INDEFINITE TRUST REGION SUBPROBLEMS AND NONSYMMETRIC EIGENVALUE PERTURBATIONS

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Abstract

This paper extends the theory of trust region subproblems in two ways: (i) it allows indefinite inner products in the quadratic constraint and (ii) it uses a two sided (upper and lower bound) quadratic constraint. Characterizations of optimality are presented, which have no

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gap between necessity and sufficiency. Conditions for the existence of solutions are given in terms of the definiteness of a matrix pencil. A simple dual program is introduced which involves the maximization of a strictly concave function on an interval. This dual program simplifies the theory and algorithms for trust region subproblems. It also illustrates that the trust region subproblems are implicit convex programming problems, and thus explains why they are so tractable.

The duality theory also provides connections to eigenvalue perturbation theory. Trust region subproblems with zero linear term in the objective function correspond to eigenvalue problems, and adding a linear term in the objective function is seen to correspond to a perturbed eigenvalue problem. Some eigenvalue interlacing results are presented.

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1 INTRODUCTION

Calculation of the step between iterates in "trust region" numerical methods for minimization problems, involves the minimization of a quadratic objective function subject to a norm constraint. This trust region subproblem is

$$(\tilde{P}) \qquad \begin{array}{lll} \min & \mu(y) := & y^t B y - 2\psi^t y \\ \text{subject to} & Ay = & b \\ & y^t D y \leq & \delta,\ y \in \Re^n, \end{array}$$

where: $\psi \in \Re^n$; $B \in \Re^{n \times n}$ is symmetric; A is $m \times n$; $b \in \Re^m$; D is a positive definite scaling matrix; and $\delta > 0$ is the trust region radius. The objective function μ provides a quadratic model of a merit function, while the linear constraint $Ay = b$ is a linear model of possibly nonlinear constraints. Note that the trust region quadratic constraint has the implicit, or hidden, constraint $0 \leq y^t D y$; while a positive δ yields the standard generalized Slater constraint qualification of convex programming.

By representing the linear constraint $Ay = b$ as $y = \hat{y} + Zw$, where the range of Z is equal to the null space of A, and $\hat{y}$ is a particular solution of $Ay = b$, we can eliminate this linear constraint. Moreover, we can also eliminate the scaling matrix D and use complementary slackness to get the simplified problem:

$$(\tilde{P}_E) \qquad \begin{array}{lll} \min & \mu(y) := & y^t B y - 2\psi^t y \\ \text{subject to} & y^t y = & 1,\ y \in \Re^n. \end{array}$$

Trust region problems have proven to be very successful and important in both unconstrained and constrained optimization. The theory, algorithms and applications have been described in many papers and textbooks, see e.g. [3, 9, 6, 10, 19, 20, 24, 25, 12, 11, 27]. A well known algorithm, for numerically approximating a global minimum, is given in e.g. [21]. Other numerical algorithms are presented in [12, 14, 11]. Recently, the trust region subproblem, with the additional linear constraint $Ax = b$, has been employed as the basic step in the affine scaling variation of interior point methods for solving linear programming problems, see e.g. [7, 2, 29]. Affine scaling methods for general quadratic programming problems, which solve a trust region subproblem at each step, are given in e.g. [15]. In addition, many continuous relaxations of discrete optimization problems result in norm constraints and therefore trust region subproblems arise, see e.g. [18] for a survey.

Generalizations of $(\tilde{P})$ are also important. Subproblems with two trust region constraints appear in sequential quadratic programming (SQP) algo-

rithms, see e.g. [4, 33, 31]. In [31], an algorithm is presented that treats the two trust region problem by restricting it to two dimensions. More recently, [34] treated the two trust region problem using a parametric approach and assuming positive definiteness of the objective function. (In both [33, 34], the condition that $B - \lambda C$ is positive definite for some λ, where C is the Hessian for the second trust region constraint, is very important. This condition is studied here for the indefinite case and shown to be equally important.) Moreover, it is often useful to consider modelling the general nonlinear programming problem using quadratic approximations for both the objective function as well as for the constraints, see e.g. [5, 22]. Such problems have up to now been considered too difficult to solve without further modelling using linear approximations for the constraints. One reason for this is that the quadratic approximations can result in indefinite Hessians for the objective function as well as for the constraints, resulting in possible unboundedness and infeasibility problems.

The success of trust region methods depends in part on the fact that one can characterize, and hence numerically approximate, the global minimum of the subproblem $(\tilde{P})$. The characterization, which has no gap between necessity and sufficiency, is independent of any convexity assumptions on the quadratic function μ; that is, B can be indefinite. The choice of the scaling matrix D can be very important. It is currently restricted to be positive definite in order to maintain tractability of the subproblem, but it would be advantageous and important to allow a larger class of matrices in order to obtain scale invariance; see e.g. p. 59 in [9]. Of more interest and importance is the fact that the feasible set $\{y : y^t y = 1\}$ being nonconvex does not present a problem in the characterization of optimality. Note that we can add $k(y^t y - 1)$, $k > 0$, to the objective function without changing the optimum. Thus if k is large, then the objective function becomes convex. This means that we can assume that the objective function is convex if desired. However, this is no longer true if the constraint $y^t y = 1$ is changed to an indefinite constraint.

In case $\psi = 0$ (no linear term) the stationary points of the trust region subproblem correspond to the eigenvalues of B. In [26], the authors related stationarity properties of $(\tilde{P})$ to spectral properties of the parametric border perturbation of B given by

$$A(t) = \begin{pmatrix} B & -\psi \\ \psi^t & t \end{pmatrix}. \tag{1.1}$$

Hence, the above perturbation of B has, as an analog, the perturbation

of the purely quadratic function y^tBy by the linear term $-2\psi^tx$ in $(\tilde{P})$. Other connections between trust region problems and eigenvalue problems are known in the literature. If one considers a symmetric perturbation in (1.1), then connections with the trust region problem are studied in [23] and show up in the theory of divide and conquer algorithms for symmetric eigenvalue problems; see e.g. [1]. Moreover, the algorithms in [12, 21] are based on finding a Lagrange multiplier smaller than the smallest eigenvalue of B, and therefore guaranteeing positive definiteness of the Hessian of the Lagrangian. The success and importance of trust region methods in both unconstrained and constrained optimization can be attributed to the fact that the subproblems can be solved very efficiently and robustly, which can be attributed to their being implicit eigenvalue problems.

In the present work we shall consider generalizing $(\tilde{P})$ in two ways and relating these trust region subproblems to eigenvalue perturbation theory. The ellipsoidal constraint $y^tDy \leq \delta$ is replaced by a two sided constraint, while the positive definite scaling matrix D is replaced by a possibly indefinite matrix C. Specifically, we shall consider the problem

$$(P) \qquad \begin{array}{lll} \min & \mu(y) = & y^tBy - 2\psi^ty \\ \text{subject to} & \beta \leq & y^tCy \leq \alpha, \ y \in \Re^n, \end{array}$$

where B and C are symmetric matrices with no definiteness assumed, and $\infty \leq \beta \leq \alpha \leq \infty$. The motivation for this paper is to extend the existing theory of trust region subproblems (in light of the above discussion on applications) in the hope that this will be a step in the direction of solving general problems with quadratic objectives and quadratic constraints. Note that unlike the definite case, a change of variables will not reduce the problem to the form $(\tilde{P})$. Moreover, it is not clear that solving the equality constrained problem is equivalent to solving the inequality constrained problem, along with a complementary slackness condition. For example, if

$$B = \begin{bmatrix} -1 & 0 \\ 0 & 3 \end{bmatrix}, \ C = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix},$$

then the equality constrained problem $y^tCy = 1$ is bounded while the inequality case, with $\beta = -\infty, \ \alpha = 1$, is unbounded.

Indefinite quadratic constraints arise when considering indefinite inner product spaces or Minkowski spaces, see e.g. [13, 8]. In this case, the generalized distance function, or norm, arising from the indefinite inner product, can be 0 and/or complex valued. The two sided constraint is a step toward

the solution of problems with two quadratic constraints and generalizes the standard problem where the left hand side constraint is implicitly understood to be ≥ 0.

In Section 2 we shall give necessary and sufficient optimality conditions for (P), as well as a general existence theorem. Then in Section 3 a further analysis is undertaken. We transform (P) to a "standard form" where the matrix pencil $B - \lambda C$ satisfies a certain regularity condition, and use this form in order to catalog the various conditions under which an optimum for (P) can exist.

In Section 4, we apply our results in order to obtain spectral information regarding the completely general parametric border perturbation of B given by

$$A(t) = \begin{pmatrix} B & \alpha \\ \beta^t & t \end{pmatrix}, \tag{1.2}$$

under the assumption that the spectral decomposition of B is known.

In Section 5 we present a general dual program for (P). This dual program is a true concave maximization problem and shows that these trust region subproblems are implicitly convex. Moreover, the dual program provides bounds on the optimal value of (P). This provides stopping criteria for algorithms for (P) based on duality gap considerations.

We conclude with an appendix to show how the algorithm and results in [12, 21] can be extended to our more general two sided indefinite trust region subproblems.

