MATRIX ALGEBRAS IN QUASI-NEWTON ALGORITHMS

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PROBLEM: Given $f : \mathbb{R}^n \to \mathbb{R}$ find x_* such that $\min_{x \in D} f(x) = f(x_*)$, where D = open, convex subset of $\mathbb{R}^n$. x_* is called a global minimizer of f. Even if it is known to exist, finding it is usually an intractable task. One generally seeks x_* among the local minimizers of f; that is, one looks for x_* in D such that, for some $\delta > 0$

$$f(x_*) \le f(x) \quad \text{if} \quad \|x - x_*\| \le \delta, \; x \in D.$$

We only consider the solution of this problem called unconstrained minimization problem, if f is differentiable, and often twice continuously differentiable.

ALGORITHMS: The problem is usually attacked by trying to approximate a zero of ∇f, the gradient of f ($\nabla f = \left[\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}\right]^T$) by an iterative method

$$x_{k+1} = x_k + \lambda_k d_k, \quad x_0 \in D$$

where $\lambda_k \in \mathbb{R}^+$ is the step length and d_k is the descent direction ($f(x_{k+1}) < f(x_k)$).

In our study of function minimization it is sufficient to look just at the critical points x where $\nabla f(x) = 0$. The gradient $\nabla f(x)$ serves as the "first derivative". But we shall need also a "directional derivative" to deal with the concept of "descente direction". The directional derivative of f at the point x in the direction of the vector d is defined by

$$\frac{\partial f}{\partial d} := \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon d) - f(x)}{\varepsilon}.$$

If f has first partial derivatives in D, then $\frac{\partial f}{\partial d}$ in $x \in D$ exists and is equal to $\nabla f(x)^T d$.

In fact, let $\varphi(\lambda) = f(x+\lambda d)$, $\lambda \in \mathbb{R}^+$, and compute $\frac{d\varphi(\lambda)}{d\lambda}$, using the chain rule. We find

$\frac{d\varphi(\lambda)}{d\lambda} = \nabla f(x+\lambda d)^T d$ and, for $\lambda = 0$, we have

$$\frac{d\varphi(0)}{d\lambda} = \lim_{\varepsilon \to 0} \frac{\varphi(0+\varepsilon) - \varphi(0)}{\varepsilon} = \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon d) - f(x)}{\varepsilon} = \frac{\partial f}{\partial d}$$

= directional derivative of f at x.

The vector d represents a descent direction of $\nabla f(x)^T d < 0$. In fact, by Newton's theorem,

$$\varphi(1) = \varphi(0) + \int_0^1 \varphi'(\lambda)\, d\lambda,$$

i.e.

$$f(x+d) = f(x) + \int_0^1 [\nabla f(x+\lambda d)^T d]\, d\lambda.$$

If d_k is a descent direction at x_k and $x_{k+1} = x_k + \lambda_k d_k$, then $\nabla f(x_k)^T d_k < 0$ implies by continuity the existence of λ_k s.t.

$$f(x_{k+1}) = f(x_k) + \int_0^{\lambda_k} [\nabla f(x_k + \lambda d_k)^T d_k]\, d\lambda < f(x_k).$$

RECALL: If x_* is a minimizer for f, then $\nabla f(x_*) = 0$. In fact, if $\nabla f(x_*) = 0$, then we are able to find a descent direction d and increments of x_*, $\bar{\lambda} d$ and λd, such that $\nabla f(x_* + \lambda d)^T d < 0$ for $\lambda \in [0, \bar{\lambda}]$. In particular we can choose $d = -\nabla f(x_*)$. The algorithms for computing a minimizer x_* are just based on this argument: if x_k is not a minimizer, then we have $\nabla f(x_k) \neq 0$ and we find a local descent direction d_k to approximate x_* step by step. (Notice here the strong link between analytical and computational argument). In the method of steepest descent (the fundamental idea goes back to Cauchy) we have $d_k = -\nabla f(x_k)$ and $\nabla f(x_k)^T d_k = -\|\nabla f(x_k)\|_2^2 < 0$.

If $\nabla f(x_*)=0$ and the Hessian $\nabla^2 f(x_*)$ is positive definite (pd) ($\nabla^2 f(x) = \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)_{i,j \in n}$), then

x_* is a local minimizer for f. In fact, for a suitable z,

$$f(x_*+d) = f(x_*) + \nabla f(x_*)^T d + \frac{1}{2} d^T \nabla^2 f(z) d$$

$$= f(x_*) + \frac{1}{2} d^T \nabla^2 f(z) d > f(x_*)$$

for <u>every</u> direction d.

The steepest descent method is a special case ($A_k = I$) of the following general formula:

$$(*) \begin{cases} x_{k+1} = x_k + \lambda_k d_k \\ d_k = -A_k^{-1} \nabla f(x_k) \end{cases}$$

Where A_k is a $n \times n$ non-singular matrix. In fact we have the following typical choices of A_k:

$A_k = I$ <u>Steepest descent method</u>

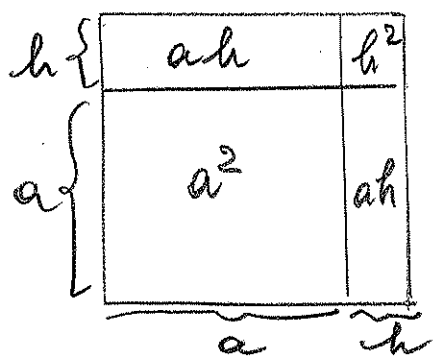
$A_k = \nabla^2 f(x_k)$ <u>Newton's method</u>

A_k = approximation of $\nabla^2 f(x_k)$ <u>Quasi-Newton method</u>

<u>Remarks</u>. One usually reads, in the standard literature, that <u>most</u> descent methods are of the form (*) (Dennis, Moré, 1977), or that the search

direction often has the form $d_k = -A_k^{-1} \nabla f(x_k)$ (Nocedal, Wright, 1999, Ch. 2). We will prove (later) that any descent direction d_k always solves equation $A_k d_k = -\nabla f(x_k)$ for some pd matrix A_k.

Remark 2. The algorithm (*) goes back to a very old scheme of computation. We have a pure geometric correspondence to this scheme in Euclid (Elements, II, 4), where the simple binomial formula is proved in a geometric version —



$$(a+h)^2 = a^2 + 2ah + h^2.$$

To solve the equation $x^2 - n = 0$, with n = integer, replace x by $a+h$, where a is a first approximation of $\sqrt{n}$, so to obtain a quadratic equation in h:

$$(a+h)^2 - n = a^2 + 2ah + h^2 - n = 0$$

Then drop the term h^2, so to obtain a linear equation in h:

$$a^2 + 2ah - n \doteq 0,$$

from which we have an approximation of h:

$$h \doteq \frac{n - a^2}{2a}.$$

Here we have the very basic idea of the main algorithms to approximate the square root of a number and then to solve numerically a singular equation or a system of equations. Problems (in modern terms: equations) of various degrees have been solved by elementary computational versions of the binomial formula in old Babylonian, Chinese and Indian mathematics, in Greek and Arabian traditions, in Fibonacci's Liber Abaci, in Italian algebraic treatises of XVI century, and finally in modern computer theory. The methods due to Viète, Newton, Raphson, as well as secant algorithm and Regula falsi depend on the same elementary construction of Euclid, II, 4.

Our main task is now to reduce the computational complexity, at each step k, of the algorithm (*) with respect to the best known Quasi-Newton methods, which require $O(n^2)$ arithmetic operations to calculate the descent direction d_k for each k. We will prove that this cost can be reduced to $O(n \log n)$ or even to $O(n)$, maintaining a significant degree of second-order

Information, and an acceptable rate of convergence. This is also an attempt to overcome the traditional gap between complexity theory and theoretical numerical analysis, as it is outlined in the following remarks due to B.N. Parlett (1992): "Numerical analysis and complexity theory are palpably different subjects. Complexity theory seeks to determine the intrinsic difficulty of certain tasks; whereas much of theoretical numerical analysis has been concerned with studying classes of algorithms, analysing convergence and stability, developing error bounds (either a priori or a posteriori), and detecting either optimal or desirable members of a class according to various criteria. Clearly complexity theory has more ambitious goals than does theoretical numerical analysis."

In the following we will use also the notations:

$g_k := \nabla f(x_k)$ for the gradient,

$H_k = H(x_k) := \nabla^2 f(x_k)$ for the Hessian,

$s_k = x_{k+1} - x_k$,

$y_k = g_{k+1} - g_k$.

We have a strong link between the unconstrained minimum problem $\min_{x \in \Omega} f(x)$ and the problem of approximating numerically the solution of a set of equations $F(x) = 0$, where $F(x) = [f_1(x)\ f_2(x)\ \cdots\ f_n(x)]^T$ and $f_i : \mathbb{R}^n \to \mathbb{R}$.

We briefly recall some features of Newton's strategy for both problems.

First consider the problem $F(x) = 0$, $F : \mathbb{R}^n \to \mathbb{R}^n$.

In the Newton's strategy we assume the linear model (assume x_k as a good approximation of the solution x_*)

$$L_k(x) = F(x_k) + F'(x_k)(x - x_k)$$

as a "good" approximation to F at x_k, where $F'(x)$ is the Jacobian matrix of F at x : $[F'(x)]_{ij} = \dfrac{\partial f_i(x)}{\partial x_j}$. Then we define x_{k+1}, from x_k, as the solution of the equation $L_k(x) = 0$:

$$x_{k+1} = x_k - F'(x_k)^{-1} F(x_k).$$

In the minimum problem we look for the solution of $\nabla f(x) = 0$. Then the previous iterative formula becomes :

$$x_{k+1} = x_k - H(x_k)^{-1} g_k.$$

We will use sometimes the symbol x_k^N to denote the k-th Newton's iterate. Notice that, in minimum problems, $d_k = -H(x_k)^{-1} g_k$ is a descent direction if $H(x_k)$ is p.d, because $g_k^T d_k = -g_k^T H(x_k)^{-1} g_k < 0$. Usually this is a local property that does not guarantee that $f(x_{k+1}) < f(x_k)$. But we will later explain how to choose a step length λ_k in order to have $f(x_{k+1}) < f(x_k)$ with $x_{k+1} = x_k - \lambda_k B_k^{-1} g_k$, where B_k is an approximation of the Hessian $H(x_k)$.

Consider the quadratic model of f at x_k:

$$M_k(x) = f(x_k) + \nabla f(x_k)^T (x - x_k) + \frac{1}{2}(x - x_k)^T H(x_k)(x - x_k).$$

Then we have:

$\nabla M_k(x) = \nabla f(x_k) + H(x_k)(x - x_k)$,

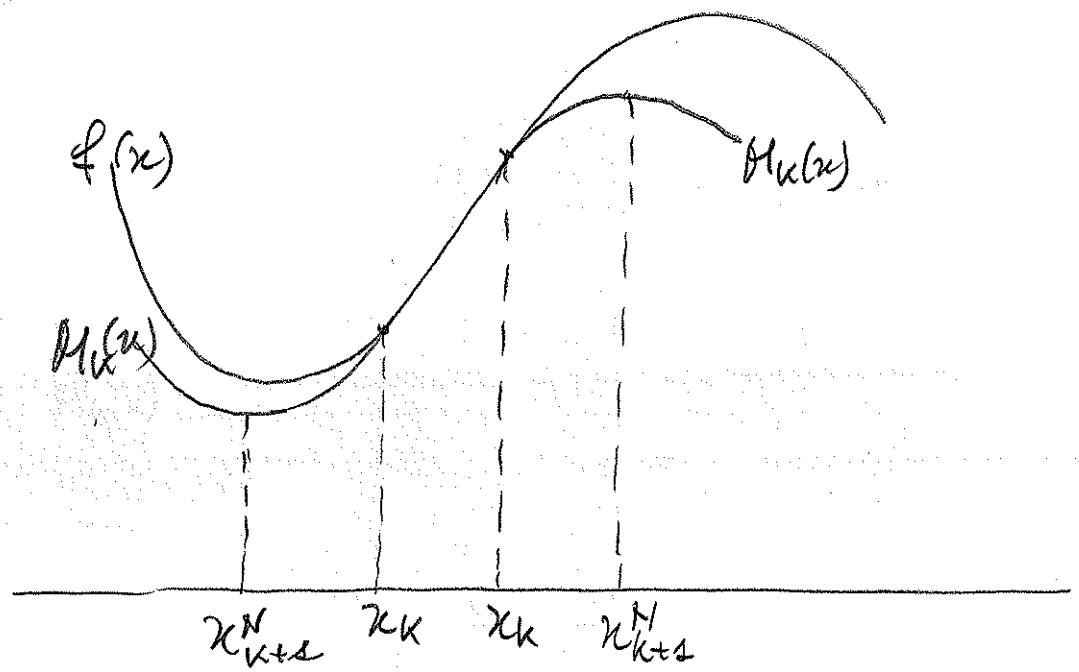
$M_k(x_k) = f(x_k)$,

$\nabla M_k(x_k) = \nabla f(x_k)$,

$\nabla M_k(x_{k+1}^N) = 0$, that is x_{k+1}^N is a stationary point of $M_k(x)$.

But x_{k+1}^N is a minimizer of $M_k(x)$ only if $\nabla^2 M_k(x_{k+1}^N)$ is positive definite. We have in any case $H(x_k) = \nabla^2 M_k(x_k)$.

