ON THE CONDITIONING OF DFP AND BFGS UPDATES FOR UNCONSTRAINED OPTIMIZATION+

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Abstract:

A necessary and sufficient condition on when the conditioning of DFP updates is better than BFGS updates is given and a line search strategy which ensures that the DFP is better conditioned than the BFGS is given.

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1. Introduction

One of the most successful classes of algorithms for the unconstrained minimization problem $\min_{x \in D} f(x)$ is the so called quasi-Newton method. They are iterative algorithms and each iteration is of the form

$$x_{k+1} = x_k - \lambda_k H_k g_k \qquad k = 1,2,\ldots \tag{1.1}$$

where $g_k = \nabla f(x_k)$ is the gradient of f at x_k. The scalar λ_k is either determined to be the exact line minimizer, that is, $\lambda_k = \min\{\lambda > 0: \langle g(x_k + \lambda d_k), d_k\rangle = 0\}$ where $d_k = -H_k g_k$ or by an inexact line search strategy which picks λ_k as an approximation to the exact line minimizer. The matrix H_k is an approximation to the inverse of the Hessian $\nabla^2 f(x_k)$ which is updated in each iteration using only the current and last gradients of f. To simplify the notation we will drop all the subscripts and put a bar over the (k+1)th term, e.g. $\bar{x} = x - \lambda Hg$.

Different updating schemes for H yield different algorithms, and among all the schemes used the most important ones are the DFP updating scheme:

$$\bar{H}_{DFP} = H - \frac{Hyy^T H}{y^T Hy} + \frac{ss^T}{y^T s}$$

$$s = \bar{x} - x \;, \; y = \bar{g} - g$$

which was introduced by Davidon (1959) and later clarified and improved by Fletcher and Powell (1963), and the BFGS updating scheme:

$$\bar{H}_{BFGS} = (I - \frac{sy^T}{y^Ts})\, H\, (I - \frac{ys^T}{y^Ts}) + \frac{ss^T}{y^Ts}$$

which was found independently by Broyden (1970), Fletcher (1970), Goldfarb (1970) and Shanno (1970). The BFGS update is sometimes called the complementary DFP update because if $B = H^{-1}$ then $\bar{B}_{BFGS} = \bar{H}^{-1}_{BFGS}$ and $\bar{B}_{DFP} = \bar{H}^{-1}_{DFP}$ can be expressed as

$$\bar{B}_{BFGS} = B + \frac{yy^T}{y^Ts} - \frac{Bss^TB}{s^TBs}$$

and

$$\bar{B}_{DFB} = (I - \frac{ys^T}{y^Ts})\, B\, (I - \frac{sy^T}{y^Ts}) + \frac{yy^T}{y^Ts}$$

Both of these formulae possesses the property that if H is symmetric and positive definite and $y^Ts > 0$ then $\bar{H}$ is also symmetric and positive definite. In the sequel we shall always assume that $y^Ts > 0$ in all the algorithms in question.

Let's now consider the following class of updates:

$$\bar{H} = (1 - \phi)\, \bar{H}_{DFP} + \phi\, \bar{H}_{BFGS} \qquad (1.2)$$

which was first introduced by Broyden (1967) and later rewritten in the form of (1.2) by Fletcher (1970).

Dixon (1972) proved a remarkable result about this ϕ-class which is the following theorem:

Theorem 1: Let $f: R^n \to R$ be differentiable on R^n and assume that for a given $x_0 \in R^n$ the level set $L(x_0)$ is bounded.

Given a symmetric positive definite $H_0 \in L(R^n)$ suppose that $\{x_k\}$ is generated by (1.1) with λ_k chosen by the exact line search and H_k chosen from (1.2). If $\phi_k \geq 0$ then the sequence $\{x_k\}$ is independent of $\{\phi_k\}$.

