AN ALL INCLUSIVE EFFICIENT REGION OF UPDATES FOR LEAST CHANGE SECANT METHODS

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Abstract

Least change secant methods, for function minimization, depend on finding a "good" symmetric positive definite update to approximate the Hessian. This update contains new curvature information while simultaneously preserving, as much as possible, the built up information from the previous update. Updates are generally derived using measures of least change based on some function of the eigenvalues of the (scaled) Hessian. A new approach for finding good least change updates is the multicriteria problem of Byrd. This uses the deviation from unity, of the n eigenvalues of the scaled update, as measures of least change. The efficient (multicriteria optimal) class for this problem is the Broyden class on the "good" side of the symmetric rank one (SR1) update. It is called the *Broyden Efficient Class.*

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This paper uses the framework of multicriteria optimization, and the eigenvalues of the scaled (sized) and inverse scaled updates, to study the question of what is a good update. In particular, it is shown that the basic multicriteria notions of efficiency and proper efficiency yield a region of updates that contains the well known updates studied to date. This provides a unified framework for deriving updates. First, the inverse efficient class is found. It is then shown that the Broyden efficient class and inverse efficient class are in fact also proper efficient classes. Then, allowing sizing and an additional function in the multicriteria problem, results in a two parameter efficient region of updates that includes many of the updates studied to date, e.g., it includes the Oren-Luenberger self-scaling updates, as well as the Broyden Efficient Class. This efficient region, called the *Self-Scaling Efficient Region*, is proper efficient and lies between two curves, where the first curve is determined by the sized SR1 updates while the second curve consists of the optimal conditioned updates. Numerical tests are included that compare updates inside and outside the efficient region.

Key words: least change secant methods, unconstrained minimization, multicriteria efficiency, proper efficiency, quasi-Newton methods, eigenvalues, sizing, scaling.

AMS 1991 Subject Classification: Primary , Secondary

1 Introduction

We consider a unified multicriteria framework for deriving updates for least change secant methods (also called quasi-Newton methods) for the unconstrained minimization problem

$$(P) \qquad \min_{x \in \Re^n} f(x),$$

where f is twice continuously differentiable. Starting with a current approximation to a local minimum for (P) (denoted x_c) and a symmetric positive definite approximation (denoted B_c) for the current Hessian, these methods perform an inexact line search in the Newton direction $d = -H_c g_c$ to find a new point x_+. (Here $g_c = \nabla f(x_c)$ and $H = B^{-1}$.)

Under the assumption that B_c is symmetric positive definite (spd) and that the line search satisfies some Wolfe-type conditions, the success of these methods depends on finding an updated spd Hessian approximation B_+, which satisfies the secant equation and preserves current built up curvature information in B_c. Various update formulae have been proposed. The updates usually arise from some proposed measure of least change, which generally depends on the eigenvalues of the scaled update $B = H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$. These updates include the well known Broyden class of updates, which then includes the DFP and BFGS updates and their convex hull, termed the convex class. The BFGS is currently the most popular update. (See e.g., [11] for details on various measures and updates.)

The fundamental concept in multicriteria decision making is that of an *efficient point*, sometimes called a *nondominated solution* or *Pareto optimum*; see e.g., [9, 22]. This refers to optimal solutions in the presence of multiple objectives. A decision maker (DM) can then choose a "best" efficient solution based on some utility function; see e.g., [19]. The framework of least change secant methods has the, possibly conflicting, objectives of minimizing the distances between 1 and each of the n eigenvalues of the scaled update. Currently, only single objectives dealing with some function of the eigenvalues have been used to derive updates.

The starting point of this paper is the result of Byrd [2]. This result states that the efficient class of updates, with respect to the multiobjective optimization problem consisting of the objective functions $|\lambda_i(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) - 1|$, $i = 1, \ldots, n$, is the Broyden class on the good side of the SR1 update.

This efficient class, called the *Broyden Efficient Class*, includes the convex class of updates. In this paper we extend the results of Byrd; we use the framework of multicriteria optimization to find a region of efficient updates, which includes the Broyden Efficient Class found by Byrd, as well as other important updates. We first find the efficient class of inverse updates and then show that both the Broyden efficient class and inverse efficient class are proper efficient classes. However, there are many important updates that are not in the Broyden class. In fact, selective sized updates (e.g., [6]) have outperformed updates in the Broyden class. By replacing the 1 in the above functions by t and adding the additional objective function $|t-1|$, we obtain a new multicriteria problem which results in a two parameter efficient region of updates. This region, called the *Self-Scaling Efficient Region* (SSER), contains the sized updates.

In particular, the following measures are functions of the eigenvalues which lead to updates which are contained in the SSER: the weighted Frobenius norm measure which results in the BFGS and DFP updates; see e.g., [11]; the measure $\psi(A) = \text{trace}(A) - \log(\det(A))$ which is used in the convergence analysis in [4] and also results in the BFGS and DFP updates, see [13]; the standard condition number measure $\kappa(A) = \lambda_1(A)/\lambda_n(A)$ which results in a curve of sized updates, see [2, 25, 18]; the uniform condition number $\omega(A) = (\text{trace}(A)/n)/(\det(A)^{\frac{1}{n}})$ which results in the sized DFP and inverse-sized BFGS updates, also called the Oren-Luenberger self-scaling updates, see [10]; the optimal volume measure $\sigma(A) = \lambda_1(A)/(\det(A)^{\frac{1}{n}})$ and the resulting optimally conditioned, sized, SR1 updates, see [25]; and the dual optimal volume measure $\tau(A) = \text{trace}(A)/\lambda_n(A)$, (see [24]) which leads to the same optimally conditioned, sized, SR1 updates, see [26]. (See [26] for results on these and other condition numbers, their relations to measures for least change, and also their relations to potential functions.)

The recent introduction and popularity of automatic differentiation [16, 12] raises questions on the importance of quasi-Newton methods in the future and, in particular, on whether it is worthwhile expending a lot of energy on finding better and improved updates. However, there are many problems where automatic differentiation is not suitable, e.g., where function evaluations may require an unknown number of iterations. Moreover, though the area of least change secant methods has been intensively studied for a long time (since [7]), there are still many fundamental unanswered questions. In fact, understanding what makes one update better than another, and whether scaling or inverse scaling is better, are still open questions. (See e.g., [3]). In addition, proper implementation of quasi-Newton methods to large sparse problems also remains an open problem.

The paper is organized as follows. We first conclude this section with some preliminary notations and results. Section 2 presents the preliminary definitions and notation for multicriteria problems. We then present and prove the above mentioned result of Byrd as well as present the inverse efficient class of updates and show that both classes are proper efficient. Section 3 presents our main result, the efficient region of updates. This region lies between two curves determined by the sized SR1 and the optimally conditioned sized updates. Moreover, by allowing sizing by t but not including the extra function $|t-1|$ in the multicriteria problem, we get an efficient curve of updates corresponding to optimally conditioned sized updates. This region and curve are also proper efficient sets. We conclude with some numerical tests illustrating the efficient region.

1.1 Preliminaries

The update at the new point x_+ (denoted B_+) satisfies the *secant equation*

$$B_+ s = y,$$

where the change in x is $s = x_+ - x_c$ and the change in the gradient is $y = g_+ - g_c$. We let H denote B^{-1} and define the curvature formulas

$$a = y^t H_c y, \;\; b = y^t s, \;\; c = s^t B_c s.$$

We assume that the current update B_c is *symmetric positive definite* (spd) and the curvature $b > 0$.

The *Broyden class* of updates is

$$B_\phi = B_c - \frac{1}{s^t B_c s} B_c s s^t B_c + \frac{1}{y^t s} y y^t + (1-\phi) s^t B_c s w w^t, \qquad (1.1)$$

where $w = \frac{1}{y^t s} y - \frac{1}{s^t B_c s} B_c s$. Since B_c spd and $b > 0$ are assumed, we have B_ϕ is spd if and only if $\phi < ac/(ac - b^2)$. Choosing $\phi = 0, 1$ yields the well known *DFP* and *BFGS* updates, respectively; the set of updates with $\phi \in [0,1]$ is called the *convex class*; while the *symmetric rank-one* update, denoted SR1, corresponds to the ϕ value $\phi_{SR1} = -c/(b-c)$. (See e.g., [11, 21] for details.) The current update is *sized* by the positive scalar t means it is changed to tB_c; see e.g. [10].

