On Sizing and Shifting the BFGS Update within
the Sized Broyden Family of Secant Updates*

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On Sizing and Shifting the BFGS Update within the Sized Broyden Family of Secant Updates

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Abstract

Recently Contreras and Tapia demonstrated that selectively sizing the BFGS secant update has numerical value. A conclusion of the current study is that there is numerical value in following a sizing of the BFGS update with a shifting of the BFGS update. Our motivation for such a strategy comes from the known fact that the BFGS update is prone to producing updates with large eigenvalues. Hence, sizing may contribute to near singularity, and shifting can help compensate for this deficiency. We follow Contreras and Tapia in our form of selective sizing. Our form of shifting can be viewed as switching from the BFGS update to an alternative member of the Broyden family of updates. Our shift is obtained by minimizing a weighted form of the Byrd-Nocedal measure over a sized Broyden family of secant updates. Numerically, our most effective shift is the one that gives the member of the class which is closest to steepest descent in the Byrd-Nocedal measure.

1 Introduction

We consider quasi-Newton methods for the unconstrained optimization problem

$$(1.1) \quad \min_{x \in \mathcal{R}^n} f(x)$$

where f is twice continuously differentiable. Given x , an approximation to a minimizer x_* , to compute x_+ , a new approximation to x_* , these methods use a local quadratic model of the form

$$(1.2) \quad f(x + s) \approx f(x) + \nabla f(x)^T s + \frac{1}{2} s^T B s$$

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where B is the current approximation to $\nabla^2 f(x)$, the Hessian of f at x , and $\nabla f(x)$ is the gradient of f at x . Our particular interest is in *secant methods*, i.e., methods that have the property that the subsequent Hessian approximation B_+ satisfies the secant equation

$$(1.3) \quad B_+ s = y \equiv \nabla f(x_+) - \nabla f(x).$$

A well-known class of such approximations is the *Broyden family*, and it is generally accepted that the BFGS method is computationally the best method among these secant methods. However, the BFGS update may be unsatisfactory when B has very large eigenvalues. In order to overcome this difficulty, two remedies have been considered. The first is *sizing* (multiplying the approximate Hessian by an appropriate scalar before it is updated), and the second is *switching* (updating the approximate Hessian by a different member of the Broyden class).

In this paper, we combine both remedies in two different ways. Thus we consider two types of *sized Broyden family updates* and propose several sizing strategies as a safeguard for the BFGS method. We present considerable numerical experimentation in an effort to determine if one particular approach is more effective than the others, and if any one of our approaches compares favorably with the numerically successful selective sizing recently suggested by Contreras and Tapia[7]. Our experimentation implies that one approach is superior to the others and this approach is also superior to the Contreras-Tapia BFGS centered Oren-Luenberger approach.

In the remainder of this section, we introduce our notation and present some history concerning sizing and switching. In Section 2, we collect our main tools and discuss some of their properties. In Sections 3 and 4, we derive our sizing strategies. In Section 5, we summarize and collect all formulas used in our new sizing strategies. Our numerical results are presented in Section 6. Finally, in Section 7 we give some concluding remarks.

Following Al-Baali[1], we consider the map

$$(1.4) \quad BFGS(X, s, y) = X - \frac{X s s^T X}{s^T X s} + \frac{y y^T}{y^T s}.$$

In terms of this map, the BFGS update of B can be written

$$(1.5) \quad \begin{aligned} B_+ &= BFGS(B, s, y) \\ &= B - \frac{B s s^T B}{s^T B s} + \frac{y y^T}{y^T s}, \end{aligned}$$

and the Broyden family of updates of B can be written

$$(1.6) \quad \begin{aligned} B_+ &= BFGS(B + \phi v v^T, s, y) \\ &= B - \frac{B s s^T B}{s^T B s} + \frac{y y^T}{y^T s} + \phi v v^T, \end{aligned}$$

where ϕ is a scalar parameter and

$$(1.7) \quad v = \sqrt{s^T B s} \left(\frac{y}{y^T s} - \frac{B s}{s^T B s} \right).$$

The equality in (1.6) is immediately transparent if one observes that $v^T s = 0$. Two important subclasses of this family are the *convex class*, $\phi \in [0, 1]$, and the *preconvex class*, $\phi < 0$. The BFGS update corresponds to the choice $\phi = 0$, and the DFP update corresponds to the choice $\phi = 1$.

Sufficient conditions for B_+ , obtained from the Broyden family given by (1.6), to be symmetric and positive definite are that B is symmetric and positive definite, $y^T s > 0$, and $\phi > \phi^\#$, where

$$(1.8) \quad \phi^\# = -\frac{1}{\tau - 1} \quad \text{with} \quad \tau = \frac{(s^T B s)(y^T B^{-1} y)}{(y^T s)^2}.$$

Note that $\tau \geq 1$, and if s and y are linearly independent, then $\tau > 1$.

In 1974, Oren and Luenberger [17] proposed a class of secant methods which they referred to as *self-scaling variable metric methods* (SSVM). They modified the convex class and obtained, for $\phi \in [0, 1]$,

$$(1.9) \quad \begin{aligned} B_+ &= \gamma \left(B - \frac{B s s^T B}{s^T B s} + \phi v v^T \right) + \frac{y y^T}{y^T s} \\ &= \text{BFGS}(\gamma(B + \phi v v^T), s, y) \\ &= \text{BFGS}(\gamma B, s, y) + \gamma \phi v v^T. \end{aligned}$$

For fixed ϕ the parameter γ was to be chosen so that $\kappa_2(Q^{-1/2} B_+ Q^{-1/2}) \leq \kappa_2(Q^{-1/2} B Q^{-1/2})$, where $\kappa_2(A)$ is the l_2 -norm condition number of A , and the matrix Q is the symmetric positive definite Hessian of f (which is constant because they assumed f to be quadratic). They suggested two choices for the parameter γ

$$(1.10) \quad \gamma_{OL} = \frac{y^T s}{s^T B s} \quad \text{and} \quad \gamma_{IOL} = \frac{y^T B^{-1} y}{y^T s}.$$

Soon after in 1976, Oren and Spedicato [18] used the ℓ_2 -norm condition number, proposed earlier by Davidon [8], to derive optimal parameters ϕ^* and γ^* for the sized Broyden family (1.9). Since these choices were in some sense optimal, they intended them to be used at each iteration. However, in 1978 Shanno and Phua [21] claimed that choosing ϕ^* and γ^* fresh at each iteration did not perform well and recommended always using the BFGS update ($\phi = 0$) and sizing only at the first iteration. They suggested sizing with γ_{OL} given in (1.10).

In 1981, Dennis, Gay, and Welsch [11] proposed their NL2SOL algorithm for the non-linear least-squares problem. Their basic algorithm was a Gauss-Newton, trust-region method. However, in order to handle large residual problems, they maintained a structured BFGS secant approximation to the second-order part of the least-squares Hessian, and adaptively decided when to use this approximation. A major concern was that since secant methods do not generate Hessian approximations that become arbitrarily accurate as the iteration proceeds, the approximation to the second-order information may impede the fast convergence for zero-residual problems. They observed that γ_{OL} in (1.10) had the property that the interval spectrum of $\gamma_{OL} B$ overlaps the interval spectrum of $\nabla^2 f(x + \theta s)$ for some $\theta \in (0, 1)$. For this reason they decided to call multiplication by γ_{OL} “sizing” instead of scaling as had previously been used. More importantly they realized

that in their application sizing with γ_{OL} would guarantee that their approximation to the second-order information would converge to zero when the second-order information was zero at the solution. In this application it was critical that the sizing was done at every iteration.

Contreras and Tapia[7] proposed a selective sizing technique in the framework of the BFGS trust-region method using the centered Oren-Luenberger sizing factor defined as

$$(1.11) \quad \gamma_{COL} = \frac{y_-^T s_- / s_-^T s_- + y^T s / s^T s}{s_-^T B s_- / s_-^T s_- + s^T B s / s^T s}.$$

Essentially, Contreras and Tapia suggested sizing only when $\gamma_{OL} < 1$. They felt that γ_{OL} sized the BFGS update too much and suggested γ_{COL} because for $\gamma_{OL} < 1$, it follows that $\gamma_{OL} < \gamma_{COL} < 1$. Hence, they viewed γ_{COL} as a dampening or softening of γ_{OL} .

Their numerical experiments showed that without sizing, DFP is vastly inferior to BFGS; however, when selectively sized, DFP is competitive with BFGS. In their experiments, DFP performed best with the Oren-Luenberger factor γ_{OL} , and BFGS fit well with the centered Oren-Luenberger factor γ_{COL} for medium dimensional problems. They concluded that their selective sizing with factor γ_{COL} was superior to the alternatives of never sizing, sizing only at the first iteration, or sizing at every iteration.

Several other measures have been used to derive similar kinds of self-scaling updates. These scalings are optimal with respect to the measures used to derive them. These measures include

$$(1.12) \quad \psi(A) = \text{Tr}(A) - \ln[\det(A)] \quad \text{Byrd and Nocedal}[4]$$

$$(1.13) \quad \omega(A) = \frac{\text{Tr}(A)}{n [\det(A)]^{1/n}} \quad \text{Dennis and Wolkowicz}[10]$$

$$(1.14) \quad \sigma(A) = \frac{\lambda_1(A)}{\det(A)^{1/n}} \quad \text{Wolkowicz}[23]$$

$$(1.15) \quad \begin{aligned} \varphi(A) &= n \ln[n \omega(A)] & \text{Todd}[22] \\ &= n \ln \text{Tr}(A) - \ln \det(A) \end{aligned}$$

In (1.14), $\lambda_1(A)$ denotes the largest eigenvalue of A .