To better understand the inconvenient of ignoring if $\nabla^2 M_k(x_{k+1}^N)$ is p.d, consider the following figure:



The iterates x_{k+1}^N on the left is a good approximation of the minimizer of $f(x)$, while the opposite holds for the iterate x_{k+1}^N on the right.

Now turn back to the problem $F(x) = 0$, $F: \mathbb{R}^n \to \mathbb{R}^n$. We have for this problem the following result, stating the rate of convergence of Newton's method:

THEOREM 1 (rate of convergence of Newton's method)

Let F be twice differentiable in D open and convex, $D \subset \mathbb{R}^n$, $x_0 \in D$. Let x_* in D satisfy the condition $\det F'(x_*) \neq 0$. Then there is an open set S such that $x_* \in S$ and, for $x_0 \in S$, the Newton's iterates are well defined, remain in S and converge to x_*. Moreover the convergence is superlinear, i.e.

$$\|x_{k+1} - x_*\| \leq \alpha_k \|x_k - x_*\|$$

with $\alpha_k \to 0$ for $k \to \infty$.

If, in addition, $F'(x)$ satisfies a Lipschitz condition at x_*, i.e.

$$\|F'(x) - F'(x_*)\| \leq c\|x - x_*\|,$$

then the convergence is quadratic, i.e.

$$\|x_{k+1} - x_*\| \leq \beta \|x_k - x_*\|^2 \text{ for a constant } \beta.$$

Remark 1 We have a linear convergence of $\|x_{k+1} - x_*\| \leq \alpha \|x_k - x_*\|$ for an $\alpha \in (0,1)$. If the convergence is superlinear, then for every $\alpha \in (0,1)$ there is a k_α such that, for $k \geq k_\alpha$ one obtains $\alpha_k \leq \alpha$ and $\|x_{k+1} - x_*\| \leq \alpha_k \|x_k - x_*\| \leq$
$\leq \alpha \|x_k - x_*\|$.

Remark 2 By the previous result there exist a domain of attraction S and all Newton's iterates land in S. This fact ensures some measure of stability of the iteration. But the convergence has a local character and the domain S may be very small.

It is important to observe that all methods with superlinear convergence for solving a system $F(x)=0$ must be compared, in a precise sense, to Newton's method. In fact we have the following

THEOREM 2 (Dennis, Moré)

Let F satisfy the same conditions of the previous theorem (F twice differentiable and $\det F'(x_*)\neq 0$). Let $\{B_k\}$ be a sequence of non singular matrices. Suppose that, for some $x_0 \in D$, the sequence

$$x_{k+1} = x_k - B_k^{-1} F(x_k)$$

remains in D, $x_k \neq x_*$ for $k \geq 0$ and $x_k \to x_*$ for $k \to \infty$. Then $\{x_k\}$ converges superlinearly if and only if

$$(\dagger) \qquad \lim_{k\to\infty} \frac{\| [B_k - F'(x_*)] s_k \|}{\| s_k \|} = 0$$

where $s_k = x_{k+1} - x_k$.

Notice that the last formula holds if $B_k \to F'(x_*)$, but this condition is not necessary. We only require that the direction $s_k = -B_k^{-1} F(x_k)$ converges to the Newton's direction $s_k^N = -F'(x_k)^{-1} F(x_k)$ as $k \to \infty$ (see next Exercise 1).

Obviously, the previous result implies that Newton's method is superlinear.

Exercise 1 Let $s_k = x_{k+1} - x_k = -B_k^{-1} F(x_k)$ and
$s_k^N = x_{k+1}^N - x_k = -F'(x_k)^{-1} F(x_k)$
where $\{B_k\}$ is the sequence of the previous theorem. If F' is continuous at x_*, prove that the condition (†) of the previous theorem implies that $\frac{\|s_k - s_k^N\|}{\|s_k\|} \to 0$ for $k \to \infty$, that is the direction s_k converges to Newton's direction.

(Sugg.: first prove that $s_k - s_k^N = F'(x_k)^{-1}[F'(x_k) - B_k] s_k$. Then use the fact that, by the continuity of $F'(x_k)$ at x_*, the norm $\|F'(x_k)^{-1}\|$ is bounded if x_k is close to x_*.)

Besides the previous attractive properties of Newton's method we have the following disadvantages:

1. A particular problem may require a very good initial approximation to x_*. In other words the set S (in Theorem 1) may be very small.
2. The computation of $F'(x_k)$, or $H(x_k)$ for minimum problem, is needed at each step k.
3. At each step we have to solve a linear system to calculate $d_k = -F'(x_k)^{-1} F(x_k)$
(or $d_k = -H(x_k)^{-1} g_k$ for minimum problem)

Exercise 2 Prove that the superlinear convergence implies that $\|x_k - x_*\|$ is small if $\|x_{k+1} - x_k\|$ is small. This lets us use a condition like $\|x_{k+1} - x_k\| < \varepsilon$, for a given $\varepsilon > 0$, as a stop criterium for a method with superlinear convergence.

We can overcome the previous inconvenients of Newton's method by exploiting a suitable approximation of the matrix $F'(x_k)$ or of the Hessian $H(x_k)$ at each step k. Here we must distinguish the two problems $F(x) = 0$ and $\min f(x)$, as the criteria for approximating the matrices involved in the search directions ($F'(x)$ or $H(x)$) are substantially different in some points.

We first consider the problem $F(x) = 0$ and recall Broyden's method for approximating the solutions x_*. To describe this method, replace the linear model of Newton's method $L_k(x) = F(x_k) + F'(x_k)(x - x_k)$ by a "simpler" model

$$M_k(x) = F(x_k) + B_k(x - x_k)$$

where B_k is an approximation of $F'(x_k)$.

Define now x_{k+1} as the solution of $m_k(x)=0$, that is

$$x_{k+1} = x_k - B_k^{-1} F(x_k).$$

In Broyden's method the construction of B_k, at each step k, is not from scratch (like $F'(x_k)$) but depends on B_k via an iterative formula. The construction of this formula depends essentially upon two criteria:

1. B_{k+1} must satisfy the equation

$$B_{k+1} s_k = y_k, \qquad s_k = x_{k+1} - x_k, \quad y_k = F(x_{k+1}) - F(x_k)$$

called "secant equation".

2. Choose $m_{k+1}(x)$ close to $m_k(x)$, that is B_{k+1} close to B_k. In fact, if $x_k \simeq x_*$, then we are in a small neighbour of x_*, the model $m_k(x)$ is sufficiently close to F and then it should not be changed.

Notice that the secant equation in 1. is the extension of the classical equation verified (for $k-1$ instead of k) by the secant method for a single equation $f(x)=0$ $(n=1)$: $x_{k+1} = x_k - \frac{f(x_k)}{a_k}$, with

$$a_k = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}.$$

Observe that $m_k(x_k) = F(x_k)$ and that the equality $B_k s_{k-1} = y_{k-1}$ is equivalent to the supplementary interpolatory property $m_k(x_{k-1}) = F(x_{k-1})$.

Now use the Negative - Broyden's formula

$$B_{k+1} = B_k + \frac{1}{s_k^T s_k}(y_k - B_k s_k) s_k^T$$

to compute the matrices of the sequence $\{B_k\}$, given an initial guess B_0 with $\det B_0 \neq 0$. This formula consists in a correction of rank 1 of the matrix B_k. It is immediate to realize that $B_{k+1} s_k = y_k$. To prove that the requirement 2. is satisfied we prove that $\|B_k - B_{k-1}\|_F \leq$ $\leq \|X - B_{k-1}\|_F$ for every matrix X satisfying the secant equation. In fact we have:
(recall that $\|X\|_F = \left[\sum |x_{ij}|^2\right]^{1/2} = \sqrt{\mathrm{tr}(X^T X)}$)

$$\|B_k - B_{k-1}\|_F = \frac{1}{s_{k-1}^T s_{k-1}} \|(y_{k-1} - B_{k-1} s_{k-1}) s_{k-1}^T\|_F$$

$$\leq \|X - B_{k-1}\|_F \cdot \frac{\|s_{k-1} s_{k-1}^T\|_F}{s_{k-1}^T s_{k-1}}$$

$$= \|X - B_{k-1}\|_F$$

as $\|s_{k-1} s_{k-1}^T\|_F = s_{k-1}^T s_{k-1}$.

Here we have the scheme of Broyden's method:

$x_0 \in \mathbb{R}^n$, B_0 non singular

$k = 0, 1, 2, \ldots$

$B_k d_k = -F(x_k)$

$x_{k+1} = x_k + d_k$

$s_k = x_{k+1} - x_k$

$y_k = F(x_{k+1}) - F(x_k)$

$$B_{k+1} = B_k + u_k s_k^T, \quad u_k = \frac{1}{s_k^T s_k}(y_k - B_k s_k)$$

The superlinear convergence of the Broyden's method is stated in the following

THEOREM 3

If $F'(x)$ is non singular in D open and convex, $F(x_*) = 0$, $\|F'(x)^{-1}\| \le \beta$ in D, $F'(x) \in \mathrm{Lip}_\gamma(x_*)$, then there are $\varepsilon, \delta > 0$ such that, for $x_0 \in I_\varepsilon(x_*)$ and $B_0 \in I_\delta(F'(x_*))$, x_{k+1} is well defined, $x_{k+1} \in I_\varepsilon(x_*)$ and

$$\|x_{k+1} - x_*\| \le \eta_k \|x_k - x_*\|, \text{ with } \eta_k \to 0$$

Main properties of Broyden's method:

1. The secant equation is verified: $B_k s_{k-1} = y_{k-1}$
2. $\|B_k - B_{k-1}\|_F \le \|X - B_{k-1}\|_F \quad \forall X : X s_{k-1} = y_{k-1}$
3. Superlinear (local) convergence
4. B_{k+1} is constructed from B_k by means of an iterative formula, a correction of rank 1 of B_k.
5. Only $O(n^2)$ (instead of $O(n^3)$) operations are sufficient at each step k.

The property 5. depends on the fact that Broyden's iterative updating of B_k can be rewritten for the matrices inverses B_k^{-1} and B_{k+1}^{-1}. This is a consequence of Sherman-Morrison theorem (1949):

THEOREM 4
Let $A \in \mathbb{R}^{n\times n}$, $\det A \neq 0$, and consider a modification of rank one of A, that is $A + uv^T$, $u, v \in \mathbb{R}^n$. If $\sigma := 1 + v^T A^{-1} u \neq 0$, then $A + uv^T$ is non singular, and

$$(A+uv^T)^{-1} = A^{-1} - \frac{1}{\sigma} A^{-1} u v^T A^{-1}.$$

Proof
First prove that $\det(I + uv^T) = 1 + v^T u$. In fact, let $u \neq 0$ and $P = I + uv^T$. Let w be an eigenvector of P: $Pw = (I + uv^T)w = \lambda w$. Then $(\lambda - 1)w = u(v^T w)$. Thus $v^T w = 0$ and $\lambda = 1$ or $v^T w \neq 0$ and w is a multiple of u, $w = ku$, with $(I + uv^T)ku = \lambda ku$, and thus $\lambda = 1 + v^T u$. Thus only one eigenvalue λ equals $1 + v^T u$, whereas the others $n-1$ eigenvalues are equal to 1, and then $\det(I + uv^T) = 1 + v^T u$. Moreover $A + uv^T = A + AA^{-1} uv^T = A(I + A^{-1} uv^T)$. Thus $\det(A + uv^T) = \det A \det(I + A^{-1} uv^T) = \det A(1 + v^T A^{-1} u) \neq 0$ iff $\sigma \neq 0$.
One can verify directly that

$$\left(A^{-1} - \frac{1}{\sigma} A^{-1} u v^T A^{-1}\right)(A + uv^T) = I.$$

By Theorem 4, the Broyden's iteration, rewritten in terms of B_k^{-1} and B_{k+1}^{-1}, becomes

$$B_{k+1}^{-1} = B_k^{-1} + \frac{1}{s_k^T B_k^{-1} y_k} [s_k - B_k^{-1} y_k] s_k^T B_k^{-1} = \psi(B_k^{-1}, s_k, y_k)$$

and the corresponding algorithm assumes the form

$$\begin{cases} x_0 \in \mathbb{R}^n, \ B_0 \text{ non singular}, \\ d_k = -B_k^{-1} F(x_k), \\ x_{k+1} = x_k + d_k, \\ s_{k+1} = x_{k+1} - x_k, \\ y_{k+1} = F(x_{k+1}) - F(x_k), \\ B_{k+1}^{-1} = \psi(B_k^{-1}, s_k, y_k), \end{cases}$$

where only $O(n^2)$ operations are required to compute B_k^{-1} and $d_k = -B_k^{-1} F(x_k)$.

Our problem is now to show how to transpose Broyden's idea to the unconstrained minimum problem.

Consider the usual scheme $x_{k+1} = x_k + d_k$, with $d_k = -B_k^{-1} g_k$ ($g_k = \nabla f(x_k)$), but a direct choice of B_{k+1} as

$$B_{k+1} = B_k + \frac{1}{s_k^T s_k} (y_k - B_k s_k) s_k^T, \quad B_k \text{ pd},$$

does not work, because B_{k+1} must be positive definite and the previous matrix calculated by Broyden's method is not pd. (even if B_k is pd). But if a simple condition holds, that is $y_k^T s_k > 0$, we can construct B_{k+1} pd.