2 OPTIMALITY CONDITIONS

Our results will generally be stated for the minimization problem

$$(P) \qquad \begin{array}{lrcl} \min & \mu(y) & = & y^t B y - 2\psi^t y \\ \text{subject to} & & \beta \leq & y^t C y \leq \alpha,\ y \in \Re^n, \end{array}$$

where $\infty \leq \beta \leq \alpha \leq \infty$, and both B and C may be indefinite. The maximization versions of the results will always be analogous in an obvious way.

We have the following theorem, which extends a result of Gay [12] and Sorensen [24], where C was assumed to be positive definite and $\beta = 0 < \alpha$ is implicitly assumed; see also Fletcher [9]. Our theorem does not tell us when problem (P) possesses a minimizing point, but rather, it tells us when

a given feasible point yields a minimum. There is no gap between the necessary and sufficient optimality conditions and there is no assumption on boundedness of the feasible set or the objective function. The four optimality conditions are respectively: stationarity, nonnegative definiteness, complementary slackness, and multiplier sign. Notationally, $M > 0$ means that a real symmetric matrix M is positive definite, while $M \geq 0$ indicates that M is positive semidefinite. (The reverse notations $M < 0$, $M \leq 0$ will later be used to denote negative definiteness and negative semidefiniteness, respectively.)

Theorem 2.1 *Let y be a feasible point for (P). Suppose that the following constraint qualification holds:*

$$Cy = 0 \quad \textit{implies } \beta < 0 < \alpha. \tag{2.1}$$

Then y gives the global minimum for (P) if and only if there exists $\lambda \in \Re$ such that

$$(B - \lambda C)y = \psi \tag{2.2}$$

$$B - \lambda C \geq 0, \tag{2.3}$$

and

$$\lambda(\beta - y^t C y) \geq 0 \geq \lambda(y^t C y - \alpha). \tag{2.4}$$

Furthermore, if

$$B - \lambda C > 0, \tag{2.5}$$

then y is the unique minimizing point.

Proof: First consider sufficiency. Let y, λ satisfy the above optimality conditions, where y is feasible. There are three cases to consider.
Case (i): Suppose that $\beta < y^t C y < \alpha$. Then, the optimality conditions imply $\lambda = 0$, μ is convex, and y is a global unconstrained minimum of the convex function μ. Therefore y solves (P).
Case (ii): Suppose that

$$y^t C y = \alpha. \tag{2.6}$$

By (2.2),(2.3), we see that y minimizes the *Lagrangian function*

$$L(z, \lambda) := \mu(z) - \lambda(z^t C z - \alpha)$$

over $\Re^n$. That is,

$$\mu(y) = L(y, \lambda) \leq L(z, \lambda), \ \ \forall z \in \Re^n.$$

Since $\beta < y^tCy$ implies $\lambda \leq 0$, it follows that $\lambda(z^tCz - \alpha) \geq 0$, for all feasible z. This in turn yields $\mu(y) \leq \mu(z)$, for all feasible z.
Case (iii): Suppose that $y^tCy = \beta$. Then the conclusion follows similarly to case (ii).

This proves the "if" part. Also, the "furthermore" part of the theorem now follows easily as well.

Now consider the necessity part of the statement. We again need to consider the same three cases. For case (i), we again conclude that the quadratic function μ must be convex. Therefore we can choose $\lambda = 0$ to satisfy the optimality conditions. For case (ii), we associate with the constraint the (isotropic) cone

$$K = \{w \in \Re^n : w^tCw = 0\}.$$

(Note that the standard linear independence constraint qualification holds, since $Cy \neq 0$ by the constraint qualification assumption.) Suppose that y solves (P). By differentiating the Lagrangian function with respect to y, we obtain the Lagrange equation (2.2) as a first order necessary condition for optimality. Hence there exists $\lambda \leq 0$ such that (2.2) holds, and it only remains to verify the second order condition (2.3). Let us denote by T_y the set of tangent directions to the constraint at y; that is,

$$T_y = \{w \in \Re^n : w^tCy = 0\}.$$

The standard second order conditions state that $B - \lambda C$ is positive semidefinite on T_y. Now let $v \in \Re^n$ be a direction such that

$$v \notin K \cup T_y. \tag{2.7}$$

For each such v, we can construct a feasible point $z = y + \theta v$, where $\theta \neq 0$ and $z^tCz = \alpha$. In order to accomplish this, consider the solvability of the equation

$$(y + \theta v)^tC(y + \theta v) = \alpha. \tag{2.8}$$

This becomes

$$y^tCy + 2\theta v^tCy + \theta^2 v^tCv = \alpha, \tag{2.9}$$

and from (2.6), this in turn becomes

$$\theta[2v^tCy + \theta v^tCv] = 0. \tag{2.10}$$

Now in view of (2.7), we see that

$$\theta = \frac{-2v^tCy}{v^tCv} \tag{2.11}$$

has the required properties.

Note that the value of the Lagrangian at a feasible point satisfying (2.6) is equal to the value of the objective function at that point. Moreover, the Lagrangian is a quadratic and so the second order Taylor expansions are exact:

$$\begin{aligned} L(z,\lambda) &= L(y,\lambda) + (z-y)^t[\nabla L(y,\lambda) + \frac{1}{2}\nabla^2 L(y,\lambda)(z-y)] \\ &= L(y,\lambda) + (z-y)^t\frac{1}{2}\nabla^2 L(y,\lambda)(z-y). \end{aligned}$$

This means that

$$\mu(z) - \mu(y) = (z-y)^t(B-\lambda C)(z-y). \tag{2.12}$$

Thus the optimality of y implies

$$v^t(B-\lambda C)v \geq 0 \quad \forall v \notin K \cup T_y. \tag{2.13}$$

Since the set K has no interior points, by analyticity of the function y^tCy, we see that (2.13), the standard second order conditions on T_y, and a continuity argument yield (2.3).

Case (iii) with $\beta = y^tCy$ follows similarly.

□

Remark 2.1 One can use homogenization in order to apply Theorem 2.1 to more general quadratic constraints; namely $y^tCy + \zeta^t y$, where C is non-singular.

Remark 2.2 The optimality conditions (2.2),(2.3),(2.4) are a compact version of the usual optimality conditions with two constraints which involve two multipliers.

- *Terminology:* If λ is such that the Lagrange equation (2.2) holds for a feasible y, then λ is called a *Lagrange multiplier* and we say that y is a *stationary point* belonging to λ. The set of all such y is denoted by $\Sigma(\lambda)$, while the set of all Lagrange multipliers is denoted by Λ.

In view of Theorem 2.1, we get the following necessary condition on the symmetric matrix pencil $B - \lambda C$ for (P) to possess a minimizing point.

Corollary 2.1 *Suppose that C is nonsingular and* $\max\{|\alpha|, |\beta|\} > 0$. *If y solves (P), then*

$$\exists\ \hat{\lambda} \in \Re \ \text{ s.t. } \ B - \hat{\lambda} C \geq 0. \tag{2.14}$$

Proof: If $y \neq 0$, then the result follows from the nonsingularity of C and Theorem 2.1. If $y = 0$, then necessarily we have $\psi = 0$, the optimal value $\mu^* = 0$, and $\beta \leq 0 \leq \alpha$. Since we cannot have both α and β equal to 0, we can assume without loss of generality that $\beta < 0$. Therefore optimality implies that the system

$$y^t C y < 0, y^t B y < 0$$

is inconsistent. The result now follows from the theorem of the alternative in [32].

□

Before stating our main existence result (Theorem 2.2 below), we distinguish between two subcases of (2.14):

- We say that we are in the *regular case* or the *positive definite pencil case* provided that (P) is feasible and

$$\exists\ \hat{\lambda} \in \Re \text{ s.t. } B - \hat{\lambda} C > 0. \tag{2.15}$$

- We are in the *irregular case* or the *positive semidefinite pencil case* if (P) is feasible and (2.14) holds, but for no $\lambda \in \Re$ do we have $B - \lambda C > 0$.

Remark 2.3 Characterizations of various definiteness properties for matrix pencils were given by Hershkowitz and Schneider [16] and by Tsing and Uhlig [28]. See also [13]. We will not make use of those results in the present work, however.

In the next section we will see that in the regular case, the set

$$J := \{\lambda \in \Re : B - \lambda C > 0\}$$

is an open subinterval of the real line which is bounded if both B and C are indefinite and unbounded if C is definite. On the other hand, in the irregular case with a nonsingular pencil $B - tC$, the number $\hat{\lambda}$ is unique. This is taken up in the following lemma. (Recall that a pencil being singular means that $\det(B - tC) \equiv 0$. The pencil is nonsingular if either B or C is a nonsingular matrix.)