Dennis and Wolkowicz [10] used the ω -measure (1.13) to give a specific sense in which γ_{OL} (see (1.10)) is the optimal sizing factor for the DFP update and γ_{IOL} (see (1.10)) is the optimal sizing factor for the BFGS update.

Byrd and Nocedal [4] introduced the ψ -measure (1.12) as a tool for analyzing the global behavior of quasi-Newton methods. The ψ -measure was a critical ingredient in the elegant global convergence theory established for methods from the convex Broyden class (except DFP) by Byrd, Nocedal, and Yuan [3].

Fletcher [12] studied the ψ -measure (1.12) and used it to establish yet another optimality characterization of the BFGS and DFP secant updates. Todd [22], following Fletcher's approach, used the φ -measure (1.15) to provide an alternative proof of a result of Dennis and Wolkowicz [10].

Byrd, Liu, and Nocedal[5] used the ψ -function to study the preconvex class. They claimed that negative values of ϕ in (1.6) are desirable. They also gave conditions on ϕ that guaranteed superlinear convergence. Moreover, they minimized $\psi(D^{-1/2} B_+ D^{-1/2})$

with respect to ϕ (with $\gamma = 1$) to obtain the optimal parameter ϕ^* . This is analogous to Strategy 1 in this paper if sizing is not used (see Section 3). Byrd et al. used $D = \nabla^2 f(x_c)$ in their numerical experiments. Clearly, this D is not available in a secant environment. However, since its use led to good numerical results, a certain validity of the theory has been demonstrated.

2 Preliminaries

The previous comments lead us to consider obtaining improved secant updates by embedding the Broyden family of updates in a larger parametric class of secant updates and then selecting the parameters which optimize a “goodness” or “conditioning” measure. Toward this end we now motivate our choice for the measure function and our choice for the parametric class.

Our choice for the measure is the Byrd-Nocedal ψ -measure

$$(2.1) \quad \psi(A) = \text{Tr}(A) - \ln[\det(A)] .$$

This measure involves all the eigenvalues of A , and not just the smallest and largest as more traditional condition measures do.

The following known properties of ψ will be important in our theory. A proof can be found in Fletcher [12].

Theorem 2.1 *The function ψ defined by (2.1) is strictly convex on the set*

$$\Gamma = \{M \in R^{n \times n} \mid M \text{ is symmetric and positive definite}\} .$$

Furthermore, $\psi(A)$ is globally and uniquely minimized by $A = I$ over the set Γ .

We now motivate our parametric family of secant updates. Historically it has been observed that the DFP update tends to produce updates with small eigenvalues, while the BFGS update tends to produce updates with large eigenvalues. Hence in working with matrices which have been generated by the BFGS update there is a danger that a particular sizing factor may be excessively small and the sized matrix γB may be nearly singular. In order to overcome this difficulty, in addition to sizing, we consider shifting the sized matrix γB , that is, we consider the following update

$$(2.2) \quad B_+ = BFGS(\gamma B + M, s, y).$$

In (2.2), γ is a sizing factor which makes the large eigenvalues small, and M is a shifting matrix which moves γB away from near singularity. Note that, for any γ and M , the update $BFGS(\gamma B + M, s, y)$ satisfies the secant condition (1.3). These motivational comments lead us to consider as our parametric family

$$(2.3) \quad \begin{aligned} B_+ &= BFGS(\gamma B + \phi v v^T, s, y) \\ &= BFGS(\gamma B, s, y) + \phi v v^T, \end{aligned}$$

where v is given by (1.7), and the matrix $\phi v v^T$ is chosen as a shifting matrix M in (2.2).

Note that the new sized Broyden family (2.3) is somewhat different from the Oren-Luenberger family (1.9). The essential difference between them is that in (2.3) the sizing and shifting are independent of each other.

For the two sized Broyden families (1.9) and (2.3), we have the following lemma. Its proof follows from the sufficient conditions stated above (see (1.8)) for B_+ in the Broyden family (1.6) to be symmetric and positive definite.

Lemma 2.1 *Assume that B is symmetric and positive definite, and $y^T s > 0$.*

1. *If $\gamma > 0$ and $\phi > \phi^\#$, then B_+ given by (1.9) is symmetric and positive definite.*
2. *If $\gamma > 0$ and $\phi > \gamma\phi^\#$, then B_+ given by (2.3) is symmetric and positive definite.*

Our objective is how to best choose parameters γ and ϕ in both (1.9) and (2.3). Oren and Spedicato[18] chose the parameters in (1.9) which minimized an upper bound of $\kappa_2(D^{-1/2}B_+D^{-1/2})$. Here $D = B$ and $\kappa_2(A)$ is the l_2 -norm condition number of A proposed by Davidon[8].

We will use the ψ -measure (2.1) instead of κ_2 to compute optimal values of γ and ϕ in (1.9) and (2.3). We consider minimizing $\psi(D^{-1/2}B_+D^{-1/2})$ for some symmetric positive definite matrix D and investigate the performance for $D = B$, I , and $\nabla^2 f(x_c)$.¹

From Theorem 2.1 we see that $B_x = D$ uniquely minimizes $\psi(D^{-\frac{1}{2}}B_xD^{-\frac{1}{2}})$ over the class of symmetric and positive definite matrices. Hence, the choice of weighting matrix $D = B$ gives a least-change secant method flavor, $D = I$ gives a gradient method flavor, and $D = \nabla^2 f(x)$ gives a Newton's method flavor.

We will consider three types of minimization problems applied to both the Oren-Luenberger sized Broyden class (1.9) and our sized Broyden class (2.3). Firstly, for a given sizing factor γ , we find the optimal secant update in the sized classes by minimizing ψ over the appropriate class to determine the optimal value of ϕ . Secondly, we do the above with the roles of γ and ϕ interchanged to find an optimal sizing factor γ for a fixed member of the Broyden class (i.e. fixed ϕ). Finally, we determine the optimal sized member of each sized Broyden class by minimizing ψ over (1.9) and over (2.3) in both γ and ϕ . Strategy 1 described in Section 3 concerns this activity for the Oren-Luenberger sized Broyden class (1.9). Strategy 2 described in Section 4 concerns this activity for our sized Broyden class (2.3).

The following algebraic properties of the map (1.4) will be very useful in the next two sections. Their proofs can be obtained from straightforward linear algebra manipulations.

Proposition 2.1 *For any $n \times n$ matrix X ,*

1. *The secant condition $[BFGS(X, s, y)]s = y$ is satisfied.*
2. *If X is symmetric, then $BFGS(X, s, y)$ is also symmetric.*
3. *If X is symmetric and positive definite, and $y^T s > 0$, then $BFGS(X, s, y)$ is also symmetric and positive definite.*

¹The matrix $D^{1/2}$ is defined as the non-singular and symmetric matrix such that $(D^{1/2})^2 = D$.

4. If X is symmetric,

$$\text{Tr}[BFGS(X, s, y)] = \text{Tr}(X) - \frac{\|Xs\|^2}{s^T X s} + \frac{\|y\|^2}{y^T s}.$$

5. We have

$$\det[BFGS(X, s, y)] = \det(X) \frac{y^T s}{s^T X s}.$$

3 Strategy 1

In this section, we derive weighted ψ -optimal values for γ and ϕ in the Oren–Luenberger sized Broyden class (1.9). Consider a given symmetric positive definite matrix D . We introduce this weight D into our optimization problem by working with the quantities

$$(3.1) \quad \hat{B}_+ = D^{-1/2} B_+ D^{-1/2}, \quad \hat{B} = D^{-1/2} B D^{-1/2}, \quad \hat{y} = D^{-1/2} y \quad \text{and} \quad \hat{s} = D^{1/2} s$$

and then considering the D -weighted Byrd–Nocedal measure $\psi(\hat{B}_+)$.

Observe that since the Byrd–Nocedal measure ψ is uniquely and globally minimized by the identity matrix, there will be a tendency to choose parameters which in some sense force $\hat{B}_+$ to approximate the identity. Now, if $\hat{B}_+ \approx I$, then $B_+ \approx D$. Hence the choice $D = B$ gives a least change or secant flavor, the choice $D = \nabla^2 f(x)$ gives a Newton’s method flavor, and the choice $D = I$ gives a steepest descent method flavor. We ask the reader to keep these comments in mind throughout the remainder of the paper and in particular in the numerical experiments section. At this point in the journey it is not at all clear which choice of D will win numerically. Indeed this was a significant part of our motivation for including the three choices in the present study.

