

COMPLEX REPRESENTATION IN THE CONSTRUCTION OF ROTATABL DESIGNS¹

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0. Summary. Response surface techniques are discussed as a generalization of factorial designs, emphasizing the concept of rotatability. It is shown that the necessary and sufficient conditions for a configuration of sample points to be a rotatable arrangement of a specified order are greatly simplified if, in the case of two factors, the factor space is considered as the complex plane. A theorem giving these conditions is proved, with an application to the conditions governing the combination of circular rotatable arrangements into configurations possessing a higher order of rotatability. This is done by showing that certain coefficients must vanish in the "design equation" whose roots are the (complex) values of the various sample points. A method is presented by which any configuration of sample points (for example, some configuration fixed by extra-statistical conditions) may be completed into a rotatable design of the first order by the addition of only two properly chosen further sample points.

1. Introduction. Response surface techniques are a generalization of the well-known factorial principle of experimental design. Since the total set of treatments in the conventional factorial is the set of all combinations of the factors taken at fixed levels, the sample points form a rectangular lattice in the factor space (whose dimension is the number of factors). The physical law relating the response with the controllable factors may be represented by a k -dimensional surface (taking k as the number of factors) in the $(k + 1)$ -dimensional space defined by the factors and the response; this is known as a "response surface". The exploration of this response surface may often be performed more efficiently if the concept of the factorial design is extended to include any configuration of sample points whatever within the factor space.

The requirements of experimental design in the chemical industry led to the work of Box and Wilson in 1951 [2]. Their problem may be stated as follows: suppose the true response surface, expressed as a function of the k controllable factors x_1, x_2, \dots, x_k , is

$$(1.1) \quad \eta = \phi(x_1, x_2, \dots, x_k),$$

i.e., the true response at the u th sample point ($u = 1, 2, \dots, N$) is

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$$(1.2) \quad \eta_u = \phi(x_{1u}, x_{2u}, \dots, x_{ku}),$$

where x_{iu} is the value of the i th factor at the u th sample point. The observed response, y_u , varies about a mean of η_u , with a common variance of σ^2 for all values of u , these N errors being uncorrelated. It is required to find, with a minimum number of experiments, a maximum or minimum of the response surface (i.e., an optimum set of operating conditions) within a region of interest in the k -dimensional factor space, which is fixed by the experimental conditions.

It is assumed that the response surface may be represented within a given sub-region by its Taylor expansion to terms of order d , that is,

$$(1.3) \quad \eta = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_{11} x_1^2 + \dots + \beta_{12} x_1 x_2 + \dots + \beta_{111} x_1^3 \dots,$$

where, in the subscript of β , the number of times each factor-number appears is the appropriate power of that factor (and x_0 is conventionally defined as unity).

This problem has been further investigated by Box and Hunter in a recent paper [1]. The notation and terminology of the Box-Wilson paper are used, but the values of the x_{iu} are subject to the scaling conventions,

$$(1.4) \quad \sum_u x_{iu} = 0, \quad \sum_u x_{iu}^2 = N, \quad \text{for all } i.$$

They have obtained a general expression for the information given by a specified design at any point of the factor space, information being defined as the reciprocal of the variance of the predicted response at that point, and have considered the advantages of using "rotatable" designs, in which the information contours are hyperspheres centered at the origin of the k -dimensional sample space. This property is not possessed by the conventional factorial designs.

They have shown that the necessary and sufficient condition for the design to be rotatable of order d is that the generating function ϕ of the moments up to order $2d$, given by

$$(1.5) \quad Q = N^{-1} \sum_{u=1}^N (1 + t_1 x_{1u} + t_2 x_{2u} + \dots + t_k x_{ku})^{2d},$$

should be of the form

$$(1.6) \quad Q = \sum_{s=0}^d a_{2s} (t_1^2 + t_2^2 + \dots + t_k^2)^s,$$

where a_{2s} are constants independent of t_1, t_2, \dots, t_k . Denoting the moment

$$(1.7) \quad N^{-1} \sum_{u=1}^N x_{1u}^{\alpha_1} x_{2u}^{\alpha_2} \dots x_{ku}^{\alpha_k}$$