Lemma 2.1 *Suppose that the irregular case holds and the function* $\det(B - tC)$ *is not identically 0 in* t. *Then there is only one value* $\hat{\lambda}$ *such that (2.14) holds.*

Proof: Suppose that $\delta \neq \hat{\lambda}$ is such that $B - \delta C \geq 0$. Then any convex combination of $B - \hat{\lambda}C$ and $B - \delta C$ is positive semidefinite. Hence

$$B - \hat{\lambda}C - \alpha(\delta - \hat{\lambda})C \geq 0 \quad \forall \alpha \in [0, 1]. \tag{2.16}$$

Now consider the analytic function

$$h(\alpha) = \det[B - \hat{\lambda}C - \alpha(\delta - \hat{\lambda})C].$$

Then $h(0) = \det(B - \hat{\lambda}C) = 0$, and the assumption on the determinant implies that there exists $\beta \in \Re$ such that $h(\beta) \neq 0$. Hence analyticity implies that $h(\alpha) \neq 0$ for all sufficiently small $\alpha > 0$. But then by (2.16), for such α we would have

$$B - \hat{\lambda}C - \alpha(\delta - \hat{\lambda})C > 0,$$

which contradicts being in the irregular case.

□

We now have the following result regarding the existence of a minimizing point for problem (P).

Theorem 2.2 *Consider problem (P) with* C *nonsingular.*

1. *If* (P) *possesses a minimizing point and* $\max\{|\alpha|, |\beta|\} > 0$, *then condition (2.14) holds.*

2. *Conversely, assume that* (P) *is feasible, (2.14) holds, and both* α *and* β *are finite. Then we have the following:*

   (a) **regular case:** (P) *possesses a minimizing point.*

   (b) **irregular case:** (P) *possesses a minimizing point if and only if the equations (2.2) – (2.4) are consistent, in which case* y *is a minimizing point with associated Lagrange multiplier* $\hat{\lambda}$.

Proof: Part 1 follows immediately from Corollary 2.1. To prove Part 2a assume that (2.15) holds and suppose, to the contrary, that (P) does not

possess a minimum. Suppose that y is a feasible point. Then there would exist a sequence of feasible vectors $\{y_i\}_{i=1}^{\infty}$ such that

$$\mu(y_i) \leq \mu(y), \ \forall i, \tag{2.17}$$

and

$$||y_i|| \longrightarrow \infty \ \text{ as } \ i \longrightarrow \infty. \tag{2.18}$$

Without loss of generality we can assume that

$$\frac{y_i}{||y_i||} \longrightarrow d \ \text{ as } \ i \longrightarrow \infty. \tag{2.19}$$

We claim that

$$d^t B d \leq 0. \tag{2.20}$$

If this did not hold, then $d^t B d = a > 0$ would imply that

$$\frac{y_i^t B y_i}{||y_i||^2} > a/2, \tag{2.21}$$

for all sufficiently large i. But then (2.18) yields $\mu(y_i) \longrightarrow \infty$, contradicting (2.17). Now (2.20) and the regularity condition (2.15) together imply

$$\hat{\lambda} d^t C d < b < 0, \tag{2.22}$$

for some b. It then follows that

$$\frac{\hat{\lambda} y_i^t C y_i}{||y_i||^2} < b/2, \tag{2.23}$$

for all sufficiently large i. But from (2.18) we then obtain $|y_i^t C y_i| \longrightarrow \infty$ as $i \longrightarrow \infty$, which contradicts the feasibility of the sequence $\{y_i\}_{i=1}^{\infty}$. This completes the proof of Part 2a.

Part 2b follows from the optimality conditions.

□

The following is an example of the irregular case, with the necessary and sufficient optimality conditions in Part 2b of the previous theorem not holding, i.e. with the problem being unbounded. Take $B = \text{diag}(2, -2)$, $C = \text{diag}(-1, 1)$ and $\psi = (1, 2)$. It is readily checked that there does not exist a minimizing y for problem (P). Now note that $\hat{\lambda} = -2$, and $B - \hat{\lambda} C = 0$. Hence the equation $(B - \hat{\lambda} C)y = \psi$ is inconsistent.

3 FURTHER ANALYSIS ($\alpha = \beta = 1$)

In this section we treat the special case of (P) where C is nonsingular and $\alpha = \beta = 1$, i.e. we have the single constraint problem

$$\begin{array}{lrcl} \min & \mu(y) & := & y^t B y - 2\psi^t y \\ \text{subject to} & y^t C y & = & 1,\ y \in \Re^n. \end{array}$$

The results will be used in our analysis of eigenvalue perturbations.

3.1 THE REGULAR CASE

The condition (2.15) implies that there exists a nonsingular real $n \times n$ matrix T such that $T^t B T = D$ and $T^t C T = S$ are both diagonal. (We here are utilizing a well–known result on simultaneous diagonalization via congruence; see e.g. Theorem 7.6.4 in Horn and Johnson [17].) By building a permutation and a scaling into T if necessary, we can without loss of generality assume that the matrices D and S are of the forms

$$D = \text{diag}(D^a, D^b) = \text{diag}(d_1^a, d_2^a, \ldots, d_{n_a}^a, d_1^b, d_2^b, \ldots, d_{n_b}^b)$$

and

$$S = \text{diag}(-I^a, I^b),$$

where

$$d_1^a \geq d_2^a \geq \ldots \geq d_{n_a}^a,$$

$$d_1^b \geq d_2^b \geq \ldots \geq d_{n_b}^b,$$

and where I^a and I^b denote identity matrices of orders n_a and n_b, respectively. Here

$$n_a + n_b = n,$$

where possibly $n_a = 0$. By Sylvester's Theorem of Inertia, see e.g. [17], feasibility of (P) is equivalent to $n_b > 0$.

We now introduce the problem

$$(P_T) \qquad \begin{array}{lrcl} \min & \mu_T(x) & := & x^t D x - 2\eta^t x \\ \text{subject to} & x^t S x & = & 1. \end{array}$$

Upon identifying

$$y = Tx$$

and

$$\eta = T^t \psi,$$

it is easy to check that

$$\mu(y) = \mu_T(x)$$

and

$$y^t C y = x^t S x.$$

Furthermore, it is clear that in the regular case, the problems (P) and (P_T) have the same Lagrange multiplier set Λ, and for each Lagrange multiplier λ we have

$$\Sigma(\lambda) = T\Sigma_T(\lambda),$$

where $\Sigma_T(\lambda)$ denotes the set of stationary points of problem (P_T) belonging to λ. Finally, it will be convenient to write

$$\eta = \begin{pmatrix} \eta^a \\ \eta^b \end{pmatrix},$$

where the number of components of η^a and η^b are n_a and n_b, respectively.

Whenever the regular case holds, we can accomplish this transformation of (P) to (P_T), which we say is a problem in *standard form*. The regular case of the standardized problem will now be discussed. Hence we shall assume that (P_T) is feasible (i.e. $n_b > 0$) and

$$\exists\ \hat{\lambda} \in \Re \ \text{ s.t. } \ D - \hat{\lambda} S > 0. \tag{3.1}$$

Two subcases of (3.1) are going to be considered. These will be referred to as the "easy" and "hard" subcases. Our analysis of these subcases generalizes that found in Gander, Golub and Von Matt [11], where it was assumed that $n_a = 0$; that is, $S = I$. (See also [27].)

3.1.1 THE EASY SUBCASE

In this subcase of (3.1), we assume feasibility and the following condition:

$$\textit{No component of } \eta \textit{ is zero.} \tag{3.2}$$

It is important to note that for $\lambda \in \Re$ we then have

$$\eta \in R(D - \lambda S) \Longrightarrow \text{rank}(D - \lambda S) = n, \tag{3.3}$$

where $R(\cdot)$ denotes range. In other words, (3.2) implies that consistency of the first order condition

$$(D - \lambda S)x = \eta \tag{3.4}$$

yields invertibility of $D - \lambda S$. (Likewise, consistency of (2.2) implies invertibility of $B - \lambda C$ when (3.2) holds.) For $\lambda \in \Lambda$, denote the unique solution to (3.4) by

$$x_\lambda = (D - \lambda S)^{-1}\eta. \tag{3.5}$$

Let us now introduce the function

$$f_T(\lambda) := 1 - \eta^t (D - \lambda S)^{-2} S\eta. \tag{3.6}$$

(Note that $f_T(\lambda) := 1 - y_\lambda^t C y_\lambda$, where $y_\lambda = (B - \lambda C)^{-1}\psi$.) Since

$$D - \lambda S = S(SD - \lambda I), \tag{3.7}$$

it follows that the singularities of $f_T(\cdot)$ are the eigenvalues of SD. We call $f_T(\cdot)$ the *secular function* for problem (P_T). It reduces to the secular function in [11] when $n_a = 0$. One can readily check that

$$f_T(\lambda) = 1 + \sum_{i=1}^{n_a} \frac{(\eta_i^a)^2}{(d_i^a + \lambda)^2} - \sum_{j=1}^{n_b} \frac{(\eta_j^b)^2}{(d_j^b - \lambda)^2}. \tag{3.8}$$

Remark 3.1 Note the use of the distinct subscripts i and j in (3.8). This is adopted here and in what follows, for notational convenience.