We have

$$(3.2) \quad \begin{aligned} \hat{B}_+ &= \gamma \left(\hat{B} - \frac{\hat{B} \hat{s} \hat{s}^T \hat{B}}{\hat{s}^T \hat{B} \hat{s}} + \phi \hat{v} \hat{v}^T \right) + \frac{\hat{y} \hat{y}^T}{\hat{y}^T \hat{s}} \\ &= BFGS(\gamma(\hat{B} + \phi \hat{v} \hat{v}^T), \hat{s}, \hat{y}), \end{aligned}$$

where

$$\hat{v} = \sqrt{\hat{s}^T \hat{B} \hat{s}} \left(\frac{\hat{y}}{\hat{y}^T \hat{s}} - \frac{\hat{B} \hat{s}}{\hat{s}^T \hat{B} \hat{s}} \right) = D^{-1/2} v$$

and v is given by (1.7). Note that some quantities are invariant under the scaling (3.1); i.e.

$$\hat{y}^T \hat{s} = y^T s, \quad \hat{s}^T \hat{B} \hat{s} = s^T B s, \quad \hat{y}^T \hat{B}^{-1} \hat{y} = y^T B^{-1} y \quad \text{and} \quad \hat{v}^T \hat{B}^{-1} \hat{v} = v^T B^{-1} v = \tau - 1.$$

However others are not invariant, i.e.,

$$\begin{aligned} \|\hat{y}\|^2 &= y^T D^{-1} y, \quad \|\hat{B} \hat{s}\|^2 = \|D^{-1/2} B s\|^2 = s^T B D^{-1} B s, \\ \|\hat{v}\|^2 &= v^T D^{-1} v = (s^T B s) \left(\frac{y^T D^{-1} y}{(y^T s)^2} - 2 \frac{y^T D^{-1} B s}{(y^T s)(s^T B s)} + \frac{s^T B D^{-1} B s}{(s^T B s)^2} \right). \end{aligned}$$

Thus an application of Proposition 2.1 to the expression (3.2) yields

$$\begin{aligned} Tr(\hat{B}_+) &= \gamma \left(Tr(\hat{B}) - \frac{\|\hat{B}\hat{s}\|^2}{\hat{s}^T \hat{B} \hat{s}} + \phi \|\hat{v}\|^2 \right) + \frac{\|\hat{y}\|^2}{\hat{y}^T \hat{s}} \\ &= \gamma \left(Tr(\hat{B}) - \frac{s^T B D^{-1} B s}{s^T B s} + \phi v^T D^{-1} v \right) + \frac{y^T D^{-1} y}{y^T s}, \end{aligned}$$

and

$$\begin{aligned} det(\hat{B}_+) &= det(BFGS(\gamma(\hat{B} + \phi \hat{v} \hat{v}^T), \hat{s}, \hat{y})) \\ &= \frac{\gamma^n}{\gamma} det(\hat{B}) det(I + \phi \hat{B}^{-1} \hat{v} \hat{v}^T) \frac{\hat{y}^T \hat{s}}{\hat{s}^T \hat{B} \hat{s}} \\ &= \gamma^{n-1} det(\hat{B}) \left(\frac{y^T s}{s^T B s} \right) (1 + \phi(\tau - 1)), \end{aligned}$$

where τ is defined in (1.8).

We will be interested in minimizing $\psi(\hat{B}_+)$ in γ or ϕ or both for a fixed matrix D . Hence we must study $\psi(\hat{B}_+)$. Using the preceding results, we have

$$\begin{aligned} (3.3) \quad \psi(\hat{B}_+) &= Tr(\hat{B}_+) - \ln(det(\hat{B}_+)) \\ &= \gamma \left(Tr(\hat{B}) - \frac{s^T B D^{-1} B s}{s^T B s} + \phi v^T D^{-1} v \right) + \frac{y^T D^{-1} y}{y^T s} \\ &\quad - (n-1) \ln \gamma - \ln(det(\hat{B})) - \ln(1 + \phi(\tau - 1)) - \ln \left(\frac{y^T s}{s^T B s} \right). \end{aligned}$$

Now, we have

$$\begin{aligned} \frac{\partial \psi}{\partial \phi} &= \gamma v^T D^{-1} v - \frac{\tau - 1}{1 + \phi(\tau - 1)}, \\ \frac{\partial \psi}{\partial \gamma} &= \xi + \phi v^T D^{-1} v - \frac{n-1}{\gamma}, \\ \frac{\partial^2 \psi}{\partial \phi^2} &= \frac{(\tau - 1)^2}{(1 + \phi(\tau - 1))^2} > 0, \\ \frac{\partial^2 \psi}{\partial \gamma^2} &= \frac{n-1}{\gamma^2} > 0, \end{aligned}$$

and

$$\frac{\partial^2 \psi}{\partial \phi \partial \gamma} = \frac{\partial^2 \psi}{\partial \gamma \partial \phi} = v^T D^{-1} v,$$

where

$$\xi = Tr(\hat{B}) - \frac{s^T B D^{-1} B s}{s^T B s}.$$

Since $Tr(\hat{B})$ is the sum of the eigenvalues of $D^{-1/2} B D^{-1/2}$ and the Rayleigh quotient

$$\frac{s^T B D^{-1} B s}{s^T B s} = \frac{(B^{1/2} s)^T B^{1/2} D^{-1} B^{1/2} (B^{1/2} s)}{(B^{1/2} s)^T (B^{1/2} s)}$$

lies between the smallest and the largest eigenvalues of $B^{1/2}D^{-1}B^{1/2}$, or equivalently of $D^{-1/2}BD^{-1/2}$,² we have

$$(3.4) \quad \xi = \text{Tr}(\hat{B}) - \frac{s^T B D^{-1} B s}{s^T B s} > 0.$$

In addition to $\phi^\#$, we define

$$(3.5) \quad \phi^{\#\#} = -\frac{\xi}{v^T D^{-1} v}.$$

Now we can consider the three types of minimization problems mentioned at the end of Section 2.

[Minimization Problem 1]

$$(3.6) \quad \min_{\phi > \phi^\#} \psi(\hat{B}_+) \quad \text{for a given } \gamma > 0.$$

Of course, we desire an optimal value ϕ^* such that $\phi^* > \phi^\#$, which will be the case. Since $d^2\psi/d\phi^2 > 0$, ψ is a strictly convex function of ϕ , hence $d\psi/d\phi = 0$ yields the unique global solution of Problem (3.6)

$$(3.7) \quad \phi^* = \frac{1}{\gamma(v^T D^{-1} v)} - \frac{1}{\tau - 1} = \frac{1}{\gamma(v^T D^{-1} v)} + \phi^\# > \phi^\#,$$

where τ and $\phi^\#$ are given in (1.8). The choice $D = B$ gives

$$(3.8) \quad \phi^* = \frac{1}{\gamma(\tau - 1)} - \frac{1}{\tau - 1} = \frac{1 - \gamma}{\gamma(\tau - 1)}.$$

Observe that here $\gamma = 1$ implies $\phi^* = 0$. So with no sizing, BFGS is optimal in this case.

Recall that the choice $D = \nabla^2 f(x)$ with $\gamma = 1$ (no sizing) was considered in the numerical experiments of Byrd et al.[5] and good numerical results were reported.

[Minimization Problem 2]

$$(3.9) \quad \min_{\gamma > 0} \psi(\hat{B}_+) \quad \text{for a given } \phi (> \phi^\#).$$

As before, since $d^2\psi/d\gamma^2 > 0$, ψ is a strictly convex function of γ , hence $d\psi/d\gamma = 0$ yields the unique global solution of Problem (3.9)

$$(3.10) \quad \gamma^* = \frac{n - 1}{\xi + \phi v^T D^{-1} v} = \frac{n - 1}{v^T D^{-1} v (\phi - \phi^{\#\#})},$$

provided $n > 1$ and $\phi > \max(\phi^\#, \phi^{\#\#})$ (to guarantee $\gamma^* > 0$).

The choice $D = B$ gives

$$\gamma^* = \frac{1}{1 + \phi \frac{\tau - 1}{n - 1}}.$$

²If (λ, x) is an eigenvalue-eigenvector pair of $B^{1/2}D^{-1}B^{1/2}$, $(\lambda, D^{1/2}B^{-1/2}x)$ is an eigenvalue-eigenvector pair of $D^{-1/2}BD^{-1/2}$.

Note that $\phi = 0$ (BFGS) implies $\gamma^* = 1$, so if we use the BFGS, then no sizing is optimal.

[Minimization Problem 3]

$$(3.11) \quad \min_{\phi > \phi^\# \quad \gamma > 0} \psi(\hat{B}_+)$$

The necessary conditions $\partial\psi/\partial\phi = 0$ and $\partial\psi/\partial\gamma = 0$ give the equations

$$\begin{aligned} \phi(v^T D^{-1} v) &= \frac{1}{\gamma} - \frac{v^T D^{-1} v}{\tau - 1}, \\ \xi + \phi v^T D^{-1} v - \frac{n-1}{\gamma} &= 0, \end{aligned}$$

where ξ is given by (3.4). Now, we have

$$(3.12) \quad \begin{aligned} \frac{1}{\gamma^*} &= \frac{1}{n-2} \left(\xi - \frac{v^T D^{-1} v}{\tau - 1} \right) \\ &= (\phi^\# - \phi^{\#\#}) \frac{v^T D^{-1} v}{n-2}, \end{aligned}$$

$$(3.13) \quad \begin{aligned} \phi^* &= \frac{\xi}{(n-2)(v^T D^{-1} v)} - \left(\frac{n-1}{n-2} \right) \frac{1}{\tau - 1} \\ &= \frac{1}{n-2} (\phi^\# - \phi^{\#\#}) + \phi^\#. \end{aligned}$$

For Problem (3.11), we must investigate the positive definiteness of $\nabla^2\psi$. Since the Hessian $\nabla^2\psi$ is represented by

$$\nabla^2\psi = \begin{pmatrix} \psi_{\phi\phi} & \psi_{\phi\gamma} \\ \psi_{\gamma\phi} & \psi_{\gamma\gamma} \end{pmatrix} = \begin{pmatrix} \frac{(\tau-1)^2}{(1+\phi(\tau-1))^2} & v^T D^{-1} v \\ v^T D^{-1} v & \frac{n-1}{\gamma^2} \end{pmatrix}$$

and $\psi_{\phi\phi} = (\tau-1)^2/(1+\phi(\tau-1))^2 > 0$, a necessary and sufficient condition for $\nabla^2\psi$ to be positive definite is

$$\det(\nabla^2\psi) > 0,$$

i.e.

$$(3.14) \quad \frac{(\tau-1)^2}{(1+\phi(\tau-1))^2} \left(\frac{n-1}{\gamma^2} \right) - (v^T D^{-1} v)^2 > 0.$$

Now it is easy to prove the following lemma.