We work in the space of symmetric matrices equipped with the *trace inner product* $\langle A, B\rangle = \text{trace}AB$. For a symmetric matrix A, we let $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A)$ denote its ordered eigenvalues. By abuse of notation, we let $\lambda_i(\phi)$ denote $\lambda_i(B(\phi))$ when $B(\phi)$ is a symmetric matrix dependent on the parameter ϕ.

2 Multicriteria Optimal Updates

In this section we introduce our first multicriteria problem and show that the efficient updates are the Broyden class updates on the good side of the SR1. We also derive the efficient class of inverse updates and show that both classes of updates are properly efficient. We first introduce the multicriteria problems and give some definitions and preliminary results.

Consider the multiobjective optimization problem

$$\begin{array}{c} \min \quad g_i(z),\ i = 1, \ldots, m, \\ \text{subject to } z \in \Omega, \end{array} \tag{2.1}$$

where $g_i : \Re^n \to \Re$, are m real valued objective functions. A point z^1 is dominated by z^2, denoted $z^2 \prec z^1$, if

$$g_i(z^2) \leq g_i(z^1),\ i = 1, \ldots, m,\ \textit{and}\ g_j(z^2) < g_j(z^1) \text{ for some } j.$$

(We use $z^2 \preceq z^1$ if z^1 is weakly dominated by z^2, i.e., if $\leq$ holds $\forall\ i$ without the possible strict $<$.) The <u>Efficient Set</u> is the set of points $z \in \Omega$ that are not dominated by any points in Ω. z^0 is said to be a <u>Properly Efficient Solution</u> of (2.1) if it is in the efficient set and if there exists a scalar $M > 0$ such that, for each i, we have:

$$g_i(z) < g_i(z^0) \Rightarrow \left\{\ \exists j \text{ s.t. } g_j(z) > g_j(z^0) \text{ and } \frac{g_i(z^0)-g_i(z)}{g_j(z)-g_j(z^0)} \leq M\ \right\}$$

(see, [15]). Thus, for any point z, we can find a constant M, such that for each gain there exists a loss where the gain over the loss is bounded above by M. Thus, the marginal improvement is bounded. Note that an efficient point that is not proper efficient allows for an arbitrarily large gain in one objective function at the expense of only a small loss in another objective function. Therefore, efficient points which are not proper are not desirable.

We now present some preliminary results on the parametrization of the Broyden class, see (1.1).

Lemma 2.1 *[21, pg. 111] The matrix $B_c^{-\frac{1}{2}} B_\phi B_c^{-\frac{1}{2}}$ has $n-2$ unit eigenvalues and the two remaining eigenvalues are*

$$\lambda_\pm(\phi) = f_1(\phi) \pm (f_1(\phi)^2 - f_2(\phi))^{\frac{1}{2}}, \tag{2.2}$$

where

$$f_1(\phi) = \frac{a(b+c) - \phi(ac - b^2)}{2b^2}, \quad f_2(\phi) = \frac{a}{b} - \frac{\phi(ac - b^2)}{bc}. \tag{2.3}$$

Every member of the Broyden class satisfies the secant equation. The following result of Davidon gives conditions for the converse.

Proposition 2.2 *[8] Suppose that B_+ is spd and satisfies the secant equation. Then the columns of $B_+ - B_c$ are in the span of $\{B_c s, y\}$ if and only if B_+ is in the Broyden class.*

Corollary 2.3 *Suppose that B_+ satisfies the secant equation. Then B_+ is in the Broyden class if and only if the matrix $B = H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ is an update of I of rank at most two and it has $n-2$ unit eigenvalues with corresponding $n-2$ dimensional eigenspace orthogonal to span$\{B_c^{\frac{1}{2}} s, H_c^{\frac{1}{2}} y\}$.*

Proof. The above Proposition 2.2 implies that B_+ is in the Broyden class if and only if the columns of $B - I$ are in span$\{B_c^{\frac{1}{2}} s, H_c^{\frac{1}{2}} y\}$, i.e., $B - I$ is at most rank two and has eigenvectors, corresponding to nonzero eigenvalues, in the above span. □

We will also need the following lemma which we call the *Perturbation Lemma*.

Lemma 2.4 *Let B be a symmetric matrix with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$. Suppose that B satisfies the scaled secant equation $B(B_c^{\frac{1}{2}} s) = H_c^{\frac{1}{2}} y$. Then*

1. *for any two eigenvalues $\lambda_k \geq \lambda_j > 1$, we can find a symmetric matrix $\bar{B}$ satisfying the secant equation $\bar{B}(B_c^{\frac{1}{2}} s) = H_c^{\frac{1}{2}} y$, such that its n eigenvalues $\bar{\lambda}_1, \ldots, \bar{\lambda}_n$ satisfy*

$$\begin{array}{ll} \lambda_i \geq \bar{\lambda}_i \geq 1 & \textit{for } i = k, j \\ \lambda_i = \bar{\lambda}_i & \textit{for } i = 1, \ldots, n \quad i \neq j, k, \end{array}$$

   with at least one of $\bar{\lambda}_k < \lambda_k$ or $\bar{\lambda}_j < \lambda_j$;

2. *for any two eigenvalues $\lambda_k \leq \lambda_j < 1$, we can find a symmetric matrix $\bar{B}$ satisfying the scaled secant equation $\bar{B}(B_c^{\frac{1}{2}} s) = H_c^{\frac{1}{2}} y$, such that its n eigenvalues $\bar{\lambda}_1, \ldots, \bar{\lambda}_n$ satisfy*

$$\begin{array}{ll} \lambda_i \leq \bar{\lambda}_i \leq 1 & \textit{for } i = k, j \\ \lambda_i = \bar{\lambda}_i & \textit{for } i = 1, \ldots, n \quad i \neq j, k, \end{array}$$

   with at least one of $\bar{\lambda}_k > \lambda_k$ or $\bar{\lambda}_j > \lambda_j$.

Proof. To prove 1., let $x_1, \ldots, x_n$ be a set of orthonormal eigenvectors corresponding to $\lambda_1, \ldots, \lambda_n$. Find $\alpha,\ \beta \in \Re$, not both 0, such that

$$(s^t B_c^{\frac{1}{2}})[x_k\ x_j] \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0,$$

i.e., $0 \neq \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in z^{\perp}$, $z^t = (s^t B_c^{\frac{1}{2}})[x_k\ x_j]$. Set

$$0 \neq w = [x_k\ x_j] \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha x_k + \beta x_j.$$

Let

$$\bar{B} = B - \epsilon w w^t \tag{2.4}$$

and denote its eigenvalues by $\bar{\lambda}_i$ with corresponding eigenvectors $\bar{x}_i$, $i = 1, \ldots, n$. We can see that $\bar{B}$ satisfies the secant equation. Moreover,

$$\bar{\lambda}_i = \lambda_i, \quad i = 1, \ldots, n, \ i \neq k, j$$

and for $\epsilon > 0$, since w is in the span of $\{x_k, x_j\}$ and $w \neq 0$,

$$\bar{\lambda}_i \leq \lambda_i, \quad i = k, j,$$

with at least one of $\bar{\lambda}_k < \lambda_k$ or $\bar{\lambda}_j < \lambda_j$.

By a similar argument with $\epsilon < 0$, we can show 2. □

2.1 Broyden Efficient Class

The general notion of least change is that we want B_+ spd such that the secant equation $B_+ s = y$ holds and B_+ is "close" to B_c. If we view B_c and B_+ as quadratic forms, then we can define close as satisfying:

$$\frac{u^t B_+ u}{u^t B_c u} \text{ is close to 1, for all } u \in \Re^n. \tag{2.5}$$

Equivalently,

$$\frac{x^t H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}} x}{x^t x} \text{ is close to 1, for all } x \in \Re^n. \tag{2.6}$$

This implies that all of the eigenvalues of $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ satisfy

$$\lambda_i \text{ is close to 1, } i = 1, \ldots, n. \tag{2.7}$$

(If we view the inverse updates instead, we would consider the eigenvalues of $B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$.) Motivated by this, Byrd [2] considers the following multiobjective least change problem, where the functions in (2.1) are $g_i(x) = |x - 1|$:

$$\begin{array}{ll} \min_{B_+} & |\lambda_i(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) - 1|, \ i = 1, \ldots, n, \\ & \text{subject to } B_+ s = y, \ B_+ = B_+^t. \end{array} \tag{2.8}$$

Let

$$\Phi = \begin{cases} [\phi_{SR1}, \infty) & \text{if } b > c \\ (-\infty, \phi_{SR1}] & \text{if } b < c \\ (-\infty, \infty) & \text{if } b = c. \end{cases} \tag{2.9}$$

We let Φ represent the subset of the Broyden class of updates $\{B_\phi, \ \phi \in \Phi\}$, and call it the *Broyden Efficient Class.* This is the set of Broyden class updates on the good side, or convex class side, of the SR1. We now state the result presented by Byrd [2]. We provide our own proof for completeness.