Dixon's result is actually more general than Theorem 1 since it allows negative values of ϕ_k with some additional assumptions on $\{H_k\}$. In particular this result shows that should exact line search be made then the algorithm which uses the DFP updates and the BFGS update perform identically. This fact and the fact that DFP and BFGS look very similar in the sense that they are the complementary updates of each other would make one think that even when an inexact line search is made in each iteration these two updates should have similar performances. However, the numerical results given by Gill, Murray and Pitfield (1972) suggest that the BFGS update is much better than the DFP update when λ_k is calculated by inexact line search and people have been trying to explain this phenomenum by investigating the relationship and differences between DFP and BFGS updates.

Davidon (1975) introduced an algorithm which chooses $\bar{H}$ from the ϕ-class to be the one which minimizes the condition number of the matrix $H^{-1}\bar{H}$. Since his new algorithm gives excellent numerical results, it is natural to think that a choice of H_ϕ which gives a smaller condition number of $H^{-1}H_\phi$ would perform better than a choice that gives a larger condition number.

We investigate this condition number for the DFP and BFGS updates and give a necessary and sufficient condition on when one is better than the other.

We shall use $[v_1,\ldots,v_n]$ to denote the vector space spanned by vectors v_i , $i = 1,\ldots n$, and $\mathrm{cond}_p(A)$ denotes the condition number of a matrix A with respect to p-norm. That is, $\mathrm{cond}_p(A) = ||A||_p \cdot ||A^{-1}||_p$.

2. The condition number of the DFP and BFGS updates.

Given a symmetric positive definite H and two $n \times 1$ vectors y and s defined as before, define the three quantities $a = y^T H y$, $b = y^T s$, $c = s^T H^{-1} s$. Then (1.2) can also be written as

$$H_\phi = H - \frac{Hyy^T H}{a} + \frac{ss^T}{b} + \phi a \left(\frac{s}{b} - \frac{Hy}{a}\right)\left(\frac{s}{b} - \frac{Hy}{a}\right)^T \qquad (2.1)$$

The DFP update corresponds to $\phi = 0$ and BFGS corresponds to $\phi = 1$. That $\det(H^{-1}H_\phi) = \frac{b}{a} + \phi\left(\frac{c}{b} - \frac{b}{a}\right)$ and H_ϕ is positive definite if and only if $\det(H^{-1}H_\phi) > 0$ follows by straightforward matrix algebra and results for similar parametrization given by Broyden (1970) and Huang (1970).

From (2.1) we see that

$$H^{-\frac{1}{2}} H_\phi H^{-\frac{1}{2}} = I - \frac{uu^T}{a} + \frac{vv^T}{b} + \phi a \left(\frac{v}{b} - \frac{u}{a}\right)\left(\frac{v}{b} - \frac{u}{a}\right)^T$$

where $u = H^{\frac{1}{2}} y$, $v = H^{-\frac{1}{2}} s$.

It is clear that if $w \perp [u,v]$ then $H^{-\frac{1}{2}} H_\phi H^{-\frac{1}{2}} w = w$

i.e. $H^{-\frac{1}{2}}H_\phi H^{-\frac{1}{2}}$ has n - 2 eigenvalues equal to 1. Let λ_1 and λ_2 be the other two eigenvalues and assume $\lambda_1 \geq \lambda_2$. Since the matrix $H^{-1}H_\phi$ is similar to $H^{-\frac{1}{2}}H_\phi H^{-\frac{1}{2}}$ we have

$$\det(H^{-1}H_\phi) = \det(H^{-\frac{1}{2}}H_\phi H^{-\frac{1}{2}}) = \lambda_1\lambda_2 = \frac{b}{a} + \phi(\frac{c}{b} - \frac{b}{a}) \tag{2.2}$$

Let $w_1 = v - \alpha u$, $w_2 = v - \beta u$ be the two eigenvectors of $H^{-\frac{1}{2}}H_\phi H^{-\frac{1}{2}}$ in [u,v] corresponding to λ_1 and λ_2 respectively. Then since $H^{-\frac{1}{2}}H_\phi H^{-\frac{1}{2}}$ is symmetric, it has n orthogonal eigenvectors which implies that $w_1{}^T w_2 = 0$ i.e.