THEOREM 5 Let B_k pd

If $y_k^T s_k > 0$, then there is a matrix B_{k+1} pd that satisfies the secant equation $B_{k+1} s_k = y_k$.

Proof (sketch)

Observe that a matrix A is p.d. iff $A = JJ^T$, with $\det J \neq 0$. Then assume $B_{k+1} = JJ^T$ and prove that there is a J such that $JJ^T s_k = y_k$. As $B_k = L_k L_k^T$, with L_k lower triangular (Cholesky factorization), set $J = L_k +$ rank one matrix (Broyden). That is we expect that B_{k+1} is close to B_k if J is close to L_k. Then write

$$J = L_k + \frac{(y_k - L_k v)}{v^T v} v^T$$

We have immediately $Jv = y_k$. Now we must choose v in order to obtain $J^T s_k = v$ and, eventually, $JJ^T s_k = y_k$. Write L instead of L_k.

Set $v = \gamma L^T s_k$ and compute $J^T s_k = L^T s_k + v\left[\frac{(y_k - Lv)^T s_k}{v^T v}\right]$.

We find

$$J^T s_k = \frac{y_k^T s_k}{\gamma s_k^T L L^T s_k} \cdot L^T s_k = v = \gamma L^T s_k$$

and then $\gamma^2 = \frac{y_k^T s_k}{s_k^T L L^T s_k}$. Thus, for $y_k^T s_k > 0$, there is a $\gamma \in \mathbb{R}^+$ and $v = \gamma L^T s_k$, and $B_{k+1} = JJ^T$.

One easily calculates $JJ^T s_k = y_k$.

Exercise 3

Prove that $J = L + \dfrac{(y_k - Lv)v^T}{v^T v}$, $v = \gamma L^T s_k$,

is now singular. (use: $\det(I + uv^T) = 1 + v^T u$)

Exercise 4

Prove that $B_{k+1} = JJ^T$ is given by the following correction of rank 2 of B_k:

$$B_{k+1} = B_k + \frac{y_k y_k^T}{y_k^T s_k} - \frac{1}{s_k^T B_k s_k}(B_k s_k s_k^T B_k) \qquad (*)$$

Now the iterative formula $(*)$ can be exploited to construct a pd matrix B_{k+1}, satisfying the secant equation, from B_k, s_k and y_k, with B_k pd. The matrices B_k, computed via $(*)$, can be used to define a descent direction d_k at each step k.

We can also construct an indipendent, alternative proof that a matrix B of the form

$$B = \tilde{B} - \frac{1}{s^T \tilde{B} s}\tilde{B} s s^T \tilde{B} + \frac{1}{y^T s} y y^T$$

is p.d. if $\tilde{B}$ is p.d. and $y^T s > 0$.

In fact, if $\tilde{B}$ is p.d., write $\tilde{B} = R^T R$, with $\det R \neq 0$

Set $q = (R^T)^{-1} y$, $p = Rs$, and then $y^T = q^T R$, $s = R^{-1} p$.

Then we obtain:

$$B = \hat{R}^T R + \frac{1}{y^T s} y y^T - \frac{1}{s^T R^T R s} R^T R s s^T R^T R$$

$$= R^T W R \quad \text{where} \quad W = I - \frac{1}{p^T p} p p^T + \frac{1}{q^T q} q q^T.$$

[Moreover, let $\Pi(A)$ denote the product of the eigenvalues of A, so we have

$$\Pi(B) = [\Pi(R)]^2 \Pi(W).$$

By the equality $B = R^T W R$ we have that B is p.d. if W is p.d. As W is a rank-two modification of I, it has $n-2$ eigenvalues equal to 1 and two remaining eigenvalues $\lambda_1, \lambda_2 \neq 1$.

Prove that (EXERCISE 5)

$$\lambda_1 + \lambda_2 = \frac{q^T p + q^T p}{q^T p},$$

$$\lambda_1 \lambda_2 = \frac{p^T q}{p^T p}.$$

Now observe that $p^T q = s^T y$. Then, if $s^T y > 0$, we have $\lambda_1, \lambda_2 > 0$ and $\lambda_1 + \lambda_2 > 0$. This implies that both eigenvalues λ_1 and λ_2 are > 0 and W is p.d.

Now we are able to define the following procedure for approximating the minimizer x_* of a function f, $f: \mathbb{R}^n \to \mathbb{R}$.

$x_0 \in \mathbb{R}^n$, B_0 = pd matrix (Ex: $B_0 = I$)

for $k = 0, 1, 2, \ldots$

$d_k = -B_k^{-1} g_k$ $\qquad g_k = \nabla f(x_k)$

$x_{k+1} = x_k - \lambda_k B_k^{-1} g_k = x_k + \lambda_k d_k$

$s_k = x_{k+1} - x_k$

$y_k = g_{k+1} - g_k$

$B_{k+1} = \phi(B_k, s_k, y_k)$

Where

$$\phi(B, s, y) = B + \frac{1}{y^T s} y y^T - \frac{1}{s^T B s} B s s^T B.$$

This procedure is known as BFGS, from the names of Broyden, Fletcher, Goldfarb, Shanno (1970)

Main properties of BFGS algorithm:

1. If $y_k^T s_k > 0$ we are able to define, by a modification of rank-2 of B_k, a matrix B_{k+1} that is pd and verifies the secant equation $B_{k+1} s_k = y_k$.
2. The complexity of each iteration is $O(n^2)$ operations. In fact we can extend the Sherman-Morrison theorem to modifications of rank 2. Then, in principle, we can replace the iterative formula $B_{k+1} = \phi(B_k, s_k, y_k)$ by an analogous iterative formula involving the inverses B_k^{-1} and B_{k+1}^{-1}, which is always a correction of rank 2. This implies that the dominant operation, at each step of

the algorithm, is a matrix × vector operation, which requires $O(n^2)$ flops. However, using Sherman-Morrison formula often implies a degree of numerical instability, so a better strategy consists in computing a Cholesky factorization of B_k at each step k, $B_k = L_k L_k^T$, deriving L_{k+1} from L_k by a process involving QR factorizations and Given's transforms. This process requires $O(n^2)$ arithmetic operations (see Dennis, Schnabel, Numerical Methods for Unconstrained Optimization and Nonlinear Equations).

A crucial problem is now the choice of the step length λ_k. We have to define λ_k in order to guarantee the following properties of BFGS algorithm:

1. A descent of f, that is $f(x_{k+1}) < f(x_k)$
2. $y_k^T s_k > 0$
3. convergence of $\{x_k\}$ to the minimizer x_*.

Now 1. and 2. are a direct consequence of two conditions, called Armijo-Goldstein conditions:

$(AG)_1$ $\quad f(x_{k+1}) = f(x_k + \lambda_k d_k) \leq f(x_k) + c_1 \lambda_k g_k^T d_k$

where $0 < c_1 < 1$;

$(AG)_2$ $\quad \nabla f(x_k + \lambda_k d_k)^T d_k \geq c_2 \nabla f(x_k)^T d_k$.

with $0 < c_1 < c_2 < 1$. (for ex.: $c_1 = 0.1$, $c_2 = 0.5$)

Both $(AG)_1$ and $(AG)_2$ are also required in convergence results.

By the condition $(AG)_1$ we want to strength the more simple requirement $f(x_{k+1}) < f(x_k)$, that does not guarantee, by itself, the convergence of $\{x_k\}$ to x_*. In fact consider the following

Exercise 6

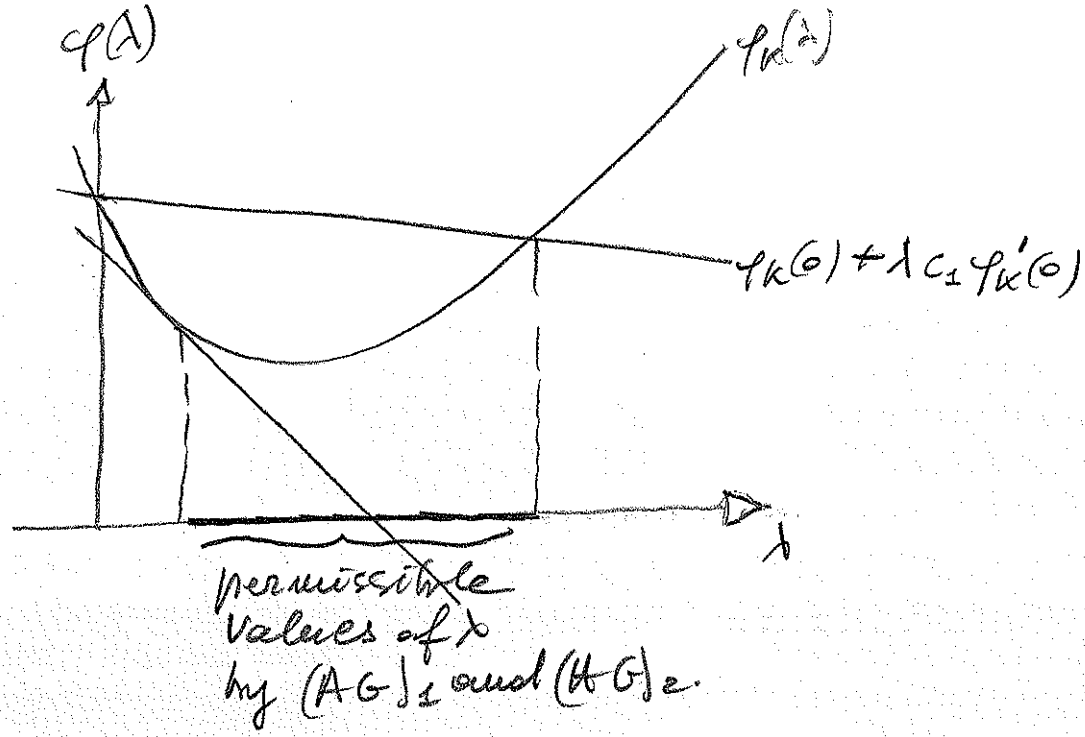
Let $f(x) = x^2$, $x_0 = 2$, $d_k = (-1)^{k+1}$, $\{\lambda_k\} = \{2 + 3(2^{-(k+1)})\}$. Verify that $f(x_k)$ is decreasing monotonically, but $\lim_{k\to\infty} f(x_k) = 1$, which is not a minimum of any sort for f. Moreover $\{x_k\}$ has limit points ± 1. Verify that we have very small decreases in f values relative to the length of the steps.

If we set $\varphi_k(\lambda) = f(x_k + \lambda d_k)$, then the Armijo-Goldstein conditions can be rewritten in the form

$(AG)_1'$ $\quad \varphi_k(\lambda) \le \varphi_k(0) + \lambda c_1 \varphi_k'(0)$,

$(AG)_2'$ $\quad \varphi_k'(\lambda) \ge c_2 \varphi_k'(0)$.

By the condition $(AG)_2$ or $(AG)_2'$, that is a condition on the curvature of $\varphi_k(\lambda)$, we require that the rate of decrease of f in the direction d at x_{k+1} be larger than some prescribed function of the rate of decrease in the direction d at x_k



The condition $(AG)_2$ implies the inequality $y_k^T s_k > 0$ and then is a crucial step for constructing a pd matrix B_{k+1} from B_k by means of the BFGS algorithm. In fact

$$(AG)_2 \Rightarrow \nabla f(x_k + \alpha_k d_k)^T \lambda_k d_k \geq c_2 \nabla f(x_k)^T \lambda_k d_k.$$

$$\Rightarrow \nabla f(x_k + \lambda_k d_k) s_k - \nabla f(x_k)^T s_k \geq (c_2 - 1) \nabla f(x_k)^T s_k$$

$$\Rightarrow y_k^T s_k \geq (c_2 - 1) \nabla f(x_k)^T \lambda_k d_k > 0$$

(because $c_2 < 1$, $\lambda_k > 0$ and d_k is a descent direction)

The following theorem states that we are always able, under suitable conditions on f, to choose λ_k, at each step k, in order to satisfy the conditions $(AG)_1$, $(AG)_2$.

THEOREM 6 (Wolfe)

Let f be continuously differentiable. Let $g_k^T d_k < 0$ (d_k = any descent direction), and let $f(x_k + \lambda d_k)$ be bounded below ($\lambda > 0$). Then we can define $\lambda_u > \lambda_\ell > 0$ such that $x_{k+1} = x_k + \lambda_k d_k$ satisfies both $(AG)_1$ and $(AG)_2$ if $\lambda_k \in (\lambda_u, \lambda_\ell)$.

The conditions $(AG)_1$ and $(AG)_2$ are required in convergence results of any method $x_{k+1} = x_k + \lambda_k d_k$, and in particular in local superlinear convergence of BFGS method. In fact, for any method satisfying the condition

1. d_k = descent direction
2. λ_k satisfies $(AG)_1$, $(AG)_2$
3. $g(x) = \nabla f(x)$ is Lipschitz in $\mathbb{R}^n$
4. f is bounded below

we have $\lim_{k \to \infty} \dfrac{\nabla f(x_k)^T s_k}{\|s_k\|} = 0$. This, in general, does not imply $\lim \nabla f(x_k) = 0$, that is the so called global convergence. To gain global convergence we must suppose the angle between g_k and $s_k = x_{k+1} - x_k$ is bounded away from $\pi/2$. In quasi-Newton iterations $x_{k+1} = x_k - B_k^{-1} g_k$, B_k p.d., this happens when the condition numbers of B_k are uniformely bounded (we will prove later this result).

