_k$  is maintained in NPSOL. After the linesearch, a BFGS update of the form

$$R_{k+1} = Q_k R_k (I + r_k s_k^T), \quad Q_k \text{ orthogonal}$$

is made to improve the quality of the Hessian approximation within some space. Various choices are possible for the vectors  $r_k$  and  $s_k$ . They reflect the change in  $x$  and the change in gradient of some modified Lagrangian  $M_k(x, y_{k+1}, \rho_{k+1})$  defined

with the latest estimate of  $y$  (but  $\rho_{k+1} = 0$  where possible).

## LSSOL

NPSOL uses the least-squares solver LSSOL [5] for the subproblems  $QP_k$ . LSSOL deals directly with the triangular factor  $R_k$ . It is virtually unique in avoiding the squared condition number that most solvers would fall prey to with Hessians of the form  $R_k^T R_k$ .

## SNOPT

The reliability of NPSOL and LSSOL allowed them to be applied to increasingly large problems (particularly at McDonnell Douglas). However, LSSOL uses orthogonal transformations of  $J(x_k)$  to solve the QP subproblems, and as problem size increases the total cost becomes dominated by the associated linear algebra.

To a large extent, SNOPT is a sparse SQP implementation that combines the virtues of MINOS and NPSOL. Sparse Jacobians are handled as in the Reduced-Gradient method (using LUSOL to maintain a sparse basis factorization), and the same merit function as in NPSOL ensures global convergence.

The primary innovation is a method for treating the QP Hessian in sparse form. Also, infeasible problems NCB are dealt with more methodically by including an  $\ell_1$  penalty term within the problem definition (where  $e$  is a vector of ones):

### The QP Subproblem

The SNOPT subproblems include the  $\ell_1$  penalty terms verbatim:



$$\begin{aligned} \text{QP}_k(\gamma) \quad & \underset{x, v, w}{\text{minimize}} \quad \phi(x_k) + g_0(x_k)^T \Delta x + \frac{1}{2} \Delta x^T H_k \Delta x + \gamma e^T (v + w) \\ & \text{subject to} \quad \bar{c}_k(x) + v - w = 0, \quad \ell \leq x \leq u, \quad v, w \geq 0. \end{aligned}$$

Initially  $\gamma = 0$ , but it is set to  $\gamma_k \equiv 10^4(1 + \|g_0(x_k)\|)$  if  $\text{QP}_k(0)$  proves to be infeasible or if the norm of the dual variables for  $\text{QP}_k(0)$  becomes larger than  $\gamma_k$ .

Optimization continues with that value of  $\gamma$  until an optimal solution of  $\text{NCB}()$  has been obtained. If the nonlinear constraints are not satisfied ( $c(x) \neq 0$ ),  $\gamma$  is increased and optimization continues. If  $\gamma$  reaches an allowable maximum value and the nonlinear constraints are still violated, the problem is declared infeasible. At this stage, SNOPT has essentially minimized  $\|c(x)\|_1$ .

## SQOPT

SNOPT includes a sparse QP solver, SQOPT, which employs a two-phase active set algorithm to achieve feasibility and optimality. SQOPT implements elastic programming implicitly. Any specified bounds on the variables or constraints may be elastic. The associated variables or slacks are given a piecewise linear objective function that penalizes values outside the "real" bounds.

If  $\gamma > 0$  in  $\text{NCB}(\gamma)$  (perhaps because previous QP subproblems were infeasible), SNOPT defines elastic bounds on the slacks associated with linearized nonlinear constraints. SQOPT then solves each  $\text{QP}_k(\gamma)$  with  $v$  and  $w$  implemented implicitly.

Separately, SNOPT can use SQOPT to find a point close to a user-provided starting point  $x_0$ . One option is to set  $\ell_j = u_j = (x_0)_j$  for the nonlinear variables and specify that those bounds are elastic. (Linear variables retain their true bounds.) SQOPT will then solve the "proximal point problem"

PP1	$\begin{aligned} &\underset{x \in \mathbb{R}^n}{\text{minimize}} && \ x - x_0\ _1 \\ &\text{subject to} && \text{the linear constraints and (modified) bounds.} \end{aligned}$
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Similarly, SNOPT's PP2 option asks SQOPT to minimize  $\frac{1}{2}\|x - x_0\|_2^2$  subject to the linear constraints and true bounds. Further details about SNOPT and SQOPT are given in [6, 7, 8].

## Limited-Memory Hessian Updates

For moderate-sized problems, SNOPT maintains a dense Hessian approximation similar to that in NPSOL. For large problems with thousands of nonlinear variables, a limited-memory procedure is used to represent  $H_k$ .

