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ORTHOGONAL AND SCALING TRANSFORMATIONS OF QUADRATIC FUNCTIONS WITH SOME APPLICATIONS

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ABSTRACT: In this paper we present a non-singular transformation that can reduce a given quadratic function defined on $\mathbb{R}^n$ to another simpler quadratic function and study the impact of the transformation in relation to the problem of minimization of the function. In particular, we construct a non-singular transformation that can reduce a quadratic function whose level surfaces are ellipsoids to another quadratic function whose level surfaces are spherical while preserving the convexity/concavity property of the given function. The relation between a minimizing point of the given function and that of the new simpler function obtained under the transformation is also described.

Key words/phrases: Level surface, minimization, non-singular transformation, quadratic function

INTRODUCTION

Consider a quadratic function $f:\mathbb{R}^n \to \mathbb{R}$ given by

$$f(x) = x^T Ax - b^T x \text{ ………………………………….}\mathbf{(1)}$$

where A is an $n \times n$ real matrix and $b \in \mathbb{R}^n$. Without loss of generality we assume that A is symmetric. If this is not the case, then it can be converted to symmetric form by replacing A by $\frac{1}{2}(A + A^T)$ which does not change the value of $f(x)$.

Quadratic functions occur very often as the objective functions of various practical optimization problems. For example, objective functions in problems of minimization of energy, portfolio optimization, optimal engineering design, and least square problems are often quadratic functions of certain variables (see, for example, Kirsch, 1981; Flaudos and Visweswaran, 1995). They also frequently appear as the objective functions of sub-problems of various nonlinear programming problems that employ methods such as sequential quadratic programming and trust-region methods (Sorensen, 1982; Eldersveld, 1991; Nocedal and Wright, 1999). Various problems in Algebra, Functional Analysis, Analytic Geometry and Computational Mathematics also involve quadratic forms of the type $x^T Ax$ (see, for instance, Murtha and Willard, 1969; Taylor and Lay, 1980; Strang, 2006). It is clear, therefore, that quadratic functions have great importance, both from mathematical and application point of views.

There are several approaches that have been proposed for solutions of optimization problems that have quadratic objective functions (Frank and Wolfe, 1956; Beale, 1959; Lemeke, 1962; Goldstein, 1965; Cryer, 1971; Benveniste, 1979; Han *et al.*, 1992). The main source of difficulties for solutions and differences in approaches is the type of definiteness of the matrix *A* which determines the type of convexity of the function.

Though strictly convex functions are also convex, in this paper, whenever we say that a quadratic function $f(x)$ is convex, we particularly mean that the involved matrix A is positive semi-definite. The same should be understood also for a concave quadratic function.

From the viewpoint of solving a minimization problem on a given subset of $\mathbb{R}^n$, the problem is relatively the easiest when the quadratic function is strictly convex and the most difficult when the quadratic function is indefinite (Simmons, 1975; Kough, 1979). A survey of solution methods for minimization of various types of problems with quadratic objective functions can be found on the paper of Flaudos and Visweswaran, 1995. The common feature in most of the solution methods is that they rely on iterative procedures.

In most non optimization problems that involve a quadratic form (or quadratic function), it is usually advantageous to use a transformation that can reduce the quadratic form into a simpler form without altering an associated geometry of the problem. Principal axis transformation, Lagrange's reduction, and Kroneker's reduction are such useful transformations (Hohn, 1964). The most important of these transformations is probably diagonalization by means of an orthogonal transformation. It is well known that for every $n \times n$ symmetric real matrix A, there exists orthogonal matrix U such that

$$U^T AU = diag(\lambda_1, \lambda_2, \cdots, \lambda_n) \quad \text{……………………… (2)}$$

where $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the eigenvalues of A, each of which are real numbers, and the matrix U is formed by the normalized eigenvectors of A. That is,

$$U = [q_1, q_2, \cdots, q_n] \quad \text{……………………..……... (3)}$$

where its j - th column, q_j, is the normalized eigenvector of A corresponding to λ_j. Thus,

$Aq_j = \lambda_j q_j$,

$q_j^T q_j = 1$ for each j, and

$q_i^T q_j = 0$ when $i \neq j$.