Theorem 2.5 *The efficient set for problem (2.8) consists of the Broyden efficient class, i.e., the Broyden class with $\phi \in \Phi$.*

Before proving the theorem, we first note that the efficient class for our multicriteria problem has the following dominating property.

Lemma 2.6 *Suppose that $B = B^t$ satisfies the secant equation. Then there exists an efficient update $\bar{B}$ for (2.8) such that $\bar{B} \preceq B$.*

Proof. The proof follows by an application of Zorn's Lemma upon noting that the set of updates $\{\bar{B} : \bar{B} \preceq B\}$ is compact; see e.g., Theorem 1 in [1]. $\square$

We now use the perturbation lemma and the above lemma to prove the theorem.

Proof. Let B_+ be in the efficient set for problem (2.8) and let $B = H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$. Then B satisfies the scaled secant equation

$$B(B_c^{\frac{1}{2}} s) = (H_c^{\frac{1}{2}} y). \tag{2.10}$$

Let $\lambda_1 \geq \ldots \geq \lambda_n$ be the eigenvalues of B with $x_1, \ldots, x_n$ a set of corresponding orthonormal eigenvectors. First we show that

$$\lambda_2 = \lambda_{n-1} = 1. \tag{2.11}$$

Suppose not and suppose that

$$\lambda_2 > 1. \tag{2.12}$$

By Lemma 2.4 we can find an update $\bar{B}$ such that $\bar{B} \prec B$. This contradicts the fact that B_+ is an efficient point. So (2.12) fails. Similarly, we cannot have $1 > \lambda_{n-1}$, i.e., (2.11) must hold and B is an update of I of at most rank 2. It remains to show that B is in the Broyden class with parameter $\phi \in \Phi$. We do this by first showing that it solves the following problem

$$\begin{array}{rrcl} \min\limits_{A} & \lambda_1(A) & & \\ \text{subject to} & AB_c^{\frac{1}{2}} s & = & H_c^{\frac{1}{2}} y \\ & \lambda_n(A) & \geq & \lambda_n(B) \\ & A & = & A^t. \end{array} \tag{2.13}$$

Since λ_1 is a convex function while λ_n is a concave function, the above is a convex programming problem. Since $||A|| = \max\{\lambda_1(A), -\lambda_n(A)\}$, we can assume that the feasible set is bounded. Therefore, the minimum is attained say at $\bar{A}$. Then, since B is feasible, we have

$$\lambda_1(B) \geq \lambda_1(\bar{A}) \geq \lambda_n(\bar{A}) \geq \lambda_n(B). \tag{2.14}$$

By Lemma 2.6, there must be an efficient update that weakly dominates $\bar{A}$ and, since any efficient update satisfies (2.11), it weakly dominates B as well. The efficiency of B now implies that $B = \bar{A}$ solves (2.13).

We now use the optimality conditions for (2.13) with Proposition 2.6 to show that the update is in the Broyden class. For some Lagrange multiplier vector u and nonnegative scalars v, w, the Lagrangian for problem (2.13) is

$$L(u, v, w, \bar{B}) = w\bar{\lambda}_1 + u^t(\bar{B}B_c^{\frac{1}{2}}s - H_c^{\frac{1}{2}}y) - v(\bar{\lambda}_n - \lambda_n),$$

where u, v, w cannot all be 0 and $\bar{\lambda}_i = \lambda_i(\bar{A})$. We have added the multiplier w to avoid assuming a constraint qualification, i.e., in the absence of a constraint qualification we necessarily have $w = 0$; while if a constraint qualification holds for (2.13), then we can assume that $w = 1$. We can differentiate the Lagrangian and set it equal to zero to get the Lagrange equation (or Fritz John stationarity condition)

$$w\bar{\lambda}_1' + us^tB_c^{\frac{1}{2}} + B_c^{\frac{1}{2}}su^t + v\bar{\lambda}_n' = 0. \tag{2.15}$$

Here $\bar{\lambda}_i'$ are subgradients; see e.g., [20]. First suppose that a constraint qualification holds, so $w = 1$, and suppose that $v > 0$. Since the rank of $B_c^{\frac{1}{2}}su^t + us^tB_c^{\frac{1}{2}}$ is at most 2, we must have the ranks of the subdifferentials equal to 1, i.e.,

$$\bar{\lambda}_1' = \bar{x}_1\bar{x}_1^t \text{ and } \bar{\lambda}_n' = \bar{x}_n\bar{x}_n^t.$$

(Note that $u = 0$ implies that $\bar{\lambda}_1 = \bar{\lambda}_n$, which would uniquely define the trivial identity update. In fact, the entire Broyden class must reduce to this trivial update in this case, since necessarily $a = b = c$.) Now (2.15) implies that $B_c^{\frac{1}{2}}s \in \text{span}\{x_1, x_n\}$. The secant equation (2.10) now implies that $H_c^{\frac{1}{2}}y$ is in this span as well. Therefore (2.11) and Corollary 2.3 implies that B is in the Broyden class.

If $v = 0$, then the Lagrange equation now implies that either $\bar{\lambda}'_1$ is rank one, so $B_c^{\frac{1}{2}} s$ and $H_c^{\frac{1}{2}} y$ are in span$\{x_1\}$, i.e., are linearly dependent, or it is rank two and the eigenvalue $\bar{\lambda}_1 = \bar{\lambda}_2 = 1$. In either case we can still apply Corollary 2.3 and we have the SR1 update. The same argument holds if $w = 0$.

Therefore, it only remains to show that B is in the efficient part of the Broyden class. If $b = c$ then there is nothing to show. If $b < c$, then from Lemma 2.1, the eigenvalues for the SR1 update satisfy $0 < \lambda_-(\phi_{SR1}) < 1 = \lambda_+(\phi_{SR1})$. If $\lambda_n < \lambda_-(\phi_{SR1})$, then we have $B_{\phi_{SR1}} \prec B$, which is a contradiction. Therefore

$$\lambda_n \geq \lambda_-(\phi_{SR1}), \tag{2.16}$$

i.e., $B = B_\phi$ with $\phi \in \Phi$, since $\lambda_-(\phi)$ is isotonic with $-\phi$, by Lemma 2.1.

The case $b > c$ follows similarly except we use the fact that B is optimal for the following problem

$$\begin{array}{cc} \max & \lambda_n(\bar{B}) \\ \text{subject to} & \bar{B} B_c^{\frac{1}{2}} s = H_c^{\frac{1}{2}} y \\ & \lambda_1(\bar{B}) \leq \lambda_1(B) \\ & \bar{B} = \bar{B}^t. \end{array}$$

Now we have shown that any efficient point B must be in the Broyden efficient class, Φ. Conversely, for any update B_ϕ in the Broyden efficient class, $\lambda_\pm(\phi)$ are isotonic with $-\phi$ and (2.11) holds. Thus B_ϕ cannot be dominated by any other updates in the Broyden efficient class, Φ. Moreover, we can restrict ourselves to Φ since any update can be dominated by an efficient update by Lemma 2.6. $\square$

Note that (2.7) is a relaxation of (2.6), which involves an infinite number of functions. One way of handling (2.6) directly is to use the volume of the ellipsoids corresponding to the quadratic forms. This is the approach in [25].

