Measures For Least Change Secant Methods

by

Qing Zhao

A thesis
presented to the University of Waterloo
in fulfilment of the
thesis requirement for the degree of
Master of Mathematics
in
Combinatorics and Optimization

Waterloo, Ontario, Canada, 1992

I hereby declare that I am the sole author of this thesis.

I authorize the University of Waterloo to lend this thesis to other institutions or individuals for the purpose of scholarly research.

I further authorize the University of Waterloo to reproduce this thesis by photocopying or by other means, in total or in part, at the request of other institutions or individuals for the purpose of scholarly research.

The University of Waterloo requires the signatures of all persons using or photocopying this thesis. Please sign below, and give address and date.

Abstract

In order to solve an unconstrained optimization problem, quasi-Newton methods are used when the Hessian matrix of the objective function can not be cheaply computed. In these methods, at each step, the current approximation to the Hessian matrix is updated to a new approximation satisfying the secant equation. The open question is how can we find a new approximation which maintains as much information as possible already built up in the current approximation. In this thesis we try to answer this question by considering various measures related to the eigenvalues of the scaled new approximation. The analysis of these eigenvalues plays an important role in our approach.

The measures can be obtained by considering the matrix condition numbers, the volume of the symmetric difference of the ellipsoids corresponding to the Hessian approximation and other concepts. We show that all the ω, σ, and τ optimal updates are also the optimally conditioned updates. Multi-criteria provides means to combine various motivational concepts and updates. We study the efficient class of updates and show that this efficient class is proper. By taking self-scaling into consideration, we present a more general multi-criteria problem, which gives an efficient region and which includes most well-known updates. Non-smooth analysis and perturbation techniques are extensively used in this thesis.

Acknowledgement

My deepest thanks go to my supervisor, Professor Henry Wolkowicz, for his excellent guidance, advice and infinite help throughout my Master's program. I learn a lot from him not only mathematics but his personality.

I would like to thank the Department of Combinatorics and Optimization, University of Waterloo, for their financial support which made my graduate study possible.

Finally, I would like to thank my wife Jiali for her love and encouragement.

Contents

Chapter 1

Introduction

We consider the unconstrained minimization problem

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

where f is twice continuously differentiable. To solve problem (P), various methods have been proposed. Among them, quasi-Newton methods introduced by Davidon in 1959 [1] are well known and successful. These methods are iterative. The required initial data is a starting point $x_0 \in \Re^n$ and an initial approximation B_0 for the Hessian $G = \nabla^2 f(x)$, which is typically chosen as $B_0 = I_{n\times n}$. Given this initial information, at each iteration we use a local quadratic model of the form

$$m_c(x) = f(x_c) + g_c^t(x - x_c) + \frac{1}{2}(x - x_c)^t B_c(x - x_c), \qquad (1.0.0)$$

where x_c is the current approximation to a minimizer x^*, B_c is symmetric positive definite ($s.p.d.$) and is the current approximation to the true Hessian at x_c, and g_c is the gradient at x_c. Let the search direction for $f(x)$ at x_c be

$$d_c = -B_c^{-1} g_c.$$

By using an inexact line search in the direction d_c, we find the steplength α_c and thus obtain a new point x_+

$$x_+ = x_c + \alpha_c d_c,$$

which is then chosen as the next point for the iteration.

A key element of each iteration is the updating of the matrix B_c which takes advantage of the new information about f gathered during the current iteration. Let B_+ be the new approximation to the Hessian at x_+. The local quadratic model at x_+ becomes

$$m_+(x) = f(x_+) + g_+^t(x - x_+) + \frac{1}{2}(x - x_+)^t B_+(x - x_+),$$

where g_+ is the gradient at x_+. The gradient of $m_+(x)$ is

$$\nabla m_+(x) = g_+ + B_+(x - x_+). \tag{1.0.1}$$

Now we can see that $m_+(x_+) = f(x_+)$ and $\nabla m_+(x_+) = g_+$. In order to make the local quadratic model $m_+(x)$ a good approximation to $f(x)$, it is natural that we would want $m_+(x)$ to also satisfy $\nabla m_+(x_c) = g_c$. We thus get the *secant or quasi-Newton equation*

$$B_+ s = y, \tag{1.0.2}$$

where $y \equiv g_+ - g_c$ and $s \equiv x_+ - x_c$. Alternatively, the secant equation can be motivated by Taylor's Formula, i.e. we have

$$y = Gs + o(\|s\|).$$

The higher order terms are zero for a quadratic function and it is convenient to neglect them. Since y and s can only be calculated after the line search is completed, the matrix B_c does not usually relate them correctly, i.e. $B_c s$ does not necessarily equal y. Thus B_+ is chosen so that it does correctly relate these differences, that is

$B_+ s = y$. The symmetric matrices B_+ that satisfy the secant equation are referred to as *updates*. The best known updates are the Broyden family of updates (see Subsection 2.1.1 below). Throughout this thesis we assume $y^t s > 0$ and B_c *s.p.d* unless otherwise noted.

1.1 Least Change Secant Methods

Least change secant methods consist in finding an updated Hessian approximation B_+ which is *s.p.d.*, satisfies the secant equation (1.0.2), and simultaneously preserves as much information as possible from the current Hessian B_c. Various measures can be used to preserve information from B_c. These measures usually define the distance in some metric of an *s.p.d.* matrix to the identity or a multiple of the identity. For example the Frobenius norm (and weighted Frobenius norm) gives rise to various rank-two updates of B_c. These include the popular BFGS and DFP updates from the Broyden class, see e.g.[2] and [3]. In [4] it is shown that the measure

$$\omega(A) = \frac{(\operatorname{trace} A)/n}{\det(A)^{1/n}}, \tag{1.1.3}$$

where det denotes determinant, gives rise to sized updates. *Sized* update means that B_+ is the update of αB_c, $\alpha > 0$, instead of B_c. In [5], a study of the volumes of the ellipsoids corresponding to B_c and B_+ give rise to the measures

$$\sigma(A) = \frac{\lambda_1(A)}{\det(A)^{1/n}} \tag{1.1.4}$$

and

$$\max\{\det(A) : \lambda_1(A) \leq 1\}. \tag{1.1.5}$$

These two measures give rise to the optimally conditioned, sized, symmetric rank-one updates (OCSSR1) and the symmetric rank-one (SR1) update, respectively.

The functions ω and σ measure how far an *s.p.d.* matrix is from a multiple of the identity. Thus they can be considered as condition numbers similar to the usual condition number

$$\kappa(A) = \frac{\lambda_1(A)}{\lambda_n(A)}. \tag{1.1.6}$$

In addition, they can be thought of as potential functions, e.g.

$$\log \omega(A) = \log(\frac{\sum \lambda_i(A)}{\Pi \lambda_i(A)})$$

is the potential function used by Karmarkar [6] after scaling the objective function.

This thesis studies the matrix design question of how to choose a good update. Though quasi-Newton methods have been extensively studied since 1959, it is still unknown what the best update is and which criterion determines a good update. Function evaluations may be very expensive, so an inexact line search is usually used. This increases the importance of obtaining good updates and also makes the analysis of a good update very hard. It is generally believed that the eigenvalues of the scaled update $B = H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ $(H_c = B_c^{-1})$ play an important role in determining whether one update is better than another. We present various measures which utilize this eigenvalue information. Thus we study problems of the type

$$\min \ f(B) \ \text{ s.t. } B(B_c^{\frac{1}{2}} s) = (H_c^{\frac{1}{2}} y), \quad B \ \ s.p.d.,$$

where f is an appropriate measure.

1.2 Overview

We now summarize the contents of the thesis. In Chapter 2, we first give some definitions and provide some basic results on the Broyden class of updates. We will also introduce various scalings and motivations. Finally, we include some numerical results, which not only present a picture of how well various quasi-Newton methods work but also provide the motivation for us to dig out the reasons behind these results by trying different least change methods.

In Chapter 3, we include Wolkowicz's work in [5] to consider the volume of the ellipsoids corresponding to B_c and B_+ as a measure for improving convergence of least change secant methods and then see how this measure provide a motivation for the σ measure.

Chapter 4 concerns condition numbers. We will see how and why condition numbers can determine the error of the solution of a linear system and see the motivation for introducing the uniform condition number. We also include some properties of κ, ω, σ and τ condition numbers.

In Chapter 5, we first include the optimal results for the κ measure from [5], and then by their properties, we will directly show that all ω, σ and τ optimal updates are κ-optimal updates and then give their expression in the scaled Broyden class.

In Chapter 6, multi-criteria analysis provides a framework to combine various motivations and updates. All well known (to us) updates fall into an efficient region. We first consider the results of a multi-criteria problem introduced by Byrd, which gives an efficient Broyden class. By using the subgradients for largest and smallest eigenvalues, we provide a proof for the results of Byrd. Furthermore, by introducing the concept of proper efficiency, we show that the efficient Broyden class is also proper. Finally, by taking the self-scaling into consideration, we present a more general multi-criteria problem and get its efficient Broyden region, which contains all of the rank-two κ-optimal updates, and among them are ω, σ and τ optimal updates.

In Chapter 7, we use a parametric approach in the case that $y^t s \leq 0$, i.e. when the hereditary positive definiteness of the updates fails.

Chapter 2

Preliminaries

2.1 Definitions

Definition 2.1 *For* $x = (x_1, x_2, \ldots, x_n)^t \in \Re^n$, $1 \le p < \infty$, *the* l_p *norm of* x *is*

$$\|x\|_p = (\sum_{i=1}^{n} |x_i|^p)^{1/p}.$$

Definition 2.2 *For a matrix* $A = (a_{ij}) \in \Re^{n \times n}$, $1 \le p < \infty$, *the induced matrix norm* $\| \ \|_p$ *of* A *is*

$$\|A\|_p = \max_{x \in \Re^n, x \ne 0} \frac{\|Ax\|_p}{\|x\|_p}.$$

Note that for a symmetric positive semi-definite matrix A, $\|A\|_2 = \lambda_1$, is the largest eigenvalue of A. Throughout this thesis, we use $\| \ \|$ for $\| \ \|_2$ when the meaning is clear.

Definition 2.3 *For a matrix* $A = (a_{ij}) \in \Re^{n \times n}$, *the Frobenius norm is*

$$\|A\|_F = (\sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|^2)^{1/2} = [\mathrm{trace}\,(A^t A)]^{1/2}.$$

Definition 2.4 *Let H denote B^{-1} and*

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

2.1.1 Broyden Family of Updates

The Broyden family of updates can be parametrized by

$$B_\phi = B_c - \frac{1}{s^t B_c s} B_c s s^t B_c + \frac{1}{y^t s} y y^t + (1-\phi) s^t B_c s w w^t, \tag{2.1.7}$$

where $w = \frac{1}{y^t s} y - \frac{1}{s^t B_c s} B_c s$. We assume that the current approximation B_c to the Hessian is *s.p.d.* and $y^t s > 0$. If $\phi = 1$ we get the BFGS update, $\phi = 0$ yields the DFP update and $\phi = \frac{c}{c-b}$ gives the SR1 update. The updates for $\phi \in [0,1]$ are called the convex class. Moreover, $\phi < \frac{ac}{ac-b^2}$ if and only if B_ϕ is *s.p.d.*

If we form the Fletcher dual updates, i.e. we exchange the roles of y and s, then we get the inverse updates

$$H_{\hat{\phi}} = H_c - \frac{1}{y^t H_c y} H_c y y^t H_c + \frac{1}{y^t s} s s^t + (1-\hat{\phi}) y^t H_c y v v^t, \tag{2.1.8}$$

where

$$v = \frac{1}{y^t s} s - \frac{1}{y^t H_c y} H_c y.$$

We now have that $\hat{\phi} = 1$, $\hat{\phi} = 0$ and $\hat{\phi} = \frac{a}{a-b}$ yield the DFP, BFGS and SR1 updates, respectively. Note that $b^2 \leq ac$ with equality if and only if $B_c^{-\frac{1}{2}} y$ and $B_c^{\frac{1}{2}} s$ are collinear, which is true if and only if y and $B_c s$ are collinear, which is true if and only if $H_c y$ and s are collinear. In general,

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

is a 1-1 and onto mapping for $\phi < \frac{ac}{ac-b^2}$. The mapping satisfies $\iota^2(\phi) = \phi$ and the convex class $\phi \in [0,1] \rightarrow \hat{\phi} \in [0,1]$. Furthermore, every member of the Broyden family of updates satisfies the secant equation, i.e., for every ϕ,

$$B_\phi s = y.$$

Unfortunately (or fortunately), the converse does not generally hold. However, the following theorem, due to Davidon [7], shows that under certain conditions the converse does hold. (We provide a proof below.)

Theorem 2.1 *Let $y^t s > 0$, B_c be s.p.d. and suppose that B_+ satisfies the secant equation (1.0.2). 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.*

Proof. Sufficiency is clear from the parametrization (2.1.7).

Now, assume that the columns of $B_+ - B_c$ are in the span of $\{B_c s, y\}$. Then B_+ can be expressed in the following form

$$B_+ = B_c + \alpha B_c s s^t B_c + \beta y y^t + \gamma(B_c s y^t + y s^t B_c) \tag{2.1.9}$$

and by multiplying (2.1.9) by s, we have

$$y = B_c s + c\alpha B_c s + b\beta y + \gamma(b B_c s + c y)$$

or $(1 - b\beta - c\gamma)y = (1 + c\alpha + b\gamma)B_c s$. If $B_c s$ and y are collinear, B_+ is the symmetric rank-one update of B_c, the SR1, which is a member of the Broyden family for $\phi = -\frac{c}{b-c}$. Thus we can assume that $B_c s$ and y are not collinear. We now have

$$1 - b\beta - c\gamma = 0 \tag{2.1.10}$$

and

$$1 + c\alpha + b\gamma = 0. \tag{2.1.11}$$

By solving (2.1.10) and (2.1.11), we have

$$\alpha = -\frac{1+b\gamma}{c} \tag{2.1.12}$$

and

$$\beta = \frac{1-c\gamma}{b}. \tag{2.1.13}$$

By substituting both (2.1.12) and (2.1.13) into (2.1.9) and letting $\phi = 1 + b\gamma$, we obtain

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

where $w = \frac{1}{y^t s} y - \frac{1}{s^t B_c s} B_c s$. ▮

Corollary 2.1 *Suppose that B_+ satisfies the secant equation. Then B_+ is in the Broyden class if and only if $B = H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ is at most a rank two update of I with $n-2$ 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 theorem 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 a rank two update of I with eigenvectors in this span. ▮

From the proof of Theorem 2.1, we can see that when B_c and B_+ are symmetric positive semi-definite and $s^t B_c s > 0$, the necessary and sufficient conditions of the theorem still hold.

Theorem 2.2 *Let $y^t s > 0$, $s^t B_c s > 0$, and both B_c and B_+ be symmetric positive semi-definite. If B_+ satisfies the secant equation, then the columns of $B_+ - B_c$ are in the span of $\{B_c s, y\}$ if and only if $B_+ = B_\phi$, given in (2.1.7).*

We include the following explicit representation of the eigenvalues of a scaled Broyden class update. This result is in Schnabel [3].

Lemma 2.1 *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*

$$\lambda_\pm(\phi) = f_1(\phi) \pm (f_1(\phi)^2 - f_2(\phi))^{\frac{1}{2}}, \tag{2.1.14}$$

where

$$\begin{cases} f_1(\phi) = \frac{a(b+c)-\phi(ac-b^2)}{2b^2} \\ f_2(\phi) = \frac{a}{b} - \frac{\phi(ac-b^2)}{bc}. \end{cases} \tag{2.1.15}$$

Furthermore, $\lambda_\pm(\phi)$ are isotonic with $-\phi$ (i.e. $\lambda_\pm(\phi)$ is a monotone decreasing function of ϕ) and

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

where

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

A detailed discussion and proof are found in [3]. From this lemma, we immediately have the following theorem. The theorem shows that the eigenvalues $\lambda_\pm$ in (2.1.14) are the largest and the smallest if and only if ϕ lies on the 'good' side of the SR1.

Theorem 2.3 *The largest and the smallest eigenvalues of the matrix $B_c^{-\frac{1}{2}} B_\phi B_c^{-\frac{1}{2}}$ are $\lambda_\pm(\phi)$, respectively, if and only if $b = c$ or ϕ satisfies*

$$\begin{cases} \phi \in [\phi_{SR1}, \infty) & \text{if } b > c \\ \phi \in (-\infty, \phi_{SR1}] & \text{if } b < c \end{cases} \tag{2.1.16}$$

where $\phi_{SR1} = -\frac{c}{b-c}$.

Proof. We assume that λ_+ and λ_- are the largest and the smallest eigenvalues, respectively. By Lemma 2.1, we have

$$\begin{cases} f_1(\phi) + (f_1(\phi)^2 - f_2(\phi))^{\frac{1}{2}} \geq 1 \\ f_1(\phi) - (f_1(\phi)^2 - f_2(\phi))^{\frac{1}{2}} \leq 1, \end{cases}$$

which is equivalent to $|f_1(\phi) - 1| \leq (f_1(\phi)^2 - f_2(\phi))^{\frac{1}{2}}$. thus, by squaring both sides, we have

$$-2f_1(\phi) + 1 \leq -f_2(\phi). \tag{2.1.17}$$

By substituting (2.1.15) into (2.1.17), we have

$$(b - c)\phi \geq -c \tag{2.1.18}$$

which implies either $b = c$ or

$$\begin{cases} \phi \geq -\frac{c}{b-c} & \text{if } c < b \\ \phi \leq -\frac{c}{b-c} & \text{if } c > b, \end{cases} \tag{2.1.19}$$

that is

$$\begin{cases} \phi \in [\phi_{SR1}, \infty) & \text{if } c < b \\ \phi \in (-\infty, \phi_{SR1}] & \text{if } c > b. \end{cases} \tag{2.1.20}$$

The sufficiency can be obtained by reversing the order of the above steps. ∎

Note from this theorem, since $\phi \in [0, 1]$ always satisfies (2.1.16), we can see that $\lambda_\pm(\phi)$ are the largest and the smallest eigenvalues of the convex class of scaled updates $B_c^{-\frac{1}{2}} B_\phi B_c^{-\frac{1}{2}}$.