Lemma 3.1 *The pair (ϕ^*, γ^*) given by (3.12)–(3.13) is the unique global solution of Problem (3.11).*

Proof: Substituting (ϕ^*, γ^*) into (3.14), we have

$$\det(\nabla^2\psi(\phi^*, \gamma^*)) = (n-2)(v^T D^{-1} v)^2 > 0.$$

Therefore $\nabla^2\psi(\phi^*, \gamma^*)$ is positive definite and (ϕ^*, γ^*) is a local solution. The uniqueness follows from the fact that (ϕ^*, γ^*) is the unique solution of the necessary conditions $\partial\psi/\partial\phi = 0$ and $\partial\psi/\partial\gamma = 0$. $\square$

The choice $D = B$ gives $\gamma^* = 1$ and $\phi^* = 0$. This implies that the BFGS update without sizing is optimal for this particular choice of weighting matrix.

Summarizing the preceding results, we obtain the following proposition.

Proposition 3.1

1. The parameter ϕ^* in Problem (3.6) is greater than $\phi^\#$.
2. If $\phi^\# > \phi^{\#\#}$, then the parameters γ^* in Problem (3.9) and (ϕ^*, γ^*) in Problem (3.11) satisfy the conditions

$$\phi^* > \phi^\# \quad \text{and} \quad \gamma^* > 0.$$

4 Strategy 2

In this section, we derive weighted ψ -optimal values for γ and ϕ in our new sized Broyden family (2.3). Recall that this new family is different from the Oren-Luenberger family (1.9). The essential difference between (1.9) and (2.3) is that in (2.3), the matrix ϕvv^T is used as a shifting operator and only the matrix B is sized. By doing so, we can separately control the sizing parameter and the shifting term. As before we work with $\psi(\hat{B}_+)$. We have

$$\begin{aligned} \hat{B}_+ &= BFGS(\gamma\hat{B} + \phi\hat{v}\hat{v}^T, \hat{s}, \hat{y}) \\ (4.1) \quad &= \gamma \left(\hat{B} - \frac{\hat{B}\hat{s}\hat{s}^T\hat{B}}{\hat{s}^T\hat{B}\hat{s}} \right) + \phi\hat{v}\hat{v}^T + \frac{\hat{y}\hat{y}^T}{\hat{y}^T\hat{s}}, \end{aligned}$$

where

$$\hat{v} = \sqrt{\hat{s}^T\hat{B}\hat{s}} \left(\frac{\hat{y}}{\hat{y}^T\hat{s}} - \frac{\hat{B}\hat{s}}{\hat{s}^T\hat{B}\hat{s}} \right).$$

Using the same arguments as in Section 3, we have

$$\begin{aligned} Tr(\hat{B}_+) &= \gamma \left(Tr(\hat{B}) - \frac{\|\hat{B}\hat{s}\|^2}{\hat{s}^T\hat{B}\hat{s}} \right) + \phi\|\hat{v}\|^2 + \frac{\|\hat{y}\|^2}{\hat{y}^T\hat{s}} \\ &= \gamma \left(Tr(\hat{B}) - \frac{s^T B D^{-1} B s}{s^T B s} \right) + \phi v^T D^{-1} v + \frac{y^T D^{-1} y}{y^T s}, \end{aligned}$$

and

$$\begin{aligned} det(\hat{B}_+) &= det(BFGS(\gamma\hat{B} + \phi\hat{v}\hat{v}^T, \hat{s}, \hat{y})) \\ &= \gamma_{n-1} det(\hat{B}) \left(\frac{y^T s}{s^T B s} \right) \left(1 + \frac{\phi}{\gamma}(\tau - 1) \right), \end{aligned}$$

where τ is defined in (1.8).

Thus,

$$(4.2) \quad \psi(\hat{B}_+) = \text{Tr}(\hat{B}_+) - \ln(\det(\hat{B}_+))$$

$$(4.3) \quad = \gamma\xi + \phi v^T D^{-1} v + \frac{y^T D^{-1} y}{y^T s} \\ - (n-2) \ln \gamma - \ln(\det(\hat{B})) - \ln(\gamma + \phi(\tau-1)) - \ln\left(\frac{y^T s}{s^T B s}\right),$$

where ξ is given by (3.4).

Then we have

$$\begin{aligned} \frac{\partial \psi}{\partial \phi} &= v^T D^{-1} v - \frac{\tau-1}{\gamma + \phi(\tau-1)}, \\ \frac{\partial \psi}{\partial \gamma} &= \xi - \frac{n-2}{\gamma} - \frac{1}{\gamma + \phi(\tau-1)}, \\ \frac{\partial^2 \psi}{\partial \phi^2} &= \frac{(\tau-1)^2}{(\gamma + \phi(\tau-1))^2} > 0, \\ \frac{\partial^2 \psi}{\partial \gamma^2} &= \frac{n-2}{\gamma^2} + \frac{1}{(\gamma + \phi(\tau-1))^2} > 0, \\ \text{and} \quad \frac{\partial^2 \psi}{\partial \phi \partial \gamma} &= \frac{\partial^2 \psi}{\partial \gamma \partial \phi} = \frac{\tau-1}{(\gamma + \phi(\tau-1))^2} > 0. \end{aligned}$$

Now, we can consider the same minimization problems for function (4.2) as we did for function (3.3).

[Minimization Problem 1]

$$(4.4) \quad \min_{\phi > \gamma\phi^\#} \psi(\hat{B}_+) \quad \text{for a given } \gamma (> 0).$$

Of course, we need an optimal value ϕ^* such that $\phi^* > \gamma\phi^\#$ (see Lemma 2.1), which will be the case. Since $d^2\psi/d\phi^2 > 0$, ψ is a strictly convex function in ϕ . Hence $d\psi/d\phi = 0$ yields the unique global solution of Problem (4.4)

$$(4.5) \quad \phi^* = \frac{1}{v^T D^{-1} v} - \frac{\gamma}{\tau-1} = \frac{1}{v^T D^{-1} v} + \gamma\phi^\# > \gamma\phi^\#.$$

The choice $D = B$ gives

$$(4.6) \quad \phi^* = \frac{1-\gamma}{\tau-1}.$$

Note that $\gamma = 1$ (no sizing) implies $\phi^* = 0$ (BFGS).

[Minimization Problem 2]

$$(4.7) \quad \min_{\gamma > 0} \psi(\hat{B}_+) \quad \text{for a given } \phi (> \gamma\phi^\#).$$

As before, since $d^2\psi/d\gamma^2 > 0$, ψ is a strictly convex function of γ , hence the equation $d\psi/d\gamma = 0$ implies

$$\xi - \frac{n-2}{\gamma} - \frac{1}{\gamma + \phi(\tau-1)} = 0.$$

This yields a quadratic equation of γ

$$\xi\gamma^2 + (\xi\phi(\tau - 1) - (n - 1))\gamma - \phi(\tau - 1)(n - 2) = 0.$$

Thus we have

$$\gamma = \frac{1}{2\xi} [(n - 1) - \xi\phi(\tau - 1) \pm \sqrt{\delta}],$$

where

$$\delta = (\xi\phi(\tau - 1) - (n - 1))^2 + 4\xi\phi(\tau - 1)(n - 2).$$

Considering the positivity of γ , we choose

$$(4.8) \quad \gamma^* = \frac{1}{2\xi} [(n - 1) - \xi\phi(\tau - 1) + \sqrt{\delta}].$$

Now we investigate the positivity of γ . In the choice $\phi > 0$, we have

$$\delta = (\xi\phi(\tau - 1) - (n - 1))^2 + 4\xi\phi(\tau - 1)(n - 2) > 0.$$

In the choice $\phi \leq 0$, we have

$$\delta = (\xi\phi(\tau - 1) + (n - 1))^2 - 4\xi\phi(\tau - 1) > 0.$$

Then, for any ϕ ,

$$\gamma^* = \gamma^*(\phi) = \frac{1}{2\xi} [(n - 1) - \xi\phi(\tau - 1) + \sqrt{\delta}] > 0,$$

so we must choose a parameter ϕ such that $\phi > \gamma^*(\phi)\phi^\#$.

The choice $D = B$ gives $\xi = n - 1$; therefore

$$(4.9) \quad \gamma^* = \frac{1}{2} \left(1 - \phi(\tau - 1) + \sqrt{(\phi(\tau - 1) - 1)^2 + 4\phi(\tau - 1)\frac{n - 2}{n - 1}} \right).$$

Note that $\phi = 0$ implies $\gamma = 1$.