by $[1^{\alpha_1}, 2^{\alpha_2}, \dots, k^{\alpha_k}]$, they deduce by equating the coefficients $t_1^{\alpha_1} t_2^{\alpha_2} \dots t_k^{\alpha_k}$ in (1.5) and (1.6), that for rotatability of order d it is necessary and sufficient that

$$[1^{\alpha_1}, 2^{\alpha_2}, \dots, k^{\alpha_k}] = 0, \quad \text{if one or more } \alpha_i \text{ are odd,}$$

$$(1.8) \quad = \lambda_\alpha \frac{\prod_{i=1}^k \alpha_i!}{2^{\alpha/2} \prod_{i=1}^k (\frac{1}{2}\alpha_i)}, \quad \text{if all } \alpha_i \text{ are even,}$$

where $\alpha = \alpha_1 + \alpha_2 + \dots + \alpha_k \leq 2d$, and λ_α is a constant depending on α , but independent of the way in which α is partitioned into $\alpha_1, \alpha_2, \dots, \alpha_k$. Note that $\lambda_0 = 1$, since $x_0 = 1$, and $\lambda_2 = 1$ by the scaling convention. A distinction is made between an "arrangement" and a "design" of order d , the former being any configuration of sample points satisfying the necessary moment properties, and the latter being an arrangement which also permits estimation of the constants in the d th order model. Arrangements not having this property may, when properly chosen, be combined to form designs. In particular, any rotatable arrangement of the second order can be converted to a design by the addition of center points.

2. Conditions for rotatability in terms of complex variables. In Box and Hunter's paper referred to, necessary and sufficient conditions for rotatability are given in terms of real variables. If, however, the factor plane, whose coordinates (x and y) are the levels of the two factors, is considered as the complex plane, some interesting and useful results may be developed. In particular, we have the following theorem, which is valid for two-factor rotatable arrangements of any configuration whatever (not necessarily based on regular figures or circles) and for rotatability of any order.

THEOREM 1. *The necessary and sufficient condition that a two-factor arrangement, in which the u th sample point is specified by (x_u, y_u) , should be rotatable of order d is*

$$(2.1) \quad \sum_u z_u^{a-b} \bar{z}_u^b = 0,$$

for all integers a and b satisfying $0 < a \leq 2d, 0 \leq b < a/2$, where z is the complex variable $x + iy$ and \bar{z} is its complex conjugate $x - iy$.³

Now from the result of Box and Hunter quoted in Section 1, the necessary and sufficient conditions for the design to be rotatable of order d are that the moment generating function

$$(2.2) \quad Q = N^{-1} \sum_{u=1}^N (1 + t_1 x_u + t_2 y_u)^{2d},$$

should be expressible in the form

$$(2.3) \quad Q = \sum_{s=0}^d a_{2s} (t_1^2 + t_2^2)^s,$$

where the constants a_{2s} depend upon the design points, but are independent of t_1 and t_2 . Put

³ The present short proof was suggested by the referee. For an alternative see [4].

$$(2.4) \quad z_u = x_u + iy_u, \quad \bar{z}_u = \bar{x}_u - i\bar{y}_u,$$

$$(2.5) \quad r_u^2 = x_u^2 + y_u^2 = z_u \bar{z}_u, \quad z_u = r_u e^{i\theta_u}, \quad \bar{z}_u = r_u e^{-i\theta_u},$$

so that (r_u, θ_u) are the polar coordinates of the point (x, y) . Similarly put

$$(2.6) \quad t = t_1 + it_2, \quad \bar{t} = t_1 - it_2,$$

$$(2.7) \quad \rho^2 = t_1^2 + t_2^2 = t\bar{t}, \quad t = \rho e^{i\phi}, \quad \bar{t} = \rho e^{-i\phi},$$

so that (ρ, ϕ) are the polar coordinates of the point t_1, t_2 . Now

$$(2.8) \quad t\bar{z}_u + \bar{t}z_u = (t_1 + it_2)(x_u - iy_u) + (t_1 - it_2)(x_u + iy_u) \\ = t_1x_u + t_2y_u.$$