Feasibility of x_λ for (P_T) is characterized by the equivalence

$$x_\lambda^t S x_\lambda = 1 \Longleftrightarrow f_T(\lambda) = 0. \tag{3.9}$$

It is now clear that in the easy subcase of (3.1),

$$\lambda \in \Lambda \Longleftrightarrow f_T(\lambda) = 0, \tag{3.10}$$

in which case x_λ, as given by (3.5), is the unique associated stationary point.

Since $n_b > 0$ (feasibility of (P_T)), the assumption that (3.1) holds implies that either

$$n_a > 0 \quad \text{and} \quad -d_{n_a}^a < d_{n_b}^b \tag{3.11}$$

or

$$n_a = 0. \tag{3.12}$$

If (3.11) holds, then

$$B - \lambda C > 0 \Longleftrightarrow D - \lambda S > 0 \Longleftrightarrow \lambda \in (-d^a_{n_a}, d^b_{n_b}), \tag{3.13}$$

while if (3.12) holds, then

$$B - \lambda C > 0 \Longleftrightarrow D - \lambda S > 0 \Longleftrightarrow \lambda \in (-\infty, d^b_{n_b}). \tag{3.14}$$

We summarize the above discussion in the following.

Lemma 3.1 *Problem (P_T) is feasible if and only if C is not negative semidefinite. Moreover, the set of t where $B - tC$ is positive definite is an open interval which is bounded if and only if C is indefinite.*

We now introduce the function

$$g_T(\lambda) := \lambda - \eta^t (D - \lambda S)^{-1} \eta, \tag{3.15}$$

which is called the *secular antiderivative function* for problem (P_T). The implicit form of this function is

$$g(\lambda) := \lambda - \psi^t (B - \lambda C)^{-1} \psi. \tag{3.16}$$

The singularities of $g_T(\cdot)$ are those of $f_T(\cdot)$, and what is more,

$$g'_T(\lambda) = f_T(\lambda) \tag{3.17}$$

at all real numbers λ which are not singularities. It is readily verified that

$$g_T(\lambda) = \lambda - \sum_{i=1}^{n_a} \frac{(\eta^a_i)^2}{(d^a_i + \lambda)} - \sum_{j=1}^{n_b} \frac{(\eta^b_j)^2}{(d^b_j - \lambda)}. \tag{3.18}$$

At nonsingular points λ we also have

$$g''_T(\lambda) = -\eta^t (D - \lambda S)^{-3} \eta. \tag{3.19}$$

Now suppose that (3.11) holds. Then, by (3.19), $g_T(\cdot)$ is strictly concave on the interval $(-d^a_{n_a}, d^b_{n_b})$, which by (3.13) is where $B - \lambda C > 0$. Furthermore,

$$g_T(\lambda) \downarrow -\infty \quad \text{as} \quad \lambda \downarrow -d^a_{n_a}$$

and

$$g_T(\lambda) \downarrow -\infty \quad \text{as} \quad \lambda \uparrow d^b_{n_b}.$$

Then there exists a unique $\lambda^* \in (-d^a_{n_a}, d^b_{n_b})$ such that $g'_T(\lambda^*) = f_T(\lambda^*) = 0$. It follows that $\lambda^* \in \Lambda$, and x_{λ^*} minimizes (P_T). Also, for indices $i < n_a$ we have

$$g_T(\lambda) \downarrow -\infty \quad \text{as} \quad \lambda \downarrow -d^a_i$$

and

$$g_T(\lambda) \uparrow \infty \quad \text{as} \quad \lambda \uparrow -d^a_i,$$

while for indices $j < n_b$ we have

$$g_T(\lambda) \downarrow -\infty \quad \text{as} \quad \lambda \uparrow d^b_i$$

and

$$g_T(\lambda) \uparrow \infty \quad \text{as} \quad \lambda \downarrow d^b_i,$$

Now suppose that (3.12) holds. Then $g(\cdot)$ is strictly concave on $(-\infty, d^b_{n_b})$,

$$g_T(\lambda) \downarrow -\infty \quad \text{as} \quad \lambda \downarrow -\infty$$

and

$$g_T(\lambda) \downarrow -\infty \quad \text{as} \quad \lambda \uparrow d^b_{n_b}.$$

Hence there exists a unique $\lambda^* \in (-\infty, d^b_{n_b})$ such that $g'_T(\lambda^*) = f_T(\lambda^*) = 0$. Then $\lambda^* \in \Lambda$, and x_{λ^*} is minimizes problem (P_T). For indices $j < n_b$ we have the same behavior as when (3.11) holds.

Remark 3.2 If one analyzes the function $g_T(\cdot)$ in the special case where $n_a = 0$, additional graphical properties may be obtained. In particular, one can exploit the fact that $g'''_T(\lambda) < 0$ at every nonsingular point λ; see [26] for the details.

We now can give the following existence and uniqueness result for the easy case. It includes a necessary and sufficient condition for the simultaneous existence of a maximizing point and a minimizing point for (P).

Theorem 3.1 *Consider the easy subcase of the regular case of problem (P); that is, (P) is feasible (i.e. $n_b > 0$), and (3.1), (3.2) hold. Then we have the following:*

1. *The set of Lagrange multipliers Λ is finite.*

2. *(P) possesses a unique minimizing point.*

3. (P) possesses a maximizing point if and only if n_a=0.

Proof: We can without loss of generality assume that (P) is in the standard form (P_T). Parts 1 and 2 of the theorem follow from the discussion above. (In Part 1 we used the analyticity of $f_T(\cdot)$ on any open interval which does not contain a singularity.) In order to prove Part 3, assume first that $n_a > 0$. For there to exist a maximizing point, there would necessarily exist $\tilde{\lambda} \in \Lambda$ such that

$$(D - \tilde{\lambda}S) \leq 0. \tag{3.20}$$

This implies

$$d_1^b \leq -d_1^a, \tag{3.21}$$

which contradicts (3.11). Sufficiency in Part 3 follows from compactness of the feasible set and continuity.

□

Remark 3.3 Let the hypotheses of Theorem 3.1 hold, with $n_a > 0$. In view of the preceeding discussion, we see that there exists at least one Lagrange multiplier $\tilde{\lambda}$ (that is, a critical point of $g_T(\cdot)$) such that $g_T''(\tilde{\lambda}) > 0$. In particular, there must be such a number in the interval (d_1^b, ∞). However, in view of the preceeding theorem, the corresponding stationary point $x_{\tilde{\lambda}}$ does not give a maximum for problem (P_T). In fact, in Example 4.1 below, it will be seen that $x_{\tilde{\lambda}}$ need not even give a local maximum.

We conclude the discussion of the easy subcase with a key lemma that will be used in the sections below. The lemma also provides a (concave) dual program. The lemma asserts that in the easy case, the values of the secular antiderivative at its critical points (which are the Lagrange multipliers) equal the values of the objective functions of (P) and its standardization at the corresponding set of stationary points. A variant of this result can be found in [10]; see also [26]. The proof is by direct substitution, and is omitted.

Lemma 3.2 *Let the hypotheses of lemma 3.1 hold, and let $\lambda \in \Lambda$. Then*

$$g_T(\lambda) = \mu_T(x_\lambda) = \mu(y_\lambda), \tag{3.22}$$

where $y_\lambda = (B - \lambda C)^{-1}\psi$.

The above results yield the following dual program, i.e. the optimal values of the primal and dual are equal. The details will be presented in Section 5.

DUAL PROGRAM

$$\begin{array}{ll} \max & g_T(\lambda) \\ \text{subject to} & B - \lambda C \geq 0 \end{array}$$

3.1.2 THE HARD SUBCASE

In this subcase of (3.1), we assume feasibility and the following condition:

$$\textit{Some components of } \eta \textit{ are zero.} \tag{3.23}$$

Let us introduce the (possibly empty) index sets

$$\Gamma_a = \{i : \eta_i^a \neq 0\}$$

and

$$\Gamma_b = \{j : \eta_j^b \neq 0\}.$$

The secular function for problem (P_T) now becomes

$$f_T(\lambda) = 1 - \sum_{\substack{i=1 \\ i \in \Gamma_a}}^{n_a} \frac{(\eta_i^a)^2}{(d_i^a + \lambda)^2} - \sum_{\substack{j=1 \\ j \in \Gamma_b}}^{n_b} \frac{(\eta_j^b)^2}{(d_j^b - \lambda)^2}, \tag{3.24}$$

and the secular antiderivative correspondingly becomes

$$g_T(\lambda) = \lambda - \sum_{\substack{i=1 \\ i \in \Gamma_a}}^{n_a} \frac{(\eta_i^a)^2}{(d_i^a + \lambda)} - \sum_{\substack{j=1 \\ j \in \Gamma_b}}^{n_b} \frac{(\eta_j^b)^2}{(d_j^b - \lambda)}. \tag{3.25}$$

Since we are still in the regular case, the interval J of real numbers λ for which the matrix pencil $D - \lambda S > 0$ is given by

$$J = (-\infty, d_{n_b}^b)$$

when $n_a = 0$, and by

$$J = (-d_{n_a}^a, d_{n_b}^b),$$

when $n_a > 0$. The following discussion deals with both forms of J at once. We introduce the index sets

$$\Delta_a = \{i : d_i^a = d_{n_a}^a\}$$

and

$$\Delta_b = \{j : d_j^b = d_{n_b}^b\}.$$

1. If J contains a critical point λ^* of $g_T(\cdot)$ (which is necessarily an isolated local maximum of $g_T(\cdot)$), then $\lambda^* \in \Lambda$, since a unique minimizing point x for problem (P_T) can be obtained by solving $(D - \lambda^* S)x = \eta$. Necessarily then $x_i \neq 0 \ \ \forall i \notin \Gamma_a, \ \ x_j \neq 0 \ \ \forall j \notin \Gamma_b$, and automatically $x^t S x = 1$ since $f_T(\lambda^*) = 0$.