[Minimization Problem 3]

$$(4.10) \quad \min_{\phi > \gamma\phi^\#} \min_{\gamma > 0} \psi(\hat{B}_+)$$

Since

$$\frac{\partial^2 \psi}{\partial \phi^2} = \frac{(\tau - 1)^2}{(\gamma + \phi(\tau - 1))^2} > 0,$$

and

$$\begin{aligned} \det(\nabla^2 \psi(\phi, \gamma)) &= \frac{(\tau - 1)^2}{(\gamma + \phi(\tau - 1))^2} \left(\frac{n - 2}{\gamma^2} + \frac{1}{(\gamma + \phi(\tau - 1))^2} \right) - \frac{(\tau - 1)^2}{(\gamma + \phi(\tau - 1))^4} \\ &= \frac{(\tau - 1)^2}{(\gamma + \phi(\tau - 1))^2} \left(\frac{n - 2}{\gamma^2} \right) > 0, \end{aligned}$$

the function $\psi(\hat{B}_+)$ given by (4.2) is strictly convex with respect to (ϕ, γ) . Thus, for Problem (4.10), a stationary point is the unique optimal point. The equations

$$\frac{\partial \psi}{\partial \phi} = 0 \quad \text{and} \quad \frac{\partial \psi}{\partial \gamma} = 0$$

yield

$$\begin{aligned} \frac{1}{\gamma + \phi(\tau - 1)} &= \frac{v^T D^{-1} v}{\tau - 1}, \\ \xi - \frac{n - 2}{\gamma} - \frac{1}{\gamma + \phi(\tau - 1)} &= 0. \end{aligned}$$

Therefore we obtain the unique global solution for Problem (4.10)

$$(4.11) \quad \gamma^* = \frac{n - 2}{\xi - \frac{v^T D^{-1} v}{\tau - 1}} = \frac{1}{\phi^\# - \phi^{\#\#}} \frac{n - 2}{v^T D^{-1} v},$$

$$(4.12) \quad \phi^* = \frac{1}{v^T D^{-1} v} - \frac{\gamma^*}{\tau - 1} = \frac{1}{v^T D^{-1} v} + \gamma^* \phi^\# > \gamma^* \phi^\#.$$

The choice $D = B$ gives $\gamma^* = 1$ and $\phi^* = 0$. This implies that the BFGS update without sizing is optimal for this choice of weighting matrix.

Summarizing the preceding results, we obtain the following proposition.

Proposition 4.1

1. The parameter ϕ^* in Problem (4.4) is greater than $\gamma \phi^\#$.
2. The parameter γ^* in Problem (4.7) is positive for all ϕ . (Recall that for B_+ to be positive definite, the parameter ϕ must be chosen so that $\phi > \gamma^*(\phi) \phi^\#$.)
3. If $\phi^\# > \phi^{\#\#}$, then the parameters (ϕ^*, γ^*) in Problem (4.10) satisfy the conditions

$$\phi^* > \phi^\# \gamma^* \quad \text{and} \quad \gamma^* > 0.$$

5 Relationships Between Strategies

In this section, we summarize the main results obtained in Sections 3 and 4 and present some relationships among them. Let the ψ -optimal values in Strategies 1 and 2 be ϕ_1^*, γ_1^* and ϕ_2^*, γ_2^* , respectively. Assuming that B is symmetric and positive definite, and y and s are linearly independent, and $y^T s > 0$, the results concerning the three minimization problems we considered are the following.

[Minimization Problem 1]

Since, for γ positive, we have

$$\phi_1^* = \frac{1}{\gamma(v^T D^{-1} v)} + \phi^\# \quad \text{and} \quad \phi_2^* = \frac{1}{v^T D^{-1} v} + \gamma \phi^\#,$$

we obtain the relationship

$$\phi_2^* = \gamma \phi_1^*.$$

Moreover, these optimal values always produce symmetric positive definite updates.

[Minimization Problem 2]

For a given ϕ , we have

$$\gamma_1^* = \frac{n-1}{\xi + \phi v^T D^{-1} v}$$

and

$$\gamma_2^* = \frac{1}{2\xi} [(n-1) - \xi\phi(\tau-1) + \sqrt{(\xi\phi(\tau-1) - (n-1))^2 + 4\xi\phi(\tau-1)(n-2)}],$$

where

$$\xi = \text{Tr}(D^{-1/2} B D^{-1/2}) - \frac{s^T B D^{-1} B s}{s^T B s} > 0.$$

In this case, these optimal values do not always produce a positive definite update. However, $\phi \geq 0$ is sufficient, but not necessary, for these optimal values to produce symmetric positive definite updates.

[Minimization Problem 3]

Since

$$\begin{aligned} \phi_1^* &= \frac{\xi}{(n-2)(v^T D^{-1} v)} + \left(\frac{n-1}{n-2}\right) \phi^\# = \frac{1}{\gamma_1^* v^T D^{-1} v} + \phi^\#, \\ \gamma_1^* &= \frac{n-2}{\xi + v^T D^{-1} v \phi^\#}, \end{aligned}$$

and

$$\begin{aligned} \phi_2^* &= \frac{1}{v^T D^{-1} v} + \gamma_2^* \phi^\#, \\ \gamma_2^* &= \frac{n-2}{\xi + v^T D^{-1} v \phi^\#}, \end{aligned}$$

we obtain the relationships

$$\phi_2^* = \gamma^* \phi_1^* \quad \text{and} \quad \gamma^* \equiv \gamma_1^* = \gamma_2^*.$$

Once again, even though these optimal values do not always produce positive definite updates, $\phi \geq 0$ is sufficient, but not necessary, for these optimal values to produce symmetric positive definite updates.

Finally, observe that, in the choice $D = B$, the standard BFGS update ($\phi = 0, \gamma = 1$) is optimal using either Strategy 1 or 2 for Problem 1 with $\gamma = 1$, for Problem 2 with $\phi = 0$, and for Problem 3. This is certainly an interesting finding and begs for more understanding.

6 Numerical Experiments

Contreras and Tapia[7] obtained impressive numerical results for the BFGS trust-region method using selective sizing and a sizing factor γ_{COL} they called *centered Oren-Luenberger*. In this section, we present considerable numerical experimentation using various forms of the sizing strategies described in Sections 3 and 4. Our objective, of course, is to determine if one particular approach is more effective than the others, and if any one of our approaches compares favorably with the Contreras-Tapia approach. Hence, we include this latter approach in our numerical studies.

Our sizing strategies were adapted to both the trust-region and line-search algorithms in an enhanced MATLAB version of the well-known Dennis-Schnabel code[9]. This code uses the double-dogleg implementation of trust-region globalization and the backtracking implementation of line-search globalization.

Our experimentation implies that one approach is superior to the others and this approach is also superior to the Contreras-Tapia BFGS approach. The best sizing procedure was derived from our new sized Broyden family (2.3) (Strategy 2) as the solution of Minimization Problem 1 given by (4.4) with $D = I$ and $\gamma = \gamma_{COL}$, the centered Oren-Luenberger sizing introduced by Contreras and Tapia. Later on, we call this approach I2-COL. In fact, Method I2-COL was efficient (see Table 3), robust to parameter changes (see Tables 5 and 6), and reliable as the problem size increased (see Table 7).³ See Section 7 for a plausible explanation as to why I2-COL is our most effective strategy.

6.1 Implementation

We incorporated into our code the options of *shifting* and *sizing* the approximation to the Hessian before it is updated. Thus, before the BFGS updating formula is applied to a matrix B , we have the option of modifying B either by

$$(6.1) \quad B \leftarrow \gamma (B + \phi vv^T) \quad (\text{Oren - Luenberger sizing (1.9)})$$

or by

$$(6.2) \quad B \leftarrow \gamma B + \phi vv^T \quad (\text{New sizing (2.3)}),$$

depending on whether Strategy 1 (Section 3) or Strategy 2 (Section 4) is being used. Here γ and ϕ are real scalars and $v \in R^n$ is given by (1.7).

We also included in the code the ability to accept an arbitrary initial matrix B_0 . Our choices for the initial matrix B_0 were

$$(6.3) \quad \begin{aligned} B_0^0 &= |f(x_0)| I, \\ B_0^1 &= \text{diag}(10, 10^4, 1, \dots, 1), \\ B_0^2 &= \text{diag}(10^{-1}, 10^{-4}, 1, \dots, 1), \\ B_0^3 &= \text{diag}(0.1, 2, 0.5, 10, 1, \dots, 1). \end{aligned}$$

In the first expression of (6.3), x_0 denotes the starting point. Observe that B_0^0 has representative eigenvalues, B_0^1 has large eigenvalues, B_0^2 has small eigenvalues, and B_0^3

³Other methods were "equally" efficient, but not as robust and reliable. See Methods BFGS-COL, I1-OL, I2-OL for example.

has moderate size eigenvalues. In all of our experiments we allowed a maximum of 500 iterations. The stopping criteria employed is the same as that used in the Dennis-Schnabel optimization code, in particular, convergence is reached when the relative gradient is less than 10^{-7} . The machine used to obtain these numerical results was a SUN SPARC-10/Model 41.

Our test set consists of five problems. Four of them are problems 1, 2, 5 and 21 (with $n=6$) from the standard set of test functions in Moré, Garbow and Hillstom[14]. The other one is the strictly convex quartic function of Byrd, Liu, and Nocedal[5]. This latter function was also used by Al-Baali[2] in similar numerical testing. For each problem, we chose the standard starting point included in the respective reference.

