CONFIDENCE REGION FOR A LINEAR RELATION

By C. Villegas

Instituto de Matemática y Estadística, Montevideo

1. Summary. The analysis of a linear relation is considered, when there are replications and all the variables involved are subject to errors or fluctuations. A test based on the F distribution is derived for testing the hypothesis that the unknown relation is a given linear relation. From this test a joint confidence region for the coefficients of the linear relation is derived. A confidence region for the linear relation is then defined as the set of all points which belong to hyperplanes not rejected by the test. The corresponding confidence coefficient is not known exactly, but it is known to be greater than a previously chosen P. In the non-degenerate case, the confidence region is a hyperboloid centered at the centroid of the given points, and it has the property that a hyperplane is not rejected by the test if and only if it is entirely contained in it. This confidence region estimation procedure is compatible with the maximum likelihood estimation of a linear relation, in the sense that the maximum likelihood hyperplane is contained in the confidence region for the linear relation, if this region is not empty.

2. Introduction. The problem of finding confidence regions for the parameters of a linear relation when all the variables are subject to error or fluctuations has been considered recently by several authors. Thus, under the usual normal theory assumptions, confidence regions have been derived by Wald (1940) and Bartlett (1949) using the method of grouping; by Creasy (1956) assuming the ratio of error variances is known a priori; and by Geary (1949) and Halperin (1961) using instrumental variables or a priori weights. Moreover, confidence intervals based on non-parametric methods have been given by Hemelrijk (1949) and Theil (1950).

In experimental work it is usually possible to replicate the observations. Replicated experiments can be analyzed without great difficulties, because we can easily derive from them valid estimates of the experimental error. However, none of the above mentioned authors considered replicated experiments in a systematic manner; rather, they considered the models with replication only as special cases of more general models. If no a priori knowledge about the ratio of the error variances is assumed, the confidence regions obtained in this way for the model with replications, using normal theory methods, are confidence regions based on a priori weights. Clearly confidence regions based on a priori weights are not the ideal confidence regions which we should try to find. Moreover, such confidence region procedures are not compatible with the maximum likelihood estimator of the linear relation, in the sense that in particular cases

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the maximum likelihood estimate may be outside the corresponding confidence region.

3. Notation and model. Let

$$\alpha + \beta_1 x^1 + \cdots + \beta_p x^p = 0 \tag{3.1}$$

be an unknown linear relation among the variables $x^1, \cdots, x^p$. Superscripts will, in general, be indexing symbols, not powers, in this paper. We shall assume that the observed values do not satisfy (3.1) because all of them are subject to errors or fluctuations. In matrix notation the linear relation is simply

$$\alpha + \boldsymbol{\beta}\mathbf{x} = 0, \tag{3.2}$$

where $\boldsymbol{\beta}$ is the row vector $(\beta_1, \cdots, \beta_p)$ and, if the prime over a matrix denotes transposition, $\mathbf{x}$ is the column vector $(x^1, \cdots, x^p)'$. Assume that we have q treatments corresponding to q points $\boldsymbol{\xi}_i$ on the hyperplane (3.2), and that, for the treatment i we have n_i observed points

$$\mathbf{x}_{ij} = \boldsymbol{\xi}_i + \boldsymbol{\varepsilon}_{ij} \qquad (i = 1, \cdots, q; j = 1, \cdots, n_i) \tag{3.3}$$

where $\boldsymbol{\xi}_i$ is a column vector of p components which satisfies the linear relation (3.2), and the errors or fluctuations $\boldsymbol{\varepsilon}_{ij}$ are column vectors with p components which are independent and have a normal distribution with zero mean and covariance matrix $\boldsymbol{\Sigma}$. Let $n = \sum n_i$ be the total number of observed vectors and let

$$\mathbf{x}_i = n_i^{-1} \sum_{j=1}^{n_i} \mathbf{x}_{ij} \tag{3.4}$$

be the average of all the observed vectors corresponding to the treatment i. Then the sample covariance matrix is

$$\mathbf{S} = (n - q)^{-1} \sum_{ij} (\mathbf{x}_{ij} - \mathbf{x}_i)(\mathbf{x}_{ij} - \mathbf{x}_i)'. \tag{3.5}$$

In this paper we shall assume also that $n - q \geqq p$. This last assumption assures us that $\mathbf{S}$ is, with probability 1, a positive definite matrix and has the Wishart distribution with mean value $\boldsymbol{\Sigma}$ and $\nu = n - q$ degrees of freedom.