2.2 Inverse Broyden Efficient Class

The inverse Broyden class updates can be parametrized by

$$H_{\hat{\phi}} = H_c - \frac{1}{y^t H_c y} H_c y y^t H_c + \frac{1}{y^t s} s s^t + (1 - \hat{\phi}) y^t H_c y v v^t,$$

where $v = \frac{1}{y^t s} s - \frac{1}{y^t H_c y} H_c y$. The BFGS and DFP updates correspond to $\hat{\phi} = 0, 1$, respectively; while the SR1 update is $\hat{\phi}_{SR1} = -\frac{a}{b-a}$. In general,

$$\hat{\phi} = \iota(\phi) = \frac{1-\phi}{1+\phi[\frac{b^2}{ac} - 1]} \tag{2.17}$$

is a 1-1 and onto mapping (c.f. [23]) that relates ϕ and $\hat{\phi}$ for which B_ϕ is spd and $B_\phi^{-1} = H_{\hat{\phi}}$. Now consider the inverse multiobjective least change problem

$$\begin{array}{ll} \min & |\hat{\lambda}_i(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) - 1|, \ i = 1, \ldots, n; \\ & \text{subject to } B_+ s = y, \ B_+ = B_+^t. \end{array} \tag{2.18}$$

Let

$$\hat{\Phi} = \begin{cases} [\hat{\phi}_{SR1}, \infty) & \text{if } b > a \\ (-\infty, \hat{\phi}_{SR1}] & \text{if } b < a \\ (-\infty, \infty) & \text{if } b = a. \end{cases} \tag{2.19}$$

We let $\hat{\Phi}$ represent the subset of the Broyden class of updates $\{B_{\hat{\phi}}\}$, $\hat{\phi} \in \hat{\Phi}$, and call it the *Inverse Broyden Efficient Class.* From the previous section, after exchanging the roles of B_+, B_c and s with H_+, H_c and y, respectively, we get the following corollary.

Corollary 2.7 *The efficient class for problem (2.18) consists of the inverse Broyden class with $\hat{\phi} \in \hat{\Phi}$.*

2.3 Proper Efficiency

As mentioned above, an efficient point that is not proper efficient is not desireable, since we can obtain an arbitrarily large marginal improvement. However, based on the results of Theorem 2.5, we can present the following theorem.

Theorem 2.8 *The Broyden efficient class Φ for problem (2.8) is also the properly efficient class for problem (2.8). The same holds true for the inverse efficient class $\hat{\Phi}$ and the problem (2.18).*

Proof. Let B_{ϕ_0} be an update in the Broyden efficient class. Without loss of generality and for simplicity of notation, we can assume that $B_c = I$. By abuse of notation, let

$$h_i(\phi_0) = |\lambda_i(B_{\phi_0}) - 1|, \quad i = 1, \ldots, n,$$

and let $h_i(+)$ denote $|\lambda_i(B_+) - 1|$. Then

$$h_i(\phi_0) = |\lambda_i(B_{\phi_0}) - 1| = 0 \text{ for } i = 2, \ldots, n-1,$$

and so, to show that B_{ϕ_0} is proper efficient, it is sufficient to only consider the two cases $i = 1$ and $i = n$. In addition, if $ac = b^2$, the entire Broyden class reduces to the SR1 update. Therefore every update is dominated by the SR1 update which must therefore be proper efficient. So we can also assume that $ac > b^2$.

Let B_+ be a symmetric update satisfying the secant equation such that

$$h_1(+) < h_1(\phi_0). \tag{2.20}$$

As in the proof of Theorem 2.5, we can use Lemma 2.4 and find a Broyden efficient class update B_{ϕ_1} such that

$$h_i(\phi_1) \le h_i(+), \quad i = 1, n. \tag{2.21}$$

Therefore, from (2.20) we have

$$h_1(\phi_1) < h_1(\phi_0),$$

which implies that $\lambda_1(B_{\phi_1}) < \lambda_1(B_{\phi_0})$. Since Lemma 2.1 implies that $\lambda_{\pm}(\phi)$ are isotonic with $-\phi$, we have $\phi_1 > \phi_0$ and hence

$$\lambda_n(B_{\phi_1}) < \lambda_n(B_{\phi_0}),$$

which is equivalent to

$$h_n(\phi_1) > h_n(\phi_0). \tag{2.22}$$

Therefore, from (2.20),(2.21) and (2.22) we have

$$\begin{cases} h_1(\phi_1) \le h_1(+) < h_1(\phi_0) \\ h_n(+) \ge h_n(\phi_1) > h_n(\phi_0). \end{cases}$$

This together with Cauchy's mean value theorem yields

$$\frac{h_1(\phi_0)-h_1(+)}{h_n(+)-h_n(\phi_0)} \le \frac{h_1(\phi_0)-h_1(\phi_1)}{h_n(\phi_1)-h_n(\phi_0)} = \frac{\lambda_+(\phi_0)-\lambda_+(\phi_1)}{\lambda_-(\phi_0)-\lambda_-(\phi_1)} = \frac{\lambda'_+(\bar\phi)}{\lambda'_-(\bar\phi)}, \qquad (2.23)$$

for some $\phi_0 < \bar\phi < \phi_1$ with $\lambda'_-(\bar\phi) \neq 0$.

From chapter 7 in [21] or Lemma 2.1, we have

$$\lambda'_\pm(\phi) = \frac{-(ac-b^2)}{2b^2}(1 \pm g(\phi)),$$

where

$$g(\phi) = \frac{(f_1(\phi)-\frac{b}{c})}{[(f_1(\phi)-\frac{b}{c})^2+\frac{ac-b^2}{c^2}]^{\frac{1}{2}}} < 1.$$

Let

$$h(\phi) = \frac{\lambda'_+(\phi)}{\lambda'_-(\phi)} = \frac{1+g(\phi)}{1-g(\phi)}. \qquad (2.24)$$

Then

$$h'(\phi) = \frac{\partial h}{\partial g}\frac{\partial g}{\partial f_1}\frac{\partial f_1}{\partial \phi} = \frac{2}{(1-g)^2}\frac{ac-b^2}{((f_1(\phi)-\frac{b}{c})^2+\frac{ac-b^2}{c^2})^{\frac{3}{2}}}\frac{-(ac-b^2)}{2b^2} < 0,$$

i.e., we obtain the upper bound for gain over loss

$$\frac{\lambda'_+(\bar\phi)}{\lambda'_-(\bar\phi)} \le \frac{\lambda'_+(\phi_0)}{\lambda'_-(\phi_0)} = \frac{1+g(\phi_0)}{1-g(\phi_0)}. \qquad (2.25)$$

For the case of $i = n$ in the definition of proper efficient, a similar argument yields the upper bound $\frac{1-g(\phi_0)}{1+g(\phi_0)}$. Therefore, B_{ϕ_0} is a properly efficient solution of problem (2.8). The proof for the inverse efficient class follows similarly. □

3 Self-Scaling Efficient Region

The above Broyden efficient class Φ of updates does not contain many important updates that have been studied in the literature, e.g., the Oren-Luenberger self-scaling updates to which we refer as sized updates. We now relax the multicriteria problem (2.8) by allowing sizing of B_c by t and adding the function $|t-1|$. The relaxation attempts to have all the eigenvalues close to a constant, where the constant is close to 1. (The constant was equal to 1 in the first multicriteria problem.) We then see that we get an efficient region that contains all the classes mentioned so far. The relaxation yields the following problem.

$$\begin{array}{ll} \min_{t,B_+} & \left\{ \begin{array}{l} |\lambda_i((tB_c)^{-\frac{1}{2}}B_+(tB_c)^{-\frac{1}{2}})-1|, \quad i=1,\ldots,n, \\ |t-1| \end{array} \right. \\ & \text{subject to } B_+s=y,\ B_+=B_+^t,\quad t>0. \end{array} \tag{3.1}$$

The self-scaling Broyden class is

$$B_+(t,\phi)=t(B_c-\frac{1}{s^tB_cs}B_css^tB_c+(1-\phi)s^tB_csww^t)+\frac{1}{y^ts}yy^t,$$

where $w=\frac{1}{y^ts}y-\frac{1}{s^tB_cs}B_cs$ and $t\in\Re$. This includes the sized DFP with $(t,\phi)=(\frac{b}{c},0)$ and the inverse sized BFGS with $(t,\phi)=(\frac{a}{b},1)$. If $ac>b^2$, then we define the region

$$\Phi_R^{>}=\left\{(t,\phi): \begin{array}{c} \min(1,\alpha_-)\le t \\ t\le\max(1,\alpha_+) \end{array} \text{ and } \left(\begin{array}{ll} \frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t}\le\phi & \text{if } 1<t \\ \phi\le\frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t} & \text{if } t<1 \\ \phi\le\frac{t}{t-\frac{b}{c}} & \text{if } \frac{b}{c}<t \\ \frac{t}{t-\frac{b}{c}}\le\phi & \text{if } t<\frac{b}{c} \\ \phi \text{ arbitrary} & \text{if } t=\frac{b}{c}=1 \end{array} \right) \right\}, \tag{3.2}$$

where

$$\alpha_\pm=\frac{a}{b}\pm\{\frac{a^2}{b^2}-\frac{a}{c}\}^{\frac{1}{2}}. \tag{3.3}$$