At certain iterations  $k = r$ , say, a positive-definite diagonal estimate  $H_r = R_r^2$  is used. In particular,  $R_0$  is a multiple of the identity. Up to  $\ell$  quasi-Newton updates (default  $\ell = 10$ ) are accumulated to represent the Hessian as

$$H_k = R_k^T R_k, \quad R_k = R_r \prod_{j=r}^{k-1} (I + r_j s_j^T)$$

SQOPT accesses  $H_k$  by requesting products of the form  $H_k v$ . The work and storage required grows linearly with  $k-r$ . When  $k = r + \ell$ , the diagonals of  $R_k$  are computed and saved to form the next  $R_r$ . Storage is then "reset" by discarding the vectors  $\{r_j, s_j\}$ .

More elaborate limited-memory methods are known; notably [13, 2]. The simple form above has an advantage for problems with purely linear constraints: the reduced Hessian required by the Reduced-Gradient implementation in SQOPT can be updated between major iterations. This is important on large problems with many superbasic variables. As the SQP iterations converge, very few minor iterations are needed to solve  $QP_k$  and the cost becomes dominated by the formation of  $Z^T H_k Z$  and its factors, but when the constraints are linear, this expense is avoided. (The LU factors of the basis can also be retained.)

Recently, the thesis research of Andrew Bradley [1] has led to a new limited-memory quasi-Newton implementation for SNOPT7 and SNOPT8. A circular buffer is used to hold the latest pairs of update vectors  $\{s_j, y_j\}$  (recording the recent changes in  $x$  and the gradient of the

Lagrangian), and the initial diagonal Hessian approximation  $H_0$  is continually updated. The resulting LMCBD procedure (limited-memory circular buffer with diagonal update) produces a robust Hessian approximation that on average outperforms SNOPT's current limited-memory implementation.

## Quasi-Newton and CG

To avoid forming and factorizing the reduced Hessian in all cases, a quasi-Newton version of SQOPT has been implemented. It maintains  $R^T R \approx Z^T H_k Z$  analogous to the RG method in MINOS.

A further option is to use the Conjugate-Gradient method to solve the reduced-Hessian system  $Z^T H_k Z \Delta x_s = -Z^T g$ . This seems to converge in remarkably few iterations even when there are many thousands of superbasic variables. The "diagonal plus low-rank" structure of  $H_k$  plus the large identity matrix in  $Z$  must be largely responsible, but it would be easier to explain if the diagonal part  $H_r = R_r^2$  were always the identity.

## Future QP Solvers

Hanh Huynh's thesis research [12] includes the development of a convex QP solver QPBLU that periodically factorizes the current KKT matrix

$$K_0 = \begin{pmatrix} H_0 & W^T \\ W & \end{pmatrix}, \quad H_0 \text{ diagonal}$$

and uses block-LU updates to accommodate 50 or 100 active-set changes to  $W$  as well as BFGS updates to  $H_0$ . The aim is to handle many degrees of freedom with a direct method rather than the CG option above (allowing  $W$  to be large with many more columns than rows).

QPBLU is implemented in Fortran 95 and is designed to use any available sparse solver to factorize the current  $K_0$ . Currently it includes interfaces to LUSOL [10], MA57 [4], PARDISO [15], SuperLU [3], and UMFPACK [16]. Such solvers are assumed to give a factorization  $K_0 = LU$  and to permit separate solves with  $L$ ,  $L^T$ ,  $U$ ,

and  $U^T$ . For example, MA57's symmetric factorization  $K_0 = LDL^T$  is regarded as

$K_0 = L(DL^T)$ . At the time, PARDISO did not separate its factors, so QPBLU uses " $L$ " =  $I$  and " $U$ " =  $K_0$ .

This work has been continued by Chris Maes for his thesis research [14]. A new QP solver QPBLUR has been developed, with modules from QPBLU serving as a valuable starting point. QPBLUR uses a BCL method to solve a sequence of regularized convex QP subproblems (in order to solve the given convex QP). It has been incorporated into SNOPT7 as an alternative to SQOPT.

QPBLUR's block-LU updates are the main hope for making use of the most advanced (possibly parallel) linear system solvers within an active-set QP solver and hence within an SQP algorithm. In May 2010, Chris installed a more recent version of PARDISO that allows separate solves with L and U and optionally uses multiple CPUs during its Factor phase.

SNOPT will continue to use SQOPT while the number of superbasic variables remains below 2000 (say), then switch to QPBLUR if necessary. With its warm-start capability, QPBLUR will bridge the gap between null-space active-set methods and full-space interior methods.

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