$$\begin{aligned}(v - \alpha u)^T(v - \beta u) &= v^Tv - \alpha u^Tv - \beta u^Tv + \alpha\beta u^Tu \\ &= a\alpha\beta - b(\alpha + \beta) + c \\ &= 0\end{aligned} \tag{2.3}$$

Now $H^{-\frac{1}{2}}H_\phi H^{-\frac{1}{2}}w_1 = \lambda_1 w_1 = \lambda_1 v - \alpha\lambda_1 u$

and
$$\begin{aligned}H^{-\frac{1}{2}}H_\phi H^{-\frac{1}{2}}w_1 &= v - \alpha u - \frac{b-\alpha a}{a}u + \frac{c-\alpha b}{b}v + \phi a(\frac{v}{b} - \frac{u}{a})(\frac{ac-b^2}{ab}) \\ &= [1 + \frac{c}{b} - \alpha + \phi(\frac{ac-b^2}{b^2})]v - [\frac{b}{a} + \phi(\frac{c}{b} - \frac{b}{a})]u\end{aligned}$$

Plugging in the value of ϕ from (2.2) we get

$$H^{-\frac{1}{2}}H_\phi H^{-\frac{1}{2}}w_1 = [\frac{c}{b} - \alpha + \frac{a}{b}\lambda_1\lambda_2]v - \lambda_1\lambda_2 u$$ which by (2.3)

and comparing coefficient implies $\alpha = \lambda_2$ and $\beta = \lambda_1$.

We are now ready to prove the following theorem.

<u>Theorem 2</u>: Given any symmetric and positive definite matrix H, define $K(A) = \mathrm{cond}_2(H^{-\frac{1}{2}} A H^{-\frac{1}{2}})$ and quantities a,b,c as at the beginning of this section. Then $K(\bar{H}_{DFP}) \geq K(\bar{H}_{BFGS})$ if and only if $c \geq a$.

<u>Proof</u>: We prove this theorem by first explicitly expressing $K(\bar{H}_{DFP})$ and $K(\bar{H}_{BFGS})$ in terms of a,b,c.

First, $\bar{H}_{DFP}$ corresponds to $\phi = 0$ and from (2.2) we get $\phi = 0 = \frac{ab}{ac-b^2}(\lambda_1\lambda_2 - \frac{b}{a})$. With (2.3) we can solve for the eigenvalues λ_1 and λ_2 as the two roots of the equation $ab\lambda^2 - a(b+c)\lambda + b^2 = 0$ which gives us λ_1 and λ_2 as

$$\lambda_{1,2} = \frac{a(b+c) \pm \sqrt{a^2(b+c)^2 - 4ab^3}}{2ab} \qquad \text{and}$$

$$\lambda_1 + \lambda_2 = \frac{a(b+c)}{ab}, \quad \lambda_1\lambda_2 = \frac{b}{a}.$$

Now, $\lambda_1 \geq 1 \geq \lambda_2$ if and only if $(\lambda_1 - 1)(\lambda_2 - 1) \leq 0$

i.e. iff $\frac{b}{a} - \frac{a(b+c)}{ab} + 1 \leq 0$ which is equivalent to $b^2 \leq ac$ and we know this is always true by an application of the Cauchy-Schwarz inequality and the fact that H is symmetric and positive definite. Therefore, the condition number of $H^{-\frac{1}{2}}\bar{H}_{DFP}H^{-\frac{1}{2}}$ is

$$K(\bar{H}_{DFP}) = \frac{\lambda_1}{\lambda_2} = \frac{a(b+c) + \sqrt{a^2(b+c)^2 - 4ab^3}}{a(b+c) - \sqrt{a^2(b+c)^2 - 4ab^3}}$$

$$= \frac{1}{4ab^3}\left[2a^2(b+c)^2 - 4ab^3 + 2a(b+c)\sqrt{a^2(b+c)^2 - 4ab^3}\right]$$