As a consequence, the transformation

$x = Uy$,

applied to the quadratic function $f(x) = x^T Ax - b^T x$ gives

$$F(y) = \sum_{i=1}^{n} \lambda_i y_i^2 - b^T Uy \quad \text{……………..…………….(4)}$$

This provides a particularly simple form in many important problems and changes the orientation of reference axes without altering an associated level surface of $f(x)$. Here, by a level surface of f we mean the set $\{x \in \mathbb{R}^n \mid f(x) = c, \quad c \in \mathbb{R}\}$

Unfortunately, however, this transformation provides no simplification for optimization problems that involve quadratic objective functions. This is because iterative solution procedures for optimization problems are more influenced by the geometry of the level surfaces of objective functions than by the orientation of the reference axes. For instance, if we consider the steepest descent method in the case of a minimization problem, it is well known that the method experiences a slow convergence when the level surfaces of $f(x)$ are ellipsoids due to zigzagging of the steepest descent direction whether the objective function is in the form of (1) or (4). Furthermore, as the ellipsoid level surfaces of the quadratic function become more elongated, the zigzagging becomes more pronounced, and the steepest descent performs more poorly (Nocedal and Wright, 1999).

However, if the level surfaces of f are spheres in $\mathbb{R}^n$, then, just one step of the steepest descent procedure with exact line search provides the minimizing point of the function on $\mathbb{R}^n$ starting from any initial point (Nocedal and Wright, 1999). The level surfaces of f can have this nice geometry (sphere) when the n eigenvalues of A are all equal.

This simplicity with the solution procedure of minimization of a quadratic function whose level surfaces are spheres, has motivated the work in this paper. In particular, our aim is to construct a non-singular transformation that can reduce a quadratic function whose level surfaces are ellipsoids to another suitable quadratic function whose level surfaces are spheres. Furthermore, it is desirable to have an easy way of recovering a minimizing (or maximizing) point of the given quadratic function from that of the new simpler quadratic function that has been obtained under the transformation. This is also illustrated in this paper.

METHODS AND NOTATIONS

We consider that, in the general case, the matrix A that defines a given quadratic function on $\mathbb{R}^n$ has k positive, r negative, and m zero eigenvalues (counting multiplicities) where $k + r + m = n$

and, hence, rank (A) = $k+r \le n$. The method employed in this paper is analytic. In particular, for a quadratic function $f(x)$ given in (1), we construct a suitable non-singular linear transformation that reduces $f(x)$ to a simpler quadratic function whose all nonzero eigenvalues are absolutely equal (i.e., their absolute values are equal). In fact, we transform $f(x)$ to a new quadratic function $g(y)$ such that the associated eigenvalues of $g(y)$ are all

- 1 (with multiplicity n), if $f(x)$ is strictly convex;
- –1 (with multiplicity n), if $f(x)$ is strictly concave;
- 1 and 0 (with multiplicity k and m, respectively), if $f(x)$ is convex;
- –1 and 0 (with multiplicity r and m, respectively), if $f(x)$ is strictly concave;
- 1 and –1 (with multiplicity k and r, respectively), if rank (A) = n and $f(x)$ is indefinite;
- 1, –1 and 0 (with multiplicity k, r and m, respectively), if rank (A) < n and $f(x)$ is indefinite.

In order to have significance in optimization, the transformation should preserve the convexity/concavity property of $f(x)$ and the nature of its critical points. Thus, the design of our transformation takes this into account. We will also show that a minimizing point of $f(x)$ can be easily recovered from that of the new simpler quadratic function. Indeed, our discussion will focus only on minimization problems as a maximization problem is equivalent to a minimization problem.

For this purpose, we will construct a non-singular linear transformation using a product of two non-singular $n \times n$ matrices formed from the eigenvectors and eigenvalues of A. This involves an orthogonal transformation followed by scaling. The orthogonal transformation that forms part of the desired transformation is the usual orthogonal transformation given by the $n \times n$ orthogonal matrix U stated in (3) above. However, as discussed above, this does not produce a change on the geometry of the level surfaces other than rotating the coordinate axes to result in separation of variables which is, of course, desirable in many applications. In optimization, however, this alone has no significant role since the geometry of the level surfaces that have key influence on solution procedures still remains the same under the orthogonal transformation.