Hence from (2.2)

$$(2.9) \quad Q = N^{-1} \sum_{u=1}^N \left[1 + \sum_{a=1}^{2d} \binom{2d}{a} (t\bar{z}_u + \bar{t}z_u)^a \right] \\ = 1 + \sum_{u=1}^N \sum_{a=1}^{2d} \left[\binom{2d}{a} \sum_{b+c=a} \binom{a}{b} t^b \bar{t}^c z_u^b \bar{z}_u^c \right] \\ = 1 + \sum_{a=1}^{2d} \left[\rho^a \sum_{b+c=a} \left(m_{b,c} e^{i(b-c)\phi} \sum_{u=1}^N \bar{z}_u^b z_u^c \right) \right],$$

where

$$(2.10) \quad m_{b,c} = \frac{2d!}{(2d - b - c)! b! c!}.$$

Again from (2.3) and (2.7)

$$(2.11) \quad Q = \sum_{s=0}^d a_{2s} \rho^{2s}.$$

Since the constants a_{2s} do not depend on t_1 and t_2 and are therefore independent of ϕ , one sees by comparing (2.9) and (2.11) that the necessary and sufficient condition for rotatability of order d is that the quantity

$$(2.12) \quad \sum_{b+c=a} m_{b,c} e^{i(b-c)\phi} \sum_{u=1}^N \bar{z}_u^b z_u^c,$$

is independent of the arbitrary angle ϕ . This is satisfied if and only if

$$(2.13) \quad \sum_{u=1}^N z_u^c \bar{z}_u^b = 0, \quad \text{unless } b = c, \quad (0 < b + c = a \leq 2d),$$

and this is precisely what Theorem 1 states.

3. The design equation. We now combine the results of the preceding section with a consideration of the elementary symmetric functions of the roots of an equation by which the design is specified. For any two-factor arrangement whatever of N sample points, whose locations in the complex factor plane are

given by z_1, z_2, \dots, z_N , the design equation is defined as that equation having these values as roots. Thus this equation may be written

$$(3.1) \quad 0 = (z - z_1)(z - z_2) \cdots (z - z_N) \\ = z^N + p_1 z^{N-1} + p_2 z^{N-2} + \cdots + p_{N-1} z + p_N.$$

The relation between the coefficients, p_u , in this equation, and the sums of the powers of its roots, $s_m = \sum_u z_u^m$, is given by Waring's formulas [3],

$$(3.2) \quad s_m = \sum (-1)^t \frac{m(t-1)!}{\prod_u t_u!} \prod_u p_u^{t_u}, \quad (u = 1, 2, \dots, N),$$

where $t = \sum_u t_u$ and the summation is over all sets of non-negative integers (t_1, t_2, \dots, t_N) such that $\sum_u u t_u = m$. Conversely,

$$(3.3) \quad p_m = \sum (-1)^q \frac{1}{\prod_v q_v! v^{q_v}} \prod_v s_v^{q_v} \quad (v = 1, 2, \dots, m),$$

where $q = \sum_v q_v$ and the summation is over all sets of non-negative integers (q_1, q_2, \dots, q_m) such that $\sum_v v q_v = m$. Alternatively, these quantities may be calculated by means of Newton's recursion,

$$(3.4) \quad s_m + p_1 s_{m-1} + p_2 s_{m-2} + \cdots + p_{m-1} s_1 + p_m m = 0, \quad m < N; \\ s_m + p_1 s_{m-1} + p_2 s_{m-2} + \cdots + p_N s_{m-N} = 0, \quad m \geq N.$$

Now by Theorem 1 the necessary and sufficient conditions for any rotatable design of the first order are

$$(3.5) \quad s_1 = \sum_u z_u = 0, \quad s_2 = \sum_u z_u^2 = 0.$$

From the formulas above, we have

$$(3.6) \quad p_1 = -s_1, \quad p_2 = (1/2)(s_1^2 - s_2).$$

Hence for any first-order rotatable design, both of these coefficients vanish, and the design equation is of the form

$$(3.7) \quad z^N + p_3 z^{N-3} + p_4 z^{N-4} + \cdots + p_{N-1} z + p_N = 0,$$

the first two powers of z below the highest power being absent.