2. Now suppose that J does not contain a critical point of $g_T(\cdot)$. Then since $g_T(\cdot)$ is strictly concave on J, we see that $g_T(\cdot)$ is strictly monotone on J. We need to consider both the monotone increasing and monotone decreasing possibilities.

   (a) If $g_T'(\lambda) > 0$ on J, then

   $$\Delta_b \cap \Gamma_b = \phi,$$

   for otherwise the assumed monotonicity is violated. (Here ϕ denotes the empty set.) Also,

   $$\lambda^* = d^b_{n_b} \in \Lambda,$$

   because a minimizing vector x for (P_T) can be found by simultaneously solving $(D - \lambda^* S)x = \eta$ and $x^t S x = 1$. Necessarily then

   $$x_i = 0 \quad \forall i \notin \Gamma_a$$

   and

   $$x_j = 0 \quad \forall j \notin \Delta_b \cup \Gamma_b.$$

   Note that selected components x_j can be nonzero for $j \in \Delta_b,\ j \notin \Gamma_b$. The set of vectors x thusly obtained is a submanifold of $\Re^{n-1}$. However, x will be unique in the special case where $g_T'(d^b_{n_b}) = 0$.

   (b) If $g_T'(\lambda) < 0$ on J, then monotonicity yields

   $$\Delta_a \cap \Gamma_a = \phi.$$

   Also,

   $$\lambda^* = d^a_{n_a} \in \Lambda,$$

   because now a minimizing vector x for (P_T) can be found by simultaneously solving $(D - \lambda^* S)x = \eta$ and $x^t S x = 1$. Then

   $$x_j = 0 \quad \forall j \notin \Gamma_b$$

   and

   $$x_i = 0 \quad \forall i \notin \Delta_a \cup \Gamma_a.$$

   Since certain components x_i may be nonzero for $i \in \Delta_a,\ i \notin \Gamma_a$, the set of vectors x obtained in this way is a submanifold of $\Re^{n-1}$, with x being unique in the special case where $g_T'(d^a_{n_a}) = 0$.

3.2 THE IRREGULAR CASE

In the irregular case it may be that (P) cannot be transformed into standard form. Nevertheless, we will study the irregular case of the standard form problem (P_T). We therefore will be assuming that

$$\exists\ \hat{\lambda} \in \Re \ \text{ s.t. } \ D - \hat{\lambda} S \geq 0, \tag{3.26}$$

and (by Lemma 2.1) that $\hat{\lambda}$ is unique. We have the following lemma.

Lemma 3.3 *In the irregular case of the feasible problem (P_T), we have*

$$n_a > 0 \tag{3.27}$$

and

$$-d^a_{n_a} = d^b_{n_b} = \hat{\lambda}. \tag{3.28}$$

Proof: If $n_a = 0$, then we would have $D - \lambda S > 0$ on the interval $(-\infty, d^b_{n_b})$, violating the uniqueness of $\hat{\lambda}$. Hence (3.27) holds. Similarly, we must have $-d^a_{n_a} \leq d^b_{n_b}$ for (3.26) to hold, and if $-d^a_{n_a} < d^b_{n_b}$, then $D - \lambda S > 0$ on the interval $(-d^a_{n_a}, \hat{d}^b_{n_b})$, which also violates the uniqueness of $\hat{\lambda}$. Consequently, (3.28) holds.

□

What follows is an existence theorem for the irregular case of the standard form.

Theorem 3.2 *Assume that we are in the irregular case of problem (P_T). Then (P_T) possesses a minimizing point if and only if*

$$\Delta_a \cap \Gamma_a = \phi \tag{3.29}$$

and

$$\Delta_b \cap \Gamma_b = \phi, \tag{3.30}$$

Proof: Suppose that (P_T) possesses a minimizing point x. We will first verify (3.29). It must be shown that

$$\eta_i = 0 \ \ \forall i \in \Delta_a.$$

To this end, let $i \in \Delta_a$. Then for the necessary condition (3.4) to hold, we must have

$$-(d_i^a + \hat{\lambda})x_i = \eta_i.$$

Since $d_i^a + \hat{\lambda} = 0$, (3.29) follows. Condition (3.4) leads to (3.30) in a similar way.

Now suppose that (3.29) and (3.30) hold. If $g_T'(\hat{\lambda}) \geq 0$, then $\hat{\lambda} \in \Lambda$, since a minimizing vector x^* may be constructed by simultaneously solving $(D - \lambda^* S)x = \eta$ and $x^t S x = 1$. Then

$$x_i = 0 \quad \forall i \notin \Gamma_a$$

and

$$x_j = 0 \quad \forall j \notin \Delta_b \cup \Gamma_b.$$

Since selected components x_j can be nonzero for $j \in \Delta_b,\ j \notin \Gamma_b$, it follows that the set of vectors x determined in this way is a submanifold of $\Re^{n-1}$, with x being unique in the special case where $g_T'(\hat{\lambda}) = 0$. The analysis for the possibility $g_T'(\hat{\lambda}) \leq 0$ is similar.

□

4 NONSYMMETRIC EIGENVALUE PERTURBATIONS

We wish to obtain spectral information about the real $n \times n$ parametric border perturbation of B given by (1.2); that is

$$A(t) = \begin{pmatrix} B & \alpha \\ \beta^t & t \end{pmatrix},$$

where B is a symmetric $(n-1) \times (n-1)$ matrix. We shall assume that the spectral decomposition of B is known. In other words, we know an orthogonal matrix P such that $P^t B P$ is diagonal. Then (after including a permutation in P if necessary) we have a unitary matrix

$$\hat{P} = \begin{pmatrix} P & 0 \\ 0 & 1 \end{pmatrix}$$

such that

$$\hat{A}(t) := \hat{P}^t A(t) \hat{P} = \begin{pmatrix} D_0 & 0 & 0 & \alpha^0 \\ 0 & D_+ & 0 & \alpha^+ \\ 0 & 0 & D_- & \alpha^- \\ (\beta^0)^t & (\beta^+)^t & (\beta^-)^t & t \end{pmatrix}, \tag{4.1}$$

where

$$\begin{aligned} D_0 &= \mathrm{diag}(\gamma_1^0, \gamma_2^0, \ldots, \gamma_{n_0}^0), \\ D_- &= \mathrm{diag}(\gamma_1^+, \gamma_2^+, \ldots, \gamma_{n_+}^+), \\ D_+ &= \mathrm{diag}(\gamma_1^-, \gamma_2^-, \ldots, \gamma_{n_-}^-), \\ \alpha_i^0 \beta_i^0 &= 0 \quad \forall i = 1, 2, \ldots, n_0, \\ \alpha_i^+ \beta_i^+ &> 0 \quad \forall i = 1, 2, \ldots, n_+, \\ \alpha_i^- \beta_i^- &< 0 \quad \forall i = 1, 2, \ldots, n_-, \end{aligned}$$

and

$$n_0 + n_+ + n_- = n - 1.$$

Note that we allow n_0, n_+ or n_- to be zero.

The spectrum of $\hat{A}(t)$ consists of the n_0 numbers γ_i^0 along with the spectrum of

$$\bar{A}(t) := \begin{pmatrix} D_+ & 0 & \alpha^+ \\ 0 & D_- & \alpha^- \\ (\beta^+)^t & (\beta^-)^t & t \end{pmatrix}. \tag{4.2}$$

Hence we will focus attention on $\bar{A}(t)$.

Without loss of generality we can assume the diagonal orderings

$$\gamma_1^+ \geq \gamma_2^+ \geq \ldots \gamma_{n_+}^+$$

and

$$\gamma_1^- \geq \gamma_2^- \geq \ldots \gamma_{n_-}^-.$$

Define

$$S = \mathrm{diag}(-1, -1, \ldots, -1, 1, 1, \ldots, 1), \tag{4.3}$$

where the number of -1's is n_+ and the number of 1's is n_-.