If $ac=b^2$, then we define the region

$$\Phi_R^{=}=\{(t,\phi):\min(1,\frac{b}{c})\le t\le\max(1,\frac{b}{c}),\ \phi \text{ arbitrary}\}. \tag{3.4}$$

We let Φ_R represent the appropriate region determined by the value of $ac-b^2$, i.e., it represents the sized Broyden class updates $B_+(t,\phi)$, $(t,\phi)\in\Phi_R$,

$$\Phi_R=\left\{ \begin{array}{ll} \Phi_R^{>} & \text{if } ac>b^2 \\ \Phi_R^{=} & \text{if } ac=b^2 \end{array} \right. .$$

We call Φ_R the *Self-Scaling Efficient Region.* The above representation illustrates that the efficient region lies between the two curves:

$$\phi = \frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t};\ \phi = \frac{t}{t-\frac{b}{c}}.$$

We also define the curve

$$\Phi_C = \left\{ (t,\phi):\ \alpha_- \le t \le \alpha_+ \text{ and } \begin{pmatrix} \phi = \frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t} & \text{if } ac-b^2>0 \\ \phi \text{ arbitrary} & \text{if } ac-b^2=0 \end{pmatrix} \right\}, \tag{3.5}$$

and call Φ_C the *Self-Scaling Efficient Curve.* Note that this curve contains optimally conditioned updates, i.e., updates optimal for the κ measure, see [2, 25, 18]. (See figures 1 and 2 for illustrations of the various efficient sets.) We now state and prove our main results.

Theorem 3.1 *The efficient updates for problem (3.1) are the self-scaling efficient region updates $B_+(t,\phi)$, with $(t,\phi)\in\Phi_R$.*

Before we prove the above theorem, we present the following preliminary results.

Lemma 3.2 *The matrix $B = (tB_c)^{-\frac{1}{2}}B_+(t,\phi)(tB_c)^{-\frac{1}{2}}$ has $n-2$ unit eigenvalues and the two remaining eigenvalues are*

$$\lambda_\pm(t,\phi) = f_1(t,\phi) \pm (f_1(t,\phi)^2 - f_2(t,\phi))^{\frac{1}{2}},$$

where

$$\begin{cases} f_1(t,\phi) = \frac{a}{2bt} + \frac{ac-\phi(ac-b^2)}{2b^2} \\ f_2(t,\phi) = \frac{1}{t}(\frac{a}{b} - \frac{\phi(ac-b^2)}{bc}). \end{cases}$$

Furthermore:

1. *$\lambda_\pm(t,\phi)$ are isotonic with $-\phi$ for any fixed t, and*

$$\frac{\partial\lambda_\pm(t,\phi)}{\partial\phi} = \frac{-(ac-b^2)}{2b^2}[1\pm g(t,\phi)],$$

where

$$g(t,\phi) = \frac{(f_1(t,\phi)-\frac{b}{tc})}{[(f_1(t,\phi)-\frac{b}{tc})^2 + \frac{ac-b^2}{t^2c^2}]^{\frac{1}{2}}},$$

and $|g(t,\phi)|\le 1$;

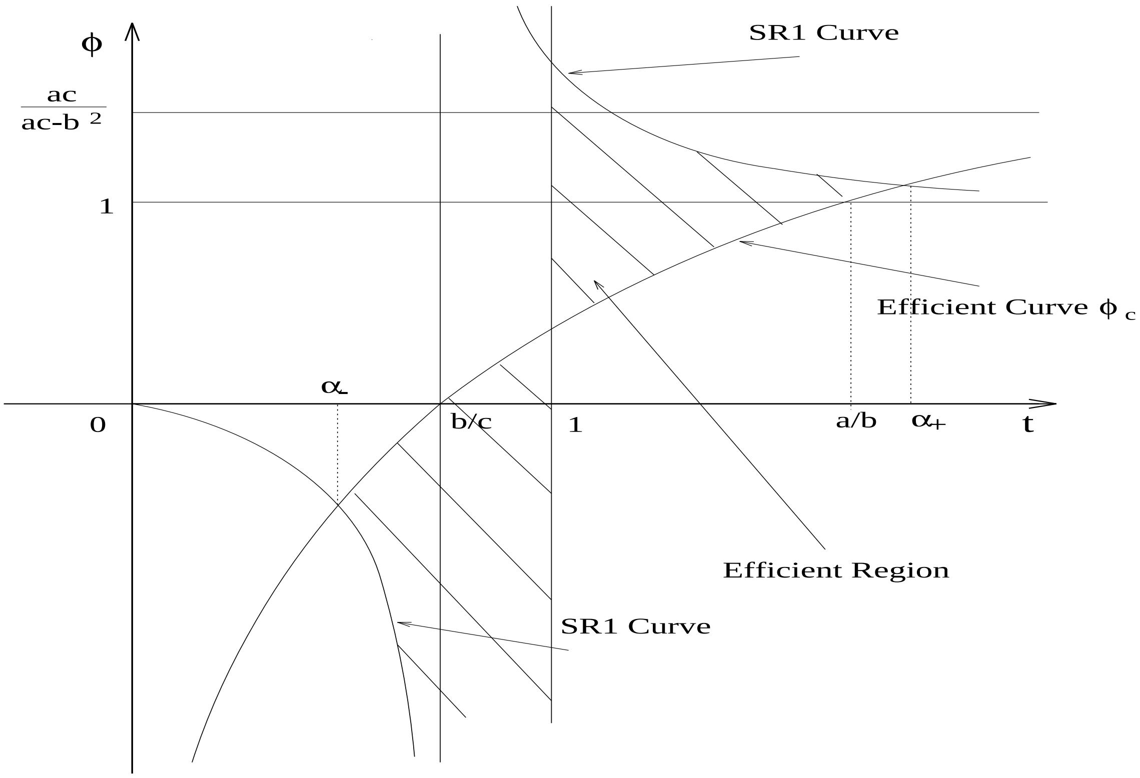

Figure 1: Efficient Region for $\frac{b}{c} < 1$.

2. $\lambda_{\pm}(t, \phi)$ *are isotonic with* $-t$ *for any fixed* ϕ*, and*

$$\frac{\partial \lambda_{\pm}(t, \phi)}{\partial t} = -\frac{a}{2bt^2}(1 \pm d(t, \phi)), \tag{3.6}$$

where

$$d(t, \phi) = \frac{f_1(t, \phi) - \frac{tb}{a} f_2(t, \phi)}{(f_1^2(t, \phi) - f_2(t, \phi))^{\frac{1}{2}}},$$

and $|d(t, \phi)| \leq 1$*.*

Proof. Note that a becomes $\frac{a}{t}$ and c becomes ct when B_c is sized with t. The results in 1. are straightforward extensions of those in [21], see also Lemma 2.1. Here we only prove 2. Differentiating $\lambda_{\pm}(t, \phi)$ yields (3.6). Now,