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Under suitable conditions on f - including $f \in L1P$, f twice differentiable, $H(x_*)$ positive definite - the BFGS method has local superlinear rate of convergence. Moreover the BFGS method is globally convergent ($\liminf \|g_k\| = 0$) under the simple assumption $\|y_k\|^2 / y_k^T s_k$ (Powell, 1976). This condition is implied by the convexity of f but is weaker than convexity. To prove global convergency $(AG)_1$ and $(AG)_2$ are also required.

The BFGS update has been considered for a long time (see Dennis, Schnabel, 1983, p. 201) as the best Hessian update known. Moreover, BFGS is competitive with a (modified) Newton method, since each iteration can be performed with only $O(n^2)$ operations and no Hessian evaluation is required. Other minimization algorithms are especially efficient when the dimension n is large. The method introduced by Shanno (1978), having $O(n)$ complexity per step, is a simple memory-less modification of the BFGS method, in which the identity matrix I is used, instead of B_k, to compute the new approximation B_{k+1}. But by the very nature of the memory-less approach, the amount of second-order information (dealing with the Hessian) is considerably

reduced in comparison with the standard BFGS method and thus the number of iterations required for the desired approximation must be increased.

In order to reduce time and space complexity of BFGS method, one can try to replace B_k, in the updating formula $B_{k+1} = \phi(B_k, s_k, y_k)$, by a suitable simpler matrix $\tilde{B}_k$, maintaing a significant degree of second order information. We could try the following strategy:

1. Construct an iterative formula, more general than $B_{k+1} = \phi(B_k, s_k, y_k)$, in terms of a generic positive definite $\tilde{B}_k$ (replacing B_k):

$$B_{k+1} = \phi(\tilde{B}_k, s_k, y_k)$$

A natural choice of $\tilde{B}_k$ could be in the set of matrices approximating B_k.

2. Look for best choices of $\tilde{B}_k$ in order to minimize the complexity by maintaining a quasi-Newtonian rate of convergence.

We exploit the fact that, to obtain a superlinear convergence, it is not necessary that $B_k \to H(x_*)$, but only that $\|[B_k - H(x_*)]s_k\| / \|s_k\| \to 0$ (see theorem 2), so we try to weaken the conditions for the convergence of $\{x_k\}$ and we look for just an approximation of B_k.

In order to have a suitable approximation of B_K, recall that the space $M_n(\mathbb{C})$ of $n \times n$ matrices on the complex field are an Hilbert space with inner product $(X, Y) = \sum_{i,j=1}^{n} \bar{x}_{ij} y_{ij}$ and a corresponding norm $\|\cdot\|_F$.

$$X \in M_n(\mathbb{C}) \to \sqrt{(X, X)} = \left(\sum_{i,j=1}^{n} \bar{x}_{ij} x_{ij} \right)^{1/2} = \sqrt{\sum_{ij} |x_{ij}|^2} := \|X\|_F,$$

called Frobenius norm.

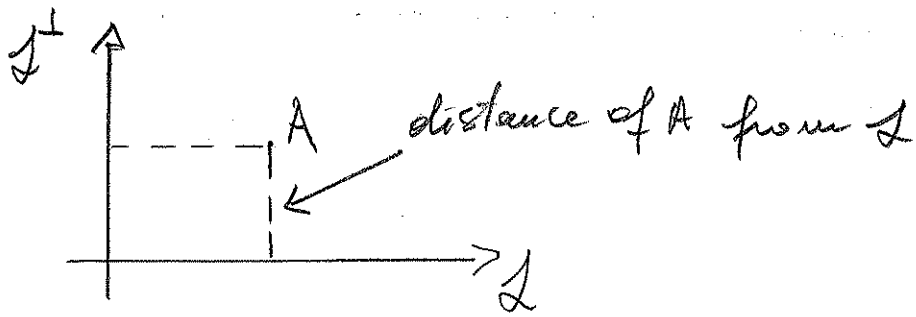
Then the Hilbert's projection theorem holds:

THEOREM 7

Let $\mathcal{L}$ be a subspace of $M_n(\mathbb{C})$. We can write any element A of $M_n(\mathbb{C})$ as the sum of an element of $\mathcal{L}$ and an element of $\mathcal{L}^\perp$, the space orthogonal with respect to $\mathcal{L}$. These two elements $\mathcal{L}_A = PA \in \mathcal{L}$ and $QA \in \mathcal{L}^\perp$ are the orthogonal projections of A and $A = PA + QA$. Moreover

$$\|\mathcal{L}_A - A\|_F \leq \|X - A\|_F \quad \forall X \in \mathcal{L},$$

that is $\mathcal{L}_A$ has the least distance of A from $\mathcal{L}$.



Consider the m-dimensional space $\mathcal{L}$ of matrices $\sum_{i=1}^{m} x_i J_i$, where $J_i \in \mathbb{R}^{n\times n}$, and let $\mathcal{L}_A$ the best approximation in $\mathcal{L}$ of a given matrix $A \in \mathbb{R}^{n\times n}$. We have to compute z_i such that $\mathcal{L}_A = \sum_{i=1}^{m} z_i J_i$. By orthogonality we have

$$(A - \mathcal{L}_A, X) = 0 \quad \forall\, X \in \mathcal{L}.$$

and, by linearity in Hilbert's space,

$$(A, X) - (\mathcal{L}_A, X) = 0.$$

For $X = J_j$ we obtain

$$(A, J_j) - (\mathcal{L}_A, J_j) = 0 \quad \text{and, for } \mathcal{L}_A = \sum_{i=1}^{m} z_i J_i,$$

$$\left(\sum_{i=1}^{m} z_i J_i, J_j\right) = (A, J_j), \quad \text{that is}$$

$$\sum_{i=1}^{m} z_i (J_i, J_j) = (A, J_j).$$

Now set $c_j := (A, J_j)$ and $w_{ij} := (J_i, J_j)$. Then the last equality becomes ($w_{ij} = w_{ji}$)

$$\sum_{j=1}^{m} w_{ij} z_j = c_i$$

which is a <u>normal system</u>. By solving the system we compute z_i s.t. $\mathcal{L}_A = \sum_{i=1}^{m} z_i J_i = \sum_{i=1}^{m} [W^{-1} c]_i J_i$ where $W = (w_{ij})$ and $c = [c_1 \cdots c_m]^T$.

Our task is now to apply the operator $\mathcal{L}$ to both sides of the equality

$$B_{k+1} = \tilde{B}_k + \frac{1}{y_k^T s_k} y_k y_k^T - \frac{1}{s_k^T \tilde{B}_k s_k} \tilde{B}_k s_k s_k^T \tilde{B}_k ,$$

In the special case where $\mathcal{L} = \{ U_z d(z) U_z^H : z \in \mathbb{C}^n \}$, $d(z) = \begin{bmatrix} z_1 & & 0 \\ & \ddots & \\ 0 & & z_n \end{bmatrix}$ and U_z = unitary matrix, and $\tilde{B}_k$ is the best approximation of B_k in $\mathcal{L}$. The effect of this application will be a reduction of arithmetic complexity from $O(n^2)$ to $O(n \log n)$ operations per step if U_z defines a fast transform. First, a set of properties of the operator $\mathcal{L}$ are to be stated.

PROPERTY 1. If $\mathcal{L} = \sum_{i=1}^{m} x_i J_i$ is a m-dimensional subspace of $\mathcal{M}_n(\mathbb{C})$, $J_i \in \mathbb{R}^{n \times n}$, we have

$$\mathcal{L}_{\alpha X + \beta Y} = \alpha \mathcal{L}_X + \beta \mathcal{L}_Y$$

where α, β = scalars and $X, Y \in \mathcal{M}_n(\mathbb{C})$. (Linearity of $\mathcal{L}$).

Proof.

Let W_k^{-1} be the row k of W^{-1}. Then we have

$$\mathcal{L}_{\alpha X + \beta Y} = \sum_k W_k^{-1} \begin{bmatrix} (\alpha X + \beta Y, J_1) \\ \hline \\ (\alpha X + \beta Y, J_n) \end{bmatrix} J_k = \sum_k W_k^{-1} \begin{bmatrix} \alpha (X, J_1) + \beta (Y, J_1) \\ \hline \\ \alpha (X, J_n) + \beta (Y, J_n) \end{bmatrix} J_k$$

$$= \alpha \sum_k W_k^{-1} \begin{bmatrix} (X, J_1) \\ \hline \\ (X, J_n) \end{bmatrix} J_k + \beta \sum_k W_k^{-1} \begin{bmatrix} (Y, J_1) \\ \hline \\ (Y, J_n) \end{bmatrix} = \alpha \mathcal{L}_X + \beta \mathcal{L}_Y .$$

The remaining Properties hold of

$$\mathcal{A} = SDU_{\mathcal{A}} = \left\{ U_{\mathcal{A}}\, d(z)\, U_{\mathcal{A}}^H : z \in \mathbb{C}^n \right\},$$

$d(z) = \mathrm{diag}(z_i, i = 1, \dots, n)$, $z = [z_1\, z_2 \cdots z_n]^T$, that is $\mathcal{A}$ is the subspace of $\mathcal{H}_n(\mathbb{C})$, of dimension n, whose elements are the matrices simultaneously diagonalized by the same unitary transform $U_{\mathcal{A}}$. set $U = U_{\mathcal{A}}$.

PROPERTY 2

We have $\mathcal{A}_A = U\, d(z_A)\, U^H$, where $(z_A)_j = [U^H A U]_{jj}$.

Proof

When U is unitary we have $\|A\|_F = \|UA\|_F$. Then $\|U\, d(z)\, U^H - A\|_F = \|d(z) - U^H A U\|_F$. Now recall that $\|A\|_F = \left(\sum_{i,j} |a_{ij}|^2 \right)^{1/2}$, so $\|d(z) - U^H A U\|_F$ is minimum when the diagonal elements of $U^H A U$ are equal to $d(z)$, that is $(U^H A U)_{ii} = [d(z)]_i$, or $(z_A)_i = (U^H A U)_{ii}$.

PROPERTY 3

$\mathcal{A}_{xy^T} = U\, d(z_{xy^T})\, U^H$, $x, y \in \mathbb{C}^n$, where

$$[z_{xy^T}]_i = [U^H xy^T U]_{ii} = U_i^H x\, y^T U_i = [d(U^H x) \cdot U^T y]_i,$$

U_i^H and U_i are the row i of U^H and the column i of U, respectively.

Proof

$$d(U^H x) = \begin{bmatrix} U_1^H x & & 0 \\ & U_2^H x & \\ 0 & & \ddots \\ & & & U_m^H x \end{bmatrix} \quad \text{and}$$

$$U^T y = \begin{bmatrix} U_1^T y \\ U_2^T y \\ \vdots \\ U_m^T y \end{bmatrix} = \begin{bmatrix} y^T U_1 \\ y^T U_2 \\ \vdots \\ y^T U_m \end{bmatrix}.$$

Then $\left[d(U^H x) \cdot U^T y \right]_i = (U_i^H x) \cdot (U_i^T y) = (U_i^H x)(y^T U_i)$

$$= U_i^H (x y^T) U_i = (U^H x y^T U)_{ii}.$$

PROPERTY 4

$A = A^H \Rightarrow \Lambda_A = \Lambda_A^H$. Moreover:

A symmetric and positive definite $\Rightarrow \Lambda_A$ symmetric and pd

Proof

$$\Lambda_A = U d(z_A) U^H = U d(e_j^T U^H A U e_j) U^H,$$

$$\Lambda_A^H = U \overline{d(z_A)} U^H = U d(e_j^T U^H A^H U e_j) U^H$$

$$= U d(e_j^T U^H A U e_j) U^H = \Lambda_A.$$

Then the eigenvalues of Λ_A are real. The eigenvalues of $\Lambda_A = U d(z_A) U^H$ are $(z_A)_j = (U^H A U)_{jj} = u_j^H A u_j > 0$, thus Λ_A is positive definite.

PROPERTY 5

If $B \in \mathcal{H}_n(\mathbb{C})$, then $tr(\mathcal{L}_B) = tr(B)$. Moreover, if B is hermitian and positive definite, then

$$\det(B) \leq \det(\mathcal{L}_B).$$

Proof

The equality $tr(\mathcal{L}_B) = tr(B)$ follows from Property 2. Moreover,

$$\det B = \det(U^H B U) \leq \prod_{i=1}^{n} [U^H B U]_{ii}$$

(as $\det B \leq \prod_{i=1}^{n} b_{ii}$ when B is hermitian and p.d.).

Thus

$$\begin{aligned} \det B &\leq \det(\operatorname{diag}[U^H B U],\ i = 1, \dots, n) \\ &= \det(U \operatorname{diag}[U^H B U]_{ii} U^H) \\ &= \det(\mathcal{L}_B). \end{aligned}$$

Notice that the inequality $\det B \leq \prod_{i=1}^{n} b_{ii}$, where B is hermitian and pd, is a special case of the inequality $\det(B) \leq \det(\mathcal{L}_B)$, for $U = I$.