This may be generalized to a rotatable arrangement of any order, d , as follows. By Theorem 1 all the sums of powers of z_u , up to order $2d$, vanish; that is, s_1, s_2, \dots, s_{2d} are all equal to zero. But (3.3) gives an expression for p_m explicitly as a polynomial in s_1, s_2, \dots, s_m . Thus p_1, p_2, \dots, p_{2d} are also all equal to zero, and we have

THEOREM 2. *A necessary condition that an arrangement be rotatable of order d is that the first $2d$ terms after the initial term in the design equation be equal to zero.*

N.B. Now when $d = 1$, as shown above, this condition is also sufficient, but,

for greater values of d , the summations involving the complex conjugate must be considered also. At this point, the importance of the circular arrangement will become apparent.

4. Rotatable circular arrangements. The arrangement formed by the N points z_1, z_2, \dots, z_N of the complex factor plane, may be called a circular arrangement if the N points lie on a circle with the origin as center. If the points also form a rotatable arrangement of order d , i.e., satisfy the moment conditions for rotatability of order d , then they may be said to form a rotatable circular arrangement of order d . We shall now prove

THEOREM 3. If the points z_1, z_2, \dots, z_N form a circular arrangement, then the necessary and sufficient conditions for them to form a rotatable circular arrangement of order d are

$$(4.1) \quad \sum_u z_u^a = 0, \quad \text{for } 0 < a \leq 2d.$$

Let r be the radius of the circle on which z_1, z_2, \dots, z_N lie. Then

$$(4.2) \quad z_u \bar{z}_u = r^2, \quad u = 1, 2, \dots, n.$$

Let a and b be integers satisfying

$$(4.3) \quad 0 < a \leq 2d, \quad 0 \leq b < a/2.$$

Then

$$(4.4) \quad \sum_u z_u^{a-b} \bar{z}_u^b = r^{2b} \sum_u z_u^{a-2b}.$$

It follows from Theorem 1, that conditions (4.1) are necessary and sufficient for a circular arrangement to be rotatable of order d , which proves Theorem 3.

Let (3.1) be the design equation of a circular arrangement. It follows from what has been shown in Section 3, that the conditions (4.1) are equivalent to $p_1 = p_2 = \dots = p_d = 0$.

Hence Theorem 3 may be stated in the alternative form

THEOREM 3A. *If N points form a circular arrangement then the necessary and sufficient conditions for them to form a rotatable circular arrangement of order d are that the first $2d$ terms after the initial term in the design equation be equal to zero.*

Suppose we combine g rotatable arrangements each of order not less than $d - 1$, where the points of the w th arrangement are

$$(4.5) \quad z_{w1}, z_{w2}, \dots, z_{wN_w}, \quad w = 1, 2, \dots, g.$$

Then by Theorem 1 we have

$$(4.6) \quad \sum_w \sum_u z_{wu}^{a-b} \bar{z}_{wu}^b = 0, \quad a = 1, 2, \dots, 2(d - 1), 0 \leq b < a/2,$$

that is, the combined arrangement satisfies the conditions for rotatability up to order $d - 1$. In order that this combined arrangement shall be a rotatable

arrangement of order d , the radii and relative orientations of the component arrangements must be adjusted so as to satisfy the remaining conditions,

$$(4.7) \quad \sum_w \sum_u z_w^{a-b} \bar{z}_{wu}^b = 0, \quad a = 2d - 1, 2d; b = 0, 1, \dots, d - 1.$$

These remaining conditions may also be written

$$(4.8) \quad \sum_w \sum_u (z_w \bar{z}_{wu})^b z_w^c = 0,$$

where $c = a - 2b$ and has the values $1, 2, \dots, 2d - 2, 2d - 1, 2d$. Now if the component rotatable arrangements are also circular arrangements, the quantity $z_w \bar{z}_{wu}$ is constant for any fixed w , and $u = 1, 2, \dots, N_w$. Let $z_w \bar{z}_{wu} = r^2$. Then (4.8) may be written as

$$(4.9) \quad \sum_w [r_w^{2b} \sum_u z_w^c] = 0.$$

But by (4.6) these conditions are already satisfied for $c = 1, 2, \dots, 2d - 2$. Hence the only further conditions are

$$(4.10) \quad \sum_w \sum_u z_w^{2d-1} = 0, \quad \sum_w \sum_u z_w^{2d} = 0.$$

Combining this result with Theorem 2 we have:

THEOREM 4. *If a number of circular rotatable arrangements of order not less than $d - 1$ are combined together, the necessary and sufficient condition that the resulting arrangement be a rotatable arrangement of order d is that the first $2d$ terms after the initial term in the design equation be equal to zero.*

5. Combination of first order rotatable circular designs. We can use Theorem 4 for obtaining rotatable arrangements of the second order by combining suitable rotatable circular arrangements of the first order. Box and Hunter [1] have shown that the points of a regular n -gon with center at the origin constitute a rotatable arrangement of the d th order if and only if $n \geq 2d + 1$. Thus points of an equilateral triangle or a square (inscribed in circle with the center at origin) constitute a rotatable arrangement of the first order but not of the second. However we can combine equilateral triangles or squares to form rotatable arrangements of second order.

Suppose, for example, that we wish to combine m equilateral triangles (each of which is a rotatable circular arrangement of the first order) in such a way that the combination is a rotatable arrangement of the second order. The design equation of the w th equilateral triangle ($w = 1, 2, \dots, m$) is

$$(5.1) \quad z^3 - a_w = 0.$$

The design equation for the combined arrangement is

$$(5.2) \quad (z^3 - a_1) (z^3 - a_2) \dots (z^3 - a_m) = 0,$$

which may be written

$$(5.3) \quad z^{3m} - (a_1 + a_2 + \cdots + a_m)z^{3m-3} + (a_1a_2 + a_1a_3 + \cdots + a_{m-1}a_m)z^{3m-6} - \cdots + (-1)^m a_1a_2 \cdots a_m = 0.$$

It follows from Theorem 4, that for the combined arrangement to be rotatable of the second order, we require only that

$$(5.4) \quad a_1 + a_2 + \cdots + a_m = 0.$$

For instance, if $m = 2$, we have $a_1 = -a_2$, and thus the triangles must form a regular hexagon.

Similarly, if we combine m squares, the m th square having the design equation,

$$(5.5) \quad z^4 - a_w = 0,$$

the design equation for the combined arrangement is

$$(5.6) \quad z^{4m} - (a_1 + a_2 + \cdots + a_m)z^{4m-4} + (a_1a_2 + a_1a_3 + \cdots + a_{m-1}a_m)z^{4m-8} - \cdots + (-1)^m a_1a_2 \cdots a_m = 0.$$

As before, for a rotatable arrangement of the second order, we require only that

$$(5.7) \quad a_1 + a_2 + \cdots + a_m = 0.$$

Thus, to any $m - 1$ squares we can always add the square whose design equation is

$$(5.8) \quad z^4 + (a_1 + a_2 + \cdots + a_{m-1}) = 0,$$

in order to make a rotatable arrangement of the second order.

Since the moments of a rotatable arrangement must equal those of a spherical distribution [1], previous work in this field has concentrated on arrangements in which the sample points are equally spaced on the surface of a hypersphere (or combinations of such arrangements). Thus in the case of two factors only regular polygons have been used. One of the authors [4] has by using an iterative process calculated a table of circular rotatable arrangements of the first order each with seven points, not situated at the vertices of a regular heptagon. It is hoped to publish the details of the computational procedure and the table of designs as a separate paper. We shall now show how these arrangements may be used as building blocks for second order rotatable arrangements.

Let the design equations of the three arbitrarily selected seven-point designs be

$$(5.9) \quad \begin{aligned} z^7 + p_{13}z^4 + p_{14}z^3 + \cdots + p_{17} &= 0, \\ z^7 + p_{23}z^4 + p_{24}z^3 + \cdots + p_{27} &= 0, \\ z^7 + p_{33}z^4 + p_{34}z^3 + \cdots + p_{37} &= 0, \end{aligned}$$

where the terms in z^6 and z^5 are absent, in virtue of Theorem 2. These designs, as tabulated, have a unit radius and one sample point on the positive x -axis. In order to combine them in such a way that the resulting arrangements is second-order rotatable, we must change the radii to r_1 , r_2 , and r_3 , and rotate

the designs through the angles ϕ_1, ϕ_2 , and ϕ_3 respectively. We define the complex variables:

$$\begin{aligned}
 (5.10) \quad v_1 &= r_1(\cos \phi_1 + i \sin \phi_1), \\
 v_2 &= r_2(\cos \phi_2 + i \sin \phi_2), \\
 v_3 &= r_3(\cos \phi_3 + i \sin \phi_3).
 \end{aligned}$$