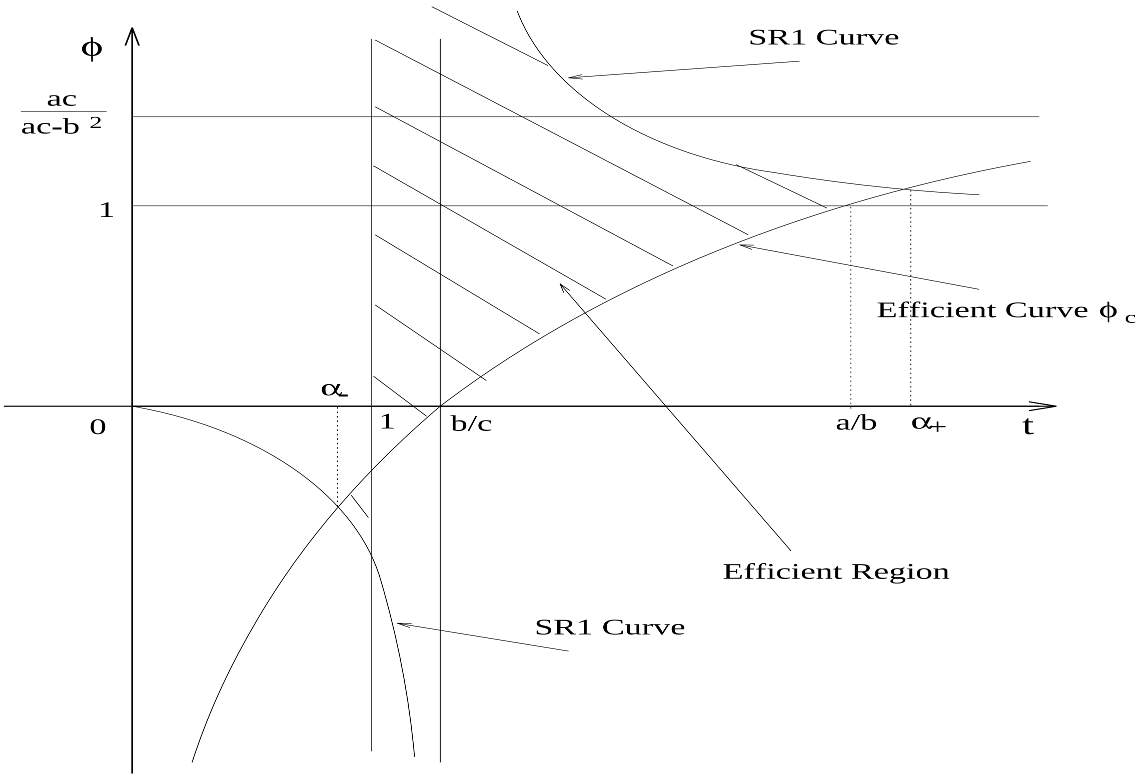

Figure 2: Efficient Region for $\frac{b}{c} > 1$.

in order to show that $\lambda_{\pm}(t,\phi)$ are isotonic with $-t$, we need only show that $|d(t,\phi)| \leq 1$. By squaring both sides, we have

$$(f_1(t,\phi) - \frac{b}{a} f_2(t,\phi))^2 \leq f_1^2(t,\phi) - f_2(t,\phi),$$

which is equivalent to

$$(1 - \frac{\phi(ac-b^2)}{ac})^2(1 - \frac{ac}{b^2}) \leq 0.$$

Therefore, we have

$$\begin{cases} d(t,\phi) = 1 & \text{if } \phi = \frac{ac}{ac-b^2} \\ d(t,\phi) < 1 & \text{otherwise.} \end{cases}$$

$\square$

Note that the derivatives may not exist in the case of multiple eigenvalues. In this case, they are subdifferentiable, since the scaled update $B(t, \phi)$ is a linear function of ϕ and $\frac{1}{t}$ and so the largest and smallest eigenvalues are convex and concave functions, respectively, of ϕ and $\frac{1}{t}$.

Lemma 3.3 *Suppose that $ac - b^2 > 0$ and $(t_1, \phi_1) \in \Phi_R$. Then the level curves for $\lambda_\pm(t, \phi)$ passing through (t_1, ϕ_1) are*

$$\phi = \frac{\lambda_+(t_1, \phi_1)b}{\lambda_+(t_1, \phi_1)ct - b} + \frac{ac - \lambda_+(t_1, \phi_1)b^2}{ac - b^2}, \quad \textit{for } t > \frac{b}{\lambda_+(t_1, \phi_1)c},$$

and

$$\phi = \frac{\lambda_-(t_1, \phi_1)b}{\lambda_-(t_1, \phi_1)ct - b} + \frac{ac - \lambda_-(t_1, \phi_1)b^2}{ac - b^2}, \quad \textit{for } t < \frac{b}{\lambda_-(t_1, \phi_1)c},$$

respectively.

Proof. Let (t, ϕ) be on the level curve for $\lambda_+(t, \phi)$ passing through (t_1, ϕ_1). Then

$$(\lambda_+(t_1, \phi_1) - f_1(t, \phi))^2 = f_1^2(t, \phi) - f_2(t, \phi),$$

which is equivalent to

$$\lambda_+^2(t_1, \phi_1) - 2\lambda_+(t_1, \phi_1)f_1(t, \phi) = -f_2(t, \phi).$$

By putting the expressions for $f_1(t, \phi)$ and $f_2(t, \phi)$ into the above equality, we have

$$\begin{aligned}
&\phi(ac - b^2)(\lambda_+(t_1, \phi_1)ct - b) \\
&= abc\lambda_+(t_1, \phi_1) + \lambda_+(t_1, \phi_1)ac^2t - \lambda_+^2(t_1, \phi_1)b^2ct - abc \\
&= (ac - b^2)\lambda_+(t_1, \phi_1)b + \lambda_+(t_1, \phi_1)ac^2t - \lambda_+^2(t_1, \phi_1)b^2ct - abc + \lambda_+(t_1, \phi_1)b^3 \\
&= (ac - b^2)\lambda_+(t_1, \phi_1)b + (\lambda_+(t_1, \phi_1)ct - b)(ac - \lambda_+(t_1, \phi_1)b^2),
\end{aligned}$$

i.e.,

$$\phi = \frac{\lambda_+(t_1, \phi_1)b}{\lambda_+(t_1, \phi_1)ct - b} + \frac{ac - \lambda_+(t_1, \phi_1)b^2}{ac - b^2}.$$

Moreover, the Raleigh quotient implies that

$$\lambda_+(t_1, \phi_1) \geq \frac{((tB_c)^{\frac{1}{2}}s)^t(tB_c)^{-\frac{1}{2}}B_+(t, \phi)(tB_c)^{-\frac{1}{2}})(tB_c)^{\frac{1}{2}}s}{||(tB_c)^{\frac{1}{2}}s)||^2} = \frac{b}{tc}.$$

Therefore, the level curve is the branch for $t > \frac{b}{\lambda_+(t_1,\phi_1)c}$.

Conversely, for any (t,ϕ) on the curve

$$\phi = \frac{\lambda_+(t_1,\phi_1)b}{\lambda_+(t_1,\phi_1)ct - b} + \frac{ac - \lambda_+(t_1,\phi_1)b^2}{ac - b^2}, \tag{3.7}$$

where $t > \frac{b}{\lambda_+(t_1,\phi_1)c}$, we have

$$|\lambda_+(t_1,\phi_1) - f_1(t,\phi)| = (f_1^2(t,\phi) - f_2(t,\phi))^{\frac{1}{2}}. \tag{3.8}$$

Now $\lambda_+(t_1,\phi_1) - f_1(t,\phi) > 0$ is equivalent to

$$\frac{\frac{ab}{t} + ac - \phi(ac - b^2)}{2b^2} < \lambda_+(t_1,\phi_1). \tag{3.9}$$

After substituting for ϕ using (3.7), and noting that $t > \frac{b}{\lambda_+(t_1,\phi_1)c}$, this is equivalent to $\lambda_+^2(t_1,\phi_1)ct^2 - 2\lambda_+(t_1,\phi_1)bt + a > 0$. This further reduces to $4\lambda_+^2(t_1,\phi_1)(b^2 - ac) < 0$, which clearly holds. Therefore (3.8) becomes

$$\lambda_+(t_1,\phi_1) - f_1(t,\phi) = (f_1^2(t,\phi) - f_2(t,\phi))^{\frac{1}{2}}$$

which yields $\lambda_+(t,\phi) = \lambda_+(t_1,\phi_1)$.

By a similar argument we obtain the level curve for λ_-. □

We now prove the above theorem.

Proof. From Theorem 2.5, for any fixed $t > 0$, we need only consider sized Broyden class updates in the set

$$\Phi_t = \left\{ \phi : \begin{array}{ll} \phi \geq \frac{ct}{ct-b} & \text{if } t < \frac{b}{c} \\ \phi \leq \frac{ct}{ct-b} & \text{if } t > \frac{b}{c} \\ \phi \text{ arbitrary} & \text{if } t = \frac{b}{c} \end{array} \right\}.$$

First suppose that $ac - b^2 > 0$. If we are given a scaled update $B(t,\phi)$ with $\phi \in \Phi_t$, then in order to check efficiency we need to see if the update can be improved with respect to the $n+1$ functions in (3.1). From the proof of Theorem 2.5, we know that (2.11) holds, i.e., $\lambda_2 = \lambda_{n-1} = 1$. Therefore, we need only consider the largest and smallest eigenvalues, $\lambda_\pm$. Moreover, if $r = \frac{1}{t}$, then the scaled update is linear in (r,ϕ), which implies that the largest and smallest eigenvalues $\lambda_\pm$ are convex and concave functions, respectively, of (r,ϕ). Therefore directions of descent correspond to negative directional derivatives. Thus it is easier to view the functions in the space (r,ϕ), which we do.