2.2 Scaling

2.2.1 Linear Equations

Consider the linear system

$$Ax = b.$$

The solution can be found by solving the scaled system

$$D_1^{-1} A D_2 y = D_1^{-1} b,$$

where D_1 and D_2 are positive diagonal matrices, and then setting $x = D_2 y$. Let Δx and Δy be the perturbations of x and y, respectively. Then we have

$$\frac{\|\Delta x\|}{\|x\|} \leq u \cdot \kappa(A)$$

and

$$\frac{\|D_2^{-1} \Delta x\|}{\|D_2^{-1} x\|} = \frac{\|\Delta y\|}{\|y\|} \leq u \cdot \kappa(D_1^{-1} A D_2),$$

where u is the relative error of data. Thus, if $\kappa(D_1^{-1} A D_2)$ can be made considerably smaller than $\kappa(A)$, we might expect a correspondingly more accurate $\hat{x} = x + \Delta x$. Therefore, ill-conditioned linear systems are usually scaled. The scaling tackles two issues: the condition number of the linear system and the estimation of the error.

A difficult problem is that of finding scaling matrices D_1 and D_2 that minimize the l_2 condition number of $D_1^{-1} A D_2$ (see, e.g. [8] and [9]). One technique is *simple row scaling.* In this scheme D_2 is the identity and D_1 is chosen so that each row in $D_1^{-1} A$ has approximately the same norm. Some results are known, see e.g. [10]. Other condition numbers are more suitable when used to find scaling matrices. Also, arguments can be made that other condition numbers are more suitable when measuring the conditioning of a matrix. The l_2 condition number only considers the largest and smallest singular values of a matrix. Other measures, such as ω, σ, take all the singular values into account.

2.2.2 Newton-type Methods

Scaling is important in minimizing a function f. After applying the invertible linear transformation T, suppose that the method of steepest descent is applied to the unconstrained minimization of the function $h(y) = f(Ty)$. The unconstrained minimum of f is then $x = Ty$, where y is the unconstrained minimum of h. The steepest descent direction for h is

$$-\nabla h(y) = -\nabla_y f(Ty) = -T^t \nabla_x f(x),$$

where $x = Ty$. In the original variable x, the direction is $-TT^t \nabla_x f(x)$, i.e. it is a 'deflected' gradient direction. Therefore, we see the steepest descent direction is affected by this transformation, i.e. the steepest descent algorithm is not scale-free.

Also, the Newton direction for h is

$$-[\nabla_y^2 h(y)]^{-1} \cdot \nabla_y h(y).$$

Since the Hessian after the scaling is

$$\nabla^2 h(y) = T^t \nabla^2 f(x) T,$$

we see that, the Newton direction in the original variable x, is

$$\begin{aligned} -T[\nabla^2 h(y)]^{-1} \nabla h(y) &= -T(T^t \nabla^2 f(x) T)^{-1} T^t \nabla f(x) \\ &= -[\nabla_x^2 f(x)]^{-1} \nabla_x f(x) \end{aligned}$$

which shows that Newton's method is scale free. The rate of convergence of steepest descent depends on the condition number of the Hessian. The Hessian after the scaling is

$$\nabla^2 h(y) = T^t \nabla^2 f(x) T.$$

The condition number of this Hessian is at its optimal value 1 when T is chosen so that

$$TT^t = [\nabla^2 f(x)]^{-1}.$$

(Assuming that the Hessian is positive definite and so has a Cholesky decomposition.) Thus the optimal scaling, or deflection, is given by e.g.

$$T = [\nabla^2 f(x)]^{-\frac{1}{2}}.$$

This gives rise to Newton's method and shows that scaling is a strong technique for improving the convergence. In this sense Newton's method possesses a better convergence property than steepest descent. (See e.g. [11].)

In quasi-Newton methods, at each iteration, any *s.p.d.* matrix satisfying the secant equation (1.0.2) is a candidate for the new update. In order to maintain as much curvature information already stored in B_c as possible, it is natural that we want to choose the "closest" matrix B_+ to B_c. However, B_+ may become ill-conditioned even though B_c is well conditioned. Therefore, we should choose the matrix B_+ which is the "closest" to B_c and is well conditioned. In order to achieve this, we can use the above idea to find a matrix T for scaling. The following two theorems support this idea. (see e.g. [2])

Theorem 2.4

$$\min_{\substack{B_+ s = y \\ B_+ s.p.d.}} \|T(H_+ - H_c)T^t\|_F,$$

where $T^tTs = y$ and T nonsingular, yields the BFGS update.

Theorem 2.5

$$\min_{\substack{B_+ s = y \\ B_+ s.p.d.}} \|W(B_+ - B_c)W^t\|_F,$$

where $W^tWy = s$ *and* W *nonsingular, yields the DFP update.*

Note that without scaling by T, the minimization problems in both Theorem 2.4 and Theorem 2.5 become

$$\min_{\substack{B_+ s = y \\ B_+ s.p.d.}} \|H_+ - H_c\|_F$$

and

$$\min_{\substack{B_+ s = y \\ B_+ s.p.d.}} \|B_+ - B_c\|_F,$$

respectively, which yield the Greenstadt update and PSB update, respectively. But as is well known, the Greenstadt update and PSB update may not be *s.p.d.* Therefore, we can see that by using the scaling matrix T, the above minimization problems 'center' the problem. This centering provides hereditary symmetric positive definiteness.

2.3 Numerical Tests

Before we further discuss these update methods and relate them to various least change measures in the following sections, let us take a look at some of the numerical test results in the literature for some of these update methods to get a picture of how well these methods work. This also provides us with a motivation to dig out the reasons behind these results by trying different least change methods.

The most famous updates are the BFGS and DFP updates and their linear combinations, i.e. the Broyden class. It is generally agreed that the BFGS is more efficient than the DFP, which has been shown by various numerical tests, see for example, Powell [12]. The numerical tests in Byrd, Nocedal and Yuan [13] showed further that the updates in the restricted $[0,1]$ Broyden class may become more and more efficient as the parameter ϕ goes increasingly from DFP ($\phi = 0$) to BFGS ($\phi = 1$) and even beyond.

In order to find a quasi-Newton update which is more efficient than the BFGS method, various methods have been tried. Davidon in [7] got the following optimal conditioned update method by minimizing the condition number of $H_c B_+$ restricted to the Broyden class:

$$B_+ = B_\phi,$$

where

$$\phi = \begin{cases} 1 - \frac{(a-b)b}{ac-b^2} & \text{if } 2ac > (a+c)b \\ \frac{c}{c-b} & \text{if } 2ac \le (a+c)b. \end{cases}$$

But numerical tests, see for example Schnabel [3], showed that this optimal condition number update does not provide a significant improvement over the BFGS method.

The analysis in [13] suggests that the BFGS method is better at correcting small eigenvalues than large ones. By similar analysis one may expect that the large eigenvalues can be corrected by choosing $\phi > 1$, as was done by Zhang and Tewarson [14]. Their numerical results show a moderate but consistent improvement over the BFGS method. However, Byrd, Liu and Nocedal in [15] show that this method is not superlinearly convergent, in general.

One can also attempt to improve quasi-Newton methods by using self-scaling or sizing strategies, i.e. update tB_c instead of B_c. The numerical results in Dennis and Wolkowicz [4] show that sizing improves the DFP update. This was also shown in Nocedal and Yuan [16]. Several choices for t have been proposed by Oren and Luenberger in [17] and [18], among them $t = b/c$ is often recommended. Dennis and Wolkowicz in [4] obtained the sizing scalars $t = a/b$ and $t = b/c$ by introducing the uniform condition number ω. Wolkowicz in [5] also gives sized SR1 updates by using the volume of ellipsoids motivation. In the numerical tests in both [4] and [5], the priority theory of Lootsma and Saaty is used. It is based on a pairwise comparison of the method iteration and function evaluation count on the various problems. These numerical test results show the importance of self-scaling. However, the numerical results in Shanno and Phua [19] show that self-scaling algorithms may perform badly. They introduce a strategy that only sizes at the first iteration. Their numerical tests show that this method is more efficient than BFGS. The numerical tests in [4] seem to support their idea. Tapia and Contreras in [20] present a selective sizing strategy, from both their numerical test results and the results in Wolkowicz [5], it seems to us that the selective sizing is presently the most efficient.

Yuan in [21] presents a modified BFGS method which does not necessarily satisfy the secant equation. Anjos [22] extended this idea to the Broyden class. From their numerical tests, we can see that the results are encouraging. Also recently factorized-selective column scaling was introduced by Siegel [23], which seems very encouraging.

There are also some interesting numerical results in Al-Baali [24], Hu and Storey [25] and Luksan [26] on optimal conditioning and self scaling. Khalfan [27] gives some numerical tests on the SR1. The above various test results are all inconclusive and many are contradictary. This motivates us to use various measures to explain these results.

Chapter 3

Volume of Ellipsoids

3.1 Motivation

In this chapter we review the volume of ellipsoids as a measure for least change discussed in [5]. In order to find an update B_+ that satisfies the secant equation while simultaneously preserving as much information already built up in the current Hessian approximation B_c as possible, B_+ and B_c should be close in some sense. We now try to find B_+ in the following sense. Assume the gradient vector g_+ can be a random direction (of norm 1 say), then we can consider that B_+ is preserving the information from B_c when the search directions H_+g_+ and H_cg_+ are close. Thus, we can regard B_+ as a least change update of B_c if the images of the unit ball under H_+ and H_c are close. Suppose that B is *s.p.d.* Denote the ellipsoid for B of radius α by

$$E_\alpha(B) = \{x \in \Re^n : ||Bx|| \leq \alpha\} = \{x \in \Re^{n\times n} : x^t B^2 x \leq \alpha^2\}. \qquad (3.1.21)$$

Note that the unit ball is $E_1(I)$ and the ellipsoid corresponding to the square root of B is

$$E_\alpha(B^{\frac{1}{2}}) = \{x \in \Re^n : x^t B x \leq \alpha^2\}. \tag{3.1.22}$$

Also note that the image of the ball under $H = B^{-1}$ is $H(E_\alpha(I)) = E_\alpha(B)$. Therefore, in order to have $H_+(E_\alpha(I))$ and $H_c(E_\alpha(I))$ close, we should make $E_\alpha(B_+)$ and $E_\alpha(B_c)$ close. Let us use the volume as a measure of closeness for ellipsoids. It would be best if we could find the update B_+ so that the volume of the symmetric difference of the updated and current ellipsoids

$$\mathrm{vol}(E_\alpha(B_+) \cup E_\alpha(B_c) - E_\alpha(B_+) \cap E_\alpha(B_c))$$

is minimized. The following presents relaxations to this problem.

3.2 Two Measures for Volume

The volume of the ellipsoid $E_\alpha(B)$ is the determinant of H times the volume of $E_\alpha(I)$, i.e.

$$\mathrm{vol}(E_\alpha(B)) = \frac{\alpha^n}{\det(B)}\mathrm{vol}(E_1(I)).$$

Given B fixed, since

$$\lambda_1(B) = \max_{x \in E_1(I)} \|Bx\|,$$

the ellipsoid of minimal volume containing $E_1(I)$ is $E_\alpha(B)$ with $\alpha = \lambda_1(B)$. Therefore, the n-th root of the volume of the ellipsoid leads to the measure

$$\sigma(B) = \frac{\lambda_1(B)}{\det(B)^{\frac{1}{n}}}.$$

We also need the measure

$$s(B) = \frac{\|B\|_2}{\det(B)^{\frac{1}{n}}},$$

where $\|B\|_2$ denotes the spectral norm of B, i.e. the largest singular value of B. Note that both measures σ and s are well defined if B has real positive eigenvalues. Moreover, in this case, $\sigma(B) \leq s(B)$ and equality holds if B is *s.p.d.*. However, it can be shown that the two measures are not necessarily isotonic.

3.3 Optimal Volume Updates

We now present two theorems and their corollaries from [5] which characterize the ellipsoids $E_\alpha(B_+)$ and $E_1(B_+)$ of minimal (maximal) volume that contain (are contained in) $E_1(B_c)$.

Theorem 3.1 *Suppose that B_c s.p.d. is given and Ω is a closed set of symmetric matrices which intersects the set of s.p.d. matrices. Then:*

a) The s.p.d. update B_+ in Ω which yields the ellipsoid $E_\delta(B_+)$ of minimal volume that contains $E_1(B_c)$ is the solution of

$$\min_{\substack{B_+ \in \Omega \\ B_+ s.p.d.}} \quad s(H_c B_+) \tag{3.3.23}$$

with $\delta = \lambda_1(H_c B_+)$. Moreover, the volume ratio satisfies

$$1 \leq \frac{\mathrm{vol}(E_\delta(B_+))}{\mathrm{vol}(E_1(B_c))} = s(H_c B_+)^n.$$

b) The s.p.d. update B_+ in Ω which yields the ellipsoid $E_\beta(B_+)$ of maximal volume contained in $E_1(B_c)$ is the solution of

$$\min_{\substack{B_+ \in \Omega \\ B_+ s.p.d.}} \quad s(H_+ B_c) \tag{3.3.24}$$

with $\beta = 1/\lambda_1(H_+B_c)$. *Moreover, the volume ratio satisfies*

$$1 \leq \frac{\mathrm{vol}(E_1(B_+))}{\mathrm{vol}(E_\beta(B_c))} = s(H_+B_c)^n.$$

c) If $\Omega = \{B = B^t : Bs = y\}$, *then the minimum in both minimization problems is attained.*

Proof. Given B_+ and B_c fixed, the ellipsoid of minimal volume for B_+ that contains $E_1(B_c)$ is $E_\delta(B_+)$, where δ is the solution of the generalized eigenvalue problem

$$\delta = \max_{\|B_cx\|\leq 1} \|B_+x\|.$$

After substituting $x = H_cy$ with $\|y\| \leq 1$, we get $\delta = \|(H_cB_+)\|_2$. Therefore, with only B_c fixed, we minimize $\frac{\|(H_cB_+)\|_2^n}{\det(B_+)}$ or equivalently $s(H_cB_+)$ to find the ellipsoid of minimal volume.

Similarly, the ellipsoid of maximum volume for B_+ that is contained in $E_1(B_c)$ is $E_\beta(B_+)$, where the fact that $E_1(B_+) \subset E_{\frac{1}{\beta}}(B_c)$ if and only if $E_\beta(B_+) \subset E_1(B_c)$ implies that $\beta = \frac{1}{\|(H_+B_c)\|_2}$, i.e. we maximize $\frac{\frac{1}{\|(H_cB_+)\|_2^n}}{\det(B_+)}$ or equivalently minimize $s(H_+B_c)$.

The volume ratios follow from the definitions. To prove c), note that the functions are bounded below by 1 and bounded above by the fact that there is a feasible *s.p.d.* matrix, since we assume that $b > 0$. Attainment follows from the restriction on the singular values by the secant equation. ▮

Corollary 3.1 *Under the hypotheses of the above Theorem, if the matrices* B_+, B_c, H_+, H_c *are replaced by their respective square roots, with* $\Omega = \{B^{\frac{1}{2}} : Bs = y\}$, *then the Theorem holds with* $\delta = \sqrt{\lambda_1(H_cB_+)}$ *and* $\beta = 1/\sqrt{\lambda(H_+B_c)}$ *and with the* *measure s replaced by* $\sqrt{\sigma}$*, the square root of the measure* σ*, so that the two volume ratios are* $\sigma(H_cB_+)^{\frac{n}{2}}$ *and* $\sigma(H_+B_c)^{\frac{n}{2}}$*, respectively.*

The above theorem provides updates H_+ so that $H_+(E_\delta(I))$ and $H_+(E_\beta(I))$ approximate $H_c(E_1(I))$. The Corollary is used to derive the optimally conditioned $SR1$ updates. However, for H_+g_+ to properly approximate H_cg_+, we would like δ and β to be 1. This is done in the following.

Theorem 3.2 *Suppose that* B_c *s.p.d. is given and* Ω *is a closed set of symmetric matrices which intersects the set of s.p.d. matrices. Then:*

a) If there exists an s.p.d. B *in* Ω *such that* $\lambda_1(H_c^{\frac{1}{2}}BH_c^{\frac{1}{2}}) \leq 1$*, then the s.p.d. update* B_+ *in* Ω *which yields the ellipsoid* $E_1(B_+)$ *of minimal volume that contains* $E_1(B_c)$ *is the solution of*

$$\max_{\substack{B_+ \in \Omega \\ B_+ s.p.d. \\ \lambda_1(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) \leq 1}} \quad \det(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}).$$

Moreover, the volume ratio satisfies

$$1 \leq \frac{\mathrm{vol}(E_1(B_+))}{\mathrm{vol}(E_1(B_c))} = \det(B_cH_+).$$

b) If there exists an s.p.d. B *in* Ω *such that* $\lambda_1(B_c^{\frac{1}{2}}HB_c^{\frac{1}{2}}) \leq 1$*, then the s.p.d. update* B_+ *in* Ω *which yields the ellipsoid* $E_1(B_+)$ *of maximal volume contained in* $E_1(B_c)$ *is the solution of*

$$\max_{\substack{B_+ \in \Omega \\ B_+ s.p.d. \\ \lambda_1(B_c^{\frac{1}{2}}H_+B_c^{\frac{1}{2}}) \leq 1}} \quad \det(B_c^{\frac{1}{2}}H_+B_c^{\frac{1}{2}}).$$

Moreover, the volume ratio satisfies

$$\frac{\mathrm{vol}(E_1(B_c))}{\mathrm{vol}(E_1(B_+))} = \det(B_+ H_c).$$

c) If $\Omega = \{B = B^t : Bs = y\}$*, then (under the feasibility assumption) the maximum in both maximization problems is attained.*

Proof. The proof for a) follows by noting that the volume of $E_1(B_+)$ is the volume of $E_1(I)$ divided by $\det(B_+)$ and that

$$E_1(B_c) \subset E_1(B_+) \Leftrightarrow \|(B_+ H_c)\|_2 \leq 1.$$

The proof of b) is similar. Attainment follows by the constraint on the norm and the fact that, on *s.p.d.* matrices, the function $\det^{\frac{1}{n}}$ is concave and increasing, or the function $\log\det$ is concave and strictly increasing. ∎

Corollary 3.2 *Under the hypotheses of the above theorem, if the matrices* B*,* B_+*,* B_c*,* H_+*,* H_c *are replaced by their respective square roots, then the Theorem holds with the spectral norm* $\|.\|$ *replaced by the square root of the largest eigenvalue* $\sqrt{\lambda_1(.)}$.

The proofs of the above two theorems can be found in [5]. The above two theorems provide updates B_+ such that the ellipsoids $E_1(B_+)$ contain, or are contained in, $E_1(B_c)$. It appears intuitively clear that convex combination of these updates should improve the value of the symmetric difference.