Therefore, in order to convert also the geometry of the level surfaces to a convenient form, we let the orthogonal transformation be accompanied by a suitable scaling that can shrink the elongation of ellipsoid level surfaces along the principal axes and convert them to the desired spherical surfaces. For this purpose, we use $n \times n$ diagonal matrix S, which we call scaling matrix of $f(x)$, given by

$$S = diag(s_{11}, s_{22}, \cdots, s_{nn}) \text{ ,……………...………} \textbf{(5)}$$

where, for each $j = 1,2,...,n,$ the j – th diagonal element s_{jj} is defined as follows:

$$s_{jj} = \begin{cases} \dfrac{1}{\sqrt{|\lambda_j|}}, & \text{if } \lambda_j \neq 0 \\ 1, & \text{if } \lambda_j = 0, \end{cases}$$

where, $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the eigenvalues of A. Note that $S^T = S$ and its inverse is obviously $S^{-1} = diag(1/s_{11}, 1/s_{22}, \cdots, 1/s_{nn})$. We will see that, the product of the two matrices, US, has the desired effect.

For convenience, we order the eigenvalues in such a way that all the positive terms appear first, followed by all the negative terms. Therefore, $\lambda_1, \lambda_2, \cdots, \lambda_k$ represent the k positive eigenvalues, $\lambda_{k+1}, \lambda_{k+2}, \cdots, \lambda_{k+r}$ represent the r negative eigenvalues, and $\lambda_{k+r+1}, \lambda_{k+r+2}, \cdots, \lambda_{k+r+m}$ represent the m zero eigenvalues of A. Of course, any one or two of $k, r,$ or m can be zero, depending on the type of definiteness of the matrix A.

We will use the following notations for subsets of the index set $\mathfrak{I} = \{1, 2, \cdots, n\}$:

$$\mathfrak{I}_{\mathrm{P}} = \{i \in \mathfrak{I} \mid \lambda_i > 0\} = \{1, 2, \cdots, k\},$$
$$\mathfrak{I}_{\mathrm{N}} = \{i \in \mathfrak{I} \mid \lambda_i < 0\} = \{k+1,\ k+2, \cdots, k+r\}, \text{ and}$$
$$\mathfrak{I}_{\mathrm{Z}} = \{i \in \mathfrak{I} \mid \lambda_i = 0\} = \{k+r+1,\ k+r+2, \cdots, k+r+m\}.$$

Again, any one or two of $\mathfrak{I}_{\mathrm{P}}$, $\mathfrak{I}_{\mathrm{N}}$ or $\mathfrak{I}_{\mathrm{Z}}$ can be empty depending upon whether A has positive, negative or zero eigenvalues or not.

RESULTS AND DISCUSSION

Let $f(x)$ be the quadratic function given in (1). That is, $f:\mathbb{R}^n \to \mathbb{R}$ such that

$$f(x) = x^T Ax - b^T x,$$

where A is an $n\times n$ symmetric real matrix and $b \in \mathbb{R}^n$. We consider the $n\times n$ orthogonal matrix U defined in (3) and the scaling matrix S defined in (5). Throughout this paper, we use the linear transformation $L:\mathbb{R}^n \to \mathbb{R}^n$ given by

$$L(y) = USy\,,$$

which will be expressed simply as $x = USy$. Since, the matrix US is non-singular, $(US)^{-1} = S^{-1}U^T$, the transformation is bijective. Hence, for any $x \in \mathbb{R}^n$ there is a unique $y \in \mathbb{R}^n$ such that

$$x = L(y) = USy\,,$$

and for any $y \in \mathbb{R}^n$ there is a unique $x \in \mathbb{R}^n$ such that

$$y = L^{-1}(x) = S^{-1}U^T x\,.$$

Theorem 1: Suppose the matrix A, given in the expression of $f(x)$, has k positive, r negative, and m zero eigenvalues. Then,

$$S(U^T AU)S = \tilde{I}_n\,,$$

where $\tilde{I}_n = diag(\underbrace{1,1,\cdots,1}_{k-terms},\ \underbrace{-1,-1,\cdots-1}_{r-terms},\ \underbrace{0,0,\cdots,0}_{m-terms})$.