In (6.1) and (6.2), two values were considered for ϕ : 0 (BFGS) and ϕ^* (minimizers given in Sections 3 and 4),⁴ and three values for γ : the Oren-Luenberger sizing factor γ_{OL} given in (1.10), the Centered Oren-Luenberger sizing factor γ_{COL} given by (1.11), and γ^* (minimizer given in Sections 3 and 4). As suggested by Contreras and Tapia[7], to prevent us from inadvertently sizing with an excessively small constant, the actual sizing factor used was $\max\{\gamma_{min}, \gamma\}$, where γ is the computed sizing factor, and γ_{min} is a small positive constant.

Our numerical experimentation concerned the following 14 sizing procedures and the standard BFGS method for comparison purposes.

0. BFGS ($\gamma = 1$, $\phi = 0$, Standard BFGS).
1. OL-BFGS ($\gamma = \gamma_{OL}$, $\phi = 0$, Standard sized BFGS).⁵
2. COL-BFGS ($\gamma = \gamma_{COL}$, $\phi = 0$, Standard sized BFGS).⁶
3. B1-OL ($\gamma = \gamma_{OL}$, $\phi = \phi^*$ given by (3.7), Strategy 1, Min. Prob. 1, $D = B$).
4. B1-COL ($\gamma = \gamma_{COL}$, $\phi = \phi^*$ given by (3.7), Strategy 1, Min. Prob. 1, $D = B$).
5. B2-OL ($\gamma = \gamma_{OL}$, $\phi = \phi^*$ given by (4.5), Strategy 2, Min. Prob. 1, $D = B$).
6. B2-COL ($\gamma = \gamma_{COL}$, $\phi = \phi^*$ given by (4.5), Strategy 2, Min. Prob. 1, $D = B$).
7. I1-OL ($\gamma = \gamma_{OL}$, $\phi = \phi^*$ given by (3.7), Strategy 1, Min. Prob. 1, $D = I$).
8. I1-COL ($\gamma = \gamma_{COL}$, $\phi = \phi^*$ given by (3.7), Strategy 1, Min. Prob. 1, $D = I$).
9. I2-OL ($\gamma = \gamma_{OL}$, $\phi = \phi^*$ given by (4.5), Strategy 2, Minimization Problem 1, $D = I$).
10. I2-COL ($\gamma = \gamma_{COL}$, $\phi = \phi^*$ given by (4.5), Strategy 2, Min. Prob. 1, $D = I$).
11. I12* ($\gamma = \gamma^*$ given by (3.10), $\phi = 0$, Strategy 1, Minimization Problem 2, $D = I$).
12. I22* ($\gamma = \gamma^*$ given by (4.8), $\phi = 0$, Strategy 2, Min. Prob. 2, $D = I$).
13. I13* ($\gamma = \gamma^*$, $\phi = \phi^*$ given by (3.12) and (3.13), Strategy 1, Minimization Problem 3, $D = I$).

⁴Since not always $\phi^* > \phi^\#$ (or $\phi^* > \gamma\phi^\#$), ϕ^* was used only if $\phi^* > 0.95\phi^\#$ (or $\phi^* > 0.95\gamma\phi^\#$).

⁵Oren-Luenberger-sized BFGS, Oren[16], and Oren and Luenberger[17].

⁶Centered Oren-Luenberger sized BFGS, Contreras and Tapia[7].

14. I23* ($\gamma = \gamma^*$, $\phi = \phi^*$ given by (4.11) and (4.12), Strategy 2, Minimization Problem 3, $D = I$).

6.2 Preliminary Results

An important observation from our initial experimentation concerns how often sizing should be performed. If used at every iteration, the sized secant strategies suggested in Sections 3 and 4 were inferior to the standard BFGS in all problems except the last one.⁷ Therefore, sizing should be used as a *safeguarding* of the BFGS secant method; in other words, we size or shift B before it is updated only when a need is detected (Selective Sizing/Shifting). It is interesting that this is what has been concluded by numerous authors including Carter[6], Contreras and Tapia[7], Al-Baali[1],[2], and Wolkowicz[23]. Following Contreras and Tapia[7], to decide when to size, we use the fact that both γ_{OL} and γ_{COL} should be “close” to 1 whenever B has “good” information relative to $\nabla^2 f(x)$ along the direction s . We consider the following two Selective Sizing/Shifting criteria:

1. Selective Sizing/Shifting Criterion 1
*For $k = 1, 2, \dots$
if $1 - \bar{\gamma} > \epsilon$ then size or shift B .*
2. Selective Sizing/Shifting Criterion 2
*For $k = 1, 2, \dots$
if $|1 - \bar{\gamma}| > \epsilon$ then size or shift B .*

We should mention that our preliminary experimentation included other choices of ϕ such as 1 (DFP) and other choices of γ such as $\gamma_{IOL} = y^T B^{-1} y / y^T s$ (inverse Oren-Luenberger[17]). The results of these experiments showed that selectively sizing the approximation matrix B using γ^* from Sections 3 or 4 as the sizing factor (see Minimization Problem 2 in Sections 3 and 4) improved the behavior of DFP much more than it improved the behavior of BFGS. However, these sizing strategies never made DFP competitive with the standard BFGS. This concurs with the common belief that BFGS is a more robust update than DFP, and therefore, DFP is more likely to be improved by a safeguarding technique such as sizing. We believe that further tuning of these sizing procedures is needed in order to obtain the competitive behavior of DFP reported by Contreras and Tapia[7]. Since no better results than those of the standard BFGS method are expected for the sized DFP method, we excluded it from further numerical experiments.

These results also showed that the choice of γ_{IOL} gave similar results to the choice of γ_{OL} . This is not surprising since both quantities contain essentially the same information concerning B relative to $\nabla^2 f(x)$. For this reason, and because it takes $O(n^2)$ more operations to compute, we excluded γ_{IOL} from further numerical experiments.

6.3 Results

⁷For this particular problem suggested by Byrd et.al.[5], sizing or shifting the matrix in the ways proposed above did improve the behavior of BFGS. This agrees with the results reported by Byrd et.al.[5] and by Al-Baali[2] using a special member of the Broyden Class different from BFGS (shifting).

Table 1: Normalized Averages, ($1 - \gamma_{OL} > 0.05$, $\gamma_{min} = 0.1$)

METHOD	LINE SEARCH			TRUST REGION		
	Iterations	Functions	Fun.-Grad.	Iterations	Functions	Fun.-Grad.
0. BFGS	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1. OL -BFGS	0.8659	0.9677	0.8662	0.9533	1.0392	0.9538
2. COL-BFGS	0.9340	0.9848	0.9337	1.0041	1.1300	1.0038
3. B1 - OL	0.9139	0.9777	0.9141	0.9551	0.9971	0.9555
4. B1 - COL	0.9248	0.9663	0.9250	0.9681	1.0115	0.9684
5. B2 - OL	0.9138	0.9747	0.9141	0.9592	1.0048	0.9596
6. B2 - COL	0.9285	0.9709	0.9287	0.9589	1.0056	0.9593
7. I1 - OL	0.8497	1.0944	0.8500	0.9577	1.1834	0.9575
8. I1 - COL	0.8919	1.0690	0.8922	1.0063	1.2197	1.0058
9. I2 - OL	0.8601	0.9917	0.8607	0.9375	1.0820	0.9378
10. I2 - COL	0.8944	0.9832	0.8949	0.9460	1.0194	0.9463
11. I12*	1.4030	1.6330	1.3930	1.0336	1.0635	1.0316
12. I22*	1.4030	1.6330	1.3930	1.0336	1.0635	1.0316
13. I13*	1.0270	1.1068	1.0269	0.9908	1.1426	0.9904
14. I23*	1.0036	1.0308	1.0038	0.9463	1.0074	0.9466

Table 2: Normalized Averages, ($|1 - \gamma_{OL}| > 0.05$, $\gamma_{min} = 0.1$)

METHOD	LINE SEARCH			TRUST REGION		
	Iterations	Functions	Fun.-Grad.	Iterations	Functions	Fun.-Grad.
0. BFGS	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1. OL -BFGS	1.2112	1.2071	1.2088	1.0961	1.1650	1.0959
2. COL-BFGS	1.1274	1.1746	1.1259	1.1440	1.2255	1.1423
3. B1 - OL	1.2679	1.2184	1.2671	1.1662	1.1671	1.1653
4. B1 - COL	1.1689	1.1364	1.1682	1.0831	1.0975	1.0825
5. B2 - OL	1.2833	1.2407	1.2823	1.1897	1.1878	1.1886
6. B2 - COL	1.1884	1.1543	1.1875	1.0821	1.0837	1.0815
7. I1 - OL	1.6885	2.0295	1.6853	1.4871	1.9763	1.4831
8. I1 - COL	1.1712	1.5095	1.1695	1.4075	1.8285	1.4048
9. I2 - OL	1.3490	1.4927	1.3462	1.2107	1.4682	1.2073
10. I2 - COL	1.1823	1.3410	1.1800	1.1997	1.4089	1.1967
11. I12*	1.2986	3.4839	1.2877	1.5460	2.1660	1.5425
12. I22*	1.2986	3.4839	1.2877	1.5460	2.1660	1.5425
13. I13*	0.9455	2.2305	0.9447	1.3927	2.0251	1.3907
14. I23*	0.9299	1.9855	0.9295	1.2172	1.4421	1.2177

Each of the 14 procedures described in the Implementation Section 6.1 was used to solve the five problems mentioned above. Each problem was solved with the four initial matrix approximations listed in (6.3) using both line-search and trust-region globalization techniques. We use three measures for comparisons: number of iterations, number of function evaluations, and number of function-gradient evaluations (function evaluations plus n times gradient evaluations, where n is the dimension of the problem). The results are presented as the average of each measure over the 20 outputs for each procedure. Our comparisons will be given relative to the control (standard BFGS). We accomplish this by listing all quantities normalized (divided) by the corresponding quantity for the BFGS control.