Chapter 4

Condition Numbers

4.1 Condition Numbers

An ill-conditioned problem is one for which the values to be computed are very sensitive to changes in the data. The amplification factors for the relative error in the computed values of a problem with respect to the relative error in the data are called *condition numbers*, see e.g. [28], [10]. For linear algebra related problems, the condition number is usually defined in conjunction with a related norm. Condition numbers and estimates for condition numbers are used to determine errors arising in algorithms, see e.g. [29].

Let us take a look at the linear system

$$Ax = b, \quad A \in \Re^{n\times n}, \quad b \in \Re^n, \ x \in \Re^n$$

It is easily shown that ill-conditioning can be detected in terms of the matrix A in the system. Let us determine the relative change in the solution x_*, given some relative change in b or in A. If we change b by Δb, then the new solution can be written as $x_* + \Delta x$, where

$$A(x_* + \Delta x) = b + \Delta b = Ax_* + \Delta b.$$

So that

$$A\Delta x = \Delta b.$$

Thus in norm $\|\cdot\|$

$$\|\Delta x\| \leq \|A^{-1}\| \cdot \|\Delta b\|.$$

Also from $Ax_* = b$,

$$\frac{1}{\|x_*\|} \leq \frac{\|A\|}{\|b\|}$$

so that

$$\frac{\|\Delta x\|}{\|x_*\|} \leq \|A\| \cdot \|A^{-1}\| \frac{\|\Delta b\|}{\|b\|}. \tag{4.1.25}$$

Similarly, if we change A by ΔA, set

$$(A + \Delta A)\hat{x} = b,$$

where $\hat{x} = x_* + \Delta\hat{x}$, then

$$(A + \Delta A)(x_* + \Delta\hat{x}) = b$$

which yields

$$\Delta\hat{x} = -\Delta A \cdot \hat{x},$$

$$\|\Delta\hat{x}\| \leq \|A^{-1}\| \cdot \|\Delta A\| \cdot \|\hat{x}\|,$$

so that

$$\frac{\|\Delta\hat{x}\|}{\|\hat{x}\|} \leq \|A\| \cdot \|A^{-1}\| \frac{\|\Delta A\|}{\|A\|}. \tag{4.1.26}$$

In both cases, the relative change in x is bounded by the relative change in the data multiplied by $\|A\|\|A^{-1}\|$. This term is know as the condition number of A

and is denoted by $\kappa(A)$. Since in a quasi-Newton method, B_+ is used in solving a linear system $B_+d_+ = -g_+$, it is reasonable to try to hold down the condition number of B_+ at each iteration. From [7] and [3], we have

$$\kappa(B_+) \leq \kappa(B_c) \cdot \kappa(B_c^{-\frac{1}{2}} B_+ B_c^{-\frac{1}{2}}),$$

thus it is reasonable for us to try to hold down $\kappa(B_c^{-\frac{1}{2}} B_+ B_c^{-\frac{1}{2}})$.

For square matrices, condition numbers usually measure the deviation of the matrix from a multiple of an orthogonal matrix. For simplicity we will consider symmetric, positive definite matrices, denoted *s.p.d.* In this case, the condition numbers measure the distance to a multiple of the identity. Let A be an $n \times n$ *s.p.d.* matrix with eigenvalues

$$\lambda_1 \geq \ldots \geq \lambda_n > 0,$$

and corresponding normalized eigenvectors $u_1, \ldots, u_n$. The l_2 condition number of the matrix A becomes

$$\kappa(A) = \lambda_1/\lambda_n = ||A||\ ||A^{-1}||.$$

We can also write A as

$$A = \sum_{i=1}^{n} \lambda_i u_i u_i^t$$

called its *spectral resolution.* Let

$$x = \sum_{i=1}^{n} \alpha_i u_i, \quad \Delta x = \sum_{i=1}^{n} \Delta\alpha_i u_i$$

and

$$b = \sum_{i=1}^{n} \beta_i u_i, \quad \Delta b = \sum_{i=1}^{n} \Delta\beta_i u_i.$$

Then, from $A(x + \Delta x) = b + \Delta b$, we have

$$\sum_{i=1}^{n} (\alpha_i + \Delta\alpha_i)\lambda_i u_i u_i^t = \sum_{i=1}^{n} (\beta_i + \Delta\beta_i) u_i,$$

which by $Ax = b$ implies that

$$\Delta\alpha_i = \frac{\Delta\beta_i}{\lambda_i}$$

and

$$\alpha_i = \frac{\beta_i}{\lambda_i},$$

for $i = 1, 2, \ldots, n$. Therefore,

$$\frac{\|\Delta x\|}{\|x\|} = \frac{\|\sum_{i=1}^{n} \frac{\Delta\beta_i}{\lambda_i} u_i\|}{\|\sum_{i=1}^{n} \frac{\beta_i}{\lambda_i} u_i\|} \leq \frac{\lambda_1}{\lambda_n} \frac{\|\Delta\beta\|}{\|\beta\|},$$

where $\beta = (\beta_1, \ldots, \beta_n)$ and $\Delta\beta = (\Delta\beta_1, \ldots, \Delta\beta_n)$.

If $\lambda_1 \gg \lambda_n$, A is an ill-conditioned matrix and the above inequality provides a worst case estimation of the error for $Ax = b$. But if

$$\Delta\beta_n = 0$$

and

$$\lambda_1 = \lambda_2 = \ldots = \lambda_{n-1},$$

then we have

$$\frac{\|\Delta x\|}{\|x\|} \leq \frac{\|\Delta\beta\|}{\|\beta\|},$$

i.e. no amplification in the error at all. Therefore, it is necessary to take into consideration the eigenvalues between the largest and smallest one, this is a motivation to consider the uniform condition number, below.

Other well known condition numbers are those arising from l_p norms, $p \geq 1$. In particular, the l_1 and l_∞ are often used. The l_1 condition number can be estimated very efficiently (see [10]).

4.1.1 Uniform Condition Number

For *s.p.d.* A, the l_2 condition number depends only on the largest and smallest eigenvalues and thus does not take into account the possible variation among the other eigenvalues. Also the condition number is invariant under scaling, i.e.

$$\kappa(\alpha A) = \kappa(A) \text{ for } \alpha > 0.$$

Since κ depends only on the largest and smallest eigenvalues, we consider the following measure which depends more uniformly on all the eigenvalues

$$\omega(A) = \frac{\operatorname{trace}(A)/n}{\det(A)^{\frac{1}{n}}}.$$

Just as the usual condition number $\kappa(A)$ is a measure of how close A is to the pencil αI, where I is the identity matrix and $\alpha > 0$, the function $\omega(A)$ similarly measures the 'distance' of A from αI. This measure takes all the eigenvalues of A into account and so is a more uniform or average indicator of the distance of A to αI.

Moreover, ω can be calculated in terms of the actual data of A rather than its spectrum and can be more easily differentiated and manipulated.

We now include some useful properties of κ and ω from [4]. Here we restrict ourselves to the *s.p.d.* matrices and use the Loewner order, i.e. $A \geq B$ means $A - B$ is positive semidefinite. See e.g. [30]. Recall that a function is pseudoconvex means:

$$(y - x)^t \nabla f(x) \geq 0 \text{ implies } f(y) \geq f(x)$$

See e.g. [31].

Proposition 4.1 *The uniform condition number $\omega(A)$ satisfies:*

(i) $1 \leq \omega(A) \leq \kappa(A) < \frac{(\kappa(A)+1)^2}{\kappa(A)} \leq 4\omega^n(A)$, *with equality in the first and second inequality if and only if A is a multiple of the identity and equality in the last inequality if and only if*

$$\lambda_2 = \ldots = \lambda_{n-1} = \frac{\lambda_1 + \lambda_n}{2};$$

(ii) $\omega(\alpha A) = \omega(A),$ *for all* $\alpha > 0$;

(iii) if $n = 2$, $\omega(A)$ *is isotonic with* $\kappa(A)$.

(iv) The measure ω is pseudoconvex on the set of s.p.d. matrices, and thus any stationary point is a global minimizer of ω.

(v) Let V be a full rank $m \times n$ matrix, $n \leq m$. Then the optimal column scaling that minimizes the measure ω, i.e.

$$\min \omega((VD)^t(VD)),$$

over D positive, diagonal, is given by

$$D_{ii} = \frac{1}{||V_i||}, \; i = 1, \ldots, n,$$

where V_i is the i-th column of V.

The proof for the proposition is found in [4]. Property (i) above shows that $\omega(A)$ is a valid condition number, e.g. we can replace $||A||\ ||A^{-1}||$ by $4\omega^n(A)$ in both (4.1.25) and (4.1.26). Property (v) shows that the measure ω predicts the best column scaling.

4.1.2 σ-Condition Number

In section 3 above, we saw that to find an ellipsoid of minimal volume containing the unit ball leads to the measure

$$\sigma(A) = \frac{\lambda_1(A)}{\det(A)^{\frac{1}{n}}}.$$

The measure σ can be considered as a condition number since σ has several interesting properties similar to the measure ω.

Proposition 4.2 *The measure $\sigma(A)$ satisfies*

(i) $1 \leq \sigma(A) \leq n\omega(A) \leq n\kappa(A) \leq 4n\omega^n(A) \leq 4n\sigma^n(A)$;

(ii) $\sigma(\alpha A) = \sigma(A)$, *for all* $\alpha > 0$;

(iii) The measure σ is a pseudoconvex function on the set of s.p.d. matrices, and thus any stationary point is a global minimizer.

The proof for this proposition is found in [5].

4.1.3 τ-Condition Number

L. Tuncel in [32] introduced the following potential function:

$$\tau(A) = \frac{\mathrm{trace}\,(A)/n}{\lambda_n}.$$

The function τ can also be considered as a condition number since τ has properties similar to the measures ω and σ.

Proposition 4.3 *The measure $\tau(A)$ satisfies* *(i)* $1 \le \omega(A) \le \tau(A) \le \kappa(A) \le 4\omega^n(A)$;

(ii) $\tau(\alpha A) = \tau(A)$, *for all* $\alpha > 0$;

(iii) The measure τ *is pseudoconvex on the set of s.p.d. matrices, and thus any stationary point is a global minimizer.*

Proof. That $\omega(A) \le \tau(A) \le \kappa(A)$ follows from the definition of τ, while $1 \le \omega(A)$ and $\kappa(A) \le 4\omega^n(A)$ is given in (i) of Proposition 4.1, therefore, (i) is true. (ii) also follows directly from the definition.

On the set of *s.p.d.* matrices, the smallest eigenvalue is a concave function, while $\mathrm{trace}\,(A)/n$ is linear and so convex. Thus τ is pseudoconvex. ∎

Chapter 5

Optimal Updates

In this section we find the optimal updates for various measures, i.e. for

(i) $\kappa(A) = \frac{\lambda_1(A)}{\lambda_n(A)}$,

(ii) $\sigma(A) = \frac{\lambda_1(A)}{\det(A)^{1/n}}$,

(iii) $\tau(A) = \frac{\mathrm{trace}\,(A)/n}{\lambda_n}$,

(iv) $\omega(A) = \frac{\mathrm{trace}\,(A)/n}{\det(A)^{1/n}}$

(v) $\max\det(A)$ $s.t$ $\lambda_1(A) \leq 1$.

5.1 κ-Optimal Updates

The κ measure is

$$\kappa(A) = \frac{\lambda_1(A)}{\lambda_n(A)},$$

where $\lambda_1(A)$ and $\lambda_n(A)$ are the largest and smallest eigenvalues of A $s.p.d$, respectively. The use of the condition number as a measure to obtain a better update has been extensively studied. The motivation to consider this measure is not only that the condition number possesses many good properties but also that it plays an important role in the class of optimal updates, since from [5], we can see that the optimal updates for each of the measures ω, σ and τ are also optimal for the κ measure. Note that the spectrum of a matrix product C_1C_2 is equal to the spectrum of C_2C_1 and $\kappa(C) = \kappa(C^{-1})$. Consequently, we can replace $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ by $B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$ for κ measure. The following theorem due to Davidon [7] gives the "optimally conditioned" update restricted to the Broyden class.

Theorem 5.1 *Let $n > 2$, $y^t s > 0$, B_c s.p.d. and $B_c s$ and y are linearly independent. Then among all positive definite B_ϕ in Broyden class (2.1.7), $\kappa(H_c^{\frac{1}{2}} B_\phi H_c^{\frac{1}{2}})$ is minimized by B_{ϕ^*}, where*

$$\phi^* = \begin{cases} 1 - \frac{(a-b)b}{ac-b^2} & \textit{if } 2ac > (a+c)b \\ \frac{c}{c-b} & \textit{if } 2ac \leq (a+c)b. \end{cases}$$

The proof of Theorem 5.1 can be found in [3]. Wolkowicz in [5] gave a general form of κ-optimal updates by considering all the *s.p.d.* updates satisfying the secant equation. Byrd independently showed that κ optimal update is a sized Broyden class update. Also, Hu and Storey in [25] gave a family of κ-optimal updates. We summarize the discussion in section 5 of [5] in the following theorem which generalizes Theorem 5.1.

Theorem 5.2 *Consider the problem*

$$\begin{array}{cc} \min & \kappa(B_+) \\ \text{subject to } \mathrm{B_+ s = y,\ B_+\ s.p.d.} & \end{array} \tag{5.1.27}$$

(i) *The optimal updates of I for (5.1.27) are of the form*

$$B_+ = B_Q + B,$$

where

$$B_Q = Q - \frac{1}{c}ss^t + \frac{1}{b}yy^t + (1-\phi)cww^t, \; w = \frac{1}{b}y - \frac{1}{c}s,$$

Q is the projection of I on span$\{s, y\}$,

$$\phi = 1 - \frac{(a-b)b}{ac-b^2},$$

$P = I - Q$, $PBP = B$, and the eigenvalues of B lie between the eigenvalues of B_Q which are

$$\lambda_\pm = \frac{a}{b} \pm \{\frac{a^2}{b^2} - \frac{a}{c}\}^{\frac{1}{2}}.$$

Moreover, for any $\lambda_2^*, \ldots, \lambda_{n-1}^* \in \Re$ such that

$$\lambda_+ \geq \lambda_2^* \geq \ldots \geq \lambda_{n-1}^* \geq \lambda_-,$$

we can find an optimal update of (5.1.27) with $\lambda_+, \lambda_2^*, \ldots, \lambda_{n-1}^*$ and λ_- as its eigenvalues.

(ii) *A κ-optimal update exists in the Broyden family if and only if*

$$2ac \geq (a+c)b$$

holds. Moreover, if $2ac < (a+c)b$, we have that the SR1 is s.p.d. and is the κ-optimal update restricted to the Broyden Family.

Proof. To prove (i), suppose that B_+ is an optimal update of (5.1.27) and let its eigenvalues be

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$$

with $x_1,\ x_2, \ldots, x_n$ its corresponding normalized eigenvectors. The Lagrangian for problem (5.1.27) is

$$L(u, B_+) = \frac{\lambda_1}{\lambda_n} - u^t(B_+ s - y).$$

Since the above Lagrangian is not differentiable in general, we will find its subgradient. Differentiating the Lagrangian and then setting it equal to zero, we have

$$\lambda_1^{'}\lambda_n - \lambda_n^{'}\lambda_1 + su^t + us^t = 0 \tag{5.1.28}$$

for some u, where $\lambda_1^{'}$ and $\lambda_n^{'}$ are subgradients. Since the rank of $su^t + us^t$ is at most 2, we must have

$$\lambda_1^{'} = x_1 x_1^t \ \text{ and } \ \lambda_n^{'} = x_n x_n^t.$$

(See Appendix A) Therefore, (5.1.28) becomes

$$\lambda_n x_1 x_1^t - \lambda_1 x_n x_n^t + su^t + us^t = 0. \tag{5.1.29}$$

By multiplying (5.1.29) by x_1 and x_n, respectively, we have

$$\begin{cases} \lambda_n x_1 = -s(u^t x_1) - u(s^t x_1) \\ \lambda_1 x_n = s(u^t x_n) - u(s^t x_n) \end{cases},$$

which implies that

$$span\{u, s\} = span\{x_1, x_n\}.$$

The secant condition now implies that y is also in span of $\{x_1, x_n\}$, therefore, we have

$$span\{x_1, x_n\} = span\{s, y\}.$$

Now let

$$Q = x_1 x_1^t + x_n x_n^t,\ P = I - Q,$$

$$B_Q = \lambda_1 x_1 x_1^t + \lambda_n x_n x_n^t$$

and

$$B = \lambda_2 x_2 x_2^t + \ldots + \lambda_{n-1} x_{n-1} x_{n-1}^t$$

then,

$$B_+ = B_Q + B, \ PBP = B.$$

Since the columns of $B_Q - Q$ are in $span\{s, y\}$ and $B_Q s = y$, by Theorem 2.2, noting that $Qs = s$ and $Qy = y$, we have

$$B_Q = Q - \frac{1}{c} s s^t + \frac{1}{b} y y^t + (1 - \phi) c w w^t, \ w = \frac{1}{b} y - \frac{1}{c} s. \tag{5.1.30}$$

Let $W = (x_1, x_n)$, $\bar{B}_Q = W^t B_Q W$, $\bar{s} = W^t s$ and $\bar{y} = W^t y$. Noting that $\bar{s}^t \bar{s} = c$ and $\bar{y}^t \bar{s} = b$, from (5.1.30) we have

$$\bar{B}_Q = \bar{B}_Q(\phi) = \begin{pmatrix} \lambda_1 & \\ & \lambda_n \end{pmatrix} = I - \frac{1}{c} \bar{s} \bar{s}^t + \frac{1}{b} \bar{y} \bar{y}^t + (1 - \phi) c \bar{w} \bar{w}^t,$$

where $\bar{w} = \frac{1}{b} \bar{y} - \frac{1}{c} \bar{s}$, for some ϕ, which shows that λ_1 and λ_n are the largest and the smallest eigenvalue of $\bar{B}_Q$ and $\bar{B}_Q$ is in the Broyden Class. Since when $n = 2$, κ is isotonic with ω, Theorem 5.6 implies that the minimum for $\kappa(\bar{B}_Q(\phi))$ is attained at

$$\phi^* = 1 - \frac{(a - b) b}{ac - b^2}$$

with

$$\lambda_1^* = \lambda_+ = \frac{a}{b} + \{\frac{a^2}{b^2} - \frac{a}{c}\}^{\frac{1}{2}}$$

and

$$\lambda_n^* = \lambda_- = \frac{a}{b} - \{\frac{a^2}{b^2} - \frac{a}{c}\}^{\frac{1}{2}}.$$

Thus we have

$$\kappa(B_+) \geq \kappa(\bar{B}_Q(\phi^*)) = \lambda_+ / \lambda_-. \tag{5.1.31}$$

Now for any $\lambda_2^*, \ldots, \lambda_{n-1}^* \in \Re$ such that

$$\lambda_1^* = \lambda_+ \geq \lambda_2^* \geq \ldots \geq \lambda_{n-1}^* \geq \lambda_- = \lambda_n^*,$$

let

$$z_1 = \frac{\lambda_n^* s - y}{\|\lambda_n^* s - y\|} \quad \text{and} \quad z_n = \frac{-\lambda_1^* s + y}{\| - \lambda_1^* s + y\|}.$$

Then we can see that z_1 and z_2 are normalized orthogonal vectors and that

$$s = \frac{\|\lambda_n^* s - y\|}{\lambda_n^* - \lambda_1^*} z_1 + \frac{\| - \lambda_1^* s + y\|}{\lambda_n^* - \lambda_1^*} z_n$$

$$y = \frac{\|\lambda_n^* s - y\|}{\lambda_n^* - \lambda_1^*} \lambda_1^* z_1 + \frac{\| - \lambda_1^* s + y\|}{\lambda_n^* - \lambda_1^*} \lambda_n^* z_n.$$

Now by finding $z_2, \ldots, z_{n-1}$ such that $z_1, z_2, \ldots, z_{n-1}, z_n$ are normalized and orthogonal, let

$$B_+^* = \lambda_1^* z_1 z_1^t + \lambda_2^* z_2 z_2^t + \ldots + \lambda_{n-1}^* z_{n-1} z_{n-1}^t + \lambda_n^* z_n z_n^t.$$

We have that $B_+^* s = y$ and $\lambda_1^*, \lambda_2^*, \ldots, \lambda_{n-1}^*, \lambda_n^*$ are the eigenvalues of B_+^*, which together with (5.1.31) implies that

$$\kappa(B_+) = \lambda_+ / \lambda_- = \kappa(B_+^*)$$

and hence $\lambda_1 = \lambda_+$ and $\lambda_n = \lambda_-$.