First suppose that an efficient point (r,ϕ) is given and that $r<1$ (or equivalently $t>1$) and $\lambda_1>1>\lambda_n$. If we hold r fixed, then we obtain $\phi\in\Phi_t$ by Theorem 2.5. Otherwise, at the point (r,ϕ), consider moving in the direction $e=(1\ x)^t\in\Re^2$. Then there is a gain in r and so efficiency implies that we cannot have a gain in both $\lambda_\pm$ as well, i.e., from Lemma 3.2, the directional derivatives (in (r,ϕ) space) cannot satisfy

$$\nabla\lambda_+^t e=\frac{a}{2b}(1+d)-x\frac{ac-b^2}{2b^2}(1+g)<0<\nabla\lambda_-^t e=\frac{a}{2b}(1-d)-x\frac{ac-b^2}{2b^2}(1-g). \tag{3.10}$$

(Note that we have used $\frac{\partial\lambda_\pm(r,\phi)}{\partial r}=\frac{\partial\lambda_\pm(t,\phi)}{\partial t}\frac{-1}{r^2}$, since $t=\frac{1}{r}$.) This reduces to

$$\frac{1+d}{1+g}<\frac{ac-b^2}{2b^2}\frac{2b}{a}x<\frac{1-d}{1-g},$$

which is feasible for x if and only if $d<g$ or equivalently $\phi<\frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t}$, i.e., if $t>1$ and $\lambda_+>1>\lambda_-$, then efficiency implies $\phi\geq\frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t}$. If $\lambda_+=1$ (resp. $\lambda_-=1$), then the left (resp. right) $<$ is replaced by $\leq$ in (3.10). Moreover, $ac-b^2>0$ implies that $\lambda_+>\lambda_-$. Thus $(\phi,t)\in\Phi_R$.

The conclusions for $t<1$ are similar, i.e., finding a direction of improvement implies that $d>g$ or $\phi>\frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t}$. Therefore, if $t<1$, then efficiency implies $\phi\leq\frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t}$. The case for $t=1$ follows from Theorem 2.5. The above argument for efficiency is reversible, since the functions $\lambda_\pm$ are convex and concave, respectively.

If $ac=b^2$, then for each fixed t, the scaled sized Broyden class reduces to the scaled sized SR1 with $n-1$ unit eigenvalues and the remaining eigenvalue given by $1+\frac{(1-\frac{c}{b}t)a}{tb}$. Therefore we need only solve the multicriteria problem with the two functions $|\frac{(\frac{1}{t}-\frac{c}{b})a}{b}|,|t-1|$. This completes the proof that Φ_R is the efficient region. $\square$

Theorem 3.4 *The proper efficient updates for problem (3.1) are the efficient region updates.*

Proof. To prove proper efficiency, we need to consider several cases arising from the definition of the efficient region. Suppose that $(t, \phi) \in \Phi_R$ is given. As in the proof of Theorem 3.1, we continue to let: (t, ϕ) represent the update $B_+(t, \phi)$; and we let $\lambda_\pm$, or $\lambda_{1,n}$, represent the largest and smallest eigenvalues, respectively, of the corresponding scaled update. As in the proof of Theorem 2.8, we can restrict ourselves to $i = 1, n$ and to efficient updates. But, we need to consider the additional objective function $|t-1|$. Moreover, we let $(\bar{t}, \bar{\phi}) \in \Phi_R$ be a given second efficient point, and consider the points and functions in (r, ϕ) space, where $r = \frac{1}{t}$. (So that $\lambda_\pm$ are convex and concave functions, respectively.)

By efficiency, we know that $\lambda_1 = \lambda_+ \geq 1 \geq \lambda_- = \lambda_n$. Therefore, a gain (resp. loss) in the first function corresponds to $\lambda_+ > \bar{\lambda}_+ \geq 1$ (resp. $\bar{\lambda}_+ > \lambda_+ \geq 1$). Similarly, a gain (resp. loss) in the n-th function corresponds to $\lambda_- < \bar{\lambda}_- \leq 1$ (resp. $\bar{\lambda}_- < \lambda_- \leq 1$). However, a gain or loss for the last function is not as simple, e.g., if $r < 1$, then a gain (resp. loss) can be $r < \bar{r} \leq 1$ or $r \leq 1 \leq \bar{r} < 2 - r$, (resp. $\bar{r} < r \leq 1$ or $r \leq 1 \leq 2 - r < \bar{r}$). We have to treat several different cases corresponding to different choices for the numerator and denominator in the gain over loss ratio. We prove the first few cases directly by finding an upper bound to the gain over loss ratio. We then complete the remaining cases by using a proof by contradiction.

Case (i): suppose that we measure a gain in the first function for $(\bar{r}, \bar{\phi})$; thus $\bar{\lambda}_1 < \lambda_1$ since efficiency implies $\lambda_1 \geq 1 \geq \lambda_n$. By efficiency of (r, ϕ) we must have a loss in r or in λ_n.

Subcase (i)(a): Suppose there is no loss in r and so there is a loss $\bar{\lambda}_n < \lambda_n$. If r stays constant, then a bound for the gain/loss ratio follows by applying Theorem 2.8 to the sized update. Otherwise, the direction between the two points must be $e = (\pm 1 \ x)^t$, for some x.

Subsubcase(i)(a)(1): Suppose first that $r < 1$ so that the direction is $e = (1 \ x)^t$. Since $\lambda_\pm$ are convex and concave functions, the ratio of directional derivatives at (r, ϕ), in the direction $-e$, provides an upper bound on gain over loss, i.e.,

$$\frac{\lambda_+ - \bar{\lambda}_+}{\lambda_- - \bar{\lambda}_-} \leq \frac{\nabla \lambda_+^t(-e)}{\nabla \lambda_-^t(-e)}. \tag{3.11}$$

If we differentiate this ratio of directional derivatives, we get

$$\frac{\partial}{\partial x}\left(\frac{\frac{a}{2b}(1+d)-x\frac{ac-b^2}{2b^2}(1+g)}{\frac{a}{2b}(1-d)-x\frac{ac-b^2}{2b^2}(1-g)}\right)=K(d-g),$$

for a positive constant K. We have seen that when $t>1$, efficiency means that $d-g\geq 0$. Therefore, we need to increase x to infinity to get the largest gain over loss ratio, i.e., this means that t stays constant and we can apply the result in Theorem 2.8 to the sized update and get a bound which depends only on (t,ϕ). In particular, the right-hand side in (3.11) yields $\frac{1+g}{1-g}$ as $x\to\infty$. (See also (2.25).)

Subsubcase(i)(a)(2): If $r=1$, then we cannot have an improvement in r and the direction must keep r constant if there is no loss in r. We can again apply Theorem 2.8.

Subsubcase(i)(a)(3): If $r>1$ and there is no loss in r, then the direction must be $e=(-1\ x)^t$. Differentiating the ratio of directional derivatives now yields $-(d-g)$ up to a positive constant. Efficiency in the case $t<1$ now implies that this derivative is nonnegative and so we again increase x to infinity, i.e., t stays constant and we apply Theorem 2.8 to obtain the upper bound for the gain over loss ratio as in (1).

The above presents a direct proof of proper efficiency in several cases, by providing upper bounds for the gain over loss ratio. The remainder of the proof is by contradiction. First, suppose that (r,ϕ) is efficient but not proper. Then there is a sequence of efficient points (r_k,ϕ_k) such that the corresponding gain over loss ratio goes to infinity. Let $e_k=((s_k,\phi_k)-(s,\phi))/||(s_k,\phi_k)-(s,\phi)||$ be the normalized direction between the points. By choosing an appropriate subsequence, we can assume that $e_k\to e$. Then the gradient of the loss functions must be orthogonal to e. For example, if the ratio is a gain for λ_+ over a loss for r, with $r_k<r\leq 1$, then

$$\frac{\lambda_+-\lambda_+^k}{\frac{1}{r_k}-\frac{1}{r}}\leq\frac{\nabla\lambda_+^t(-e_k)}{(\frac{1}{r^2}\ 0)(-e_k)}.$$