For each method and each globalization technique, the tables in this section present the average of the normalized data for each of our three measures. Tables 1 and 2 use $\bar{\gamma} = \gamma_{OL}$ in the Selective Sizing/Shifting Criteria 1 and 2, respectively. Similarly, Tables 3 and 4 use $\bar{\gamma} = \gamma_{COL}$. All four tables use $\epsilon = 0.05$ and $\gamma_{min} = 0.1$ in the selective sizing/shifting criteria as suggested by Contreras and Tapia[7].

From these results, we can see that in general:

1. The improvement for the line-search globalization technique is better than it is for the trust-region globalization technique, which indicates that trust region is a more robust technique, and therefore less sensitive to changes such as selective sizing or shifting.
2. The Selective Sizing/Shifting Criterion 1 (Tables 1 and 3) is much better than Criterion 2 (Tables 2 and 4). This supports Contreras-Tapia's reason for sizing only when the sizing factor is less than one [7].
3. The number of iterations and function-gradient evaluations (which are similar) improved much more than the number of function evaluations. This further supports the explanation mentioned above because both globalization techniques are implemented to take care of "large" steps ("small" B 's or $\bar{\gamma} > 1$) at the expense of more than one function evaluation per iteration. Sizing only when $\bar{\gamma} < 1$ increases the number of "large" steps, which decreases the number of iterations, but it may increase the total number of function evaluations.
4. Using the identity matrix as a weighting matrix in the computation of the optimal values γ^* or ϕ^* gives better results than using the matrix B . A plausible reason for this is that when $\bar{\gamma} \neq 1$, the matrix B does not have "good" information relative to $\nabla^2 f(x)$. Therefore it is desirable to de-emphasize the role of B and use a step that has a some "gradient" flavor (weighted matrix equal to the identity) to safeguard the BFGS method.
5. The optimal sizing factors given by Minimization Problem 2 in Sections 3 and 4 (Methods 11 and 12) always failed as a safeguard for the BFGS method. However, Minimization Problem 1 and 3 (Methods 3-10, 13 and 14) sometimes improved the behavior of the standard BFGS method, and slightly more than standard sizing techniques (Methods 1 and 2). This says that to safeguard the BFGS method, it is better to size another member of the Broyden class of secant updates than to just size the BFGS itself, i.e., when the BFGS is not performing well "move on" to

Table 3: Normalized Averages, ($1 - \gamma_{COL} > 0.05$, $\gamma_{min} = 0.1$)

METHOD	LINE SEARCH			TRUST REGION		
	Iterations	Functions	Fun.-Grad.	Iterations	Functions	Fun.-Grad.
0. BFGS	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1. OL -BFGS	0.9336	1.0110	0.9337	0.9706	1.0501	0.9710
2. COL-BFGS	0.8686	0.9613	0.8692	0.9430	1.0633	0.9429
3. B1 - OL	0.9851	1.0050	0.9853	0.9828	1.0087	0.9832
4. B1 - COL	0.9029	0.9651	0.9032	0.9651	1.0101	0.9654
5. B2 - OL	0.9326	0.9869	0.9328	0.9729	1.0083	0.9732
6. B2 - COL	0.8989	0.9619	0.8992	0.9713	1.0138	0.9717
7. I1 - OL	1.0802	1.3142	1.0796	1.0255	1.1725	1.0251
8. I1 - COL	0.8791	1.1248	0.8791	0.9837	1.1691	0.9836
9. I2 - OL	0.9895	1.1661	0.9887	1.0047	1.1365	1.0044
10. I2 - COL	0.8524	1.0177	0.8556	0.9442	1.0900	0.9463
11. I12*	1.4086	1.6368	1.3984	1.0454	1.0798	1.0431
12. I22*	1.4086	1.6368	1.3984	1.0454	1.0798	1.0431
13. I13*	1.0227	1.1233	1.0222	0.9864	1.1181	0.9861
14. I23*	1.0044	1.0307	1.0043	0.9854	1.0342	0.9854

Table 4: Normalized Averages, ($|1 - \gamma_{COL}| > 0.05$, $\gamma_{min} = 0.1$)

METHOD	LINE SEARCH			TRUST REGION		
	Iterations	Functions	Fun.-Grad.	Iterations	Functions	Fun.-Grad.
0. BFGS	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1. OL -BFGS	1.2112	1.2071	1.2088	1.0961	1.1650	1.0959
2. COL-BFGS	1.1274	1.1746	1.1259	1.1440	1.2255	1.1423
3. B1 - OL	1.2747	1.2165	1.2740	1.1430	1.1212	1.1420
4. B1 - COL	1.1329	1.1056	1.1322	1.0978	1.0956	1.0970
5. B2 - OL	1.1704	1.1270	1.1696	1.1465	1.1388	1.1454
6. B2 - COL	1.1606	1.1315	1.1596	1.1228	1.1151	1.1220
7. I1 - OL	1.9117	2.3055	1.9075	1.5109	2.0212	1.5054
8. I1 - COL	1.2292	1.6407	1.2266	1.5080	1.9200	1.5027
9. I2 - OL	1.2907	1.4182	1.2876	1.2032	1.3705	1.1999
10. I2 - COL	1.1703	1.3073	1.1679	1.2347	1.4600	1.2307
11. I12*	1.3083	3.5063	1.2973	1.6134	2.3020	1.6086
12. I22*	1.3083	3.5063	1.2973	1.6134	2.3020	1.6086
13. I13*	0.9656	2.2585	0.9642	1.4929	2.2196	1.4886
14. I23*	0.9481	2.0051	0.9471	1.2705	1.5207	1.2690

Table 5: Normalized Averages, ($1 - \gamma_{COL} > 0.1$, $\gamma_{min} = 0.1$)

METHOD	LINE SEARCH			TRUST REGION		
	Iterations	Functions	Fun.-Grad.	Iterations	Functions	Fun.-Grad.
0. BFGS	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1. OL -BFGS	0.9303	1.0077	0.9305	0.9834	1.0682	0.9837
2. COL-BFGS	0.8745	0.9678	0.8747	0.9776	1.0473	0.9775
3. B1 - OL	0.9369	0.9917	0.9371	0.9700	1.0190	0.9703
4. B1 - COL	0.9059	0.9686	0.9062	0.9577	1.0108	0.9580
5. B2 - OL	0.9279	0.9891	0.9281	0.9666	0.9971	0.9669
6. B2 - COL	0.9027	0.9672	0.9030	0.9646	1.0203	0.9649
7. I1 - OL	0.9920	1.1871	0.9915	1.0113	1.1796	1.0109
8. I1 - COL	0.8732	1.1066	0.8733	0.9670	1.1475	0.9669
9. I2 - OL	0.9746	1.1410	0.9738	1.0090	1.1335	1.0087
10. I2 - COL	0.8540	1.0057	0.8543	0.9456	1.0897	0.9457
11. I12*	1.2608	1.6543	1.2508	1.0602	1.2437	1.0577
12. I22*	1.2608	1.6543	1.2508	1.0602	1.2437	1.0577
13. I13*	0.8634	1.0813	0.8634	0.9347	1.1377	0.9349
14. I23*	0.8549	1.0034	0.8552	0.9605	1.0601	0.9608

another update instead of trying to patch up the BFGS. A similar conclusion was reached by Al-Baali[2] in his numerical experimentation using his *switching methods*.

6. The best results are obtained when there is a direct correlation between $\bar{\gamma}$, the quantity used to decide when to size or shift, and γ , the sizing factor actually used. When $\bar{\gamma} = \gamma_{OL}$, Methods 7 and 9, which used $\gamma = \gamma_{OL}$ as the sizing factor, saved 15% and 6.3% over BFGS with line search and trust region, respectively (Table 1). Similarly, when $\bar{\gamma} = \gamma_{COL}$, the best method, I2-COL, used γ_{COL} as the sizing factor and saved 14.5% and 5.4% (Table 3). Notice that the same is true not only for the choices that gave the best results.
7. Notice that the results given above are slightly better than those for Method 2, which was the choices considered by Contreras and Tapia[7] (see Tables 1 and 3).

6.4 More Results

Further numerical experimentation was done to determine the sensitivity of our results to both the dimension of the problems and choices of ϵ and γ_{min} . For the second analysis, we computed the same type of information as the tables above for different values of ϵ and γ_{min} using Selective Sizing/Shifting Criterion 1. Tables 5 and 6 show this information for $\gamma = \gamma_{COL}$ and (ϵ, γ_{min}) equal to $(0.1, 0.1)$ and $(0.05, 0.001)$, respectively. These are typical results for this sensitivity analysis.