To prove (ii), let

$$B_{\phi^*} = I - \frac{1}{c} s s^t + \frac{1}{b} y y^t + (1 - \phi^*) c w w^t, \; w = \frac{1}{b} y - \frac{1}{c} s.$$

Since any update with $\lambda_\pm$ as its largest and smallest eigenvalues is a κ-optimal update and

$$\begin{cases} \lambda_+ \geq 1 \\ \lambda_- \leq 1 \end{cases} \Leftrightarrow 2ac \geq (a + c) b,$$

therefore, the first part of (ii) is true. By Theorem 5.1, the remaining part of (ii) is also true. ▮

If we replace B_+ with $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$, s with $B_c^{\frac{1}{2}} s$ and y with $H_c^{\frac{1}{2}} y$, then by Theorem 5.2 we have the following corollary.

Corollary 5.1 *Consider problem*

$$\begin{array}{cc} \min & \kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\textit{subject to } B_+ s = y, \ B_+ \ \textit{s.p.d}} \end{array} \tag{5.1.32}$$

(i) The largest and the smallest eigenvalues of $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ *are*

$$\lambda_\pm = \frac{a}{b} \pm \{\frac{a^2}{b^2} - \frac{a}{c}\}^{\frac{1}{2}}.$$

Moreover for any $\lambda_2^*, \ldots, \lambda_{n-1}^* \in \Re$ *such that*

$$\lambda_+ \geq \lambda_2^* \geq \ldots \geq \lambda_{n-1}^* \geq \lambda_-,$$

we can find an optimal update of (5.1.32) B_+^* *such that* $\lambda_+, \lambda_2^*, \ldots, \lambda_{n-1}^*$ *and* λ_- *are the eigenvalues of* $H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}$.

(ii) A κ*-optimal update exists in the Broyden Family if and only if*

$$2ac \geq (a+c)b$$

holds. Moreover, if $2ac < (a+c)b$*, then we have that the* $SR1$ *is s.p.d. and is the* κ*-optimal update restricted the Broyden Family.*

If we replace B_+ with $B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$, s with $H_c^{\frac{1}{2}} y$ and y with $B_c^{\frac{1}{2}} s$, then by Theorem 5.2 we have the following corollary.

Corollary 5.2 *Consider problem*

$$\begin{array}{cc} \min & \kappa(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\textit{subject to } B_+ s = y, \ B_+ \ \textit{s.p.d}} \end{array} \tag{5.1.33}$$

(i) The largest and the smallest eigenvalues of $B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$ *are*

$$\hat{\lambda}_\pm = \frac{1}{\lambda_\mp} = \frac{c}{b} \pm \{\frac{c^2}{b^2} - \frac{c}{a}\}^{\frac{1}{2}}.$$

Moreover for any $\lambda_2^*, \ldots, \lambda_{n-1}^* \in \Re$ *such that*

$$\lambda_+ \geq \lambda_2^* \geq \ldots \geq \lambda_{n-1}^* \geq \lambda_-,$$

we can find an optimal update of (5.1.33) H_+^* *such that* $\lambda_+, \lambda_2^*, \ldots, \lambda_{n-1}^*$ *and* λ_- *are the eigenvalues of* $B_c^{\frac{1}{2}} H_+^* B_c^{\frac{1}{2}}$.

(ii) A κ*-optimal update exists in the Broyden Family (2.1.8) if and only if*

$$2ac \geq (a+c)b$$

holds. Moreover, if $2ac < (a+c)b$*, then we have that the* $SR1$ *is s.p.d. and is the* κ*-optimal update restricted the Broyden Family.*

From the above theorem and corollary, we see that for any $\lambda_2^*, \ldots, \lambda_{n-1}^* \in \Re$ such that

$$\lambda_+ \geq \lambda_2^* \geq \ldots \geq \lambda_{n-1}^* \geq \lambda_-,$$

we can find an optimal update of (5.1.32) B_+^* such that $\lambda_+, \lambda_2^*, \ldots, \lambda_{n-1}^*$ *and* λ_- are the eigenvalues of $H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}$. Since we are more interested in rank-two updates, we would like to consider the case

$$\lambda_+ \geq \alpha = \lambda_2^* = \ldots = \lambda_{n-1}^* \geq \lambda_-.$$

From the proof of Theorem 5.2, we can find a κ-optimal update B_+^* such that

$$\begin{aligned} H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}} &= \lambda_1^* z_1 z_1^t + \lambda_2^* z_2 z_2^t + \ldots + \lambda_{n-1}^* z_{n-1} z_{n-1}^t + \lambda_n^* z_n z_n^t \\ &= \alpha I + (\lambda_+ - \alpha) z_1 z_1^t + (\lambda_- - \alpha) z_n z_n^t, \end{aligned} \tag{5.1.34}$$

where

$$z_1 = \frac{\lambda_n^* B_c^{\frac{1}{2}} s - H_c^{\frac{1}{2}} y}{\|\lambda_n^* B_c^{\frac{1}{2}} s - H_c^{\frac{1}{2}} y\|}$$

$$z_n = \frac{-\lambda_1^* B_c^{\frac{1}{2}} s + H_c^{\frac{1}{2}} y}{\| - \lambda_1^* B_c^{\frac{1}{2}} s + H_c^{\frac{1}{2}} y\|},$$

and $z_1, z_2, \ldots, z_{n-1}$ and z_n are normalized orthogonal vectors. Thus multiplying (5.1.34) by $B_c^{\frac{1}{2}}$, we have

$$B_+^* = \alpha B_c + (\lambda_+ - \alpha) x_1 x_1^t + (\lambda_- - \alpha) x_n x_n^t,$$

where

$$x_1 = \frac{\lambda_n^* B_c s - y}{\|\lambda_n^* B_c^{\frac{1}{2}} s - H_c^{\frac{1}{2}} y\|}$$

$$x_n = \frac{-\lambda_1^* B_c s + y}{\| - \lambda_1^* B_c^{\frac{1}{2}} s + H_c^{\frac{1}{2}} y\|}.$$

Since the columns of $B_+^* - \alpha B_c$ are in the span of $\{\alpha B_c, y\}$, by Theorem 2.1, we have B_+^* is in the scaled Broyden class

$$B_+^* = \alpha B_c - \alpha \frac{1}{c} B_c s s^t B_c + \frac{1}{b} y y^t + (1 - \phi^*) \alpha c w w^t, \ w = \frac{1}{b} y - \frac{1}{c} B_c s.$$

We summarize the above discussion in the following theorem.

Theorem 5.3 *All κ-optimal rank two updates are in the scaled Broyden class.*

5.2 σ-Optimal Updates

Let

$$\alpha_\pm = \frac{c}{b} \pm \{\frac{c^2}{b^2} - \frac{c}{a}\}^{1/2},$$

$$\hat{\alpha}_\pm = \frac{a}{b} \pm \{\frac{a^2}{b^2} - \frac{a}{c}\}^{1/2},$$

and A be *s.p.d.* We also restrict $b > 0$, $ac \neq b^2$, B_+ *s.p.d.*, and $B_+ s = y$. Note that

$$\frac{1}{\alpha_-} = \hat{\alpha}_+, \ \frac{1}{\alpha_+} = \hat{\alpha}_-.$$

Recall that the minimal volume measure is

$$\sigma(A) = \frac{\lambda_1(A)}{\det(A)^{1/n}},$$

see Chapter 3 and [5].

Theorem 5.4 *Consider problem*

$$\begin{array}{cc} \min & \sigma(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\text{subject to } \mathrm{B_+ s = y, \ B_+ \ s.p.d..}} \end{array} \tag{5.2.35}$$

Then

(i) the σ-optimal update is a κ-optimal update;

(ii) the unique optimal solution of (5.2.35) gives rise to the SR1 update of $\frac{1}{\alpha} B_c$, i.e. the inverse sized SR1 update

$$H_+ = \alpha H_c + vv^t/(v^t y),$$

where $v = s - \alpha H_c y$, $\alpha = \alpha_-$ or

$$B_+ = \hat{\alpha}_+ B_c + \tilde{v}\tilde{v}^t/(\tilde{v}^t s), \ \tilde{v} = y - \hat{\alpha}_+ B_c s$$

and the optimal value is

$$\sigma(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = (\frac{\alpha_+}{\alpha_-})^{1/n}.$$

Moreover, $\frac{1}{\alpha} = \lambda_1(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})$ is of multiplicity $n-1$ and the other eigenvalue of $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ is $\lambda_n(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = \frac{1}{\alpha_+}$.

(Note: $v^t y$ and $\tilde{v}^t s$ can be zero only when $ac = b^2$ in which case B_+ is the SR1 update.)

Proof. To prove (i), let B_+ be an optimal update of (5.2.35) with its eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{n-1} \geq \lambda_n.$$

Then

$$\begin{aligned}\sigma(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) &= \frac{\lambda_1}{(\lambda_1\lambda_2\ldots\lambda_{n-1}\lambda_n)^{\frac{1}{n}}} \geq \frac{\lambda_1}{(\lambda_1\lambda_1\ldots\lambda_1\lambda_n)^{\frac{1}{n}}} \\ &= (\frac{\lambda_1}{\lambda_n})^{\frac{1}{n}} = \kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})^{\frac{1}{n}},\end{aligned} \tag{5.2.36}$$

with equality if and only if $\lambda_1 = \lambda_2 = \ldots = \lambda_{n-1}$.

Since $\hat{\alpha}_+ = \lambda_+$ and $\hat{\alpha}_- = \lambda_-$, by Corollary 5.1, we can find a κ-optimal update B_+^* such that $\hat{\alpha}_+, \ldots, \hat{\alpha}_+, \hat{\alpha}_-$ are the n eigenvalues of $H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}$, and we can see that B_+^* is a SR1 update of $\hat{\alpha}_+ B_c$. It immediately follows that

$$\kappa(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}})^{\frac{1}{n}} = \sigma(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}). \tag{5.2.37}$$

Also we have

$$\sigma(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \leq \sigma(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}) \text{ and } \kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \geq \kappa(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}),$$

thus together with (5.2.36) and (5.2.37) we have

$$\sigma(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \geq \kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})^{\frac{1}{n}} \geq \kappa(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}})^{\frac{1}{n}} = \sigma(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}) \geq \sigma(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}),$$

which implies

$$\sigma(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = \sigma(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}})$$

and

$$\kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = \kappa(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}})$$

with $\lambda_1 = \lambda_2 = \ldots = \lambda_{n-1}$, i.e. B_+ is a sized SR1 update of $\lambda_1 B_c$.

To prove (ii), from (i) since B_+ is a κ-optimal update, we have

$$\lambda_1 = \hat{\alpha}_+, \ \lambda_2 = \ldots = \lambda_n = \hat{\alpha}_-,$$

therefore, we have

$$B_+ = B_+^*,$$

i.e. $B_+ = \hat{\alpha}_+ B_c + \tilde{v}\tilde{v}^t/(\tilde{v}^t s), \ \tilde{v} = y - \hat{\alpha}_+ B_c s.$ ∎

By replacing $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ with $B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$, from Theorem 5.4, we have the following corollary

Corollary 5.3 *Consider problem*

$$\begin{array}{cc} \min & \sigma(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\text{subject to } \mathrm{H_+ y = s, \ H_+ s.p.d..}} \end{array} \tag{5.2.38}$$

Then

(i) the optimal update of (5.2.38) is also a κ-optimal update;

(ii) the unique optimal solution of (5.2.38) gives rise to the SR1 update of $\frac{1}{\hat{\alpha}} H_c$, i.e. sized SR1 update

$$B_+ = \hat{\alpha} B_c + \hat{v}\hat{v}^t/(\hat{v}^t s),$$

where $\hat{v} = y - \hat{\alpha} B_c s, \ \hat{\alpha} = \hat{\alpha}_-$ or

$$H_+ = \alpha_+ H_c + ww^t/(w^t y), \ w = s - \alpha_+ H_c y$$

and the optimal value is

$$\sigma(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) = (\frac{\alpha_+}{\alpha_-})^{1/n}.$$

Moreover, $\frac{1}{\hat{\alpha}} = \lambda_1(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}})$ *is of multiplicity n-1 and equals* α_+*; the other eigenvalue of* $B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$ *is* $\lambda_n(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) = \frac{1}{\hat{\alpha}_+}$ *and equals* α_-*.*

If we compute the arithmetic mean of both optimal updates for Theorem 5.4 and Corollary 5.3, we have

$$\begin{aligned} \bar{B} &= \tfrac{1}{2}[(\hat{\alpha}_+ B_c + \tilde{v}\tilde{v}^t/(\tilde{v}^t s)) + (\hat{\alpha}_- B_c + \hat{v}\hat{v}^t/(\hat{v}^t s))] \\ &= \tfrac{a}{b} B_c - \frac{\frac{a}{b} B_c s s^t \frac{a}{b} B_c}{s^t \frac{a}{b} B_c s} + \frac{y y^t}{y^t s}, \end{aligned}$$

and similarly

$$\begin{aligned} \bar{H} &= \tfrac{1}{2}[(\alpha_- H_c + v v^t/(v^t y)) + (\alpha_+ H_c + w w^t/(w^t y))] \\ &= \tfrac{b}{c} H_c - \frac{\frac{b}{c} H_c y y^t \frac{b}{c} H_c}{y^t \frac{b}{c} H_c y} + \frac{s s^t}{y^t s}, \end{aligned}$$

which leads to the following corollary.

Corollary 5.4 *The mean of the two* σ*-optimal updates is the inverse-sized BFGS update. The mean of the inverses of the two* σ*-optimal updates is the inverse of the sized DFP update.*

5.3 τ-Optimal Updates

As in Section 5.2, let

$$\alpha_\pm = \frac{c}{b} \pm \{\frac{c^2}{b^2} - \frac{c}{a}\}^{1/2},$$

$$\hat{\alpha}_\pm = \frac{a}{b} \pm \{\frac{a^2}{b^2} - \frac{a}{c}\}^{1/2},$$

and A be *s.p.d.* We also restrict $b > 0$, $ac \neq b^2$, B_+ *s.p.d.*, and $B_+ s = y$. Note that

$$\frac{1}{\alpha_-} = \hat{\alpha}_+, \; \frac{1}{\alpha_+} = \hat{\alpha}_-.$$

The measure to be minimized is

$$\tau(A) = \frac{\operatorname{trace}(A)/n}{\lambda_n}.$$

Theorem 5.5 *Consider problem*

$$\begin{array}{cc} \min & \tau(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\text{subject to } \mathrm{B_+ s = y},\ \mathrm{B_+} \text{ s.p.d.}.} \end{array} \tag{5.3.39}$$

Then

(i) the optimal update of (5.3.39) is also a κ-optimal update of

$$\begin{array}{cc} \min & \kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\text{subject to } \mathrm{B_+ s = y},\ \mathrm{B_+} \text{ s.p.d.};} \end{array}$$

(ii) the unique optimal solution of (5.3.39) gives rise to the SR1 update of αB_c, i.e. the inverse sized SR1 update

$$B_+ = \alpha B_c + vv^t/(v^t s),$$

where $v = y - \alpha B_c s$, $\alpha = \hat{\alpha}_-$, and the optimal value is

$$\tau(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = \frac{(n-1) + \frac{\hat{\alpha}_+}{\hat{\alpha}_-}}{n}.$$

Moreover, $\hat{\alpha}_- = \lambda_n(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})$ is of multiplicity n-1 and the other eigenvalue of $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ is $\lambda_1(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = \hat{\alpha}_+$.

Proof. To prove (i), let B_+ be an optimal update of (5.3.39) with its eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{n-1} \geq \lambda_n.$$

Then

$$\tau(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) = \frac{(\lambda_1+\ldots+\lambda_n)/n}{\lambda_n} \geq \frac{\lambda_1}{n\lambda_n} + \frac{n-1}{n} = \frac{1}{n}\kappa(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) + \frac{n-1}{n}, \tag{5.3.40}$$

with equality if and only if $\lambda_2 = \ldots = \lambda_{n-1} = \lambda_n$.