4. Joint confidence region for the coefficients α, $\boldsymbol{\beta}$. Consider the hypothesis H: $\alpha = \mathrm{A}$, $\boldsymbol{\beta} = \mathbf{B}$, where A is a number and $\mathbf{B}$ is a row vector with q components. Under the hypothesis H, the true hyperplane is the hyperplane

$$A + \mathbf{B}\mathbf{x} = 0. \tag{4.1}$$

Consider the distances

$$d_i = (A + \mathbf{B}\mathbf{x}_i)/\|\mathbf{B}\| \tag{4.2}$$

from the points $\mathbf{x}_i$ to the hyperplane (4.1). Obviously, under the hypothesis H, the random variables d_i are independently and normally distributed with mean values equal to zero. The variance of d_i is equal to

$$\sigma_i^2 = \sigma^2/n_i, \tag{4.3}$$

where

$$\sigma^2 = \mathbf{B\Sigma B}'/\|\mathbf{B}\|^2. \tag{4.4}$$

An unbiased estimator of σ^2 is obviously

$$s^2 = \mathbf{BSB}'/\|\mathbf{B}\|^2, \tag{4.5}$$

where $\mathbf{S}$ is the sample covariance matrix (3.5). Note that $\mathbf{S} = \nu^{-1} \sum \mathbf{z}_j\mathbf{z}_j'$, where the $\mathbf{z}_j$ are ν column vectors, independently and normally distributed, with mean value 0 and covariance matrix $\mathbf{\Sigma}$. Hence, $s^2 = \nu^{-1} \sum v_j^2$, where $v_j = \mathbf{Bz}_j/\|\mathbf{B}\|$ are independent random variables, normally distributed with mean value 0 and variance σ^2. If $\nu < p$, there are always non null vectors $\mathbf{B}$ such that $\mathbf{Bz}_j = 0$ for all j, and for such vectors $\mathbf{B}$, we have $s^2 = 0$, which implies that $\mathbf{S}$ is a singular matrix. In what follows, therefore, we shall assume that $\nu \geqq p$, in which case, with probability 1, $\mathbf{S}$ is a positive definite matrix and $s^2 > 0$. Note that, if $q \geqq p$ and $n_i \geqq 2$ for every i, the condition $\nu \geqq p$ is satisfied.

Clearly, the quotient $q^{-1} \sum n_i d_i^2/s^2$ has then an F-distribution with q and ν degrees of freedom, and an F-test of the hypothesis H can be derived in the usual way. More precisely, we shall not reject the hypothesis H, at the level of significance P, if

$$\sum n_i(A + \mathbf{Bx}_i)^2/\mathbf{BSB}' \leqq qF, \tag{4.6}$$

where F is the $(1 - P)$-point of the F-distribution with q and ν degrees of freedom.

The set of values of A, $\mathbf{B}$ which satisfy this inequality is a confidence region for the coefficients α, $\boldsymbol{\beta}$ with confidence coefficient P. Since the left hand member of (4.6) is obtained from the expression (3.8) of [8] by substitution of $\mathbf{S}$ for $\mathbf{\Sigma}$, it follows that the values of A, $\mathbf{B}$ which minimize the left hand member of (4.6) are the maximum likelihood estimates $\hat{\alpha}$, $\hat{\boldsymbol{\beta}}$. Therefore, the confidence region for α, $\boldsymbol{\beta}$ is compatible with the maximum likelihood estimates $\hat{\alpha}$, $\hat{\boldsymbol{\beta}}$ in the sense that if it is not empty, it contains them. The sum of products for treatments matrix is

$$(\mathbf{SP}) = \sum n_i(\mathbf{x}_i - \mathbf{x}.)(\mathbf{x}_i - \mathbf{x}.)', \tag{4.7}$$

where $\mathbf{x}.$ is the centroid of the points $\mathbf{x}_i$ with weights n_i. Then, the condition (4.6) can be written also as

$$(A + \mathbf{Bx}.)^2 + \mathbf{BMB}' \leqq 0, \tag{4.8}$$

where

$$\mathbf{M} = [(\mathbf{SP}) - qF\mathbf{S}]/n. \tag{4.9}$$

It is clear that (4.6) or, equivalently (4.8), do not provide limits for the $p + 1$ coefficients of the linear relation (3.1) but only for the ratios of p of them with respect to a $(p + 1)$th; it is also clear that this is all one really requires. Similarly, as was pointed out in [8], the maximum likelihood estimators $\hat{\alpha}$, $\hat{\boldsymbol{\beta}}$ are also determined up to a scale factor.

5. Confidence region for a linear relation. We shall say that a region in the p-dimensional space is a confidence region for a linear relation, with confidence coefficient greater than P, if it covers the true hyperplane with a probability greater than P. Let R be the set of all points $\mathbf{x}$ in p-dimensional space which belong to hyperplanes which are not rejected by the F-test at a given level of significance $1 - P$. Clearly R is a confidence region for the linear relation with confidence coefficient greater than P, because it covers the true hyperplane each time that it is not rejected by the F-test, which happens with probability P, but it may cover also the true hyperplane even if it is rejected by the F-test, as will be seen more clearly later. Moreover, since the maximum likelihood coefficients minimize the left hand member of (4.6), it follows that, if the confidence region is not empty, then it contains the maximum likelihood hyperplane.