From this data, we can see that the results obtained from the standard sizing procedures (Methods 1 and 2) became worse as ϵ increased or γ_{min} decreased, while the other

Table 6: Normalized Averages, ($1 - \gamma_{COL} > 0.05$, $\gamma_{min} = 0.001$)

METHOD	LINE SEARCH			TRUST REGION		
	Iterations	Functions	Fun.-Grad.	Iterations	Functions	Fun.-Grad.
0. BFGS	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1. OL -BFGS	0.9856	1.0245	0.9857	1.0100	1.0670	1.0103
2. COL-BFGS	0.8714	0.9584	0.8716	0.9728	1.0542	0.9727
3. B1 - OL	0.9387	0.9859	0.9388	0.9731	1.0167	0.9734
4. B1 - COL	0.9067	0.9671	0.9070	0.9651	1.0101	0.9654
5. B2 - OL	0.9380	0.9920	0.9382	0.9729	1.0083	0.9732
6. B2 - COL	0.9075	0.9659	0.9078	0.9713	1.0138	0.9717
7. I1 - OL	1.0337	1.2743	1.0331	1.0255	1.1725	1.0251
8. I1 - COL	0.8849	1.1249	0.8848	0.9837	1.1691	0.9836
9. I2 - OL	1.0352	1.2263	1.0340	1.0047	1.1365	1.0044
10. I2 - COL	0.8721	1.0278	0.8722	0.9462	1.0900	0.9463
11. I12*	1.2284	1.9570	1.2184	1.1360	1.3849	1.1332
12. I22*	1.2284	1.9570	1.2184	1.1360	1.3849	1.1332
13. I13*	0.8648	1.3652	0.8647	0.9857	1.1960	0.9857
14. I23*	0.8523	1.2269	0.8525	0.9960	1.1475	0.9961

procedures remained mostly unchanged (with exception of Methods 13 and 14, which improved with these changes). Of course, this holds within some ranges of ϵ and γ_{min} . In fact, with $\epsilon > .2$, the normalized data is close to one,⁸ and it is greater than one when γ_{min} goes to zero.⁹

To check the sensitivity of our results to the dimension of the problems, we ran our code for problem number 21 with several values of n between 10 and 30, and the starting points and initial matrices used by Contreras and Tapia[7]. Again, we used the Selective Sizing/Shifting Criterion 1 with $\bar{\gamma} = \gamma_{COL}$ and $\gamma_{min} = 0.1$.

Since now the issue is reliability rather than efficiency, Table 7 presents, for $n = 20$, the number of iterations used by each procedure to converge for the different starting points and initial matrices used in trust-region sized BFGS methods. Here, the starting points are

$$\begin{aligned}
 x_0^1 &= (-1.2, 1, \dots, -1.2, 1), \\
 x_0^2 &= (-4000, 1, -1.2, 1, \dots, -4000, 1, -1.2, 1), \\
 x_0^3 &= (-100.5, 40, \dots, -100.5, 40), \\
 x_0^4 &= (-40, 20, 20, 20, \dots, -40, 20, 20, 20), \\
 x_0^5 &= (-300, -100, \dots, -300, -100),
 \end{aligned}
 \tag{6.4}$$

⁸This means that if ϵ is not small enough, there is not enough sizing to really safeguard (improve) the behavior of the standard BFGS method.

⁹This shows the importance of preventing the sizing strategies from using too small sizing factors.

Table 7: Number of Iterations. (Problem 21 with $n = 20$, $1 - \gamma_{COL} > 0.05$, $\gamma_{min} = 0.1$)

INITIAL VALUES		M E T H O D S														
		BFGS			B1		I1		I12*	I13*	B2		I2		I22*	I23*
x_0	B_0	Stand	OL	COL	OL	COL	OL	COL			OL	COL	OL	COL		
x_0^1	B_0^1	138	147	140	149	142	144	139	142	138	152	147	146	137	142	169
	B_0^2	F	197	149	167	146	G**	152	G**	143	157	143	197	147	G**	G**
	B_0^3	183	375	360	286	384	206	292	F*	356	219	394	196	313	F*	348
	B_0^4	206	279	382	294	345	219	293	407	350	301	334	212	297	407	346
x_0^2	B_0^1	F	F	F	F	F	F	F	F	F	F	F	F	F	F	F
	B_0^2	F	284	253	204	221	425	298	F	F	213	218	284	294	F	F
	B_0^3	F	F	F	F	F	F	F	F	F	F	F	F	F	F	F
	B_0^4	F	F	F	F	F	F	F	F	F	F	F	F	F	F	F
x_0^3	B_0^1	F	472	487	F**	464	498	413	F	F*	F**	486	472	487	F	F**
	B_0^2	F	372	393	417	344	446	373	280	G**	392	342	442	364	280	295
	B_0^3	F	F	F	F*	F*	F	F**	F	F	F	F*	F	F*	F	F
	B_0^4	F	F	F*	463	447	F*	465	489	F	472	423	498	484	489	F
x_0^4	B_0^1	334	258	263	267	259	264	263	247	238	251	255	257	261	247	250
	B_0^2	F	367	291	319	268	367	310	221	216	319	255	367	291	221	221
	B_0^3	416	F	F	359	426	335	446	F*	F*	391	443	389	430	F*	F
	B_0^4	372	453	440	314	317	332	328	339	338	299	339	325	317	339	333
x_0^5	B_0^1	F*	430	390	397	365	428	390	330	348	382	363	430	390	330	369
	B_0^2	F	414	274	303	245	231	343	F	F	331	245	237	346	F	F
	B_0^3	F	F	F	F	F	F	F	F	F	F	F	F	F	F	F
	B_0^4	F*	F	F	413	386	381	377	375	385	407	390	393	372	375	384

F: Maximum number of iterations (500) reached.

G: Global strategy failed to compute a "good" step.

*: Last iterate was "close" to the solution ($error < 10^{-2}$).

** : Last iterate was "very close" to the solution ($error < 10^{-5}$).

and the initial matrices are

$$\begin{aligned}
 (6.5) \quad B_0^1 &= I, \\
 B_0^2 &= I + (10^{12} - 1) * \text{diag}(1 - \frac{i-1}{n-1}), \\
 B_0^3 &= \text{diag}(10^7, 10^{-7}, \dots, 10^7, 10^{-7}), \\
 B_0^4 &= \text{diag}(10^5, 10^{-5}, \dots, 10^5, 10^{-5}).
 \end{aligned}$$

From these results, we can see that an appropriate sizing procedure is needed to improve the reliability of the standard BFGS method, as was also concluded by Contreras and Tapia[7]. Even though none of the 14 procedures tested here were 100% reliable, the most reliable procedures were those derived from Minimization Problem 1 in Sections 3 and 4 (columns 6-9 and 12-15 in Table 7). This fact further supports Observation 5 made above, which says that BFGS should be safeguarding by sizing another update instead of patching up the BFGS.

Observe also that, ignoring the cases for which all procedures failed,¹⁰ these most reliable procedures were "close" or "very close" to the solution in the cases they failed, and in these cases, the standard BFGS completely failed. It should be noticed that this was not true for Method 2, the Contreras-Tapia choice (see case x_0^4 with B_0^3).

7 Summary and Concluding Remarks

In this study we have presented considerable theoretical and numerical discussion concerning sizing members of the Broyden family of secant updates. This study has led us to the following conclusions. The BFGS secant update should continue to be the secant method of choice for unconstrained optimization. However, the BFGS update, on occasion, produces a faulty update. This occurrence can be detected using either the Oren-Luenberger sizing factor (1.10) or the centered Oren-Luenberger sizing factor (1.11). When such a situation is detected the approximate Hessian should be sized with the sizing factor used to detect this anomaly. These findings mirror those of Contreras and Tapia [7]. However, we have discovered more.

The BFGS update is prone to producing updates with large eigenvalues. Indeed, in some way it was designed to do this, since it was presented as a fix for the DFP method which produced excessively small eigenvalues: Hence sizing the BFGS update may lead to an excessively small sizing factor and near singularity of the sized matrix. Contreras and Tapia were aware of this deficiency and suggested a safeguard for their sizing strategy. Another way to compensate for this negative feature is to shift, i.e., add a matrix to the sized matrix. The effective implementation of this shift has been the primary subject of the present study. We first considered a two-parameter family consisting of sized Broyden family secant updates. It was instructive for us to view this two-parameter family as a BFGS update of a matrix $\gamma B + \phi vv^T$ which had been sized and then shifted. The shift is of the form ϕvv^T and corresponds to switching from the BFGS update ($\phi = 0$) to an alternative member of the Broyden family of updates ($\phi \neq 0$). Considerable theory and validating numerical experimentation was performed in an effort to find good choices for

¹⁰In one of these cases, x_0^3 with B_0^3 , Procedure II-COL was the only one that almost solved the problem.

the sizing parameter γ and the shifting parameter ϕ . After much study we concluded (as mentioned above) that the sizing factor should be either the Oren-Luenberger or the centered-Oren-Luenberger sizing factor and the sizing should be done selectively as suggested by Contreras and Tapia [7]. Our numerical experimentation indicated that an effective way of determining the shift factor ϕ was to minimize the Byrd-Nocedal ψ -measure over our sized Broyden family with the sizing factor fixed. We considered weighting the Byrd-Nocedal ψ -measure by a matrix D and studied the following three choices for D : $D = I$ the identity, $D = B$ the approximate Hessian, and $D = \nabla^2 f(x)$ the exact Hessian. The choice $D = I$ gives the member of the sized Broyden family which is nearest the method of steepest descent (in the Byrd-Nocedal measure), the choice $D = B$ gives the least-change member, and the choice $D = \nabla^2 f(x)$ gives the member which is nearest to Newton's method. We therefore were rather surprised to find that our numerically most effective choice was $D = I$. In retrospect we see that there is considerable consistency in this choice. Our sizing indicator has told us that we should size; hence there is a bad match of information in the pair B and $\nabla^2 f(x)$. The choice $D = I$ prevents this faulty information from further contaminating our update.

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