Since $\hat{\alpha}_+ = \lambda_+$ and $\hat{\alpha}_- = \lambda_-$, by Corollary 5.1, we can find a κ-optimal update B_+^* such that $\hat{\alpha}_+, \hat{\alpha}_-, \ldots, \hat{\alpha}_-$ are the n eigenvalues of $H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}}$, and we can see that B_+^* is a SR1 update of $\hat{\alpha}_-B_c$. It immediately follows that

$$\frac{1}{n}\kappa(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}}) + \frac{n-1}{n} = \tau(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}}). \tag{5.3.41}$$

Also we have

$$\tau(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) \leq \tau(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}}) \text{ and } \kappa(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) \geq \kappa(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}}),$$

thus together with (5.3.40) and (5.3.41) we have

$$\begin{aligned}\tau(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) \quad &\geq \tfrac{1}{n}\kappa(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) + \tfrac{n-1}{n} \geq \tfrac{1}{n}\kappa(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}}) + \tfrac{n-1}{n} \\ &= \tau(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}}) \geq \tau(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}),\end{aligned}$$

which implies

$$\tau(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) = \tau(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}})$$

and

$$\kappa(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) = \kappa(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}})$$

with $\lambda_2 = \ldots = \lambda_{n-1} = \lambda_n$, i.e. B_+ is a sized SR1 update of $\lambda_n B_c$.

To prove (ii), from (i) since B_+ is a κ-optimal update, thus we have

$$\lambda_1 = \hat{\alpha}_+,\ \lambda_2 = \ldots = \lambda_n = \hat{\alpha}_-,$$

therefore, we have

$$B_+ = B_+^*,$$

i.e. $B_+ = B_+ = \alpha B_c + vv^t/(v^t s)$, where $v = y - \alpha B_c s,\ \alpha = \hat{\alpha}_-$. ▮

If we replace $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ with $B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$ in Theorem 5.5, then we have the following corollary.

Corollary 5.5 *Consider problem*

$$\begin{array}{cc} \min & \tau(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\text{subject to } \mathrm{H_+ y = s,\ H_+ s.p.d.}} \end{array} \tag{5.3.42}$$

Then

(i) the optimal update of (5.3.42) is also a κ-optimal update;

(ii) the unique optimal solution of (5.3.42) gives rise to the SR1 update of $\frac{1}{\hat{\alpha}} B_c$, i.e. sized SR1 update

$$B_+ = \hat{\alpha} B_c + \hat{v}\hat{v}^t/(\hat{v}^t s),$$

where $\hat{v} = y - \hat{\alpha} B_c s,\ \hat{\alpha} = \hat{\alpha}_+$ and the optimal value is

$$\tau(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) = \frac{(n-1) + \alpha_+/\alpha_-}{n}.$$

Moreover, $\frac{1}{\hat{\alpha}} = \lambda_n(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}})$ is of multiplicity n-1 and equals α_-; the other eigenvalue of $B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$ is $\lambda_1(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) = \frac{1}{\hat{\alpha}_-}$ and equals α_+.

From Theorem 5.5 and Corollary 5.5, we can see that the optimal update for $\tau(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})$ is the optimal update for $\sigma(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}})$ and the optimal update for $\tau(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}})$ is the optimal update for $\sigma(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})$, therefore, we can regard τ as a conjugate to σ. Also, the arithmetic mean of both optimal updates for Theorem 5.5 and Corollary 5.5 is the inverse-sized BFGS update.

5.4 ω- Optimal Updates

The measure given in [4] to be minimized is

$$\omega(A) = \frac{\text{trace}\,(A)/n}{\det(A)^{1/n}}.$$

The motivation to consider this measure is that ω is a more uniform condition number since it uses all the eigenvalues.

If we let $A = H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ and $A = B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}$, respectively, by restricting update B_+ into the Broyden Family, we have the following theorem and its corollary due to Dennis and Wolkowicz [4].

Theorem 5.6 *The minimum over ϕ of $\omega(B_c^{-\frac{1}{2}} B_+ B_c^{-\frac{1}{2}})$ is attained at*

$$\phi^* = 1 + \frac{(a-b)b}{(1-n)(ac-b^2)}. \tag{5.4.43}$$

Furthermore, B_{ϕ^*} is s.p.d. and

$$\iota(\phi^*) = \frac{\frac{-(a-b)b}{(1-n)(ac-b^2)}}{1 + (1 + \frac{(a-b)b}{(1-n)(ac-b^2)})(\frac{b^2}{ac} - 1)}. \tag{5.4.44}$$

Corollary 5.6 *The minimum over $\hat{\phi}$ of $\omega(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}})$ is attained at*

$$\hat{\phi}^* = 1 + \frac{(c-b)b}{(1-n)(ac-b^2)}. \tag{5.4.45}$$

Furthermore, $H_{\hat{\phi}^*}$ is s.p.d. and

$$\iota(\hat{\phi}^*) = \frac{\frac{-(c-b)b}{(1-n)(ac-b^2)}}{1 + (1 + \frac{(c-b)b}{(1-n)(ac-b^2)})(\frac{b^2}{ac} - 1)}. \tag{5.4.46}$$

The proof for both Theorem 5.6 and its corollary are found in [4]. Now among all of symmetric positive definite updates satisfying the secant equation, the optimal update of $\omega(B_c^{-\frac{1}{2}} B_+ B_c^{-\frac{1}{2}})$ is given in the following theorem due to Dennis and Wolkowicz [4].

Theorem 5.7 *Consider problem*

$$\begin{array}{cc} \min & \omega(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\text{subject to } \mathrm{B_+ s = y,\ B_+ \ s.p.d.}} \end{array} \tag{5.4.47}$$

Then

(i) the optimal update of problem (5.4.47) is also an optimal update of

$$\begin{array}{cc} \min & \kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\text{subject to } \mathrm{B_+ s = y,\ B_+ \ s.p.d.;}} \end{array}$$

(ii) the optimal solution of problem (5.4.47) gives rise to the BFGS update of $\frac{a}{b}B_c$*, i.e. the inverse sized BFGS update,*

$$B_+ = \frac{a}{b}B_c - \frac{a}{b}\frac{1}{s^t B_c s}B_c s s^t B_c + \frac{1}{y^t s}yy^t$$

and the optimal value is

$$\omega(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = (\frac{ac}{b^2})^{1/n}.$$

Proof.

To prove (i), let B_+ be an optimal update of (5.4.47) and denote

$$\lambda_\pm = \frac{a}{b} \pm \{\frac{a^2}{b^2} - \frac{a}{c}\}^{1/2}.$$

Then we have $\lambda_+ > \frac{a}{b} > \lambda_-$. By Corollary 5.1, we can find a κ-optimal update B_+^* such that $\lambda_+, \frac{a}{b}, \ldots, \frac{a}{b}, \lambda_-$ are the n eigenvalues of $H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}$. It immediately follows that

$$\omega(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \le \omega(H_c^{\frac{1}{2}} B_+^* H_c^{\frac{1}{2}}). \tag{5.4.48}$$

Since by Proposition 4.1

$$\omega^n(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \ge \frac{(\kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) + 1)^2}{4\kappa(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})},$$

with equality if and only if $\lambda_2 = \ldots = \lambda_{n-1} = \frac{\lambda_1+\lambda_n}{2}$, and since $\frac{(\kappa+1)^2}{4\kappa}$ is isotonic with κ, it follows that

$$\frac{(\kappa(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}})+1)^2}{4\kappa(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}})} \geq \frac{(\kappa(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}})+1)^2}{4\kappa(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}})} = \omega(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}}).$$

Therefore, together with (5.4.48), we have

$$\omega(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) = \omega(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}})$$

and

$$\kappa(H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}) = \kappa(H_c^{\frac{1}{2}}B_+^*H_c^{\frac{1}{2}})$$

with $\lambda_2 = \ldots = \lambda_{n-1} = \frac{\lambda_1+\lambda_n}{2}$.

The proof for (ii) is found in [4]. ∎

If we replace $H_c^{\frac{1}{2}}B_+H_c^{\frac{1}{2}}$ in Theorem 5.7 with $B_c^{\frac{1}{2}}H_+B_c^{\frac{1}{2}}$, we have the following corollary.

Corollary 5.7 *Consider problem*

$$\begin{array}{cc} \min & \omega(B_c^{\frac{1}{2}}H_+B_c^{\frac{1}{2}}) \\ \multicolumn{2}{c}{\text{subject to } \mathrm{H_+y = s,\ H_+\ s.p.d.}} \end{array} \tag{5.4.49}$$

Then

(i) the optimal update of problem (5.4.49) is also a κ-optimal update;

(ii) the optimal solution of problem (5.4.49) gives rise to the DFP update of $\frac{b}{c}B_c$, i.e. the sized DFP update

$$B_+ = \frac{b}{c}B_c + uy^t + yu^t,\ u = \frac{y - \frac{b}{c}B_cs}{b},$$

and the optimal value is

$$\omega(B_c^{\frac{1}{2}}H_+B_c^{\frac{1}{2}}) = (\frac{ac}{b^2})^{1/n}.$$

Numerical tests (See e.g. [5]) show that the inverse-sized BFGS update is better than the two σ-updates or τ-updates. Thus, we can see that to be the optimal update of κ is not sufficient to be a good update for our purposes. This explains why we should take the eigenvalues between the largest and smallest eigenvalues into account, and why the uniform condition number ω is better than κ. Also, from the volume of ellipsoids motivation, we expect that a proper convex combination of the two updates may lead to a good update.

5.5 Optimal Updates for A General Measure

After discussing the ω, κ, σ and τ optimal updates in the above subsections, now we look at a general measure. Consider a function f of the eigenvalues, $\lambda_1, \lambda_2, \ldots, \lambda_n$ of A, where

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n, \quad \text{and}$$

f has the following properties:

(i) $f(\alpha A) = f(A)$, for all $\alpha > 0$;

(ii) $f(A)$ is a pseudoconvex function;

(iii) for any n values $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, there exists a function of the largest and smallest eigenvalues $a(\lambda_1, \lambda_n)$, $\lambda_n < a(\lambda_1, \lambda_n) < \lambda_1$, such that for any n values $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$

$$\hat{f}(\lambda_1, \lambda_n, a(\lambda_1, \lambda_n)) \equiv f(\lambda_1, a(\lambda_1, \lambda_n), \ldots, a(\lambda_1, \lambda_n), \lambda_n) \leq f(\lambda_1, \lambda_2, \ldots, \lambda_n),$$

and $\hat{f}(\lambda_1, \lambda_n, a(\lambda_1, \lambda_n))$ is isotonic with λ_1/λ_n.

We can see ω, κ, σ and τ possess the properties (i), (ii) and (iii).

Theorem 5.8 *Let f be as given above. Then the problem*

$$\begin{aligned} \min \quad & f(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \\ B_+ s = y, \quad & B_+ \ s.p.d. \end{aligned} \tag{5.5.50}$$

has an optimal update which is a rank two κ-optimal update i.e. is in the sized Broyden class with the largest and smallest eigenvalues

$$\lambda_{\pm} = \frac{a}{b} \pm \{\frac{a^2}{b^2} - \frac{a}{c}\}^{\frac{1}{2}}.$$

Proof. From property (ii), there must exist an optimal update for (5.5.50). Let B_+ be an optimal update of (5.5.50) and $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ be the eigenvalues of $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$. Then by (iii), there exists $a(\lambda_1, \lambda_n)$, $\lambda_n < a(\lambda_1, \lambda_n) < \lambda_1$, such that

$$\hat{f}(\lambda_1, \lambda_n, a(\lambda_1, \lambda_n)) \leq f(\lambda_1, \lambda_2, \ldots, \lambda_n).$$

Since $\lambda_1/\lambda_n \geq \lambda_+/\lambda_-$,

$$\hat{f}(\lambda_+, \lambda_-, a(\lambda_+, \lambda_-)) \leq f(\lambda_1, \lambda_2, \ldots, \lambda_n).$$

∎

5.6 Restricted Max Determinant Updates

Another minimal volume measure given in [5] is

$$\max \det(A) \ s.t. \ \lambda_1(A) \leq 1.$$

Before we include the main results given in Wolkowicz [5], we have the following lemma.

Lemma 5.1 *For any s.p.d. update B_+ satisfying the secant equation*

$$B_+ s = y,$$

we have

$$\lambda_n \leq \frac{b}{c} \leq \frac{a}{b} \leq \lambda_1,$$

where λ_n and λ_1 are the smallest and largest eigenvalues of $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$.

Proof. First we show that $\lambda_n \leq \frac{b}{c}$. Suppose not, i.e. $\lambda_n > \frac{b}{c}$. Then $A \equiv H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}} - \frac{b}{c} I$ is *s.p.d.*. By secant equation, we have

$$(A + \frac{b}{c} I) B_c^{\frac{1}{2}} s = H_c^{\frac{1}{2}} y.$$

Multiplied by $s^t B_c^{\frac{1}{2}}$, the above equation becomes

$$s^t B_c^{\frac{1}{2}} A B_c^{\frac{1}{2}} s = 0,$$

which contradicts to the fact that A is *s.p.d.*. Therefore, $\lambda_n \leq \frac{b}{c}$.

By same argument, we can show that $\frac{a}{b} \leq \lambda_1$. ∎

The optimal updates for this restricted determinant measure are given in the following theorem.

Theorem 5.9 *Consider the two maximum determinant problems*

$$(i) \qquad \max\{\det(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) : \ B_+ \in \Omega, \ B_+ \ s.p.d., \ \lambda_1(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \leq 1\},$$

and

$$(ii) \qquad \max\{\det(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) : \ B_+ \in \Omega, \ B_+ \ s.p.d., \ \lambda_1(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) \leq 1\},$$

where $\Omega = \{B : \ Bs = y\}$. then:

a) $b > a$ *if and only if the SR1 update* B_+ *is the unique solution of problem* (i)*; in which case* $\lambda_1(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = 1$*, and problem* (ii) *is infeasible;*

b) $b > c$ *if and only if the SR1 update* B_+ *is the unique solution of problem* (ii)*; in which case* $\lambda_n(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = 1$*, and problem* (i) *is infeasible;*

c) $b \leq \min\{a, c\}$ *if and only if either the SR1 update is not s.p.d. or* B_c *is the unique optimal solution for both (i) and (ii) if and only if the feasible sets of (i) and (ii) are either the empty set or* B_c *is the unique optimal solution for both (i) and (ii).*

The proof for this theorem is found in [5]. Here we give a similar proof.

Proof. To prove a), if the SR1 update B_+ is the unique solution of problem (i). Then B_+ is *s.p.d.*, thus, from Subsection 2.1.1, we have

$$\phi_{SR1} = \frac{c}{c-b} < \frac{ac}{ac-b^2}. \tag{5.6.51}$$

Since the largest eigenvalue $\lambda_1(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \leq 1$, we have $c > b$, thus multiplying by $(c-b)(ac-b^2)$, (5.6.51) becomes

$$c(ac-b^2) < ac(c-b),$$

which implies that $b > a$.

Conversely, if $b > a$. Then $b < c$, thus by reversing the above argument, we can see that SR1 update is a feasible solution to problem (i). By Lemma 5.1, we have

$$\lambda_n(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \leq \frac{b}{c} < 1 \quad \text{and} \quad \lambda_1(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) \geq \frac{a}{b},$$

which implies that

$$\lambda_1(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) = \frac{1}{\lambda_n(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})} > 1,$$

thus problem (ii) is infeasible. Now we claim that the SR1 update B_+ is the unique solution of problem (i). Suppose not, i.e. there exists an optimal update of problem (i), B_+, which is not a SR1 update. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}$ with $x_1, \ldots, x_n$ as the corresponding eigenvectors, then we must have one of the following two cases

(1)

$$\lambda_n \leq \lambda_{n-1} < \lambda_1 = 1 \quad \text{or}$$

(2)

$$\lambda_n < \lambda_1 < 1.$$

For case (1), find $\alpha, \beta \in \Re$, not both 0, such that

$$(s^t B_c^{\frac{1}{2}})[x_n \ x_{n-1}] \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \ \text{ i.e.}$$

$$0 \neq \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in z^{\perp}, \quad z^t = (s^t B_c^{\frac{1}{2}})[x_n \ x_{n-1}].$$

Set

$$0 \neq w = [x_n \ x_{n-1}] \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha x_n + \beta x_{n-1}.$$

Let

$$B' = H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}} + \epsilon w w^t$$

and denote its eigenvalues by $\lambda_1', \ldots, \lambda_n'$. Then we can see that $B_+' = B_c^{\frac{1}{2}} B' B_c^{\frac{1}{2}}$ satisfies the secant equation and is $s.p.d$ when ϵ is small enough. Moreover,

$$\lambda_j' = \lambda_j \ , \ j = 1, \ldots, n-2;$$

and for $\epsilon > 0$, since ww^t $s.p.d$ $\lambda'_j \geq \lambda_j$ with at least one of

$$\lambda'_n > \lambda_n$$

or

$$\lambda'_{n-1} > \lambda_{n-1}.$$

Therefore, we have

$$\det(H_c^{\frac{1}{2}} B'_+ H_c^{\frac{1}{2}}) > \det(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}),$$

which is a contradiction.

For case (2), by similar argument to (1) we can also draw a contradiction.

Similarly by replacing c by a, a by c and B by H, we can show that b) holds.

To prove c), (1) if $ac > b^2$, we have

$$b \leq \min\{a, c\} \Leftrightarrow \begin{cases} \phi_{SR1} = \frac{c}{c-b} \geq \frac{ac}{ac-b^2} \\ \hat{\phi}_{SR1} = \frac{a}{a-b} \geq \frac{ac}{ac-b^2} \end{cases},$$

which is equivalent to that the SR1 updates for both (i) and (ii) are not s.p.d. This is equivalent to that the feasible sets of both (i) and (ii) are empty by noting that feasible SR1 update can be obtained from any feasible solution for (i) and (ii) by using the above perturbation technique.

(2) if $ac = b^2$, then we have y and B_c are collinear. From $b \leq \min\{a, c\}$, we can see that $a = b = c$, which implies that B_c is a feasible update for (i) and (ii). It is obvious that B_c is the unique solution for (i) and (ii). ∎

Chapter 6

Multi-criteria Optimal Updates

In this chapter we will use the concept of efficient class to discuss how close a symmetric matrix is to the identity. Our starting point will be the result presented in [33] on the efficient Broyden class. First we consider the multiobjective optimization problem

$$\begin{array}{c} \min \quad g_i(z),\ i = 1, \dots, m; \\ \text{subject to } z \in \Omega, \end{array} \tag{6.0.52}$$

where $g_i : \Re^n \to \Re$, are m real valued objective functions.

A point z^1 is <u>dominated</u> by z^2, denoted $z^2 \prec z^1$, if

$$g_i(z^2) \leq g_i(z^1), \quad i = 1, \dots, m;$$

and

$$g_j(z^2) < g_j(z^1) \ \text{ for some } j.$$

(We use $z^2 \preceq z^1$ if $\leq$ holds for any i without the possible strict $<$.)