We associate with $\bar{A}(t)$ the following problem in $\Re^{\bar{n}}$, where $\bar{n} = n_+ + n_-$:

$$(\bar{P}) \qquad \begin{array}{lll} \min & \bar{\mu}(x) := & \bar{x}^t S D \bar{x} - 2\bar{\eta}^t \bar{x} \\ \text{subject to} & \bar{x}^t S \bar{x} = & 1 \end{array}$$

Here

$$\bar{\eta} = \begin{pmatrix} \eta^+ \\ \eta^- \end{pmatrix},$$

$$
\begin{aligned}
D &= \mathrm{diag}(D^+, D^-), \\
\eta_i^+ &= (\alpha_i^+ \beta_i^+)^{1/2} \quad \forall i = 1, 2, \ldots, n_+,
\end{aligned}
$$

and

$$
\eta_i^- = (-\alpha_i^- \beta_i^-)^{1/2} \quad \forall i = 1, 2, \ldots, n_-.
$$

It is readily checked that the secular antiderivative associated with $(\bar{P})$ is given by

$$
\bar{g}(\lambda) = \lambda + \sum_{i=1}^{n_+} \frac{(\eta_i^+)^{1/2}}{(\gamma_i^+ - \lambda)} - \sum_{j=1}^{n_-} \frac{(-\eta_j^-)^{1/2}}{(\gamma_j^- - \lambda)}. \tag{4.4}
$$

We require the following lemma. The proof, which relies on Schur complements, is similar to that of Lemma 3.1 in [26], and is therefore omitted.

Lemma 4.1 *The real eigenvalues of $\bar{A}(t)$ which differ from the $\bar{n}$ diagonal entries γ_i^+ and γ_j^- are the solutions of*

$$
\bar{g}(\lambda) = t. \tag{4.5}
$$

The next theorem follows from the discussion in Subsection 3.1.1. (Only the minimization version is stated here; the maximization version is analogous.) The theorem gives sufficient conditions for realness of the spectrum of $A(t)$, and describes the associated interlacing.

Theorem 4.1 *Assume that problem $(\bar{P})$ is feasible; that is, $n_- > 0$, and that either*

$$
n_+ > 0 \quad \text{and} \quad \gamma_1^+ < \gamma_{n_-}^- \tag{4.6}
$$

or

$$
n_+ = 0. \tag{4.7}
$$

Then problem $(\bar{P})$ possesses a unique minimizing point, and the following hold:

1. *The matrix $A(t)$ has $n-2$ real eigenvalues, including all the eigenvalues of D_0 and $\bar{n}-1$ eigenvalues of $\bar{A}(t)$, which interlace the $n-1$ eigenvalues of B.*

2. *Suppose that (4.6) holds. Let λ_α denote the unique critical point of $\bar{g}(\cdot)$ in the interval $(\gamma_1^+, \gamma_{n_-}^-)$. A sufficient condition for the other two eigenvalues of $A(\bar{t})$, say $\delta_a \leq \delta_b$, to be real is that*

$$t \leq \bar{g}(\lambda_\alpha). \tag{4.8}$$

If the inequality is strict, we get the interlacing

$$\gamma_1^+ < \delta_a < \lambda_\alpha < \delta_b < \gamma_{n_-}^-. \tag{4.9}$$

If the inequality is not strict, then

$$\gamma_1^+ < \delta_a = \lambda_\alpha = \delta_b < \gamma_{n_-}^-. \tag{4.10}$$

3. *Now suppose that (4.7) holds, and let λ_α denote the unique critical point of $\bar{g}(\cdot)$ in the interval $(-\infty, \gamma_{n_-}^-)$. A sufficient condition for the other two eigenvalues of $\bar{A}(t)$, again denoted $\delta_a \leq \delta_b$, to be real, is that (4.8) holds. In case (4.8) holds strictly, we obtain the interlacing*

$$-\infty < \delta_a < \lambda_\alpha < \delta_b < \gamma_{n_-}^-. \tag{4.11}$$

If the inequality (4.8) is not strict, then

$$-\infty < \delta_a = \lambda_\alpha = \delta_b < \gamma_{n_-}^-. \tag{4.12}$$

Remark 4.1

1. Suppose that problem (P_T) is infeasible. (This includes the case of a purely symmetric border perturbation.) Then

$$\bar{g}(\lambda) = \lambda + \sum_{i=1}^{n_+} \frac{(\eta_i^+)^{1/2}}{(\gamma_i^+ - \lambda)}. \tag{4.13}$$

   From the graphical analysis of this function, one can prove the classical result that for every value t, the spectrum of B interlaces that of $A(t)$. (See Wilkinson [30], Section 2.39.)

2. A specialized version of Theorem 4.1 appears in [26], where it was assumed that $n_+ = 0$.

The following example illustrates Lemma 4.1 and the preceeding theorem.

Example 4.1 Let

$$A(t) = \bar{A}(t) = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & -1 & t \end{pmatrix}.$$

Then

$$\bar{g}_T(\lambda) = \lambda + \frac{1}{(1-\lambda)} - \frac{1}{(2-\lambda)}.$$

The spectral decomposition and graph were obtained via MATLAB. The graph is shown in Figure 1. In view of Theorem 3.1, there is no maximizing point for problem $(\bar{P})$. There is a minimizing point, however, with corresponding Lagrange multiplier $\lambda_\alpha = 1.5$ and critical value -2.5. The other critical point is $\lambda_\beta = 2.9$ with critical value 3.5. (If one uses MATLAB in order to graph $\mu_T(\cdot)$, then it is seen that λ_β does not correspond to a local maximum, even though one might suspect this from the graph of $g_T(\cdot)$.) The eigenvalues of $A(t)$ are real if $t \leq -2.5$ or if $t \geq 3.5$. For the selected value $t = -3$, the spectrum of $A(-3)$ is $\{-3.11, 1.33, 1.68\}$. The interlacing is of type (4.9).

5 A GENERAL DUAL PROGRAM

We now return to studying the general program (P):

$$(P) \qquad \begin{array}{lll} \min & \mu(y) = & y^t B y - 2\psi^t y \\ \text{subject to} & \beta \leq & y^t C y \leq \alpha, \ y \in \Re^n. \end{array}$$

In this section we derive a dual problem for (P) which is a true concave maximization programming problem. This illustrates that (P) is an implicit convex program and shows why the global minimum can be characterized and found. Note that if y^* solves (P), then being in the *easy case* means that $y^* = (B - \lambda^* C)^{-1}\psi$; otherwise we are in the *hard case*. Moreover, the existence of λ such that $B - \lambda C > 0$ indicates the regular case.

Theorem 5.1 *Suppose that y^* solves (P) with optimal value $\mu^* = \mu(y^*)$ and optimal Lagrange multiplier λ^*. Let*

$$L(y, \nu, \omega) = \mu(y) + \nu(\alpha - y^t C y) + \omega(y^t C y - \beta) \tag{5.1}$$

Figure 1: Secular antiderivative

denote the Lagrangian function for (P); let

$$\phi(\nu,\omega) = \inf L(y,\nu,\omega) \tag{5.2}$$

denote the Lagrange dual functional; and let

$$h(\nu,\omega) = \nu\alpha - \omega\beta - \psi^t(B - \nu C + \omega C)^{-1}\psi \tag{5.3}$$

denote the quadratic dual functional. Then the optimal value of (P) satisfies

$$\begin{array}{rcl} \mu^* & = & \max_{\nu\le 0,\omega\le 0}\phi(\nu,\omega) \\ & = & \sup_{\substack{B-\nu C+\omega C>0 \\ \nu\le 0,\omega\le 0}} h(\nu,\omega), \end{array} \tag{5.4}$$

where the latter equality requires that the regular case holds. Moreover, the first equality is attained by

$$\nu^* = -(-\lambda^*)_+ \quad \textit{and}\ \omega^* = -(\lambda^*)_+, \tag{5.5}$$

where

$$(\lambda)_+ = \begin{cases} \lambda & \textit{if } \lambda \ge 0 \\ 0 & \textit{otherwise.} \end{cases}$$

Proof: If $B - \nu C + \omega C > 0$, then $\phi(\nu,\omega)$ in (5.2) is finite. Moreover, $L(y,\nu,\omega) = \phi(\nu,\omega)$ for $y = (B - \nu C + \omega C)^{-1}\psi$. Substituting for y in L yields

$$h(\nu,\omega) = \phi(\nu,\omega). \tag{5.6}$$

Now if z is feasible for (P), then for all nonpositive ν,ω we have $\phi(\nu,\omega) \le L(z,\nu,\omega) \le \mu(z)$. We now have

$$\begin{array}{rcl} \mu^* & = & \min_{z\ \textit{feasible}}\mu(z) \\ & \ge & \sup_{\nu\le 0,\omega\le 0}\phi(\nu,\omega), \\ & = & \sup_{\substack{B-\nu C+\omega C\ge 0 \\ \nu\le 0,\omega\le 0}}\phi(\nu,\omega) \\ & \ge & \sup_{\substack{B-\nu C+\omega C>0 \\ \nu\le 0,\omega\le 0}} h(\nu,\omega). \end{array} \tag{5.7}$$

Now, from Theorem 2.1, there exists an optimal multiplier λ^*. Let ν^* and ω^* be chosen as in (5.5). Then

$$\begin{array}{rcl} \mu^* & = & L(y^*,\nu^*,\omega^*) \\ & = & \phi(\nu^*,\omega^*) \\ & \le & \max_{\nu\le 0,\omega\le 0}\phi(\nu,\omega), \end{array}$$

i.e. this and (5.7) imply that the first equality in (5.4) holds.