EXERCISE 7

Prove that, if B is hermitian and pd, then

$$\det B \leq \prod_{i=1}^{n} b_{ii}$$

Now consider the iterative formula (generalized BFGS)

$$B_{k+1} = \tilde{B}_k + \frac{1}{y_k^T s_k} y_k y_k^T - \frac{1}{s_k^T \tilde{B}_k s_k} \tilde{B}_k s_k s_k^T \tilde{B}_k = \phi(\tilde{B}_k, s_k, y_k).$$

Set $\tilde{B}_k = \mathcal{L} B_k$ and apply to both sides of the matrices equality the operator $\mathcal{L}$. We obtain by the linearity (Property 1)

$$\mathcal{L} B_{k+1} = \mathcal{L}\mathcal{L} B_k + \left(\frac{1}{y_k^T s_k}\right) \mathcal{L} y_k y_k^T - \frac{1}{s_k^T \mathcal{L} B_k s_k} \mathcal{L}\mathcal{L} B_k s_k s_k^T \mathcal{L} B_k .$$

From $\mathcal{L}\mathcal{L} B_k = \mathcal{L} B_k$ and $\mathcal{L} A = U\, d(z_A)\, U^H$ we obtain

$$U\, d(z_{B_{k+1}})\, U^H = U\, d(z_{B_k})\, U^H + \frac{1}{y_k^T s_k} U\, d(z_{y_k y_k^T})\, U^H - \frac{1}{s_k^T \mathcal{L} B_k s_k} U\, d(z_{\mathcal{L} B_k s_k s_k^T \mathcal{L} B_k})\, U^H$$

and thus

$$d(z_{B_{k+1}}) = d(z_{B_k}) + \frac{1}{y_k^T s_k} d(z_{y_k y_k^T}) - \frac{1}{s_k^T \mathcal{L} B_k s_k} d(z_{\mathcal{L} B_k s_k s_k^T \mathcal{L} B_k}),$$

or in terms of vectors z,

$$z_{B_{k+1}} = z_{B_k} + \frac{1}{y_k^T s_k} z_{y_k y_k^T} - \frac{1}{s_k^T \mathcal{L} B_k s_k} z_{\mathcal{L} B_k s_k s_k^T \mathcal{L} B_k}.$$

By Property 3 we have

$$z_{y_k y_k^T} = d(U^H y_k) \cdot (U^T y_k) = \text{vector whose component } i \text{ is}$$

$$\left(\sum_h u_{ih}^H y_{kh}\right) \cdot \left(\sum_j u_{ij}^T y_{kj}\right) = \left(\sum_h u_{ih}^H y_{kh}\right)\left(\overline{\sum_h u_{ih}^H y_{kh}}\right)$$

(recall that $y_{kh} \in \mathbb{R}$)

Where u^H_{ih} = component h of u^H_i (= row i of U^H),

u^T_{ij} = component j of u^T_i (= row i of U^T),

u^T_{ij} = element ij of U^T; $u^T_{ij} = \overline{u}^H_{ij}$.

Then Property 3 implies

$$z_{y_k y_k^T} = |U^H y_k|^2$$

where $|z|^2$ denotes the vector whose component i is $|z_i|^2$.

We have also, by Property 3,

$$z_{\mathcal{L}_{B_k} s_k s_k^T \mathcal{L}_{B_k}} = z_{(\mathcal{L}_{B_k} s_k)(\mathcal{L}^T_{B_k} s_k)^T} = d(U^H \mathcal{L}_{B_k} s_k) \cdot (U^T \mathcal{L}^T_{B_k} s_k)$$

$$= d(U^H U\, d(z_{B_k})\, U^H s_k)(U^T (U^T)^H d(z_{B_k})\, U^T s_k)$$

$$= d(d(z_{B_k})\, U^H s_k) \cdot d(z_{B_k})\, U^T s_k$$

$$= \begin{bmatrix} [d(z_{B_k}) U^H s_k]_1 & & \\ & [d(z_{B_k}) U^H s_k]_2 & \\ & & \ddots \\ & & [d(z_{B_k}) U^H s_k]_M \end{bmatrix} \cdot \begin{bmatrix} [d(z_{B_k}) U^T s_k]_1 \\ \vdots \\ [d(z_{B_k}) U^T s_k]_M \end{bmatrix}$$

$$= \begin{bmatrix} d(z_{B_k})_1^2 & & \\ & d(z_{B_k})_2^2 & \\ & & \ddots \\ & & d(z_{B_k})_M^2 \end{bmatrix} \begin{bmatrix} (U^H s_k)_1 \cdot (U^T s_k)_1 \\ \vdots \\ (U^H s_k)_M \cdot (U^T s_k)_M \end{bmatrix} = d(z_{B_k})^2 \cdot |U^H s_k|^2 .$$

Moreover

$$S_k^T \mathcal{L}_{B_k} S_k = S_k^T U \, d(z_{B_k}) \, U^H S_k = S_k^T U \, d\left[(U^H B_k U)_{jj}\right] U^H S_k$$

$$= S_k^T U \begin{bmatrix} e_1 U^H B_k U e_1 & & & \\ & e_2 U^H B_k U e_2 & & \\ & & \ddots & \\ & & & e_m U^H B_k U e_m \end{bmatrix} \cdot U^H S_k$$

where $S_k^T U = (U^T S_k)^T$. Thus

$$S_k^T \mathcal{L}_{B_k} S_k = \left[(U^T S_k)_1 \; (U^T S_k)_2 \; \cdots \; (U^T S_k)_m\right] \begin{bmatrix} (z_{B_k})_1 & & & \\ & (z_{B_k})_2 & & \\ & & \ddots & \\ & & & (z_{B_k})_m \end{bmatrix} \begin{bmatrix} (U^H S_k)_1 \\ (U^H S_k)_2 \\ \vdots \\ (U^H S_k)_m \end{bmatrix}$$

$$= \overline{(U^H S_k)_1} \; \overline{(U^H S_k)_2} \cdots \overline{(U^H S_k)_m} \begin{bmatrix} (z_{B_k})_1 & & \\ & \ddots & \\ & & (z_{B_k})_m \end{bmatrix} \begin{bmatrix} (U^H S_k)_1 \\ \vdots \\ (U^H S_k)_m \end{bmatrix}$$

$$= z_{B_k}^T \left| U^H S_k \right|^2 .$$

Now apply the 3 equalities

$$z_{y_k} y_k^T = |U^H y_k|^2,$$

$$z_{\mathcal{L}_{B_k} S_k} S_k^T \mathcal{L}_{B_k} = d(z_{B_k})^2 \cdot |U^H S_k|^2,$$

$$S_k^T \mathcal{L}_{B_k} S_k = z_{B_k}^T |U^H S_k|^2,$$

to the iterative computation of z_{B_k} to obtain, eventually,

$$z_{B_{k+1}} = z_{B_k} + \frac{1}{y_k^T s_k}\,|U^H y_k|^2 - \frac{1}{z_{B_k}^T |U^H s_k|}\,d(z_{B_k})^2 \cdot |U^H s_k|^2 .$$

The previous iteration gives, at each step k, the eigenvalues of $\tilde{B}_{k+1} = \mathcal{L}_{B_{k+1}}$ in terms of the eigenvalues of $\tilde{B}_k = \mathcal{L}_{B_k}$. These eigenvalues are all the information one needs to define $\tilde{B}_k$ at each step, once the "structure" of the space $\mathcal{L}$, consisting in the matrix U, is given. Dividing this structure from the "information content" of each single $\tilde{B}_k = \mathcal{L}_{B_k}$ is the best way to obtain the previous updating formula. This formula is a single, one-dimensional array iteration, replacing the two-dimensional array iteration of the BFGS procedure. This reduces space complexity to $O(n)$, instead of $O(n^2)$ memory units required by BFGS. Moreover, notice that $z_{B_{k+1}}$ is real when z_{B_k} is real. This implies that all z_{B_k} are real when $x_0 \in \mathbb{R}^n$ and $B_0 \in \mathbb{R}^{n\times n}$.

The new iteration, involving the eigenvalues of B_k and B_{k+1}, let us define two possible quasi-Newton procedure for unconstrained minimization, depending on the choice of the descent direction d_k. In fact we can choose $d_{k+1} = -\tilde{B}_{k+1}^{-1} g_{k+1} = -U\, d(z_{B_{k+1}})^{-1} U^H g_{k+1}$ as well as

$$d_k = -B_{k+1}^{-1} g_k .$$

The first choice leads to a Non-Secant (NS) algorithm because the matrix $\tilde{B}_{k+1}$ does not satisfy the secant equation. The second choice leads to a Secant algorithm (S), because the matrix

$$B_{k+1} = \mathcal{L}_{B_k} + \frac{1}{y_k^T s_k} y_k y_k^T - \frac{1}{s_k^T \mathcal{L}_{B_k} s_k} \mathcal{L}_{B_k} s_k s_k^T \mathcal{L}_{B_k}$$

satisfy the secant equation : $B_{k+1} s_k = y_k$.

We can describe this new class of procedures, called LQN algorithms, as follows, with the two possible choices of the direction d_k :

$x_0 \in \mathbb{R}^n$, B_0 symmetric pos. def.

$U^H d_0 = - d(z_{B_0}^{-1}) U^H g_0$ (NS) or $U^H d_0 = - U^H B_0^{-1} g_0$ (S)

$d_0 = U(U^H d_0)$

For $k = 0, 1, 2, \dots$

$x_{k+1} = x_k + \lambda_k d_k$

$s_k = x_{k+1} - x_k$, $y_k = g_{k+1} - g_k$.

$$z_{B_{k+1}} = z_{B_k} + \frac{1}{y_k^T s_k} |U^H y_k|^2 - \frac{1}{z_{B_k}^T |U^H s_k|^2} d(z_{B_k})^2 |U^H s_k|^2$$

$$\begin{cases} U^H d_{k+1} = - d(z_{B_{k+1}}^{-1}) U^H g_{k+1} & (NS) \\ U^H d_{k+1} = - U^H B_{k+1}^{-1} g_{k+1} & (S) \end{cases}$$

$d_{k+1} = U(U^H d_{k+1})$

EXERCISE 8

Prove that the secant direction $d_k = -B_{k+1}^{-1} g_{k+1}$ can be computed through the formula

$$U^H d_{k+1} = -d(z_{B_k}^{-1}) U^H g_{k+1} + \frac{s_k^T g_{k+1}}{y_k^T s_k} d(z_{B_k}^{-1}) U^H y_k$$

$$+ \left[-\left(1 + \frac{(z_{B_k}^{-1})^T |U^H y_k|^2}{y_k^T s_k}\right) \frac{s_k^T g_{k+1}}{y_k^T s_k} + \frac{(z_{B_k}^{-1})^T d(U^T y_k) U^H g_{k+1}}{y_k^T s_k} \right] U^H s_k$$

(Suggr: use a Sherman - Morrison formula for a modification of rank 2 of B_k, given by the iteration $B_{k+1} = \mathcal{L}_{B_k} + \frac{1}{y_k^T s_k} y_k y_k^T - \frac{1}{s_k^T \mathcal{L}_{B_k} s_k} \mathcal{L}_{B_k} s_k s_k^T \mathcal{L}_{B_k}$ where $\mathcal{L}_{B_k} = U d(z_{B_k}) U^H$.)

Notice that, if U defines a fast transform (FFT, Hartley or others) then only two fast transforms are required at each step of the Non-Secant (NS) LQN algorithm, so the cost of each step is $O(n \log n)$ flops. The two fast transforms required are:

1. $U^H g_{k+1}$, from which we obtain also $U^H y_k = U^H (g_{k+1} - g_k)$.
2. $U(U^H d_{k+1})$, where $U^H d_{k+1}$ is obtained by multiplying $-d(z_{B_{k+1}}^{-1})$ by $U^H g_{k+1}$.

EXERCISE 8' How many fast transforms are required in the secant algorithm?

Now global convergence properties of the NS LQN algorithm will be investigated. The final result is an extension of a well known result of Powell (1976) on global convergence of the BFGS method to the NS BFGS-type algorithm, where B_k is replaced by $\tilde{B}_k$, under some new simple supplementary assumptions on $\tilde{B}_k$.

Consider the basic scheme

$$\begin{cases} x_0 \in \mathbb{R}^n, \; B_0 \in \mathbb{R}^{n\times n} \text{ pd} \\ \text{for } k = 0, 1, 2, \dots \\ \text{If } g_k \neq 0 \text{ then} \\ \text{define a pd matrix } \tilde{B}_k \in \mathbb{R}^{n\times n} \\ d_k = -\tilde{B}_k g_k \quad \text{(Non secant directions!)} \\ x_{k+1} = x_k + \lambda_k d_k, \\ B_{k+1} = \phi(\tilde{B}_k, s_k, y_k) \end{cases}$$

Assume that the step-lengths λ_k satisfy the Armijo-Goldstein conditions $(AG)_1$ and $(AG)_2$. Moreover, let $f: \mathbb{R}^n \to \mathbb{R}$ be a lower bounded, continuously differentiable function. Denote by I_0 the level set $\{x : f(x) \leq f(x_0)\}$. The previous non secant algorithm yields a sequence of points x_{k+1}, $k = 0, 1, 2, \dots$ such that $f(x_{k+1}) < f(x_0)$ (consequence of $(AG)_1$) and $y_k^T s_k > 0$ (consequence of $(AG)_2$). Therefore, x_{k+1} belongs to the set I_0 and $B_{k+1} = \phi(\tilde{B}_k, s_k, y_k)$ is well defined and pd, until $\nabla f(x_k) = 0$. □

From now on assume that $\nabla f(x_k) \neq 0$, otherwise the algorithm terminates in a finite number of steps at a stationary point for f. Since $\{f(x_k)\}$ is a lower bounded strictly decreasing sequence, obviously $\lim_{k\to\infty} f(x_k) \geq \inf f(x)$.