Secondly, $\bar{H}_{BFGS}$ corresponds to $\phi = 1$ and from (2.2) again we get $\phi = 1 = \frac{ab}{ac-b^2}(\lambda_1\lambda_2 - \frac{b}{a})$ and together with (2.3) we find λ_1 and λ_2 are the roots of the equation

$b^2\lambda^2 - c(a+b)\lambda + bc = 0$ which gives us

$$\lambda_{1,2} = \frac{c(a+b) \pm \sqrt{c^2(a+b)^2 - 4b^3c}}{2b^2}$$

and

$$\lambda_1 + \lambda_2 = \frac{c(a+b)}{b^2}, \quad \lambda_1\lambda_2 = \frac{c}{b}.$$

Again $\lambda_1 \geq 1 \geq \lambda_2$ if and only if $(\lambda_1-1)(\lambda_2-1) \leq 0$ i.e. $\frac{c}{b} - \frac{c(a+b)}{b^2} + 1 \leq 0$, i.e. $b^2 \leq ac$ and hence

$$K(\bar{H}_{BFGS}) = \frac{\lambda_1}{\lambda_2} = \frac{c(a+b) + \sqrt{c^2(a+b)^2 - 4b^3c}}{c(a+b) - \sqrt{c^2(a+b)^2 - 4b^3c}}$$

$$= \frac{1}{4b^3c}\left[2c^2(a+b)^2 - 4b^3c + 2c(a+b)\sqrt{c^2(a+b)^2 - 4b^3c}\right]$$

Finally, it is straight forward to find that

$$K(\bar{H}_{DFP}) - K(\bar{H}_{BFGS}) = \frac{1}{2b^3}\left[(c-a)(ac-b^2) + \sqrt{D} - \sqrt{E}\right]$$

where $D = (a^2(b+c)^2 - 4ab^3)(b+c)^2$, $E = (a+b)^2(c^2(a+b)^2 - 4b^3c)$.
Adding and subtracting the term $(a+b)^2(a^2(b+c)^2 - 4ab^3)$ gives us
$D-E = (a^2(b+c)^2-4ab^3)(2b+a+c)(c-a)+(a+b)^2[a^2(b+c)^2-4ab^3-c^2(a+b)^2+4b^3c$

Adding and subtracting $c^2(b+c)^2$ from the term in the square bracket yields

$$
\begin{aligned}
&4b^3(c-a) + (b+c)^2(a+c)(a-c) + c^2(2b+a+c)(c-a) \\
&= (c-a)[4b^3 - (a+c)(b+c)^2 + c^2(2b+a+c)] \\
&= (c-a)[4b^3 - ab^2 - 2abc - b^2c]
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
D - E &= (c-a)[(a^2b^2 + 2a^2bc + a^2c^2 - 4ab^3)(2b+a+c) \\
&\qquad + (a+b)^2\ (4b^3 - ab^2 - 2abc - b^2c)] \\
&= (c-a)[4b(ac-b^2)^2 + (a+c)(a^2c^2 - b^4)]
\end{aligned}
$$

We have thus proved the theorem. ▫

Note that $c = \Delta x^T H^{-1} \Delta x = \lambda^2 g^T H g$ and hence both a and c are readily available in every iteration. Therefore, Theorem 2 provides us with a switching algorithm which chooses either DFP or BFGS depending on whether c is less than a or not. We modified our hybrid method MINOP which uses Davidon's OC update (Dennis & Mei, 1975) so that it does exactly as mentioned above. The test results turned out to be worse than those of MINOP as we expected. Because choosing an update with the smallest $K(\bar{H})$ is certainly better than just choosing the one among DFP and BFGS that has the smaller value of $K(\bar{H})$.

Theorem 2 has not explained why BFGS performed better than DFP but we believe that the inexact line search routine has something to do with it.

Let's now look at some existing inexact line routines and see what effect they have on the conditioning of DFP and BFGS updates.