If the easy case holds, i.e. $y^* = (B - \lambda^* C)^{-1}\psi$, then (5.6) implies

$$h(\nu^*, \omega^*) = L(y^*, \nu^*, \omega^*) = \mu^*;$$

so (5.7) implies that equality holds in (5.4). Now suppose that the hard case holds, i.e. $B - \lambda^* C$ is singular. Equivalently, $D - \lambda^* S$ is singular, where $T^t B T = D$ and $T^t C T = S$ are both diagonal, T nonsingular. Let $\bar{y} = T(D - \lambda^* S)^{\dagger} T^t \psi$, where $\dagger$ denotes the Moore-Penrose generalized inverse. From the optimality conditions, we have that $\psi \in R(B - \lambda^* C)$. Let $\lambda_k \to \lambda^*$ with $B - \lambda_k C$ positive definite (see Lemma 3.1). Let ν_k, ω_k correspond to λ_k as ν^*, ω^* corresponds to λ^*. Then, from the simultaneous diagonalization, we conclude that

$$y_k = (B - \lambda_k C)^{-1}\psi = T(D - \lambda_k S)^{-1} T^t \psi \to \bar{y}. \tag{5.8}$$

Moreover, $y^* = \bar{y} + z$ for some z in the null space of $B - \lambda^* C$, and we also have $z \perp \psi$. Now $L(y, \nu, \omega) = y^t(B - \nu C - \omega C)y - 2\psi^t y + \nu\alpha - \omega\beta$. So

$$h(\nu_k, \omega_k) = L(y_k, \nu_k, \omega_k) \to L(\bar{y}, \nu^*, \omega^*) = L(y^*, \nu^*, \omega^*) = \mu^*,$$

i.e. this and (5.7) yields (5.4). Attainment follows directly from Theorem 2.1.

□

The first equality in (5.4) provides the standard Lagrangian dual program without any duality gap, while the second equality provides a quadratic program type dual. Both duals have no duality gap and both duals are maximizing a concave function over a convex set and so illustrate that the trust region subproblems are implicit convex programs. The constraint qualification avoids trivial exceptional cases such as minimizing x subject to $x^2 \leq 0$. Unfortunately, it can rule out cases where α or β is 0 and 0 is optimal for (P) as well as being an unconstrained minimum for μ, e.g. when $\psi = 0$, $B \geq 0$. The key observation is that there is no duality gap for the above dual programs. Therefore, we can use a dual algorithm to find the optimal Lagrange multiplier and then worry about the primal optimum point.

The hard case illustrates the difficulty that can arise in duality, i.e. a Lagrange multiplier may exist such that the dual is attained, but the infimum of the Lagrangian is not attained at a feasible point of the original primal problem.

We can obtain a duality result with only one multiplier.

Corollary 5.1 *Suppose that we are in the regular case and y solves (P) with optimal Lagrange multiplier λ. Define*

$$\bar{h}(\lambda) = -(-\lambda)_+\alpha + (\lambda)_+\beta - \psi^t(B - \lambda C)^\dagger\psi. \tag{5.9}$$

Then the optimal value of (P) satisfies

$$\mu^* = \sup_{B-\lambda C>0} \bar{h}(\lambda). \tag{5.10}$$

Moreover, in the easy case, the maximum is attained, while in the hard case it is attained for λ with $B - \lambda C$ positive semidefinite and singular.

Proof: From the three cases in Theorem 2.1, we see that at least one side of the constraint of (P) can be discarded. Therefore we can assume that at least one of ν or ω is 0 in Theorem 5.1. This yields (5.10). Attainment also follows directly from Theorem 2.1.

□

Corollary 5.2 *Suppose that $C = I$ and $\beta < 0 < \alpha$, i.e. (P) is the standard trust region subproblem. Let*

$$\bar{g}(\lambda) = \lambda\alpha - \psi^t(B - \lambda C)^\dagger\psi. \tag{5.11}$$

Then

$$\mu^* = \sup_{B-\lambda C>0} \bar{g}(\lambda). \tag{5.12}$$

Moreover, the maximum is attained in the easy case, while it is attained for λ, $B - \lambda C \geq 0$ and singular, in the hard case. In addition, in the hard case,

$$\mu^* = \sup_{B-\lambda C>0} \bar{g}(\lambda) = \max_{B-\lambda C\geq 0} \bar{g}(\lambda). \tag{5.13}$$

Proof: The proof is similar to that of Corollary 5.1. The final statement follows from Theorem 2.1 since the optimum multiplier λ^* is the only point where $B - \lambda C$ is positive semidefinite and singular.

□

Note that in the standard version of (P), we could just as well choose $\beta < 0$, which implies that the constraint qualification is automatically satisfied.

6 APPENDIX

We now follow some of the development in [21] and outline an algorithm for (P) which exploits the Cholesky factorization of $B - \lambda C$. (See Algorithm 6.3 below.) We assume that C is nonsingular and that the regular case holds, i.e. there exits λ such that $B - \lambda C > 0$. In our framework, the algorithm is a primal-dual type algorithm. We maximize the dual function in order to solve the dual problem. Therefore each such iteration provides an improved Lagrange multiplier estimator λ and, by weak duality, an improved lower bound on the optimal value. In addition, if the corresponding solution x_λ is feasible, we get an upper bound on the optimal value. This upper bound is then further improved by moving along a direction of negative curvature toward the boundary of the feasible set. When the gap between lower and upper bounds is small enough, the algorithm stops. Convergence of the algorithm follows immediately from the concavity of the dual function.

This framework also simplifies the description of the algorithm in [21], where the special case that $C = I$ and $0 < \alpha$ is treated. (β can be set to any negative number.) Note that in this case, feasibility of x_λ is a necessary condition of the hard case and is used as an indicator that the hard case might have occurred. (Recall that the hard case means that $B - \lambda^* I$ is singular.) The Newton step in the hard case will generally be too large which results in slow convergence. However, only in this case do we get the added improvement in the upper bound. A log barrier penalty function can to added to avoid the large step. Thus it appears that the hard case might actually be preferable.

Many of the statements and results are straightforward extensions from [21] and we include some of them for completeness. We include results involving our dual function (see (5.9))

$$\bar{h}(\lambda) = \begin{cases} \lambda\alpha - \psi^t (B - \lambda C)^\dagger \psi, & \text{if } \lambda < 0 \\ \lambda\beta - \psi^t (B - \lambda C)^\dagger \psi, & \text{if } \lambda \geq 0; \end{cases}$$

and we discuss some of the advantages that occur by using this dual. This dual function is concave on the interval where $B - \lambda C$ is positive definite. It is differentiable if $\lambda \neq 0$ with derivative

$$\bar{h}'(\lambda) = \begin{cases} \alpha - x_\lambda^t C x_\lambda, & \text{if } \lambda < 0 \\ \beta - x_\lambda^t C x_\lambda, & \text{if } \lambda > 0. \end{cases}$$

(Recall that $x_\lambda = (B - \lambda C)^{-1}\psi$.) The subdifferential at $\lambda = 0$ is the interval

$$\partial\bar{h}(0) = [\alpha - x_0^t C x_0, \beta - x_0^t C x_0].$$

The signs of $\bar{h}'(\lambda)$ and λ tell us which side of the trust region constraint is becoming active. For example, if $\lambda < 0$ and $\alpha > 0$, then we maximize $\bar{h}(\lambda)$ by solving

$$0 = \bar{h}'(\lambda) = \alpha - x_\lambda^t C x_\lambda, \tag{6.1}$$

and exploit the rational structure of this equation by applying Newton's method to solve

$$\phi(\lambda) := \frac{1}{\sqrt{\alpha}} - \frac{1}{\sqrt{x_\lambda^t C x_\lambda}} = 0, \; x_\lambda = (B - \lambda C)^{-1}\psi, \tag{6.2}$$

i.e. we iterate using $\lambda \leftarrow \lambda - \frac{\phi(\lambda)}{\phi'(\lambda)}$. The function ϕ is almost linear but has a singularity where $x_\lambda^t C x_\lambda = 0$. The algorithm is based on solving for feasibility of x_λ, while maintaining the optimality conditions. In our framework we are solving the simple dual problem, which means that we are equivalently maximizing the function $\bar{h}(\lambda)$ rather than just solving (6.1). The dual function does not have the singularity at $x_\lambda^t C x_\lambda = 0$. By using implicit differentiation on the Lagrange equation (2.2), we see that

$$\frac{\partial x_\lambda}{\partial \lambda} = (B - \lambda C)^{-1} C x_\lambda,$$

$$\phi'(\lambda) = \frac{\partial \phi(\lambda)}{\partial \lambda} = \frac{x_\lambda^t C (B - \lambda C)^{-1} C x_\lambda}{(x_\lambda^t C x_\lambda)^{\frac{3}{2}}},$$

$$\bar{h}''(\lambda) = \frac{\partial \bar{h}'(\lambda)}{\partial \lambda} = -2 x_\lambda^t C (B - \lambda C)^{-1} C x_\lambda,$$

and

$$\frac{\phi(\lambda)}{\phi'(\lambda)} = \frac{((x_\lambda^t C x_\lambda)^{\frac{1}{2}} - \sqrt{\alpha})}{\sqrt{\alpha}} \frac{x_\lambda^t C x_\lambda}{x_\lambda^t C (B - \lambda C)^{-1} C x_\lambda}.$$

If both α and $x_\lambda^t C x_\lambda$ are negative, then we can replace them by their negative values in the definition of ϕ. We exploit the Cholesky factorization of the positive definite pencil $B - \lambda C = R^t R$, where R is upper triangular. The following algorithm applies Newton's method to update λ.