Definition 6.1 *The <u>Efficient</u> Set is the set of points $z \in \Omega$ that are not dominated by any feasible point.*

Definition 6.2 *z^0 is said to be a* <u>*Properly Efficient Solution*</u> *of (6.0.52) if it is in the efficient set and if there exists a scalar $M > 0$ such that, for each i, we have*

$$\frac{g_i(z^0) - g_i(z)}{g_j(z) - g_j(z^0)} \leq M$$

for some j such that (loss for z) $g_j(z) > g_j(z^0)$ whenever $z \in \Omega$ and (gain for z) $g_i(z) < g_i(z^0)$ (see, [34]).

Thus, for any point z, for each gain there exists a loss such that the gain over the loss is bounded above. Now we present the following lemma which we call the *Perturbation Lemma.* We use this repeatedly in the proofs that follow.

Lemma 6.1 *Suppose that B is a symmetric matrix satisfying the secant equation $B(B_c^{\frac{1}{2}} s) = H_c^{\frac{1}{2}} y$, with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$. 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 eigenvalues $\bar{\lambda}_1, \ldots, \bar{\lambda}_n$ satisfy*

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

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 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*

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

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

$$\bar{B} = B - \epsilon w w^t \tag{6.0.53}$$

and denote its eigenvalues by $\bar{\lambda}_i$ with corresponding eigenvectors $\bar{x}_i,\ i = 1, \ldots, n$. We can see that 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, we can show (2). ▮

6.1 Efficient Broyden Class

The general notion of least change is that, given B_c $s.p.d$, and assuming $b = y^t s > 0$, we want B_+ such that

$$B_+ s = y$$

and

$$B_+ \text{ close to } B_c.$$

Viewing B_c and B_+ as quadratic forms, we want

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

which is equivalent to

$$\frac{x^t B_c^{-\frac{1}{2}} B_+ B_c^{-\frac{1}{2}} x}{x^t x} \text{ close to 1 for } x \in \Re^n,$$

which implies that all of the eigenvalues of $B_c^{-\frac{1}{2}} B_+ B_c^{-\frac{1}{2}}$

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

Therefore, it is natural that we consider the following multiobjective least change problem

$$\begin{array}{ll} \min & |\lambda_i(B_c^{-\frac{1}{2}} B_+ B_c^{-\frac{1}{2}}) - 1|, \ i = 1, \ldots, n; \\ & \text{subject to } B_+ s = y, \ B_+ = B_+^t. \end{array} \tag{6.1.54}$$

Let

$$\Phi = \begin{cases} [\phi_{SR1}, \infty) & \text{if } b > c \\ (-\infty, \phi_{SR1}] & \text{if } b < c \\ (-\infty, \infty) & \text{if } b = c. \end{cases} \tag{6.1.55}$$

We call the subset of the Broyden class of updates $B_\phi, \phi \in \Phi$, the *efficient Broyden class.* This class has the following dominating property.

Lemma 6.2 *Suppose that $B = B^t$ satisfies the secant equation. Then there exists an efficient Broyden class update $\bar{B}$ such that $\bar{B} \preceq B$.*

Proof. The proof follows by noting that $\{\bar{B} : \bar{B} \preceq B\}$ is compact, see e.g. [35]. ∎

We now state the result presented by Byrd [33]. We provide our own proof for completeness.

Theorem 6.1 *The efficient set for problem (6.1.54) consists of the Broyden class*

$$B_c - \frac{1}{s^t B_c s} B_c s s^t B_c + \frac{1}{y^t s} y y^t + (1-\phi) s^t B_c s w w^t$$

where $w = \frac{1}{y^t s} y - \frac{1}{s^t B_c s} B_c s$ *and* $\phi \in \Phi$.

Proof. Let B_+ be in the efficient set for problem (6.1.54) and

$$B = H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}.$$

Then the secant equation becomes

$$B(B_c^{\frac{1}{2}} s) = (H_c^{\frac{1}{2}} y). \tag{6.1.56}$$

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

$$\lambda_2 = \lambda_{n-1} = 1. \tag{6.1.57}$$

Suppose not and suppose that

$$\lambda_1 \geq \lambda_2 > 1. \tag{6.1.58}$$

By the Perturbation Lemma we can find an update $\bar{B}$ such that $\bar{B} \prec B$. This contradicts the fact that B_+ is an efficient point. So (6.1.58) fails. Similarly, we can not have $1 > \lambda_{n-1} \geq \lambda_n$ i.e. (6.1.57) must hold and B is at most a rank-2 update of I. We now have shown that every update in the efficient set is a rank-2 update. It remains to show that B is in the Broyden class with parameter $\phi \in \Phi$.

We first show that B is in the Broyden class by using the fact that it solves the following problem

$$\begin{array}{rrcl} \min_{\bar{B}} & \lambda_1(\bar{B}) & & \\ \text{subject to} & \bar{B}B_c^{\frac{1}{2}}s & = & H_c^{\frac{1}{2}}y \\ & \lambda_n(\bar{B}) & \geq & \lambda_n(B) \\ & \bar{B} & = & \bar{B}^t. \end{array} \tag{6.1.59}$$

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

$$\lambda_1(B) \geq \lambda_1(\hat{B}) \geq \lambda_n(\hat{B}) \geq \lambda_n(B). \tag{6.1.60}$$

If B does not solve (6.1.59), then by Lemma 6.2, there must be an efficient update that dominates or equals to $\hat{B}$, by noting that an efficient update is a rank-2 update, so dominates B, a contradiction to efficiency of B. Thus we can assume that $B = \hat{B}$.

For some Lagrange multiplier vector u and nonnegative scalars v, w, the Lagrangian for the above problem 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. 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 (6.1.59), 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 conditions)

$$\bar{\lambda}_1' + us^t B_c^{\frac{1}{2}} + B_c^{\frac{1}{2}} su^t + v\bar{\lambda}_n' = 0. \tag{6.1.61}$$

Here $\bar{\lambda}_i'$ are subgradients, see e.g. [36]. First suppose that a constraint qualification holds, so $w = 1$, and suppose that $v \neq 0$. Since the rank of $B_c^{\frac{1}{2}} su^t + us^t B_c^{\frac{1}{2}}$ is at most 2, we must have the ranks of the subdifferentials equal to 1, i.e.

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

(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.) Now (6.1.61) implies that $B_c^{\frac{1}{2}} s \in span\{x_1, x_n\}$. The secant equation (6.1.56) now implies that $H_c^{\frac{1}{2}} y$ is in this span as well. Therefore we have

$$span\{\bar{x}_1, \bar{x}_n\} = span\{B_c^{\frac{1}{2}} s, H_c^{\frac{1}{2}} y\},$$

and Corollary 2.1 implies that B is in the scaled Broyden class. Also noting that $\lambda_n \leq \lambda_{n-1} = 1 = \lambda_2 \leq \lambda_1$, by Lemma 2.1, we must have

$$\lambda_1 = \lambda_+(\phi) \quad \text{and} \quad \lambda_n = \lambda_-(\phi),$$

thus by Theorem 2.3, we have the parameter ϕ corresponding to B must be on the right side of SR1, i.e. $\phi \in \Phi$.

If $v = 0$, then the Lagrange equation now implies that either $\bar{\lambda}_1'$ is rank-one so $H_c^{\frac{1}{2}} y$ is linearly dependent on $B_c^{\frac{1}{2}} s$ or it is rank two and the eigenvalue is 1. In either case we have the SR1 update. The same argument holds if $w = 0$.

Now we have shown that any efficient point B must be in the efficient Broyden class. Conversely, since for any update B_ϕ in the efficient Broyden class, $\lambda_\pm(\phi)$ are isotonic with $-\phi$, thus, B_ϕ can not be dominated by any other updates in the efficient Broyden class. Moreover, any update not in the Broyden class can be dominated by an efficient update by Lemma 6.2 above. ∎

Now we consider the following inverse multiobjective least change problem

$$\begin{aligned} \min \quad & |\hat{\lambda}_i(B_c^{\frac{1}{2}} H_+ B_c^{\frac{1}{2}}) - 1|, \ i = 1, \ldots, n; \\ & \text{subject to } B_+ s = y, \ B_+ = B_+^t. \end{aligned} \tag{6.1.62}$$

Let

$$\hat{\Phi} = \begin{cases} [\hat{\phi}_{SR1}, \infty) & \text{if } b > a \\ (-\infty, \hat{\phi}_{SR1}] & \text{if } b < a \\ (-\infty, \infty) & \text{if } b = a. \end{cases} \tag{6.1.63}$$

We call (6.1.63) the *inversed efficient Broyden class* and denote it by $\hat{\Phi}$.

By just changing B_+, B_c and s to H_+, H_c and y, respectively, from the above theorem, we can have the following corollary.

Corollary 6.1 *The efficient class for problem (6.1.62) consists of the inverse Broyden class*

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

where $v = \frac{1}{y^t s} s - \frac{1}{y^t H_c y} H_c y$ *and* $\hat{\phi} \in \hat{\Phi}$.

From the above Theorem 6.1, we immediately have the following corollary.

Corollary 6.2 *The optimal solution of*

$$\begin{aligned} \min \quad & \textstyle\sum_{i=1}^n \psi(\lambda_i(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})) \\ & \textit{subject to } B_+ s = y \\ & B_+ = B_+^t, \end{aligned} \tag{6.1.64}$$

where ψ *is a pseudoconvex function with its unique minimizer at* $\lambda = 1$, *must be in the efficient Broyden class.*

Proof. Since ψ has a unique minimizer at $\lambda = 1$, we have that ψ is strictly decreasing for $\lambda \leq 1$ and strictly increasing for $\lambda \geq 1$.

Now we suppose the theorem is not true, i.e. there exists an optimal update B_+ for (6.1.64) which is not in the efficient Broyden class. Then by Lemma 6.2, we can find an update $\bar{B}_\phi, \phi \in \Phi$ such that

$$\bar{B} \equiv H_c^{\frac{1}{2}} B_\phi H_c^{\frac{1}{2}} \prec H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}} \equiv B.$$

Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of B and $\bar{\lambda}_1, \ldots, \bar{\lambda}_n$ be the eigenvalues of $\bar{B}$. Then

$$|\bar{\lambda}_i - 1| \leq |\lambda_i - 1| \ \text{ for } \ i = 1, \ldots, n$$

and

$$|\bar{\lambda}_k - 1| < |\lambda_k - 1| \ \text{ for some } k,$$

which implies that

$$\psi(\bar{\lambda}_i) \leq \psi(\lambda_i) \ \text{ for } \ i = 1, \ldots, n$$

and

$$\psi(\bar{\lambda}_k) < \psi(\lambda_k) \ \text{ for some } k,$$

which implies that

$$\sum_{i=1}^{n} \psi(\bar{\lambda}_i) < \sum_{i=1}^{n} \psi(\lambda_i),$$

which is a contradiction to the fact that B_+ is an optimal update. ∎

Now let us see the following examples for different ψ. From these examples we will see that Corollary 6.2 is very useful at solving some least change problems.

1. $\psi(\lambda) = \frac{1}{\lambda} + \log \lambda$;

since trace $(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = \sum_{i=1}^n \lambda_i$ and $\det(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) = \prod_{i=1}^n \lambda_i$, the problem

$$\begin{aligned} \min \;\; & [\text{trace}\,((H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})^{-1}) + \log\det(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})] \\ & \text{subject to} \;\; B_+ s = y \\ & B_+ \;\; s.p.d. \end{aligned}$$

becomes problem (6.1.64). By Corollary 6.2, we have an update $B_\phi, \phi \in \Phi$ which solves the above problem. By Lemma 2.1, we have

$$\text{trace}\,((H_c^{\frac{1}{2}} B_\phi H_c^{\frac{1}{2}})^{-1}) + \log\det(H_c^{\frac{1}{2}} B_\phi H_c^{\frac{1}{2}}) = \frac{2f_1(\phi)}{f_2(\phi)} + n - 2 + \log f_2(\phi),$$

which gets its minimum at $\phi = 0$, i.e. DFP update.

2. $\psi(\lambda) = \lambda - \log\lambda$;

   by similar argument to 1, we can see that the problem

$$\begin{aligned} \min \;\; & [\text{trace}\,(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}}) - \log\det(H_c^{\frac{1}{2}} B_+ H_c^{\frac{1}{2}})] \\ & \text{subject to} \;\; B_+ s = y \\ & B_+ \;\; s.p.d., \end{aligned}$$

   becomes problem (6.1.64), which gives rise to BFGS update $(\phi = 1)$.

6.2 Proper Efficiency

Recall a proper efficient point x_0 is such that it is efficient and if there exists a scalar $M > 0$ such that, for each i, we have

$$\frac{g_i(x) - g_i(x_0)}{g_j(x_0) - g_j(x)} \leq M$$

for some j such that $g_j(x) > g_j(x_0)$ whenever $x \in \Omega$ and $g_i(x) < g_i(x_0)$. Based on the results of Theorem 6.1, we now present the following theorem.

Theorem 6.2 *The efficient Broyden class* Φ *for problem (6.1.54) is also the properly efficient class for problem (6.1.54).*

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

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

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 two cases $i = 1$ or $i = n$ in the definition. If $ac = b^2$, the entire Broyden class reduces to SR1 update. Therefore every update is dominated by the SR1 update which must therefore be efficient. So we can assume that $ac > b^2$.

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

$$h_1(+) < h_1(\phi_0). \tag{6.2.65}$$

As in the proof of Theorem 6.1, by Lemma 6.2 we can find an efficient Broyden class update B_{ϕ_1} such that

$$h_i(\phi_1) \leq h_i(+), \quad i = 1, n. \tag{6.2.66}$$

Therefore, from (6.2.65) we have

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

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

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

which is equivalent to

$$h_n(\phi_1) > h_n(\phi_0). \tag{6.2.67}$$

Therefore, from (6.2.65), (6.2.66) and (6.2.67) we have

$$\begin{cases} h_1(\phi_1) \leq h_1(+) < h_1(\phi_0) \\ h_n(+) \geq h_n(\phi_1) > h_n(\phi_0), \end{cases}$$

thus, we have

$$\frac{h_1(\phi_0) - h_1(+)}{h_n(+) - h_n(\phi_0)} \leq \frac{h_1(\phi_0) - h_1(\phi_1)}{h_n(\phi_1) - h_n(\phi_0)} = \frac{\lambda_+(\phi_1) - \lambda_+(\phi_0)}{\lambda_-(\phi_1) - \lambda_-(\phi_0)}. \tag{6.2.68}$$

From Lemma 2.1, (the proof can be found in [3]) we have

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

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

$$h(\phi) \equiv \frac{\lambda'_+(\phi)}{\lambda'_-(\phi)} = \frac{1 + g(\phi)}{1 - g(\phi)}. \tag{6.2.69}$$

Then

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

i.e.

$$\frac{\lambda'_+(\bar{\phi})}{\lambda'_-(\bar{\phi})} \leq \frac{\lambda'_+(\bar{\phi}_0)}{\lambda'_-(\bar{\phi}_0)} = \frac{1 + g(\bar{\phi}_0)}{1 - g(\bar{\phi}_0)}.$$

For the case of $i = n$ in the definition of proper efficiency, a similar argument yields the upper bound $\frac{1-g(\bar{\phi}_0)}{1+g(\bar{\phi}_0)}$. Therefore, B_{ϕ_0} is a properly efficient solution of problem (6.1.54). ∎

From the proof of Theorem 6.2, we can see although the whole efficient Broyden class (6.1.55) is the properly efficient class, i.e. for any $\phi_0 \in \Phi$, whenever

$$h_1(\phi) < h_1(\phi_0) \quad \text{or} \quad h_n(\phi) < h_n(\phi_0),$$

we have

$$\frac{h_i(\phi_0) - h_i(\phi)}{h_j(\phi) - h_j(\phi_0)} \leq \max\{\frac{1 + g(\phi_0)}{1 - g(\phi_0)}, \frac{1 - g(\phi_0)}{1 + g(\phi_0)}\} \equiv M(\phi_0),$$

where $i, j \in \{1, n\}$, but the upper-bound $M(\phi_0)$ is determined by ϕ_0. From the definition of $M(\phi_0)$ we can see that the upper bound $M(\phi_0)$ can be decreased by letting $g(\phi_0)$ close to zero, i.e. letting ϕ_0 close to $\phi_p \equiv (abc + ac^2 - 2b^3)/((ac - b^2)c)$ which can be obtained by setting $g(\phi) = 0$.

Since the measurement of gain/loss is given by $M(\phi)$, we see that ϕ closer to ϕ_p yield a smaller ratio, i.e. ϕ closer to ϕ_p are more efficient. Moreover, taking the difference of gain and loss as $1 + g(\phi) - (1 - g(\phi))$ or $1 - g(\phi) - (1 + g(\phi))$, we see we always have a net marginal gain $|2g(\phi)|$, which gets close to zero as ϕ aproaches ϕ_p.

Also it is worthwhile noting that the optimally conditioned, unsized update is in the efficient Broyden class, and moreover, we have the following result.

Theorem 6.3 *(i) The κ-optimal update*

$$B_{\phi^*}, \ \phi^* = \begin{cases} 1 - \frac{(a-b)b}{ac-b^2} & \textit{if } 2ac > (a+c)b \\ \frac{c}{c-b} & \textit{if } 2ac \leq (a+c)b \end{cases}$$

where $ac - b^2 > 0$, is in the efficient Broyden class.

(ii) B_{ϕ^*} dominates all of the κ-optimal updates given in Theorem 5.2, thus, dominates the ω optimal update, σ-optimal update and τ-optimal update.

Proof. To prove (i), for $2ac > (a+c)b$, if $b = c$, then of course B_{ϕ^*} is in the efficient Broyden class. If $b < c$, then we can get

$$\frac{ac - ab}{ac - b^2} \in (-\infty, \phi_{SR1})$$

and if $b > c$,

$$\frac{ac - ab}{ac - b^2} \in [\phi_{SR1}, \infty).$$

For $2ac \leq (a+c)b$, we have either $b > a$ or $b > c$, and $\phi^* = \phi_{SR1}$.