That is, $\tilde{I}_n$ is $n\times n$ diagonal matrix with all the first k diagonal elements are 1, the next r diagonal elements are -1 and the last m diagonal elements are 0.

Proof: Since $U^T AU = diag(\lambda_1,\lambda_2,\cdots,\lambda_n)$ and also S is a diagonal matrix, the product $S(U^T AU)S$ is an $n\times n$ diagonal matrix. In particular,

$$S(U^T AU)S = diag(d_{11}, d_{22},\cdots, d_{nn})\,,$$

where $d_{jj} = \lambda_j s_{jj}^2$, for each $j = 1,2,\cdots n$. ……………………………….… **(6)**

Since, from the definition of S given in (5), $s_{jj} = 1/\sqrt{|\lambda_j|}$ if $\lambda_j \neq 0$ and $s_{jj} = 1$ when $\lambda_j = 0$, (6) becomes

$$d_{jj} = \lambda_j / |\lambda_j| = \begin{cases} 1, & \text{if } j \in \mathfrak{I}_{\mathrm{P}} = \{1, 2, \cdots, k\} \\ -1, & \text{if } j \in \mathfrak{I}_{\mathrm{N}} = \{k+1,\ k+2,\cdots, k+r\} \end{cases}$$

and, $d_{jj} = \lambda_j = 0$, for each $j \in \mathfrak{I}_{\mathrm{Z}} = \{k+r+1,\ k+r+2,\cdots,n\}$. Hence, we have

$$S\left(U^T AU\right)S = diag(\underbrace{1,1,\cdots,1}_{k-terms},\ \underbrace{-1,-1,\cdots-1}_{r-terms},\ \underbrace{0,0,\cdots,0}_{m-terms}).$$

Thus, the theorem is proved.

Note that rank $(\tilde{I}_n)$ = rank(A) since the number of nonzero diagonal elements of $\tilde{I}_n$ is equal to the number of nonzero eigenvalues of A.

Corollary 2: a. If A is positive definite, then

$$S(U^T AU)S = I_n\,,$$

b. If A is negative definite, then

$$S(U^T AU)S = -I_n\,,$$

where I_n is the $n\times n$ identity matrix.

Proof: If A is positive definite, then, in Theorem 1, we get $\tilde{I}_n = I_n$, since $\lambda_j > 0$ for all j =1,2, …,n, so that $k = n$, $r = 0 = m$. Similarly, If A is negative definite, then in Theorem 1, we get $\tilde{I}_n = -I_n$, since $\lambda_j < 0$ for all j =1,2, …,n. Hence, the proof is completed.

Theorem 3: Consider the quadratic function $f(x) = x^T Ax - b^T x$, defined in (1) above. If we use the non-singular transformation given by

$$x = USy, \quad \text{………………………………} \quad \textbf{(7)}$$

where U and S are as given in (2) and (5), respectively, then the quadratic function $f(x)$ becomes

$$g(y) = y^T \tilde{I}_n y - \bar{b}^T y = \sum_{i \in \mathfrak{I}_P} y_i^2 - \sum_{i \in \mathfrak{I}_N} y_i^2 - \bar{b}^T y, \quad \text{……..}\textbf{(8)}$$

where $\bar{b}^T = b^T US$, y_i is the i-th component of y, and $\tilde{I}_n$ is as given in Theorem 1.

Proof: Using the transformation (7) and Theorem 1 we get

$$\begin{aligned} x^T Ax &= (USy)^T A(USy) \\ &= y^T (SU^T AUS) y \\ &= y^T \tilde{I}_n y \\ &= \sum_{i \in \mathfrak{I}_P} y_i^2 - \sum_{i \in \mathfrak{I}_N} y_i^2 \quad \text{…………………………}\textbf{(9)} \end{aligned}$$

Moreover, since (7) implies $b^T x = b^T USy$, setting

$$\bar{b}^T = b^T US, \quad \text{…………………………………}\textbf{(10)}$$

we get $b^T x = \bar{b}^T y$. This, together with (9), gives us

$$x^T Ax - b^T x = y^T \tilde{I}_n y - \bar{b}^T y = \sum_{i \in \mathfrak{I}_P} y_i^2 - \sum_{i \in \mathfrak{I}_N} y_i^2 - \bar{b}^T y$$