Algorithm 6.1 *Let λ and x be given with $B - \lambda C = R^t R$ positive definite and $R^t R x = \psi$. Let $y = Cx$ and $\gamma = y^t x$. Solve $R^t q = y$.*

If $\lambda < 0$ or ($\lambda = 0$ and $\gamma > \alpha$),

If $\alpha\gamma > 0$, let $\lambda = \lambda - \frac{(|\gamma|^{\frac{1}{2}} - \sqrt{|\alpha|})}{\sqrt{|\alpha|}} \frac{\gamma}{q^t q}$.

If $\alpha\gamma \leq 0$, *let* $\lambda = \lambda - (\gamma - \alpha)\frac{1}{2q^tq}$.

Else if $\lambda > 0$ *or* $(\lambda = 0$ *and* $\gamma < \alpha)$,

If $\beta\gamma > 0$, *let* $\lambda = \lambda - \frac{(|\gamma|^{\frac{1}{2}} - \sqrt{|\beta|})}{\sqrt{|\beta|}}\frac{\gamma}{q^tq}$.

If $\beta\gamma \leq 0$, *let* $\lambda = \lambda - (\gamma - \beta)\frac{1}{2q^tq}$.

End

If C is positive definite, then α is positive and this algorithm reduces to that presented in [21]. Note that the algorithm stops if $\psi = 0$. However, this is not a failure, since this indicates that we have solved the dual problem if we solve an eigenvalue problem, e.g. if $\alpha \geq \beta > 0$ we need to solve $\sup_{B-\lambda C>0} \lambda$. We have therefore found the optimal value of the primal problem.

The following lemma is a generalization of Lemma 3.4 in [21]. We have modified the results and added comments to include the role of our dual function. We include the proof for completeness. Note that for $\lambda < 0$, the dual function satisfies

$$\bar{h}(\lambda) = \lambda\alpha - ||Rx||^2,$$

with $\bar{h}(\lambda) = h(\lambda)$ if $B - \lambda C > 0$. (The case $\lambda > 0$ follows similarly.)

Lemma 6.1 *Let* $0 < \sigma < 1$ *be given and suppose that*

$$B - \lambda C = R^tR,\ (B - \lambda C)x = \psi,\ \lambda < 0,$$

where $x = (B - \lambda C)^\dagger\psi$ *when* $B - \lambda C$ *is singular. Let* $z \in \Re^n$ *satisfy*

$$(x + z)^tC(x + z) = \alpha,\ ||Rz||^2 \leq \sigma|\ ||Rx||^2 - \lambda\alpha\ |\ \ (= \sigma|\bar{h}(\lambda)|). \tag{6.3}$$

Then

$$\bar{h}(\lambda) = \lambda\alpha - ||Rx||^2 \leq \mu^* \leq \mu(x + z) \leq \bar{h}_t(\lambda) + \sigma|\bar{h}_t(\lambda)| \tag{6.4}$$

where μ^* *is the optimal value of* (P).

Proof: For any $z \in \Re^n$ we have

$$\mu(x + z) = -(||Rx||^2 - \lambda(x + z)^tC(x + z)) + ||Rz||^2. \tag{6.5}$$

Then for any z which satisfies (6.3), we have

$$\mu(x + z) = \bar{h}(\lambda) + ||Rz||^2 \leq \bar{h}(\lambda) + \sigma|\bar{h}(\lambda)|.$$

Moreover, if $\mu^* = \mu(x + z^*)$, where $x + z^*$ is feasible, then (6.5) implies

$$\mu(x + z^*) \geq -(||Rx||^2 - \lambda) = \bar{h}(\lambda),$$

i.e. weak duality holds. The last two inequalities yield the lemma. □

From the lemma we now conclude that if $\mu^* \leq 0$, then $-\mu(x + z) \geq (1 - \sigma)(-\bar{h}(\lambda))$ and so

$$|\mu(x + z) - \mu^*| = \mu(x + z) - \mu^* \leq \sigma(-\mu^*) = \sigma|\mu^*|.$$

Similarly, if $\mu^* > 0$, then for good approximations λ we have $\bar{h}(\lambda) > 0$ and $-\mu(x + z) \geq (1 + \sigma)(-\bar{h}(\lambda)) \geq (1 + \sigma)(-\mu^*)$. Therefore, in both cases we conclude that

$$|\mu(x + z) - \mu^*| \leq \sigma|\mu^*|,$$

i.e. the lemma yields a nearly optimal solution to (P). Alternatively, we get the interval

$$\bar{h}(\lambda) \leq \mu^* \leq \mu(x + z) \leq \bar{h}(\lambda) + \sigma|\bar{h}(\lambda)|. \tag{6.6}$$

(Note that the error $\sigma|\mu^*| \leq \sigma|\bar{h}(\lambda)|$ if $\mu^* \leq 0$, which is the case if e.g. $y = 0$ is feasible as in the standard trust region subproblem. This is reversed if $\bar{h}(\lambda) > 0$.)

The lemma is used in the case that the current iterate yields a strictly feasible estimate, i.e. $\beta < x_\lambda C x_\lambda < \alpha$. Then a vector z with $||z|| = 1$ and $||Rz||$ small, is computed using a Linpack routine for estimating the smallest singular value. From (6.5), we see that if we can find τ such that $x + \tau z$ satisfies the constraint with equality, then we should get a good improvement in our estimate of the optimum. In addition, note that x_λ is optimal for a subproblem, e.g. if $\lambda < 0$, then x_λ is optimal for (P) with α replaced by $x_\lambda C x_\lambda$. We can therefore continue with a new modified problem with β replaced by $x_\lambda C x_\lambda$. In addition, if we know that the optimal Lagrange multiplier is negative, then we can actually replace β by α.

The lemma provides a stopping criterion since we can conclude that the duality gap is bounded by $\sigma|\mu^*|$. However, a smaller gap is obtained from $|\mu(x + z) - \bar{h}(\lambda)|$.

Safeguarding must be done in order to maintain positive definiteness of the pencil during the iterations. The safeguarding procedure needs parameters $\lambda_L, \lambda_U, \lambda_S$, and λ, such that $[\lambda_L, \lambda_U]$ is an interval of uncertainty which contains the optimal Lagrange multiplier λ^*, while $-\infty \leq \lambda_S \leq \lambda_T \leq \infty$ with the interval $[\lambda_S, \lambda_T]$ containing the interval of positive definiteness. For

example, given $B - \lambda C > 0$, updating λ_L, λ_U follows from the concavity of the dual function:

Algorithm 6.2 *Safeguarding λ:*

If $\bar{h}'_T < 0$,

$\lambda_U = \min\{\lambda_U, \lambda\}$

Else

$\lambda_L = \max\{\lambda_L, \lambda\}$

End

Note that we do not have to consider $\lambda = 0$ as a special case unless it is the optimal multiplier, in which case the algorithm stops. However, updating λ_S and λ_T does not follow as easily. It is not immediately clear how to use the information from the Cholesky factorization to improve the estimates for the interval of positive definiteness. Note that only one of these needs to be updated since we can immediately determine which side of the current λ the optimal λ^* is on. Initial estimates can be calculated from

$$\lambda_S = \max_{c_{ii}<0} \frac{b_{ii}}{c_{ii}}, \quad \lambda_T = \min_{c_{ii}>0} \frac{b_{ii}}{c_{ii}}.$$

The following outlines an iteration for an algorithm for (P). Convergence is guaranteed by the properties of the dual program. We have not included the instances where safeguarding and updating of the safeguarding parameters are done.

Algorithm 6.3 *Suppose λ and x are given with $B - \lambda C = R^t R$ positive definite and $R^t R x = \psi$.*

1. *If the convergence criteria is satisfied, then STOP.*
2. *Take a Newton step as described in Algorithm 6.1.*
3. *Backtrack if necessary until the dual functional is improved and the pencil is positive definite. (Find the Cholesky factorization $B - \lambda C = R^t R$.)*
4. *If $\beta < x^t C x < \alpha$, then $\mu(x)$ provides an upper bound on the optimal value; improve this upper bound using e.g. $\tau, \hat{z}$ or use some other technique for the primal problem.*

A Matlab program has been written and tested on randomly generated problems which satisfy our assumptions. The test results showed an average of 3.4 iterations for convergence. This program can be obtained using anonymous ftp from princeton.edu in the directory pub/henry. See the readme file for the description of the contents of this directory. A detailed numerical study of this algorithm is currently being done.

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