Since the left-hand side goes to infinity, and $e_k\to e$, we conclude that e is orthogonal to $(\frac{1}{r^2}\ 0)^t$ and $\nabla\lambda_+^t(-e)\geq 0$, which means $e=(0,1)^t$. But then e is a direction of decrease, or loss, for λ_-, so that the bound for the gain over loss ratio should use λ_-. Moreover, $\nabla\lambda_-^t e\neq 0$, a contradiction to

the ratio being unbounded. We have therefore proven subsubcase(i)(b)(1), where there is a gain in λ_+, a loss in r, and $r_k < r \leq 1$. To complete this special case we have to consider $r \leq 1 \leq 2 - r < r_k$. This is covered in the case $r > 0$ when we replace r by $2 - r$, since $|r - 1| = |2 - r - 1|$.
The case(ii), where there is a gain in λ_-, follows similarly. Note that the gain over loss is $\frac{\bar{\lambda}_- - \lambda_-}{\bar{\lambda}_+ - \lambda_+}$, which is a concave over a convex function.
Case(iii): If we measure a gain in r, then there is a loss in λ_+ (or λ_-). As above, there is a direction $e = (\pm 1 \;\; x)$ such that e is orthogonal to $\nabla\lambda_+$. If $r < 1$, then $e = (1 \;\; x)$ and $x = \frac{a}{2b}\frac{2b^2}{ac-b^2}\frac{1+d}{1+g}$ so that $\nabla\lambda_-^t e = \frac{a}{2b}(1-d) - \frac{a}{2b}\frac{1+d}{1+g}(1-g) = \frac{a}{2b}2(g-d) < 0$, i.e., e is a direction of decrease or loss for λ_- and $\nabla\lambda_-^t e \neq 0$, a contradiction. Therefore, the ratio is bounded again. The other cases follow similarly.

The ratio of gain in t over loss in one of the eigenvalues follows similarly, as does the converse, upon noting that the function in t is linear. $\square$

Corollary 3.5 *The efficient updates for problem (3.1) without the function $|t-1|$ are the self-scaling efficient curve updates, i.e., the sized Broyden class updates $B_+(t, \phi)$, with $(t, \phi) \in \Phi_C$.*

Proof. The proof follows from the proof of the above theorem by combining the two cases $t > 1$ and $t < 1$. $\square$

As was the case for the Broyden efficient class of updates, there is a corresponding inverse efficient region which can be found by scaling the inverse updates and exchanging roles appropriately.

4 Conclusion

We have used multicriteria objectives, based on the eigenvalues of the scaled Hessian, to find an efficient region of updates. We have shown that this region contains the well known updates used to date. Since it is generally acknowledged that the scaled eigenvalues are the determining factor in selecting good updates, we see that we have found a general framework for deriving good updates. Moreover, we have shown that the efficient region is proper efficient.

This region does *not* certify that each update in it is better than all the updates outside the region. However, it *does* guarantee that, for each update outside, there is an update inside that is better. The decision maker (DM) can now chose between different efficient updates; see e.g. [19].

Known results from the theory of multicriteria optimization can now be applied to quasi-Newton updates. For example, we can use the characterization of proper efficiency [15] to show that, for a given efficient update, there corresponds weights w_i, $i = 1, \ldots, n+1$ such that the update is the optimal solution of the *single* objective optimization problem

$$\begin{array}{ll} \min_{t,B_+} & \sum_i^n w_i |\lambda_i((tB_c)^{-\frac{1}{2}} B_+ (tB_c)^{-\frac{1}{2}}) - 1| + w_{n+1}|t-1| \\ \text{subject to} & B_+ s = y, \ B_+ = B_+^t, \ \ t > 0. \end{array} \tag{4.1}$$

This provides new utility functions for deriving updates. Furthermore, by calculating the weights, we can find the relative importance that different updates assign to different eigenvalues.

Up until now, our derivation of the updates has not taken into consideration modern techniques for finding search directions and stepsizes, e.g. using trust regions and inexact linesearches. However, the recent success of the selective sizing updates in a trust region framework (Contreras and Tapia [6]), suggests that these techniques should not be ignored. In both the linesearch and trust region techniques, lower and upper bounds are found for the stepsize in order to guarantee both sufficient decrease of the objective function, as well as convergence. (We restrict ourselves to the linesearch algorithm.) Slow convergence can result if guaranteeing sufficient decrease continually forces the stepsize close to its lower bound. For linesearch algorithms that use only backtracking to guarantee sufficient decrease, it can be advantageous to avoid search directions of small length. This can be done if the eigenvalues of the current Hessian approximation matrix are not too large relative to the eigenvalues of the true Hessian. This is indicated by avoiding $b/c < 1$.

In order to correct the large eigenvalues, Contreras and Tapia used b/c to size B_c, whenever $b/c < 1$. Byrd, Nocedal and Yuan [5] showed that the BFGS update can rapidly correct large eigenvalues. This property is diminished as ϕ is decreased in $[0, 1]$. In particular, the DFP update has no such property. Recall that

$$B_+(t,\phi) = tH_c^{\frac{1}{2}} B H_c^{\frac{1}{2}},$$

where B has $n-2$ unit eigenvalues and the two remaining eigenvalues $\lambda_\pm(t,\phi)$ are isotonic with $-\phi$ and $-t$. From this we can see that in order to decrease the eigenvalues of $B_+(t,\phi)$ we should increase ϕ and t. Moreover, in order to avoid excess function evaluations caused by an overly large quasi-Newton step, we also have to make sure that the eigenvalues are not too small. The efficient region provides a balance among these multiple objectives.

To illustrate how the efficient region works in practice, we choose updates inside, close to the boundary and far away from the efficient region. For comparison, we also include the BFGS update and the selective sizing update of Contreras and Tapia. (Except for BFGS, all the methods size the Hessian approximation by b/c at the initial iteration. Here $\Phi_C(t)$ is the ϕ value corresponding to t on the efficient curve.) The six updating methods we compare are:

(inside region) BFGS

(inside region) if $b/c < 1$, use sized DFP with b/c; otherwise, use DFP

(inside region) if $b/c < 1$, use $B_+(t,\phi)$, where t is randomly selected from $[b/c, 1]$ with $\phi = 0.9\Phi_C(t)$ when $t < 0.9$ and $\phi = 1$ when $t \geq 0.9$; otherwise use DFP

(outside region) if $b/c < 1$, use $B_+(t,\phi)$, where t is randomly selected from $[b/c, 1]$ with $\phi = 1.1\Phi_C(t)$ when $t < 0.9$ and $\phi = 1$ when $t \geq 0.9$; otherwise use DFP

(inside region) if $b/c < 1$, use $B_+(t,\phi)$, where t is randomly selected from $[b/c, 1]$ with $\phi = 0.5\Phi_C(t)$ when $t < 0.9$ and $\phi = 1$ when $t \geq 0.9$; otherwise use DFP

(outside region) if $b/c < 1$, use $B_+(t,\phi)$, where t is randomly selected from $[b/c, (1 + b/c)/2]$ with $\phi = 0.5(\Phi_C(t) + 1)$; otherwise use DFP

We use the standard set of 18 test problems from [14] with initial estimates scaled by: $.1, .5, 1, 2, 3, 4, 5, 6, 7, 8, 10, 20$. The tests were done on a

SUN SPARC station 1 using a MATLAB translation of the codes in [11]. We set 450 as a limit on the number of iterations. Failures were a result of too many iterations. In the case of a failure, we added twice the standard deviation of the successes to the maximum of the successes. We have used the priority theory of Lootsma and Saaty to obtain expected values for iteration and function evaluation counts. (See e.g., Hock and Schittkowski [17].) The given expected values are relative to a value of 1 for the BFGS method with an unscaled initial point. The numerical results and summary are in the following two tables.

Methods:	1	2	3	4	5	6
Iterations:	1.1748	0.9840	0.9577	0.9583	0.9984	0.9267
Fn. eval.:	1.1642	1.0655	0.9281	0.9387	0.9662	0.9372
Fails:	4.0833	1.3333	1.0000	1.2500	1.0833	1.4167

order of best methods for:						
Iterations:	6	3	4	2	5	1
Funtion evaluations:	3	6	4	5	2	1
Failures:	3	5	4	2	6	1

The best method for expected iterations is method 6; while the best for function evaluations is method 3. (Since method 3 was better for failures, this result is dependent on the penalty we assigned for a failure.) This supports our argument that large quasi-Newton steps are obtained by increasing ϕ or decreasing t and that an overly large quasi-Newton step could result in more function evaluations. The best methods for failures are method 3 and method 5. Method 4 also did well. However, method 6 did badly for failures. This shows that the risk of failures is larger for updates far from the efficient region than for those in the efficient region. The bad performance of BFGS emphasizes the importance of sizing.

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