To prove (ii), since all of the κ-optimal updates given in Theorem 5.2 are also κ-optimal updates and their largest and smallest eigenvalues are

$$\lambda_{\pm} = \frac{a}{b} \pm \{\frac{a^2}{b^2} - \frac{a}{c}\}^{\frac{1}{2}},$$

thus, for $2ac > (a+c)b$, we have 1 lies between λ_- and λ_+ and hence B_{ϕ^*}, $\phi^* = 1 - \frac{(a-b)b}{ac-b^2}$ dominates all these κ-optimal updates, for $2ac \leq (a+c)b$, we have either

$$1 \geq \lambda_+ \quad \text{or} \quad \lambda_- \geq 1,$$

in either cases, we can see all these κ-optimal updates can be dominated by SR1 update. Since ω-optimal update, σ-optimal update and τ-optimal update are κ-optimal updates, thus they are dominated by B_{ϕ^*}. ∎

6.3 Self-Scaling Efficient Region

The above Broyden efficient class Φ of updates does not contain many important updates that have proven to be better in numerical tests than the Broyden class, e.g. the Oren-Luenberger self-scaling updates. Also Tapia [20] tests show sized update better. Therefore, it seems to us that the updates in the scaled Broyden class possess some special convergence property that the updates in the efficient Broyden class do not possess. But self-scaling sometimes damages the curvature information already built up in B_c as seen by numerical tests by Shanno and Phua in [19]. Shanno and Phua tests results in the 'folk theorem' that sizing only at the first step is better than sizing at every step. Also Nocedal and Yuan in [16] showed that the self-scaled BFGS update of $\frac{b}{c}B_c$ does not possess the superlinear convergence property. Thus it will be very interesting to find the self-scaling updates which possess this special convergence property but do minimal damage to the curvature information built up in B_c. Also the numerical results in Hu and Storey [25] indicate that although optimal conditioning is important, it is also important to force the scaling factors to be close to unity. As a result, it is natural for us to consider the following multi-criteria problem

$$\min \quad \begin{cases} |\lambda_i((tB_c)^{-\frac{1}{2}}B_+(tB_c)^{-\frac{1}{2}}) - 1|, & i = 1, \ldots, n; \\ |t-1| \end{cases} \tag{6.3.70}$$
$$\text{subject to } B_+s = y, \; B_+ = B_+^t, \quad t > 0.$$

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 $t \in \Re$. If $ac > b^2$, then we define the region

$$\Phi_S^{>} = \left\{ (t,\phi): \; \min(1,\alpha_-) \le t \le \max(1,\alpha_+) \text{ and } \phi \in \left(\begin{array}{ll} \frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t} \le \phi & \text{if } 1 < t \\ \phi \le \frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t} & \text{if } t < 1 \\ \phi \le \frac{t}{t-\frac{b}{c}} & \text{if } \frac{b}{c} < t \\ \frac{t}{t-\frac{b}{c}} \le \phi & \text{if } t < \frac{b}{c} \\ \phi \text{ arbitrary} & \text{if } t = \frac{b}{c} = 1 \end{array} \right) \right\}, \tag{6.3.71}$$

where $\alpha_\pm = \frac{a}{b} \pm \{\frac{a^2}{b^2} - \frac{a}{c}\}$. If $ac = b^2$, then we define the region

$$\Phi_S^{=} = \{(t,\phi) : \min(1, \frac{b}{c}) \leq t \leq \max(1, \frac{b}{c}),\ \phi \text{ arbitrary}\}. \tag{6.3.72}$$

We let Φ_S represent the appropriate region determined by the value of $ac - b^2$. We call Φ_S the *Efficient Self-Scaling Broyden Region.* The above representation illustrates that the efficient region is determined by 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

$$\Phi_C = \left\{ (t,\phi) :\ \alpha_- \leq t \leq \alpha_+ \text{ and } \phi \in \left(\begin{array}{ll} \phi = \frac{ac}{ac-b^2}\frac{t-\frac{b}{c}}{t} & \text{if } ac - b^2 > 0 \\ \phi \text{ arbitrary} & \text{if } ac - b^2 = 0 \end{array} \right) \right\}, \tag{6.3.73}$$

and call Φ_C the efficient curve. Note that this curve contains the set of optimally conditioned updates, i.e. the updates optimal for the κ measure.

Theorem 6.4 *The efficient updates for problem (6.3.70) are the self-scaling Broyden class updates with* $(t,\phi) \in \Phi_S$.

Before we prove the above theorem, we present the following preliminary results. We assume that $ac > b^2$.

Lemma 6.3 *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,

(i) $\lambda_\pm(t,\phi)$ *is 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

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

(ii) $\lambda_\pm(t,\phi)$ *is isotonic with* $-t$ *for any fixed* ϕ*, and*

$$\frac{\partial\lambda_\pm(t,\phi)}{\partial t} = -\frac{a}{2bt^2}(1 \pm d(t,\phi)), \tag{6.3.74}$$

where

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

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

Proof. Note that a becomes $\frac{a}{t}$ and c becomes ct when B_c is sized with t. The results in (i). are straightforward extensions of those in [3], see e.g. Lemma 2.1. Here we only prove (ii). Differentiating $\lambda_\pm(t,\phi)$ yields (6.3.74). Now, in order to show that $\lambda_\pm(t,\phi)$ is isotonic with $-t$, we need only to show that $|d(t,\phi)| \le 1$. By squaring both sides, we have

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

which is equivalent to

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

Therefore, we have

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

∎

From Lemma 6.3, we can easily obtain the following result.

Corollary 6.3

$$(\frac{\partial \lambda_+(t,\phi)}{\partial \phi})(\frac{\partial \lambda_-(t,\phi)}{\partial t}) \geq (\frac{\partial \lambda_-(t,\phi)}{\partial \phi})(\frac{\partial \lambda_+(t,\phi)}{\partial t}) \quad if \ \phi \leq \frac{act-ab}{(ac-b^2)t} \tag{6.3.75}$$

and

$$(\frac{\partial \lambda_+(t,\phi)}{\partial \phi})(\frac{\partial \lambda_-(t,\phi)}{\partial t}) \leq (\frac{\partial \lambda_-(t,\phi)}{\partial \phi})(\frac{\partial \lambda_+(t,\phi)}{\partial t}) \quad if \ \phi \geq \frac{act-ab}{(ac-b^2)t}, \tag{6.3.76}$$

and the equality holds in both if and only if $\phi = \frac{act-ab}{(ac-b^2)t}$.

Proof. The inequality in (6.3.75) holds if and only if

$$(1+g(t,\phi))(1-d(t,\phi)) \geq (1-g(t,\phi))(1+d(t,\phi)),$$

which is equivalent to $g(t,\phi) \geq d(t,\phi)$, which is equivalent to $\phi \leq \frac{act-ab}{(ac-b^2)t}$. (Note: $(f_1(t,\phi) - \frac{b}{ct})^2 + \frac{ac-b^2}{c^2t^2} = f_1^2(t,\phi) - f_2(t,\phi)$.) By similar argument we can show (6.3.76). ∎

From this corollary, we can see that both λ_+ and λ_- have the same gradient directions if and only if (t,ϕ) is on the κ-optimal curve $\phi = \frac{act-ab}{(ac-b^2)t}$.

Lemma 6.4 *1. The level curves for $\lambda_\pm(t,\phi)$ passing through (t_1,ϕ_1) are*

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

and

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

respectively.

2.

$$\phi(A) = \frac{Ab}{Act-b} + \frac{ac-Ab^2}{ac-b^2}, \qquad A \neq \frac{b}{ct}$$

is isotonic with $-A$*.*

Proof. (1) Let (t,ϕ) be on the level curve for $\lambda_+(t,\phi)$ passing through (t_1,ϕ_1). Then

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

which implies

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

Squaring both sides, we get

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

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

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

Therefore, we have

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

Since the above hyperbola has two branches for $t > \frac{b}{\lambda_+(t_1,\phi_1)c}$ and $0 < t < \frac{b}{\lambda_+(t_1,\phi_1)c}$, respectively, and by Lemma 5.1 (we regard $t_1 c$ as c) or directly checking we have

$$t_1 > \frac{b}{\lambda_+(t_1,\phi_1)c},$$

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

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

$$\phi = \frac{\lambda_+(t_1,\phi_1)b}{\lambda_+(t_1,\phi_1)ct - b} + \frac{ac - \lambda_+(t_1,\phi_1)b^2}{ac - b^2}, \tag{6.3.77}$$

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

$$|\lambda_+(t_1,\phi_1) - f_1(t,\phi)| = (f_1^2(t,\phi) - f_2(t,\phi))^{\frac{1}{2}}. \tag{6.3.78}$$

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

$$\frac{\frac{ab}{t} + ac - \phi(ac - b^2)}{2b^2} < \lambda_+(t_1,\phi_1), \tag{6.3.79}$$

by putting (6.3.77) into (6.3.79), and noting that $t > \frac{b}{\lambda_+(t_1,\phi_1)c}$, we can see that $\lambda_+(t_1,\phi_1) - f_1(t,\phi) > 0$ is equivalent to

$$\lambda_+^2(t_1,\phi_1)ct^2 - 2\lambda_+(t_1,\phi_1)bt + a > 0,$$

which is equivalent to

$$4\lambda_+^2(t_1,\phi_1)(b^2 - ac) < 0.$$

Therefore from (6.3.78) we have

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

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

By the same argument as above, we have

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

where $0 < t < \frac{b}{\lambda_-(t_1,\phi_1)c}$, is the level curve for $\lambda_-(t,\phi)$ passing through (t_1,ϕ_1).

(2) Since

$$\frac{d\phi(A)}{dA} = -\frac{b^2}{(Act - b)^2} - \frac{b^2}{ac - b^2} < 0,$$

thus $\phi(A)$ is isotonic with $-A$. ∎

We now prove the above theorem.

Proof. From Theorem 6.1, for any fixed $t > 0$, we need only to consider the region

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

And for $(t,\phi) \in \bar{R}$, by Theorem 2.3, $\lambda_+(t,\phi)$ and $\lambda_-(t,\phi)$ are the largest and smallest eigenvalues of $(tB_c)^{-\frac{1}{2}}B_+(t,\phi)(tB_c)^{-\frac{1}{2}}$, and its remaining $n-2$ eigenvalues are unit. First suppose that $ac - b^2 > 0$. We consider the following four regions in Φ_t.

(1) $t > 1$ and $\phi < \frac{ac-(ab)/t}{ac-b^2}$

Let us consider an update $B_+(t_1,\phi_1)$ with $t_1 > 1$ and

$$\phi_1 < \frac{ac - (ab)/t_1}{ac - b^2}.$$

By choosing the right level curve passing through (t_1,ϕ_1), we can have (t_2,ϕ_2) on it such that $1 \leq t_2 < t_1$, $(t_2,\phi_2) \in \Phi_t$ and

$$\phi_2 \leq \frac{ac - (ab)/t_2}{ac - b^2}.$$

Say the right level curve is for $\lambda_+(t,\phi)$, then

$$\lambda_+(t_2,\phi_2) = \lambda_+(t_1,\phi_1) \tag{6.3.80}$$

and $|t_2 - 1| < |t_1 - 1|$, thus, in order to show that $B_+(t_2,\phi_2)$ dominates $B_+(t_1,\phi_1)$, we need only to show that

$$\lambda_-(t_2,\phi_2) \geq \lambda_-(t_1,\phi_1). \tag{6.3.81}$$

By Lemma 6.4, (6.3.81) is equivalent to

$$\frac{\lambda_+(t_1,\phi_1)b}{\lambda_+(t_1,\phi_1)ct_2 - b} + \frac{ac - \lambda_+(t_1,\phi_1)b^2}{ac - b^2} \leq \frac{\lambda_-(t_1,\phi_1)b}{\lambda_-(t_1,\phi_1)ct_2 - b} + \frac{ac - \lambda_-(t_1,\phi_1)b^2}{ac - b^2},$$

which is equivalent to

$$(\frac{t_2}{t_1} - 1)(\frac{t_2\phi_1}{b}(ac - b^2) - \frac{ac}{b}t_2 + a) \geq 0,$$

which is equivalent to

$$\phi_1 \leq \frac{ac - (ab)/t_2}{ac - b^2}. \quad \text{(Note: } t_2 < t_1\text{)}$$

But since $\lambda_+(t_1,\phi_1) = \lambda_+(t_2,\phi_2)$ and $t_2 < t_1$, by Lemma 6.3, we have $\phi_1 < \phi_2$. Thus,

$$\phi_1 < \phi_2 \leq \frac{ac - (ab)/t_2}{ac - b^2}.$$

Therefore we can see that $\lambda_-(t_2,\phi_2) > \lambda_-(t_1,\phi_1)$. Therefore, (t_1,ϕ_1) is not an efficient point.

(2) $t < 1$ and $\phi > \frac{ac-(ab)/t}{ac-b^2}$

Let us consider an update $B_+(t_1,\phi_1)$ with $t_1 < 1$ and

$$\phi_1 > \frac{ac - (ab)/t_1}{ac - b^2}.$$

By the same argument as (1), we can see that (t_1, ϕ_1) is also not an efficient point. Therefore, we can see the above two regions are not in the efficient region. We now show that the following two regions consist of the efficient region.

(3) $t \geq 1$ and $\phi \geq \frac{ac-(ab)/t}{ac-b^2}$

Now let us consider an update $B_+(t_1, \phi_1)$ with $t_1 \geq 1$ and

$$\phi_1 \geq \frac{ac-(ab)/t_1}{ac-b^2}.$$

If $t_1 = 1$, obviously, $B_+(t_1, \phi_1)$ is an efficient point, thus we assume $t_1 > 1$.

Suppose $B_+(t_1, \phi_1)$ be dominated by $B_+(t_2, \phi_2)$, then

$$\begin{cases} \lambda_+(t_2, \phi_2) \leq \lambda_+(t_1, \phi_1) \\ \lambda_-(t_2, \phi_2) \geq \lambda_-(t_1, \phi_1) \\ t_2 < t_1, \end{cases} \tag{6.3.82}$$

By Lemma 6.4, (6.3.82) implies

$$\phi_2 \geq \frac{\lambda_+(t_1, \phi_1)b}{\lambda_+(t_1, \phi_1)ct_2 - b} + \frac{ac - \lambda_+(t_1, \phi_1)b^2}{ac-b^2}$$

and

$$\phi_2 \leq \frac{\lambda_-(t_1, \phi_1)b}{\lambda_-(t_1, \phi_1)ct_2 - b} + \frac{ac - \lambda_-(t_1, \phi_1)b^2}{ac-b^2},$$

which gives

$$\frac{\lambda_-(t_1, \phi_1)b}{\lambda_-(t_1, \phi_1)ct_2 - b} + \frac{ac - \lambda_-(t_1, \phi_1)b^2}{ac-b^2} \geq \frac{\lambda_+(t_1, \phi_1)b}{\lambda_+(t_1, \phi_1)ct_2 - b} + \frac{ac - \lambda_+(t_1, \phi_1)b^2}{ac-b^2}.$$

By the same argument as in the proof for region (1), we have

$$\phi_1 \leq \frac{ac-(ab)/t_2}{ac-b^2}.$$

Since $t_2 < t_1$, we have

$$\frac{ac-(ab)/t_2}{ac-b^2} < \frac{ac-(ab)/t_1}{ac-b^2},$$

thus

$$\phi_1 < \frac{ac - (ab)/t_1}{ac - b^2},$$

which is contradiction. Therefore, (t_1, ϕ_1) is an efficient point.

(4) $t \leq 1$ and $\phi \leq \frac{ac-(ab)/t}{ac-b^2}$

Let us consider an update $B_+(t_1, \phi_1)$ with $t_1 \leq 1$ and

$$\phi_1 \leq \frac{ac - (ab)/t_1}{ac - b^2}.$$

By the same argument as in (3), we can see (t_1, ϕ_1) is an efficient point.

If $ac = b^2$, then for each fixed t, the sized Broyden class reduces to the 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 multi-criteria problem with the two functions $|\frac{(1-\frac{c}{b}t)a}{tb}|, |t-1|$. This yields the desired result. ∎

Note from this theorem, we can easily see that all rank-two κ-optimal updates are in the efficient Broyden region. Furthermore, we have the following corollary.

Corollary 6.4 *The efficient updates for problem (6.3.70) without the function $|t - 1|$ are the κ-optimal 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 $t < 1$. ∎

Chapter 7

Parametric Optimal Updates

Above we have found optimal, least change, *s.p.d.* updates which satisfy the secant equation (1.0.2). In each case, a necessary and sufficient condition for the existence of a *s.p.d.* B_+ has been

$$y^t s > 0. \tag{7.0.83}$$

The curvature condition $y^t s > 0$ is guaranteed by the successful completion of most inexact line search algorithms. In this case a *s.p.d.* update B_+ exists which satisfies (1.0.2). The curvature condition in conjunction with the secant equation and a sufficient decrease condition can be used to prove convergence results.

However, (7.0.83) may fail or may be costly to satisfy while a sufficient decrease in the objective function is readily found. (For example, f may be an oscillating sinusoidal type function.) In this case, it has been suggested to replace y in (1.0.2) by $y + \alpha Bs$, for some appropriate positive scalar α. Moreover, we may get a better least change update without *s.p.d* assumption.

We know that B is *s.p.d.* and the search direction is found from $B^{-1}g$. If we were using the true Hessian and a trust region approach, then we would expect

$$B = G + \alpha D, \tag{7.0.84}$$

where D is the current 'scaling' matrix and $\alpha > 0$. Therefore, we would expect the update B_+ to satisfy a perturbed secant equation

$$(B_+ - \alpha D_+)s = y, \tag{7.0.85}$$

where D_+ is an updated scaling matrix.

In this chapter we examine how to best choose α and B_+ for the perturbed secant equation

$$B_+ s = y + \alpha D s, \tag{7.0.86}$$

where $D(= D_+)$ is the current 'scaling' matrix. We assume that $B - \gamma D$, for some $\gamma \geq 0$, is a 'good' current approximation to the true Hessian and so we still minimize the various measures considered in the previous sections. Perturbation analysis now yields the 'best' values for α.