The following theorem states that under special prescriptions on the trace and on the determinant of $\tilde{B}_k$, a subsequence of $\{g_k\}$ converges to the null vector, provided that the ratios $\frac{\|y_k\|^2}{y_k^T s_k}$ are upper bounded.

THEOREM 8

Let $\tilde{B}_k$ in the previous NS algorithm satisfy the conditions

$$\operatorname{tr} B_k \geq \operatorname{tr} \tilde{B}_k,$$

$$\det B_k \leq \det \tilde{B}_k.$$

If $\exists\, M > 0$ such that

$$(*) \qquad \frac{\|y_k\|^2}{y_k^T s_k} \leq M,$$

then

$$\liminf \|\nabla f(x_k)\| = 0.$$

We recall that the assumption (*) on the current guesses x_k and x_{k+1} is automatically satisfied if $f(x)$ is a convex function [Powell, 1976]. So (*) can be seen as a sort of discrete weak convexity assumption.

Proof

The method of the proof does not help our understanding of the algorithm very much. We must consider the behaviour of the product

$$\prod_{j=0}^{k} \frac{\|g_j\|^2}{s_j^T(-g_j)},$$

because we are interested on the behaviour of $\|g_j\|^2$ and we are able to know easily the behaviour of $s_j^T(-g_j)$. We have to prove that the previous product is bounded by C^{k+1}, C = constant:

$$\prod_{j=0}^{k} \frac{\|g_j\|^2}{s_j^T(-g_j)} = \prod_{j=0}^{k} \frac{\|g_j\|}{\|s_j\| \cdot \cos\vartheta_j} \leq C^{k+1}$$

In fact:

Let $\|g_j\|$ be bounded away from zero. If we prove that $\|s_j\| \cdot \cos\vartheta_j \to 0$, then the terms $\frac{\|g_j\|}{\|s_j\| \cdot \cos\vartheta_j}$ goes to ∞ and we have a contradiction with the previous bound.

Thus we have to prove:

i) $\prod_{j=0}^{k} \frac{\|g_j\|^2}{s_j^T(-g_j)} \leq C^{k+1}$,

ii) $\|s_j\| \cdot \cos\vartheta_j \to 0$.

The limit ii) follows from $(AG)_2$:

$f(x_{j+1}) \leq f(x_j) + \lambda_j c_2 g_j^T d_j$. Add with respect to j:

$$\Rightarrow \quad c_2 \sum_{j=0}^{k} \lambda_j (-g_j^T d_j) \leq f_0 - f_{k+1} \leq f_0 - \inf[f(x)].$$

Thus the series $\sum_{j=0}^{\infty} \lambda_j (-g_j^T d_j)$ is convergent and

$\lambda_j (-g_j^T d_j) = -g_j^T s_j \to 0$.

To prove i) start from the iteration

$$B_{k+1} = \tilde{B}_k + \frac{1}{y_k^T s_k} y_k y_k^T - \frac{1}{s_k^T \tilde{B}_k s_k} \tilde{B}_k s_k s_k^T \tilde{B}_k$$

and from the inequality

$$\operatorname{tr} B_k \geq \operatorname{tr} \tilde{B}_k$$

to obtain

$$\operatorname{tr}(B_{j+1}) = \operatorname{tr}(\tilde{B}_j) + \frac{1}{y_j^T s_j} y_j^T y_j - \frac{1}{s_j^T \tilde{B}_j s_j} (\tilde{B}_j s_j)^T (\tilde{B}_j s_j)$$

$$\leq \operatorname{tr}(B_j) + \frac{\|y_j\|^2}{y_j^T s_j} - \frac{\|\tilde{B}_j s_j\|^2}{s_j^T \tilde{B}_j s_j}, \quad j = 0, 1, \ldots, k.$$

Now apply recursively this inequality and add for $j = 0, 1, \ldots, k$. We obtain

$$\operatorname{tr}(B_{k+1}) \leq \operatorname{tr}(B_0) + \sum_{j=0}^{k} \frac{\|y_j\|^2}{y_j^T s_j} - \sum_{j=0}^{k} \frac{\|\tilde{B}_j s_j\|^2}{s_j^T \tilde{B}_j s_j}$$

and, by the assumption $\|y_k\|^2 / (y_k^T s_k) \leq M$,

$$\operatorname{tr}(B_{k+1}) \leq \operatorname{tr}(B_0) + (k+1) M \leq c_3 (k+1).$$

Let $\nu_i(B_{k+1})$ be the eigenvalues of B_{k+1}. Then, by the geometric–arithmetic mean inequality, we have

$$\prod_i \nu_i(B_{k+1}) = \det(B_{k+1}) \leq \left(\frac{\sum_i \nu_i(B_{i+1})}{n} \right)^n$$

Thus

$$\det(B_{k+1}) \le \left(\frac{c_3(k+1)}{n}\right)^n, \text{ where } c_3 \ge \nu_i(B_{k+1}) \ \forall i.$$

Moreover

$$\sum_{j=0}^{k} \frac{\|\tilde{B}_j s_j\|^2}{s_j^T \tilde{B}_j s_j} \le \operatorname{tr}(B_0) - \operatorname{tr}(B_{k+1}) + \sum_{j=0}^{k} \frac{\|y_j\|^2}{y_j^T s_j}$$

$$\le \operatorname{tr}(B_0) + \sum_{j=0}^{k} \frac{\|y_j\|^2}{y_j^T s_j} \le \operatorname{tr}(B_0) + (k+1)M \le c_3(k+1).$$

Again, by the geometric-arithmetic inequality,

$$\prod_{j=0}^{k} \frac{\|\tilde{B}_j s_j\|^2}{s_j^T \tilde{B}_j s_j} \le \left[\sum_{j=0}^{k} \frac{\|\tilde{B}_j s_j\|^2}{s_j^T \tilde{B}_j s_j} \Big/ (k+1)\right]^{k+1}$$

and then

$$(\dagger) \quad \prod_{j=0}^{k} \frac{\|\tilde{B}_j s_j\|^2}{s_j^T \tilde{B}_j s_j} \le \left[\frac{c_3(k+1)}{(k+1)}\right]^{k+1} = c_3^{k+1},$$

which is the very key inequality of the proof.

We have also (see EXERCISE 9)

$$\det(B_{j+1}) = \frac{s_j^T y_j}{s_j^T \tilde{B}_j s_j} \det(\tilde{B}_j) \ge \frac{s_j^T y_j}{s_j^T \tilde{B}_j s_j} \det(B_j). \quad j = 0, 1, \ldots, k$$

and then

$$\frac{s_j^T y_j}{s_j^T \tilde{B}_j s_j} \le \frac{\det(B_{j+1})}{\det(B_j)} \quad \text{and} \quad \prod_{j=0}^{k} \frac{s_j^T y_j}{s_j^T \tilde{B}_j s_j} \le \frac{\det B_{k+1}}{\det B_0}.$$

From $(A6)_2$ we have $g_{j+1}^T d_j \ge c_2 g_j^T d_j$ and

$s_j^T y_j \ge (1 - c_2)(-g_j^T s_j)$, that is $(1 - c_2) \le \dfrac{s_j^T y_j}{s_j^T (-g_j)}$.

In the NS LQN algorithm we have

$$\tilde{B}_j s_j = \tilde{B}_j (x_{j+1} - x_j) = \tilde{B}_j \left(-\lambda_j \tilde{B}_j^{-1} g_j \right) = -\lambda_j g_j$$

and so, by the previous inequality (†), we obtain

$$(1-c_2)^{k+1} \prod_{j=0}^{k} \frac{\|g_j\|^2}{s_j^T(-g_j)} = \prod_{j=0}^{k} \frac{\|g_j\|^2 (1-c_2)}{s_j^T(-g_j)} \leq \prod_{j=0}^{k} \frac{\|g_j\|^2 (y_j^T s_j)}{s_j^T(-g_j)\, s_j^T(-g_j)}$$

$$= \prod_{j=0}^{k} \frac{\|-\lambda_j g_j\|^2 s_j^T y_j}{s_j^T(-\lambda_j g_j)\, s_j^T(-\lambda_j g_j)} = \prod_{j=0}^{k} \frac{\|\tilde{B}_j s_j\|^2 s_j^T y_j}{s_j^T \tilde{B}_j s_j\, s_j^T \tilde{B}_j s_j}$$

$$\leq c_3^{k+1} \frac{\det(B_{k+1})}{\det(B_0)} \leq c_3^{k+1} \frac{1}{\det(B_0)} \left(\frac{c_3(k+1)}{n} \right)^n \leq c_4^{k+1}$$

and finally

$$\prod_{j=0}^{k} \frac{\|g_j\|^2}{s_j^T(-g_j)} \leq c^{k+1}.$$

For a full understanding of the Goldstein theorem we should compare it with the following standard result on global convergence of sequences $\{x_k\}$ generated by iterations of the form $x_{k+1} = x_k + \lambda_k d_k$.

THEOREM 9 (Nocedal, Wright, 1999)

Consider any iteration of the form

$$x_{k+1} = x_k + \lambda_k d_k \,, \quad x_0 \in D \text{ open and convex}$$

where d_k is a descent direction ($g_k^T d_k < 0$) and λ_k satisfies $(AG)_1$ and $(AG)_2$. Suppose that f is bounded below in $\mathbb{R}^n$ and $g(x) = \nabla f(x)$ satisfies a Lipschitz condition in D, that is

$$\|g(x) - g(x')\| \le L \|x - x'\|, \quad x, x' \in D.$$

Then

$$(\dagger) \qquad \sum_{k \ge 0} \cos^2 \vartheta_k \|g_k\|^2 < \infty \,, \quad \text{where } \vartheta_k = -\widehat{g_k d_k}.$$

CONSEQUENCE: If the choice of d_k ensures that ϑ_k is bounded away from $\pi/2$, ie. there is a positive δ such that $\cos \vartheta_k \ge \delta > 0$ for every k, then $(\dagger)$ implies global convergence, that is

$$\lim_{k \to \infty} \|g_k\| = 0 \,.$$

Remark. The condition $\cos \vartheta_k \ge 1/M$ is satisfied when $d_k = -B_k^{-1} g_k$ for a sequence $\{B_k\}$ of pd matrices B_k with $\|B_k\| \cdot \|B_k^{-1}\| \le M \ \forall k$.

(see EXERCISE 12)

Proof of THEOREM 9 :

The condition $(AG)_2$, that is

$$\nabla f(x_k + \lambda_k d_k)^T d_k \geq c_2 \nabla f(x_k)^T d_k ,$$

implies (subtract $\nabla f(x_k)^T d_k$ from both sides)

$$(1) \quad \nabla f(x_{k+1})^T d_k - \nabla f(x_k)^T d_k \geq (c_2 - 1) \nabla f(x_k)^T d_k .$$

By the Lipschitz condition we have

$$\| \nabla f(x_{k+1}) - \nabla f(x_k) \| \leq L \| x_{k+1} - x_k \| = L \lambda_k \| d_k \| .$$

Thus

$$\| \nabla f(x_{k+1}) - \nabla f(x_k) \| \| d_k \| \leq \lambda_k L \| d_k \|^2 .$$

Now Apply the Cauchy - Schwarz inequality and obtain

$$(2) \quad \left[\nabla f(x_{k+1}) - \nabla f(x_k) \right]^T d_k \leq \lambda_k L \| d_k \|^2$$

Compare (1) and (2) to deduce

$$(c_2 - 1) \nabla f(x_k)^T d_k \leq \lambda_k L \| d_k \|^2$$

and

$$\lambda_k \geq \frac{(c_2 - 1) \nabla f(x_k)^T d_k}{L \| d_k \|^2} .$$

By $(AG)_1$ we have also

$$f(x_k + \lambda_k d_k) \leq f(x_k) + c_1 \frac{(c_2 - 1)}{L} \frac{(g_k^T d_k)^2}{\| d_k \|^2}$$

$$= f(x_k) - c_1 \frac{(1 - c_2)}{L} \frac{(g_k^T d_k)^2}{\| d_k \|^2} .$$

Set $c = c_1 \frac{(1 - c_2)}{L}$.

Then we have

$$f(x_{k+1}) \leq f(x_k) - \cos^2\vartheta_k \cdot \|g_k\|^2 \cdot c$$

$$\leq f(x_{k-1}) - \cos^2\vartheta_{k-1} \cdot \|g_{k-1}\|^2 \cdot c - \cos^2\vartheta_k \cdot \|g_k\|^2 \cdot c$$

$$\leq f(x_0) - c \sum_{j=0}^{k} \cos^2\vartheta_j \|g_j\|^2.$$

As f is bounded below, we have the thesis.