(1) Goldstein-Amijo line search: Given $c_1 \in (0,\frac{1}{2})$ and $q > 1$, it determines λ to be the first of q^{-j}, $j=0,1,\ldots$ such that

$$f(x+\lambda d) - f(x) \leq c_1 \lambda < g,d> .$$

Since $b - c = \lambda[(1-\lambda) g^T Hg - \bar{g}^T Hg]$ and $0 < \lambda < 1$, it is clear that whenever we overshoot at the minimum, i.e. $<\bar{g},d>$ or $-\bar{g}^T Hg$ is positive, $c < a$ and DFP update should be used.

(2) The algorithm which uses BFGS updates incorporated with the line search routine which with given $c_1 \in (0,\frac{1}{2})$ and $0 < c_1 < c_2 < 1$ finds a step-size λ such that

$$\text{(i)} \quad f(x+\lambda d) - f(x) \leq c_1 \lambda <g,d>$$

$$\text{(ii)} \quad <g(x+\lambda d), d> \geq c_2 <g,d>$$

and it always tests $\lambda = 1$ first.

Powell (1975) showed that if $f(x)$ is convex with bounded level set $L(x_0)$ and if $\nabla^2 f(x)$ exists and is bounded in $L(x_0)$ then $\{x_k\}$ converges to the minimum x^* of $f(x)$. He also proved that if further $\nabla^2 f(x)$ satisfies the Lipschitz condition and is positive definite at x^*, then the rate of convergence is superlinear and there exists a $k_0 > 0$ such that if $k > k_0$, $\lambda_k = 1$ is always chosen.

Now $b-c = \lambda[(1-\lambda)g^T Hg - \bar{g}^T Hg] \geq \lambda[(1-\lambda)g^T Hg - c_2 g^T Hg]$. Therefore, whenever $\lambda \neq 1$ but $(1-\lambda) \geq c_2$ or $\lambda = 1$ but $\bar{g}^T Hg \leq 0$ (i.e. we overshoot) we have $c < a$, DFP update is better conditioned and we believe that switching to DFP at this iteration should yield better results.

(3) The Curry-Altmann technique: This is the line search routine Stoer (1975) used to prove convergence for algorithms using updates in ϕ-class with $\phi \in [0,1]$. It defines λ_k as $\lambda_k = \min\{\lambda \geq 0 \mid \langle g(x+\lambda_k d), d\rangle = \mu_k \langle g,d\rangle\}$ for a given μ_k such that $0 < \mu_k < \bar{\mu} < 1$.

In this case $b-c = \lambda[(1-\lambda)g^T Hg - \mu_k g^T Hg]$ and DFP is better conditioned than BFGS whenever $1 - \lambda \geq \mu_k$. We do not know which is better when this does not occur.

Finally we give an inexact line search routine which would always cause the DFP update to have a smaller condition number than the BFGS update.

Consider the iteration $\bar{x} = x + \lambda d$ where λ is chosen to satisfy (1) $F(\bar{x}) \leq F(x) + c_1 \langle\lambda d, g\rangle$, $c_1 \in (0,\frac{1}{2})$

(2) $\langle g(\bar{x}), d\rangle \geq (1-\lambda)\langle g,d\rangle$

and the sequence of test values of λ in $\{1,\frac{1}{q},\frac{1}{q^2},\ldots\}$ for some integer q.

Note that if condition (2) is dropped, this is just the Goldstein-Amijo line search routine. Also note that the condition (2) ensures $y^T s > 0$.

<u>Lemma</u> If the above line search routine is incorporated in every iteration then it is always the case that $K(\bar{H}_{DFP}) \leq K(\bar{H}_{BFGS})$.

<u>Proof</u> Since $b^2 \leq ac$ it is clear that b can be greater than at most one of a and c.

Now $b-c = \lambda[(1-\lambda)g^T Hg - \bar{g}^T Hg] \geq 0$ and therefore $c < a$ and by Theorem 2 we have $K(\bar{H}_{DFP}) \leq K(\bar{H}_{BFGS})$. ▫

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