Lemma 7.1 *Suppose that the s.p.d. matrix C and the vectors s and y are given with $y^t s > 0$. Then the optimal solution to the problem*

$$\begin{array}{cc} \min & \frac{1}{2}\|B - C\|_F^2 \\ \textit{subject to} & Bs = y, \ B \ \textit{s.p.d.} \end{array} \tag{7.0.87}$$

is the PSB update

$$B = C + \frac{su^t + us^t}{s^t s} - \gamma s s^t, \tag{7.0.88}$$

with

$$u = y - Cs, \quad \gamma = \frac{u^t s}{(s^t s)^2},$$

and unique Lagrange multiplier vector

$$\lambda = \frac{2u}{s^t s} - \gamma s.$$

Proof. The derivative of the Lagrangian for problem (7.0.87) is

$$0 = B - C - (s\lambda^t + \lambda s^t)/2. \tag{7.0.89}$$

The secant equation (the constraint) yields

$$Bs = Cs + \frac{s\lambda^t + \lambda s^t}{2} s = y \tag{7.0.90}$$

or

$$\frac{\lambda}{2} = \frac{y - Cs}{s^t s} - (\frac{\lambda^t s}{2s^t s})s.$$

Let

$$\beta = \frac{\lambda^t s}{2s^t s}.$$

Substituting for $\lambda/2$ in (7.0.90) yields

$$2\beta s s^t s = \frac{sy^t s - ss^t Cs}{s^t s}$$

or

$$\beta = \gamma/2. \tag{7.0.91}$$

The expressions for B in (7.0.88) and λ now follow from (7.0.89) and (7.0.91). ∎

We now find an optimal update in the case that $y^t s < 0$ when we are given the current update B and a scaling matrix D.

Theorem 7.1 *Suppose that $y^t s < 0$. Then the parametric optimal s.p.d. update that solves*

$$\begin{aligned} \min \quad & \|D^{-\frac{1}{2}}(B_+ - B)D^{-\frac{1}{2}}\| \\ \textit{subject to} \quad & B_+ s = y + \alpha Ds, \quad B_+ \ \textit{s.p.d.} \end{aligned} \tag{7.0.92}$$

is given by

$$\alpha = \frac{s^t Bs - s^t y}{s^t Ds}$$

and

$$B_+ = B + \frac{Dsv^t + vs^tD}{s^tDs} - \gamma Dss^tD,$$

where

$$v = y_\alpha - Bs,\ y_\alpha = y + \alpha Ds,\ \gamma = \frac{y_\alpha^t s - s^tBs}{(s^tDs)^2}.$$

Proof. The problem (7.0.92) is equivalent to minimizing

$$\begin{aligned} \mu_\alpha = \min \quad & \tfrac{1}{2}\|D^{-\frac{1}{2}}B_+D^{-\frac{1}{2}} - D^{-\frac{1}{2}}BD^{-\frac{1}{2}}\|^2 \\ \text{subject to} \quad & (D^{-\frac{1}{2}}B_+D^{-\frac{1}{2}})(D^{\frac{1}{2}}s) = D^{-\frac{1}{2}}y_\alpha \\ & D^{-\frac{1}{2}}B_+D^{-\frac{1}{2}} \quad s.p.d. \end{aligned} \tag{7.0.93}$$

where $y_\alpha = y + \alpha Ds$. From Lemma 7.1, we get

$$D^{-\frac{1}{2}}B_+D^{-\frac{1}{2}} = D^{-\frac{1}{2}}BD^{-\frac{1}{2}} + \frac{D^{\frac{1}{2}}su^t + us^tD^{\frac{1}{2}}}{s^tDs} - \gamma D^{\frac{1}{2}}ss^tD^{\frac{1}{2}},$$

$$u = D^{-\frac{1}{2}}y_\alpha - D^{-\frac{1}{2}}Bs,\quad \gamma = \frac{u^tD^{\frac{1}{2}}s}{(s^tDs)^2},$$

$$\lambda = \frac{2u}{s^tDs} - \gamma D^{\frac{1}{2}}s.$$

Then

$$\begin{aligned} B_+ &= B + \tfrac{Dsu^tD^{\frac{1}{2}} + D^{\frac{1}{2}}s^tD}{s^tDs} - \gamma Dss^tD \\ &= B + \tfrac{Dsv^t + vs^tD}{s^tDs} - \gamma Dss^tD, \end{aligned}$$

where $v = y_\alpha - Bs$.

$$\gamma = \frac{y_\alpha^t s - s^tBs}{(s^tDs)^2}.$$

The derivative of the optimal value of (7.0.93), call it μ_α, is the Lagrange multiplier times the direction of the perturbation, i.e.

$$\begin{aligned} 0 = \mu_\alpha' &= (s^tD^{\frac{1}{2}})(\tfrac{2u}{s^tDs} - \gamma D^{\frac{1}{2}}s) \\ &= \tfrac{s^tD^{\frac{1}{2}}u}{s^tDs} \\ &= \tfrac{s^ty_\alpha - s^tBs}{s^tDs} \\ &= \tfrac{s^ty + \alpha s^tDs - s^tBs}{s^tDs}. \end{aligned}$$

After multiplying by s^tDs, we get

$$s^ty + \alpha s^tDs - s^tBs = 0,$$

which implies that

$$\alpha = \frac{s^tBs - s^ty}{s^tDs}.$$

∎

Chapter 8

Summary and Future Work

In this thesis, we considered various least change measures in order to try to understand the numerical results of some well-known quasi-Newton methods for unconstrained optimization. By doing so, we want to find some new quasi-Newton methods which have better convergence properties. In Chapter 2, we introduced the Broyden class of updates and by analysis of their eigenvalues, we got some basic results which have been used throughout the thesis. We also introduced various scalings and by showing that the steepest descent direction becomes the Newton's search direction by scaling and that the weighted Frobenius norms as measures give better updates than the Frobenius norms do, we showed that scaling is a strong technique for improving least change measures. Finally we gave an overview of the numerical results of some quasi-Newton methods.

In Chapter 3, we used the volume of the symmetric difference of the ellipsoids as motivation to give two measures: the σ-measure and the restricted max determinant measure.

In Chapter 4, motivated by the fact that a bound on the error of the solution of a linear system can be determined by condition numbers, we argued that condition numbers can be used as least change measures. By further analysis of the error of solution of a linear system, we provided the motivation for introducing the uniform condition number. Finally by giving some properties of κ, ω, σ and τ measures, we argued that we can regard σ and τ as condition numbers as well.

In Chapter 5, we included the optimal results for the κ-measure from [5], and then we showed that all ω, σ and τ optimal updates are κ-optimal updates and gave their optimal updates. Also by giving the lower bound for the largest eigenvalue and the upper bound for the smallest eigenvalue for the *s.p.d.* scaled updates satisfying the secant equation and by using perturbation, we gave another proof for the optimal update of the restriced max determinant problem.

In Chapter 6, we first introduced the multi-criteria problem given by Byrd and then provided a proof for the efficient class by using the subgradients for the largest and smallest eigenvalues. We then showed that the efficient class is in fact a properly efficient class. Finally, by taking the self-scaling into consideration, we introduced a general multi-criteria measure and got its efficient region, which contains all the updates considered in this thesis. Also, this result shows us why, although there are a lot of matrices satisfying secant equation, all of the updates of these well known quasi-Newton methods are in the scaled Broyden class.

In Chapter 7, we tried to use parametric updates to solve the weighted Frobenius problem in the case of $y^t s < 0$.

Finally, we list some suggestions for related further research:

1. trying some numerical tests for the updates in the efficient region to decide which efficient region updates to choose;

2. improving the efficient region by finding a properly efficient region;

3. trying to have some convergence analysis for the updates in the efficient region.

Appendix A

Subgradients for Largest and Smallest Eigenvalues

We include the results in [37] and [38] and also see reference [39] and [40]. Let X be the space of $n \times n$ symmetric matrices A. Define the inner-product for X by

$$\operatorname{trace}(A^t B), \quad \text{where } A, B \in X.$$

Denote $B \geq 0$ if $B \in X$ is positive semi-definite. Consider the function

$$\lambda_1(A)$$

which is the largest eigenvalues of $A \in X$. For the smallest eigenvalue of $A \in X$, we can consider $\lambda_1(-A)$.

Theorem A.1 $\lambda_1(A)$ *is convex.*

Proof. The Rayleigh quotient form of $\lambda_1(A)$ is

$$\lambda_1(A) = \max\{x^t A x : \ \|x\| = 1\}.$$

Since x^tAx is a linear function of A for each x, thus the $\max\{x^tAx: \ \|x\|=1\}$ is convex. ∎

Corollary A.1 $\lambda_n(A)$ *is concave.*

Theorem A.2

$$\partial\lambda_1(A) = \{B | B \geq 0, \mathrm{trace}\,(B) = 1, \ \mathrm{trace}\,(B^tA) = \lambda_1(A)\}. \tag{A.0.94}$$

Proof. B is a subgradient of $\lambda_1(A)$ if and only if

$$\mathrm{trace}\,(B^tA) = \lambda_1(A) + \sup_{C\in X}(\mathrm{trace}\,(B^tC) - \lambda_1(C)). \tag{A.0.95}$$

Let $\Omega = \mathrm{diag}\,(\omega_1, \ldots, \omega_n)$, where $\omega_1 \geq, \ldots, \geq \omega_n$ are the eigenvalues of B. Then since $\mathrm{trace}\,(B^tC) = \mathrm{trace}\,(\Omega^tC)$, we have

$$\sup_{C\in X}(\mathrm{trace}\,(B^tC) - \lambda_1(C)) = \sup_{C\in X}(\mathrm{trace}\,(\Omega^tC) - \lambda_1(C)).$$

By the same reason, we can assume that

$$C = \mathrm{diag}\,(c_1, \ldots, c_n), \quad c_1 \geq \ldots \geq c_n.$$

Thus,

$$\begin{aligned} \sup\nolimits_{C\in X}(\mathrm{trace}\,(B^tC) - \lambda_1(C)) &= \sup\nolimits_{C=\mathrm{diag}\,(c_1,\ldots,c_n)}(\mathrm{trace}\,(\Omega^tC) - c_1) \\ &= \sup\nolimits_{C=\mathrm{diag}\,(c_1,\ldots,c_n)}(\textstyle\sum \omega_i c_i - c_1). \end{aligned}$$

But since

$$\sup_{C=\mathrm{diag}\,(c_1,\ldots,c_n)}(\textstyle\sum \omega_i c_i - c_1) = \begin{cases} \infty \ \text{ if any } \omega_i < 0 \ (\text{let } c_i \to -\infty), \\ \infty \ \text{ if } \sum \omega_i > 1 \ (\text{let } c_i = \alpha \to \infty), \\ \infty \ \text{ if } \sum \omega_i < 1 \ (\text{let } c_i = \alpha \to -\infty), \\ 0 \ \text{ if } \omega_i \geq 0 \text{ and } \sum \omega_i = 1, \end{cases}$$

from (A.0.95), we have

$$\text{trace}\,(B^t A) = \lambda_1(A), \quad B \geq 0, \quad \text{trace}\,(B) = 1.$$

∎

Corollary A.2 *Let $A \in X$ and $\lambda_1 \geq \ldots \geq \lambda_n$ be its eigenvalues with corresponding eigenvectors $x_1, \ldots, x_n$, respectively. Let m be the multiplicity of λ_1. Then*

$$B \in \partial\lambda_1(A)$$

if and only if

$$B = \sum_{i=1}^{m} \theta_i x_i x_i^t, \quad \theta \geq 0, \quad \sum_{i=1}^{m} \theta_i = 1.$$

Proof. Let $B \in \partial\lambda_1(A)$, then from Theorem A.2, we have

$$B = bb^t, \quad b^t b = 1, \quad b \in \Re^n.$$

Let $b = \sum_{i=1}^n \mu_i x_i$ and $\theta_i = \mu_i^2 \;\; i = 1, \ldots, n$, then

$$B = \sum_{i=1}^{n} \theta_i x_i x_i^t, \quad \sum_{i=1}^{n} \theta_i = 1,$$

and

$$\begin{aligned} \text{trace}\,(B^t A) &= \text{trace}\,(bb^t \textstyle\sum_{i=1}^n \lambda_i x_i x_i^t) \\ &= \textstyle\sum_{i=1}^n \lambda_i (x_i^t b)^2 \\ &= \textstyle\sum_{i=1}^n \lambda_i \theta_i \\ &\leq \lambda_1, \end{aligned}$$

where the equality holds if and only if

$$\theta_i = 0, \quad i = m+1, \ldots, n.$$

∎

Bibliography

[1] W.C. DAVIDON. Variable metric methods for minimization. Technical Report ANL-5990, Argonne National Labs, Argonne, IL, 1959.

[2] J. E. DENNIS JR. and ROBERT. B. SCHNABEL. *Numerical Methods for Unconstrained Optimization and Nonlinear Equations.* Prentice-Hall, 1983.

[3] R.B. SCHNABEL. *Analysing and improving quasi-Newton methods for unconstrained optimization.* PhD thesis, Department of Computer Science, Cornell University, Ithaca, NY, 1977. Also available as TR-77-320.

[4] J.E. DENNIS and H. WOLKOWICZ. Sizing and least change secant methods. Technical Report CORR 90-02, Department of Combinatorics and Optimization, University of Waterloo, Waterloo, Ontario, 1990. To appear in SIAM J. Numerical Analysis.

[5] H. WOLKOWICZ. Measures for symmetric rank-one updates. Technical Report CORR 90-03, Department of Combinatorics and Optimization, University of Waterloo, Waterloo, Ontario, 1990. Forthcoming in Mathematical Programming.

[6] N. KARMARKAR. A new polynomial-time algorithm for linear programming. *Combinatorica*, 4:373–395, 1984.

[7] W.C. DAVIDON. Optimally conditioned optimization algorithms without line searches. *Math. Prog.*, 9:1–30, 1975.

[8] A. SHAPIRO. Optimal block diagonal l_2-scaling of matrices. *SIAM J. Numerical Analysis*, 22:81–94, 1985.

[9] A. SHAPIRO. Upper bounds for nearly diagonal scaling of matrices. *Linear and Multilinear Algebra*, 29:145–148, 1991.

[10] G.H. GOLUB and C.F. VAN LOAN. *Matrix Computations.* Johns Hopkins University Press, Baltimore, Maryland, 1989.

[11] D.G. LUENBERGER. *Linear and Nonlinear Programming.* Reading. Addison-Wesley, Massachusetts, second edition, 1984.

[12] M.J.D. POWELL. How bad are the BFGS and DFP methods when the objective function is quadratic. *Math. Prog.*, 34:34–47, 1986.

[13] R.H. BYRD, R.H. NOCEDAL, and Y.YUAN. Global convergence of a class of quasi-Newton methods on convex problems. *SIAM J. Numer. Anal.*, 24:1171–1191, 1987.

[14] YIN ZHANG and R.P. TEWARSON. Quasi-Newton algotithms with updates from the preconvex part of Broyden's family. *IMA Journal of Numerical Analysis*, 8, 1988.

[15] R.H. BYRD, D.C. LIU, and R.H. NOCEDAL. On the behaviour of Broyden's class of quasi-Newton methods. Technical Report NAM 01, Department of Electrical Engineering and Computer Science, Northwestern University, 1990.

[16] J. NOCEDAL and Y. YUAN. Analysis of a self-scaling quasi-newton method. Technical Report NAM-02, Department of Electrical Engineering and Computer Science, Northwestern University, 1991.

[17] S.S. OREN and D.G. LUENBERGER. Self-scaling variable metric (SSVM) algorithms, part I. Criteria and sufficient conditions for scaling a class of algorithms. *Manage. Sci.*, 20:845–862, 1974.

[18] S.S. OREN. Perspectives on self-scaling variable metric algorithms. *J. Opt. Theory and Appl.*, 37:137–147, 1982.

[19] K.H. PHUA and D.F. SHANNO. Matrix conditioning and nonlinear optimization. *Math. Prog.*, 14:145–160, 1984.

[20] M. CONTRERAS and R.A. TAPIA. Sizing the BFGS and DFP updates: A numerical study. Technical Report TR91-19, Department of Mathematical Sciences, Rice University, Houston, TX, 1991.

[21] Y. YUAN. A modified BFGS algorithm for unconstrained optimization. *IMA Journal of Numerical Analysis*, 11:325–332, 1991.

[22] M. ANJOS. A note on interpolation and quasi-Newton updates. 1991.

[23] D. SIEGEL. Modifying the BFGS update by column scaling techniques. Presented at 4th SIAM Conference on Optimization, Chicago, May 1992.

[24] M. AL-BAALI. Partial self scaling variable metric algorithms. Technical Report 80, Dipartimento di Sistemi, Universita della Calabria, 1988.

[25] Y. F. HU and C. STOREY. A family of optimally conditioned quasi-newton updates for unconstrained optimization. Technical Report Mathematics Re-

port Number A151, Department of Mathematical Sciences, Loughborough University of Technology, 1991.

[26] L. LUKSAN. Computational experience with improved variable metric methods for unconstrained minimization. *Kybernetika*, 5:415–431, 1990.

[27] H.F.H. KHALFAN. *Topics in quasi-Newton methods for unconstrained optimization.* PhD thesis, University of Colorado, 1989.

[28] G.W. STEWART III. *Introduction to Matrix Computations.* Academic Press, New York, NY, 1973.

[29] N.J. HIGHAM. A survey of condition number estimation for triangular matrices. *SIAM Rev.*, 29:575–596, 1987.

[30] A.W. MARSHALL and I. OLKIN. *Inequalities: Theory of Majorization and its Applications.* Academic Press, New York, NY, 1979.

[31] O.L. MANGASARIAN. *Nonlinear Programming.* McGraw-Hill, New York, NY, 1969.

[32] L. TUNCEL. On the convergence of primal-dual interior-point methods with wide neighborhoods. Technical Report TR 1003, Cornell University, Ithaca, NY, 1992.

[33] R.H. BYRD. A multiobjective characterization of the Broyden class. In preparation. Presented at ORSA/TIMS, New York, Sept. 1990.

[34] M. GEOFFRION. Proper efficient and the theory of vector maximization. *Journal of Mathematical Analysis and Applications*, 22:618–630, 1968.

[35] J. JAHN. *Mathematical Vector Optimization in Partially Ordered Linear Spaces*. Peter Lang, Frankfurt am Main, 1986.

[36] R.T. ROCKAFELLAR. *Convex Analysis*. Princeton University Press, Princeton, NJ, 1970.

[37] M.L. OVERTON. Large-scale optimization of eigenvalues. *SIAM J. Optimization*, 2:88–120, 1992.

[38] R. FLETCHER. Semi-definite matrix constraints in optimization. *SIAM J. Control and Optimization*, 23:493–513, 1985.

[39] A.R. CONN. Nonlinear programming, exact penalty functions and projection techniques for non-smooth functions. In P.T. BOGGS, R. BYRD, and R.B. SCHNABEL, editors, *Numerical Optimization 1984*, pages 3–25. SIAM, 1984.

[40] F.H. CLARKE. *Optimization and Nonsmooth Analysis*. Canadian Math. Soc. Series of Monographs and Advanced Texts. John Wiley & Sons, 1983.