Hence, the theorem is proved.
Noting that

$$\mathfrak{I}_P = \{i \in \mathfrak{I} \mid \lambda_i > 0\} = \{1, 2, \cdots, k\}, \quad \text{and}$$
$$\mathfrak{I}_N = \{i \in \mathfrak{I} \mid \lambda_i < 0\} = \{k+1, \ k+2, \cdots, k+r\},$$

we may express the new quadratic function $g(y)$ in (8) as

$$g(y) = \sum_{i=1}^{k} y_i^2 - \sum_{i=1}^{r} y_{k+i}^2 - \bar{b}^T y$$

Corollary 4: If the transformation of variables given by (7) is applied to the quadratic function $f(x) = x^T Ax - b^T x$, then $f(x)$ becomes

a. $g(y) = y^T I_n y - \bar{b}^T y = \sum_{i=1}^{n} y_i^2 - \bar{b}^T y$, if A is positive definite,

b. $g(y) = -y^T I_n y - \bar{b}^T y = -\sum_{i=1}^{n} y_i^2 - \bar{b}^T y$, if A is negative definite,

where $\bar{b}^T = b^T US$, and y_i is the i-th component of y.

The proof of Corollary 4 follows directly from Theorem 3 and Corollary 2. Note that, for the functions $g(y)$ given in Corollary 4(a) and (b), the level surfaces are spherical while the level surfaces of a strictly convex (or concave) function $f(x)$ are, in general, ellipsoids. Thus, the results in Corollary 4 show that the transformation converts ellipsoid level surfaces of a quadratic function to spherical level surfaces. The next theorem shows another useful property of the transformation: the transformation preserves the convexity property of a quadratic function.

Theorem 5: Consider a quadratic function $f(x)$ defined by (1) and the transformation $x = USy$ that transforms $f(x)$ to $g(y)$ as stated in Theorem 3. Then, the following hold:

a. If $f(x)$ is strictly convex, then $g(y)$ is strictly convex, too.
b. If $f(x)$ is convex, then $g(y)$ is convex, too.

Proof: **(a).** If $f(x)$ is strictly convex, i.e., A is positive definite, then by Corollary 4 (a)

$$g(y) = \sum_{i=1}^{n} y_i^2 - \bar{b}^T y,$$

which is obviously strictly convex, where $\bar{b}$ is as in (10).

(b). Suppose $f(x)$ is convex, i.e., A is positive semi-definite. In this case, $\mathfrak{I}_P$ ={1,2,…,k}, $\mathfrak{I}_N = \varnothing$ (so, r =0), $\mathfrak{I}_Z$ ={k+1, k+2,…,k+ m} ≠ ∅, and $k + m = n$. Hence, from (8) we get

$$g(y) = y^T \tilde{I}_n y - \bar{b}^T y = \sum_{i=1}^{k} y_i^2 - \bar{b}^T y$$

which is convex since, in this case, rank $(\tilde{I}_n) = k < n$.

Thus, the theorem is proved.

Analogously, the transformation preserves concavity property of $f(x)$. Furthermore, with similar argument, we can conclude that if $f(x)$ is indefinite so is $g(y)$. Now the question is: what if we minimize the simpler function $g(y)$ instead of the given function $f(x)$? In the next theorem, we show that a minimizing point of $f(x)$ can be easily recovered from that of $g(y)$. Indeed, we next show that if y^* is a minimizing point of $g(y)$, then $x^* = USy^*$ is a minimizing point of $f(x)$.

Theorem 6: Consider the quadratic function $f(x) = x^T Ax - b^T x$ and the transformation $x = USy$ that converts $f(x)$ to $g(y)$ as stated in Theorem 3. Then we have the followings:

a. $g(\bar{y}) = f(\bar{x})$ for every $\bar{y}, \bar{x} \in \mathbb{R}^n$ such that $\bar{x} = US\bar{y}$.

b. Given $M_x \subseteq \mathbb{R}^n$, suppose $M_y = \{ y \in \mathbb{R}^n \mid x = USy,\ x \in \mathbb{R}^n \}$. Then, $y^* \in M_y$ is a minimizer of $g(y)$ on M_y if and only if $x^* = USy^*$ is a minimizer of $f(x)$ on M_x.