Thus the required transformation is equivalent to multiplying the roots of the design equations by v_1, v_2 , and v_3 respectively, and the design equations for the transformed designs are

$$\begin{aligned}
 (5.11) \quad z^7 + p_{13}v_1^3z^4 + p_{14}v_1^4z^3 + \dots + p_{17}v_1^7 &= 0, \\
 z^7 + p_{23}v_2^3z^4 + p_{24}v_2^4z^3 + \dots + p_{27}v_2^7 &= 0, \\
 z^7 + p_{33}v_3^3z^4 + p_{34}v_3^4z^3 + \dots + p_{37}v_3^7 &= 0.
 \end{aligned}$$

The design equation for the combined arrangement of transformed designs is the product of these three equations,

$$\begin{aligned}
 (5.12) \quad z^{21} + (p_{13}v_1^3 + p_{23}v_2^3 + p_{33}v_3^3)z^{18} \\
 + (p_{14}v_1^4 + p_{24}v_2^4 + p_{34}v_3^4)z^{17} + \dots + p_{17}p_{27}p_{37}v_1^7v_2^7v_3^7 = 0.
 \end{aligned}$$

But, by Theorem 4, in order for the combined arrangement to be rotatable of the second order, the terms in z^{18} and z^{17} must vanish. Thus the transformations must be such as to satisfy the equations

$$\begin{aligned}
 (5.13) \quad p_{13}v_1^3 + p_{23}v_2^3 + p_{33}v_3^3 &= 0, \\
 p_{14}v_1^4 + p_{24}v_2^4 + p_{34}v_3^4 &= 0.
 \end{aligned}$$

These equations may be written

$$\begin{aligned}
 (5.14) \quad p_{33}^4v_3^{12} &= (p_{13}v_1^3 + p_{23}v_2^3)^4, \\
 p_{34}^3v_3^{12} &= -(p_{14}v_1^4 + p_{24}v_2^4),
 \end{aligned}$$

or, eliminating v_3 from between them,

$$(5.15) \quad (P_{11}v_1^3 + P_{12}v_2^3)^4 = -(P_{21}v_1^4 + P_{22}v_2^4)^3,$$

where $P_{11} = p_{13}/p_{33}, P_{12} = p_{23}/p_{33}, P_{21} = p_{14}/p_{34}$, and $P_{22} = p_{24}/p_{34}$. The transformations corresponding to the values of v_1 and v_2 which satisfy this equation will yield a rotatable arrangement of the second order; without loss of generality, v_3 may be taken as unity.

6. Completion of designs. It frequently occurs in experimental practice that sample points cannot easily be taken in accordance with a prescribed design, but must rather be taken at locations dictated by the experimental conditions. Again, the statistician is often faced with the problem of analyzing data collected in a manner over which he has had no control. In such cases, it is of importance

to consider applications of the methods of Section 3 to the specification of a few additional sample points which, combined with those already utilized, will result in a rotatable arrangement (thereby providing circular information contours).

For example, suppose that N observations have been made at the points $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$. It will be shown that we may complete this configuration into a rotatable design of the first order by taking observations at two more points, (x_a, y_a) and (x_b, y_b) . We define

$$(6.1) \quad A = \sum_u (x_u + iy_u) = \sum_u z_u, \quad B = \sum_u (x_u + iy_u)^2 = \sum_u z_u^2,$$

where $u = 1, \dots, N$. Since in the final (first-order rotatable) design we must have, by Theorem 1,

$$(6.2) \quad \sum_v z_v = 0, \quad \sum_v z_v^2 = 0, \quad (v = 1, 2, \dots, N, a, b),$$

we set $-A = z_a + z_b$, $-B = z_a^2 + z_b^2$. Thus we have:

$$(6.3) \quad z_a z_b = (1/2)(A^2 + B).$$

Hence z_a and z_b are the complex roots of the equation

$$(6.4) \quad z^2 + Az + (1/2)(A^2 + B) = 0.$$

(If the roots are equal, two observations are made at the corresponding sample point.)

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