For search methods of the general form $x_{k+1} = x_k + \lambda_k d_k$ The limit $\lim_{k\to\infty} \|g_k\| = 0$ is the strongest global convergence result that we are able to obtain. This result does not guarantee that the method converges to a minimizer, but only that it is attracted by stationary points. Only by making additional requirement on d_k and $H(x_k)$ - like $d_k^T H(x_k) d_k < 0$ - we can gain some information on a possible convergence to a local minimum (see Nocedal, Wright, § 3.2)

It would seem, from Theorem 9, that all we need to ensure is that the direction d_k does not tend to become orthogonal to the gradient g_k. We could simply compute $\cos\vartheta_k$ at every step k and turn d_k toward the direction $-g_k$ if $\cos\vartheta_k$ is too small. Angle tests of this type ensure global convergence but they are undesiderable because they destroy the invariance properties of quasi-Newton methods (see Nocedal, Wright, § 3.3).

Requirement of global convergence can sometimes conflict with requirement of fast convergence. For example, the steepest descent method is typically a globally convergent method, as $d_k = -g_k$ and then $\cos\vartheta_k = 1$, but the convergence can be too slow. The pure Newton iteration has a local fast convergence, but its search direction may not even be descent direction when we are away from the solution.

REMARK 1 (convergence of Secant LQN Algorithms)

The condition $\frac{\|y_k\|^2}{y_k^T s_k} \le M$, which is the key assumption in Theorem 8, implies the (discrete) Lipschitz condition on g: $\|g_{k+1} - g_k\| \le M \|x_{k+1} - x_k\|$. This is a consequence of the Cauchy-Schwarz inequality:

$\|y_k\|^2 \le M\, y_k^T s_k \le M \|y_k\| \cdot \|s_k\| \Rightarrow \|y_k\| \le M \cdot \|s_k\|$.

Thus, by Theorem 9, the conditions $\frac{\|y_k\|^2}{y_k^T s_k} \le M$ and $\cos\vartheta_k \ge c > 0$, together with the basic assumptions on λ_k and on f ($(A\,G)_1$, $(A\,G)_2$, f bounded below), imply the global convergence of $\{x_k\}$ for any descent direction d_k. In particular

$\frac{\|y_k\|^2}{y_k^T s_k} \le M$ and $\cos\vartheta_k \ge c > 0 \Rightarrow$ S LQN algorithm converges globally.

In other words, a weak convexity assumption together with a lower boundedness of $\cos\vartheta_k$ guarantees the global convergence of S LQN algorithms.

REMARK 2 (convergence of Non Secant LQN Algorithms)

By the Property 5 of $\mathcal{L}_B$, which states the link between spectral structure of B and $\mathcal{L}_B$, we have immediately that the NS Secant algorithms are globally convergent under the sole condition $\frac{\|y_k\|^2}{y_k^T s_k} \leq M$. (Theorem 8).

The Theorem 8 states that

$$\liminf_{k \to \infty} \|g_k\| = 0,$$

in other words, just a subsequence of the gradient norms $\|g_k\|$ converges to zero, rather than the whole sequence (as in Theorem 9). This is a weaker result, analogous to global convergence result proved for BFGS algorithm (Powell, 1976) or for conjugate gradient methods (see Nocedal Wright, 1999, § 3.2).

A very interesting aspect of Theorem 8 is that the convexity of the function f is replaced by the weaker discrete condition $\frac{\|y_k\|^2}{y_k^T s_k} \leq M$. This condition is weaker in the following precise sense [Powell, 1976]:

Assume that f is convex and has continuous and bounded second derivatives in a convex set $D \subset \mathbb{R}^n$. Then, for all $x, y \in D$, $\|\nabla f(x) - \nabla f(y)\|^2 \leq M (\nabla f(x) - \nabla f(y))^T (x - y)$ where $\|H(x)\| = \|\nabla^2 f(x)\| \leq M$ in D.

EXERCISE 9

Prove that, for $u_1, u_2, u_3, u_4 \in \mathbb{R}^n$,

$$\det\left(I + u_1 u_2^T + u_3 u_4^T\right) = (1 + u_1^T u_2)(1 + u_3^T u_4) - (u_1^T u_4)(u_2^T u_3).$$

Use this equality to prove that, for

$$B = \tilde{B} + \frac{1}{y^T s} y y^T - \frac{1}{s^T \tilde{B} s} \tilde{B} s s^T \tilde{B},$$

we have $$\det B = (\det \tilde{B}) \frac{s^T y}{s^T B s}.$$

EXERCISE 10

Prove that, when the eigenvalues of B_{k+1} are bounded, the ratio $\frac{\|y_k\|^2}{y_k^T s_k}$ is bounded, if B_{k+1} satisfies the secant equation: $B_{k+1} s_k = y_k$. (Recall that B_{k+1} is s.p.d, and $\sqrt{B_{k+1}}\, B_{k+1} = B_{k+1} \sqrt{B_{k+1}}$).

EXERCISE 11 (easy!)

Prove that, if g is Lipschitz and θ_k remains away from $90°$, then the ratio $\frac{\|y_k\|^2}{y_k^T s_k}$ is bounded.

EXERCISE 12 (important!)

Prove that, if B_k is pd with condition number bounded by M, then $\cos\theta_k = \cos\left(-\widehat{g_k, B_k^{-1} g_k}\right) \geq \frac{1}{M} > 0$.

We will give a characterization of descent direction by exploiting the iteration of BFGS-type algorithm.

Given any (secant or not secant) minimization iterative procedure

$$x_{k+1} = x_k + \lambda_k d_k$$

the search direction is required to be a descent direction, that is $g_k^T d_k < 0$. In the following Theorem we observe that any descent direction d_k always solves an equation $A_k d_k = -g_k$ for some pd A_k. We also show that if the angle between $-g_k$ and d_k is uniformly less than $90°$, then the matrices A_k can be chosen with bounded condition number.

THEOREM 10

If d_k is a descent direction at x_k for a function f, i.e. $g_k^T d_k < 0$, then $d_k = -A_k^{-1} g_k$ for some positive definite matrix A_k. Moreover, if $\cos \widehat{-g_k, d_k} \geq c > 0$, then A_k can be chosen such that $\text{cond}(A_k) \leq M_c$.

Proof.
The first assertion is proved by choosing

$$A_k = \phi(\alpha_k I, d_k, -g_k)$$

where $\phi(B, s, y) = B + \frac{1}{y^T s} yy^T - \frac{1}{s^T B s} Bss^T B$

(just verify directly that $\phi(\alpha_k I, d_k, -g_k) d_k = -g_k$).

For the second assertion choose the same A_k, with $\alpha_k = \frac{\|g_k\|}{\|d_k\|}$.

In fact, let λ be an eigenvalue of $\phi(\alpha_k I, d_k, -g_k)$ and let x be the corresponding eigenvector:

$$(1) \quad \left(\alpha_k I + \frac{1}{-g_k^T d_k} g_k g_k^T - \frac{\alpha_k}{d_k^T d_k} d_k d_k^T\right) x = \lambda x.$$

If $g_k^T x = d_k^T x = 0$, then $\alpha_k x = \lambda x$ and $\lambda = \alpha_k$.
Thus $\phi(\alpha_k I, d_k, -g_k)$ has $n-2$ eigenvalues equal to α_k.
Let λ_1 and λ_2 be the remaining two eigenvalues.
The characteristic polynomial of $\phi(\alpha_k I, d_k, -g_k)$ is
$\in(\lambda) = (\lambda - \alpha_k)^{n-2}(\lambda^2 + c_1\lambda + c_2)$ where $c_1 = -(\lambda_1 + \lambda_2)$ and $c_2 = \lambda_1 \cdot \lambda_2$. We find the value of $\lambda_1 + \lambda_2$ by computing the trace of $\phi(\alpha_k I, d_k, -g_k)$:

$$\operatorname{tr}[\phi(\alpha_k I, d_k, -g_k)] = (n-2)\alpha_k + \lambda_1 + \lambda_2 = n\alpha_k - \frac{g_k^T g_k}{g_k^T d_k} - \alpha_k.$$

$$\Rightarrow \quad \lambda_1 + \lambda_2 = \alpha_k - \frac{g_k^T g_k}{g_k^T d_k}.$$

To compute $\lambda_1 \cdot \lambda_2$ observe that the eigenvector x is a linear combination of g_k and d_k. By replacing this linear combination $x = \gamma_1 g_k + \gamma_2 d_k$ in (1) we find a quadratic equation in λ and $\lambda_1 \cdot \lambda_2 = -\alpha_k \frac{d_k^T g_k}{d_k^T d_k}$. Then λ_1, λ_2 are the solutions of the problem

$$\begin{cases} \lambda_1 + \lambda_2 = \alpha_k - \dfrac{g_k^T g_k}{g_k^T d_k}, \\ \lambda_1 \cdot \lambda_2 = -\alpha \dfrac{d_k^T g_k}{d_k^T d_k}. \end{cases}$$

We calculate $\lambda_1 = \lambda_-$ and $\lambda_2 = \lambda_+$ where

$$\lambda_\pm = \alpha_k + \frac{1}{2}\left[p_k - \alpha_k \pm \sqrt{(p_k-\alpha_k)^2 - 4\alpha_k(q_k - p_k)} \right.$$

where $p_k = \frac{\|g_k\|^2}{d_k^T(-g_k)}$, $q_k = \frac{d_k^T(-g_k)}{\|d_k\|^2}$, $q_k - p_k \leq 0$.

If $q_k - p_k = 0$, then $\lambda_\pm = \alpha_k$. If $q_k - p_k < 0$, then $\lambda_- < \alpha_k$ and $\alpha_k < \lambda_+$. This implies that

$$\text{Cond}(A_k) = \frac{\lambda_+}{\lambda_-} = \frac{\lambda_2}{\lambda_1}.$$

One computes, eventually,

$$\text{Cond}(A_k) = \frac{(p_k+\alpha_k)^2}{2\alpha_k q_k}(1+\omega) - 1$$

where $\omega = \sqrt{1 - 4\alpha_k q_k/(p_k+\alpha_k)^2}$.

Now we have $\text{Cond}(A_k) \leq M$ if $\frac{(p_k+\alpha_k)^2}{\alpha_k q_k} \leq \hat{M}$.

Prove, finally, that the last inequality holds when there are 3 constants M_1, M_2, M_3 such that

$$\frac{1}{\cos\text{-}\widehat{g_k, d_k}} \leq M_1, \quad \alpha_k \frac{\|d_k\|}{\|g_k\|} \frac{1}{\cos\text{-}\widehat{g_k, d_k}} \leq M_2, \quad \frac{1}{\alpha_k}\frac{\|g_k\|}{\|d_k\|}\frac{1}{\cos\text{-}\widehat{g_k d_k}} \leq M_3.$$

If $\cos\text{-}\widehat{g_k, d_k} \geq c > 0$, then the latter inequalities are satisfied for $\alpha_k = \frac{\|g_k\|}{\|d_k\|}$.

Recall that, if B_k is pd with condition number bounded by M, then $\cos(-g_k, -B_k^{-1}g_k) \geq \frac{1}{M} > 0$ (see EXERCISE 12). So we have the following

THEOREM 11

A sequence d_k is such that $\cos(-g_k, d_k) \geq c > 0$ iff $d_k = -B_k^{-1} g_k$ for some sequence $\{B_k\}$ of pd matrices satisfying the inequality

$$\|B_k\| \cdot \|B_k^{-1}\| \leq M.$$

The previous result suggests that a suitable choice of B_k, step by step, could give to the sequence $\{x_k\}$ a global convergence property.

Some rather restrictive results have been obtained concerning the <u>local</u> convergence properties of LQN methods (a local superlinear convergence holds for BFGS: see Powell, 1976). It is proved, in particular, that LQN converges to a minimizer x_* of f with a superlinear rate of convergence whenever $\nabla^2 f(x_*) \in \mathcal{L}$, with $B_k \in \mathcal{L}$. Despite its insufficient effectiveness this result suggests that, in order to improve LQN efficiency, one might look for an <u>algebra</u> $\mathcal{L}^k$, at each step k, that is "close", in some sense, to B_k, and consequently to $H(x_k)$. Two important properties of B_k are that B_k is pd and B_k satisfies the secant equation: $B_k s_{k-1} = y_{k-1}$.

So, we claim that a structured algebra $\mathcal{L}^K$ is "close" to B_K if $\mathcal{L}^K$ includes matrices satisfying the latter properties, i.e. if the set

$$\{ X \in \mathcal{L}^K : X \text{ is pd and } X s_{k-1} = y_{k-1} \}$$

is not empty.
Once such a space $\mathcal{L}^K$ is introduced, we can conceive at least two $L^K QN$ algorithms, based on the updating formula $B_{k+1} = \phi(A_k, s_k, y_k)$, $A_k \in \mathcal{L}^K$.

Algorithm 1 : $A_k = \mathcal{L}^K_{sy}$, where $\mathcal{L}^K_{sy} \in \mathcal{L}^K$ is pd and solves the secant equation $X s_{k-1} = y_{k-1}$.

Algorithm 2 : $A_k = \mathcal{L}^K_{Bk}$, where $\mathcal{L}^K_{Bk}$ is the best least squares fit to B_k in $\mathcal{L}^K$.