Proof: **(a)** For any $\bar{y}, \bar{x} \in \mathbb{R}^n$ such that $\bar{x} = US\bar{y}$, we have

$$f(\bar{x}) = \bar{x}^T A\bar{x} - b^T\bar{x} = \bar{y}^T(SU^T AUS)\bar{y} - b^T US\bar{y} = g(\bar{y}).$$

Thus, (a) is true.

(b) Since the transformation is non-singular (bijective) on $\mathbb{R}^n$ and by the definition of M_y, for every $\bar{x}, \bar{y} \in \mathbb{R}^n$ such that $\bar{x} = US\bar{y}$, it holds that $\bar{x} \in M_x$ if and only if $\bar{y} \in M_y$.

Now suppose $y^* \in M_y$ is a minimizer of $g(y)$ on M_y and $x^* = USy^*$. Then,

$g(y^*) \le g(y)$ for all $y \in M_y$ ………………………… **(11)**

Next take arbitrary $\bar{x} \in M_x$ such that $\bar{x} \ne x^*$ (If there is no such $\bar{x}$, then x^* is obviously the minimizer of f on M_x). Since the transformation is bijective, there is $\bar{y} \in M_y$ such that $\bar{x} = US\bar{y}$ and $\bar{y} \ne y^*$. Now using Theorem 6(a) and (11) we have:

$$f(x^*) = g(y^*) \le g(\bar{y}) = f(\bar{x}).$$

Thus, since $\bar{x} \in M_x$ is arbitrary, $f(x^*) \le f(x)$ for all $x \in M_x$. That is, $x^* = USy^*$ is a minimizer of $f(x)$ on M_x.

Conversely, suppose $x^* \in M_x$ is a minimizer of $f(x)$ on M_x. That is,

$f(x^*) \le f(x)$ for all $x \in M_x$ ………………………(12)

We want to show that y^* is a minimizer of $g(y)$ on M_y where $y^* = S^{-1}U^T x^*$; *i.e.*, $x^* = USy^*$. To show this, with the same argument as for the case above, take arbitrary $\bar{y} \in M_y$ such that $\bar{y} \ne y^*$. Then, there is $\bar{x} \in M_x$ such that $\bar{x} = US\bar{y}$. Hence, using again Theorem 6 (a) and (12) we get

$$g(y^*) = f(x^*) \le f(\bar{x}) = g(\bar{y}).$$

Therefore, since $\bar{y} \in M_y$ is arbitrary, we conclude that $g(y^*) \le g(y)$ for all $y \in M_y$. That is, y^* is a minimizer of $g(y)$ on M_y where $x^* = USy^*$. This completes the proof of also part (b) of the theorem. Therefore, the theorem is proved.

Corollary 7 Consider the quadratic function $f(x) = x^T Ax - b^T x$ and the transformation $x = USy$ that converts $f(x)$ to $g(y)$ as stated in Theorem 3. Then, $y^* \in \mathbb{R}^n$ is a minimizing point of $g(y)$ on $\mathbb{R}^n$ if and only if $x^* = USy^*$ is a minimizing point of $f(x)$ on $\mathbb{R}^n$.

Note that Corollary 7 follows directly from Theorem 6, since, in Theorem 6 (b), $M_x = \mathbb{R}^n$ if and only if $M_y = \mathbb{R}^n$.

CONCLUSION

In this paper, we presented a non-singular linear transformation that can convert a quadratic function whose level surfaces are ellipsoids to a simpler quadratic function whose level surfaces are spherical. In particular, the transformation reduces any strictly convex quadratic function to another strictly convex, but simpler, quadratic function whose associated eigenvalues are all 1. Similarly, the transformation reduces any strictly concave quadratic function to another strictly concave quadratic function whose associated eigenvalues are all -1. It is also demonstrated that an extremum point of the given quadratic function can be easily recovered from that of the new simpler function obtained under the transformation. We hope that this approach is useful since it is significantly easier to find a minimizing point of a strictly convex function (or a maximizing point of a strictly concave function) using, say, the steepest descent (or ascent) method when all associated eigenvalues of the quadratic function are equal. It will be our next task to study the practical impact of this approach on quadratic programming problems as well as on the solution procedures of other general nonlinear programming problems.

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