Note that the choice $A_k = \mathcal{L}^K_{sy}$ may yield a matrix A_k which is not the best approximation in Frobenius norm of B_k in $\mathcal{L}^K$, i.e. in general $A_k \neq \mathcal{L}^K_{Bk}$.
Since A_k must be an element of $\mathcal{L}^K$ it will have the form $U_k d(W_k) U_k^H$ for some vector W_k. Then, the secant condition $U_k d(W_k) U_k^H s_{k-1} = y_{k-1}$ can be rewritten in order to determine W_k via U_k^H, i.e.

$$(W_k)_i = \frac{(U_k^H y_{k-1})_i}{(U_k^H s_{k-1})_i}, \qquad (U_k^H s_{k-1})_i \neq 0 \ \forall i$$

Finally, A_K is pd if $(W_K)_i > 0$. So, the basic criterion for choosing $\mathcal{L}^K$ is the following one:

choose U_K such that

$$(*) \qquad (W_K)_i = \frac{(U_K^H y_{K-1})_i}{(U_K^H s_{K-1})_i} > 0 \quad \forall i$$

and define $\mathcal{L}^K = SDU_K = \{ U_K d(z) U_K^H : z \in \mathbb{C}^n \}$,

U_K $n \times n$ unitary.

Once U_K is found, the corresponding space $\mathcal{L}^K$ includes the desired matrix A_K of Algorithm 1, i.e. $A_K = \mathcal{L}^K_{sy}$ and the criterium of "closeness" is satisfied. The updating formula becomes $B_{K+1} = \phi(\mathcal{L}^K_{sy}, s_K, y_K)$, $\mathcal{L}^K_{sy} s_{K-1} = y_{K-1}$.

and the two possible descent directions are

$$d_{K+1} = \begin{cases} -B_{K+1}^{-1} g_{K+1} \,, \\ -(\mathcal{L}^{K+1}_{sy})^{-1} g_{K+1} \,. \end{cases}$$

Both directions satisfy the secant equation.

Now we ask if there exists a unitary matrix U_K satisfying the condition $(*)$. The following theorem answers the question:

THEOREM 11

The existence of a matrix U_K^H satisfying $(*)$ is guaranteed if and only if

$$y_{K-1}^T s_{K-1} > 0.$$

Recall that $(AG)_2 \Rightarrow y_{K-1}^T s_{K-1} > 0$.

To prove Theorem 11 we need the following preliminary LEMMA:

Let $H(z)$ denote the Householder matrix corresponding to the vector z, i.e.

$$H(z) = I - \frac{2}{\|z\|^2} zz^H, \quad z \in \mathbb{R}^n.$$

LEMMA

Given two vectors $s, y \in \mathbb{R}^n \setminus \{0\}$, let $u, x \in \mathbb{R}^n$ be such that $\|u\| \cdot \|x\| \neq 0$, $u_i \neq 0$ and $\cos \hat{us} = \cos \hat{xy}$, i.e.

$$(**) \qquad \frac{u^T s}{\|u\| \cdot \|s\|} = \frac{x^T y}{\|x\| \cdot \|y\|}.$$

Set: $v = s - y - \left(\frac{\|s\|}{\|u\|} u - \frac{\|y\|}{\|x\|} x \right)$,

$$P = H(v)s - \frac{\|s\|}{\|u\|} u = H(v)y - \frac{\|y\|}{\|x\|} x,$$

$$U^H = H(P) \cdot H(v).$$

Then

$$U^H s = \frac{\|s\|}{\|u\|} u, \quad U^H y = \frac{\|y\|}{\|x\|} x$$

and $$w_i = \frac{(U^H y)_i}{(U^H s)_i} = \frac{\|y\|}{\|s\|} \cdot \frac{\|u\|}{\|x\|} \frac{x_i}{u_i}.$$

Proof

First observe that, if $p = v - \frac{\|v\|}{\|z\|} z$, $z \neq 0$, then

$$H(p)v = \frac{\|v\|}{\|z\|} z .$$

In fact

$$H(p)v = \left[I - \frac{2}{\|p\|^2} pp^T\right] v = \left[I - \frac{2}{\|p\|^2} pp^T\right]\left[p + \frac{\|v\|}{\|z\|} z\right]$$

$$= p - \frac{2}{\|p\|^2} p(p^T p) + \frac{\|v\|}{\|z\|} z - \frac{2}{\|p\|^2} \frac{\|v\|}{\|z\|} pp^T z$$

$$= -p + \frac{\|v\|}{\|z\|} z - 2\left[\frac{1}{\|p\|^2} \frac{\|v\|}{\|z\|} p^T z\right] p$$

$$= -p + \frac{\|v\|}{\|z\|} z - 2\left(-\frac{1}{2}\right) p = \frac{\|v\|}{\|z\|} z$$

(check that $\frac{(p^T z)}{\|p\|^2} \cdot \frac{\|v\|}{\|z\|} = -\frac{1}{2}$)

Now, for a unitary matrix Q, set

$$P_1 = Qs - \frac{\|s\|}{\|x\|} x , \qquad P_2 = Qy - \frac{\|y\|}{\|x\|} x .$$

Then we have (recall that $\|Qs\| = \|s\|$ and $\|Qy\| = \|y\|$)

$$H(P_1)Qs = \frac{\|s\|}{\|x\|} x , \qquad H(P_2)Qy = \frac{\|y\|}{\|x\|} x$$

Choose Q such that $P_1 = P_2 = P$ which is equivalent to

$$Q(s-y) = \frac{\|s\|}{\|x\|} x - \frac{\|y\|}{\|x\|} x .$$

Such choice is possible provided that

$$\|s-y\| = \left\| \frac{\|s\|}{\|x\|} x - \frac{\|y\|}{\|x\|} x \right\| .$$

A matrix Q that satisfies the previous equality is $Q = I - \frac{2}{\|u\|^2} uu^T$, where

$$u = s - y - \left(\frac{\|s\|}{\|z\|} z - \frac{\|y\|}{\|x\|} x \right)$$

(by the first remark in the previous page).

The conditions

$$H(P)\, Q\, s = \frac{\|s\|}{\|z\|} z \quad \text{and} \quad H(P)\, Q\, y = \frac{\|y\|}{\|x\|} x$$

imply that we have defined a unitary matrix U such that

$$(\dagger) \qquad U^H s = \frac{\|s\|}{\|z\|} z \quad \text{and} \quad U^H y = \frac{\|y\|}{\|x\|} x .$$

From $(U^H s)^H (U^H s) = \frac{\|s\|}{\|z\|} z^T \frac{\|y\|}{\|x\|} x = z^T x \frac{\|s\|}{\|z\|} \frac{\|y\|}{\|x\|}$

$= s^T U U^H y = s^T y$ we deduce

$$(**) \qquad \frac{z^T x}{\|z\| \cdot \|x\|} = \frac{s^T y}{\|s\| \cdot \|y\|}$$

(observe that $s^T y > 0 \iff z^T x > 0$).

The equality $(\dagger)$ implies

$$\frac{(U^H s)_i}{(U^H y)_i} = \frac{\|s\|}{\|z\|} \cdot \frac{\|x\|}{\|y\|} \frac{z_i}{x_i} ,$$

so we need only to prove the effective existence of $z, s \in \mathbb{R}^n$ such that $(**)$ holds with $z_i x_i > 0$.

Proof of the Theorem 11

$y_{k-1}^T s_{k-1}$ is a necessary condition for the existence of a unitary matrix U_k satisfying (*). In fact, if (*) holds, then $U_k d(W_k) U_k^H s_{k-1} = y_{k-1}$

and $s_{k-1}^T U_k d(W_k) U_k^H s_{k-1} = s_{k-1}^T y_{k-1} > 0$.

In order to prove that the condition $y_{k-1}^T s_{k-1} > 0$ implies the existence of U such that (*) holds we have to prove that, given two vectors s_{k-1} and y_{k-1}, we are able to define $u, x \in \mathbb{R}$ such that

$$\frac{u^T x}{\|u\| \cdot \|x\|} = \frac{s_{k-1}^T y_{k-1}}{\|s_{k-1}\| \cdot \|y_{k-1}\|} \equiv \sqrt{\beta_{k-1}},$$

with $u_i x_i > 0 \ \forall i$.

An example of u, x is the following:

$$x = [1 \ \varepsilon \ \cdots \ \varepsilon]^T, \quad u = [\varepsilon \ \cdots \ \varepsilon \ 1]^T,$$

EXERCISE 13

Verify that the previous equality, with the choice $x = [1 \ \varepsilon \ \cdots \ \varepsilon]^T$, $u = [\varepsilon \ \cdots \ \varepsilon \ 1]^T$, implies

$$\varepsilon = \varepsilon(\sqrt{\beta_{k-1}}) = \frac{\sqrt{\beta_{k-1}}}{1 + \sqrt{1 - \beta_{k-1}(n-1)} + \sqrt{\beta_{k-1}(n-2)}}$$

and that $\beta > 0$ when $s_{k-1}^T y_{k-1} > 0$.

Now we have proved that the matrix $H(p)Q = H(p)H(u)$ is precisely the matrix U_k^H that maps s_{k-1} and y_{k-1} into two vectors whose directions are the same of z and x, respectively. So, by the condition $x_i z_i > 0$, the ratio of the two transformed vectors has positive entries:

$$(w_k)_i = \frac{(U_k^H y_{k-1})_i}{(U_k^H s_{k-1})_i} = \frac{\|y_{k-1}\|}{\|s_{k-1}\|} \frac{\|z\|}{\|x\|} \frac{x_i}{z_i} > 0 \quad \forall i.$$

Note that if we define U_k^H as the product of two Householder matrices $H(p)$ and $H(u)$ (as above suggested), then the corresponding L-QN method can be implemented with only $O(n)$ arithmetic operations per step and $O(n)$ memory allocations. This result is a consequence of the double possible choice of d_{k+1}:

$$d_{k+1} = -\phi(U_k D(w_k) U_k^H, s_k, y_k)^{-1} g_{k+1}$$ (by applying the Sherman-Morrison formula)

or

$$d_{k+1} = -(\mathcal{L}_{sy}^{k+1})^{-1} g_{k+1}.$$

REMARK 1

An alternative L^kQN method can be obtained in order to regain the best least squares fit condition.
Let U_k be a unitary matrix satisfying the condition (*), so that the corresponding matrix algebra $\mathcal{L}^k$ includes a pd matrix $\mathcal{L}^k_{sy}$ solving the previous secant equation $X s_{k-1} = y_{k-1}$. Pick up in $\mathcal{L}^k$ the best approximation $\mathcal{L}^k_{B_k}$ in the Frobenius norm of B_k and apply ϕ to $\mathcal{L}^k_{B_k}$.
Then

$$B_{k+1} = \phi(\mathcal{L}^k_{B_k}, s_k, y_k)$$

Since

$$B_k \text{ pd} \Rightarrow \left.\begin{array}{l} \mathcal{L}^k_{B_k} \text{ pd} \\ s_k^T y_k > 0 \end{array}\right\} \Rightarrow B_{k+1} \text{ pd} \Rightarrow \mathcal{L}^{k+1}_{B_{k+1}} \text{ pd},$$

the latter definition of B_{k+1} leads to two possible descent directions:

$$d_{k+1} = \begin{cases} -B_{k+1}^{-1} g_{k+1} & S\ L^kQN \\ -\left(\mathcal{L}^{k+1}_{B_{k+1}}\right)^{-1} g_{k+1} & NS\ L^kQN. \end{cases}$$

By the theorem 8, if the NS L^kQN algorithm iterates $\{x_k\}$, defined with $\lambda_k \in (AG)_1, (AG)_2$ satisfy the condition $\frac{\|y_k\|^2}{y_k^T s_k} \le M$, then $\liminf_{k\to\infty} g_k = 0$.

REMARK 2

The technique for defining LQN and L^{k}QN algorithms recalls, in spirit, the distinction between structure and information content of a matrix (Bini, Capovani, 1983 and Fasino, Zellini, 1989). In the split

$$\mathcal{L} = U\, d(z)\, U^H,$$

U is the same unitary transform for all matrices A of $\mathcal{L}$ (i.e. $U \simeq$ structure), whereas z defines a particular matrix A in the space $\mathcal{L}$ ($z \simeq$ information content). The information content W_i in $\mathcal{L}^k_{B_k}$ (Remark 1), regains the correspondent information of B_k, whereas the structure defined by U_k reproduces the fundamental structure of secant methods.

The distribution of the eigenvalues of $\mathcal{L}_{B_k}$ (or $\mathcal{L}^k_{B_k}$) is strictly related to that of B_k. In particular, the following result holds (Tyrtyshnikov, 1992): If B is hermitian and $\mathcal{L}$ is a space of matrices simultaneously diagonalized by a unitary matrix $U_{\mathcal{L}}$ ($\mathcal{L} = SDU_{\mathcal{L}}$), then $\mathcal{L}_B$ is hermitian and,

$$\nu_1(B) + \dots + \nu_i(B) \le \nu_1(\mathcal{L}_B) + \dots + \nu_i(\mathcal{L}_B)$$

$$\nu_i(\mathcal{L}_B) + \dots + \nu_n(\mathcal{L}_B) \le \nu_i(B) + \dots + \nu_n(B)$$

where $\nu_i(X)$, $i = 1, \dots, n$ denote the eigenvalues of X in non decreasing order. For this reason, the search directions in LQN and L^{k}QN methods appears to be strictly related to optimization strategy of the BFGS method.

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