THEOREM 1. (i) *If the proper values of the matrix* $\mathbf{M}$ *are all positive, then the confidence region* R *is empty.*

(ii) *If all the proper values of* $\mathbf{M}$ *are positive with the only exception of one which is equal to zero, or one which is negative, then the confidence region is, respectively, the maximum likelihood hyperplane or the hyperboloid*

$$(\mathbf{x} - \mathbf{x}.)'\mathbf{M}^{-1}(\mathbf{x} - \mathbf{x}.) + 1 \geqq 0. \tag{5.1}$$

(iii) *If two or more of the proper values of* $\mathbf{M}$ *are negative or equal to zero, then the confidence region is all the space.*

PROOF. Let $\mathbf{x} \in R$, and let A, $\mathbf{B}$ be solutions of (4.8) such that $A + \mathbf{Bx} = 0$. By substitution of $A = -\mathbf{Bx}$ in (4.8) we get

$$\mathbf{B}[\mathbf{M} + (\mathbf{x} - \mathbf{x}.)(\mathbf{x} - \mathbf{x}.)']\mathbf{B}' \leqq 0. \tag{5.2}$$

The set R is therefore the set of all points $\mathbf{x}$ such that the matrix $\mathbf{M} + (\mathbf{x} - \mathbf{x}.)(\mathbf{x} - \mathbf{x}.)'$ is not a positive definite matrix. Since $\mathbf{M}$ is a real, symmetric matrix, there is an orthogonal matrix $\mathbf{U}$ such that $\mathbf{UMU}'$ is a diagonal matrix, whose diagonal elements are the proper values $m_1, \cdots, m_p$ of $\mathbf{M}$. Consider the change of variables

$$\mathbf{y} = \mathbf{U}(\mathbf{x} - \mathbf{x}.).$$

Then, in the new variables, the region R is the set of all points $\mathbf{y}$ such that the matrix $\mathbf{UMU}' + \mathbf{yy}'$ is not a positive definite matrix. Equivalently, R is the set of all points $\mathbf{y} = (y_1, \cdots, y_p)'$ such that the determinant

$$D = \begin{vmatrix} 1 & -y_1 & -y_2 & \cdots & -y_p \\ y_1 & m_1 - \lambda & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ y_p & 0 & 0 & \cdots & m_p - \lambda \end{vmatrix}$$

vanishes for some $\lambda \leqq 0$. If we develop this determinant by the first row, we have

$$D = (m_2 - \lambda) \cdots (m_p - \lambda)y_1^2 + \cdots \\ + (m_1 - \lambda) \cdots (m_{p-1} - \lambda)y_p^2 + (m_1 - \lambda) \cdots (m_p - \lambda). \tag{5.3}$$

Assume that the m_i have been numbered in such a way that $m_1 \geqq \cdots \geqq m_p$. We have several cases to consider.

(a) Assume that all the proper values are positive. Then, for any point $\mathbf{y}$, and for any $\lambda \leqq 0$, we have $D > 0$. Consequently, the region R is empty.

(b) Consider the case $m_p = 0$, $m_{p-1} > 0$. Then, if $\lambda < 0$, we have $m_h - \lambda > 0$ for all h and therefore there is no solution $\mathbf{y}$. If $\lambda = 0$, then we have simply $D = m_1 \cdots m_{p-1}y_p^2$, and therefore the region is the hyperplane $y_p = 0$.

(c) Consider the case $m_p \leqq m_{p-1} \leqq 0$. If $m_p = m_{p-1}$, the equation $D = 0$ with $\lambda = m_p = m_{p-1}$ is verified for any $\mathbf{y}$, and therefore the region is all the space. If, on the contrary, $m_p < m_{p-1}$, for any λ such that $m_p < \lambda < m_{p-1}$, the differences $m_h - \lambda$ will all be different from zero and the equation $D = 0$ can be written as

$$\frac{y_1^2}{m_1 - \lambda} + \cdots + \frac{y_{p-1}^2}{m_{p-1} - \lambda} + \frac{y_p^2}{m_p - \lambda} + 1 = 0. \tag{5.4}$$

When λ goes from m_p to m_{p-1}, the first member of this equation goes from $-\infty$ to $+\infty$ if y_{p-1} and y_p are both different from zero. Hence, for any $\mathbf{y}$ with non-vanishing components y_{p-1}, y_p there is a root in the interval $m_p < \lambda < m_{p-1}$, and therefore the region R contains all points $\mathbf{y}$ which do not lie on the hyperplanes $y_{p-1} = 0$, $y_p = 0$. Consider now a point $\mathbf{y}$ of the hyperplane $y_p = 0$. The expression (5.3) vanishes then for $\lambda = m_p$, and therefore the hyperplane $y_p = 0$ belongs also to the region R. Similarly, it can be shown that the hyperplane $y_{p-1} = 0$ also belongs to the region R. Therefore, in the case $m_p \leqq m_{p-1} \leqq 0$, the region R is all the space.

(d) Finally, consider the remaining case: $m_p < 0$ and all the other proper values m_j greater than zero. If $y_p = 0$, then the expression (5.3) vanishes for $\lambda = m_p$, and therefore the hyperplane $y_p = 0$ is contained in R. Consider now the case $y_p \neq 0$. Then, for $\lambda \neq m_p$, $\lambda \leqq 0$, the equation $D = 0$ can be written as in (5.4). The first member of this equation is, in the interval $-\infty \leqq \lambda < m_p$, an increasing function of λ which goes from 1 to $+\infty$, and therefore in that interval there are no roots. In the interval $m_p < \lambda \leqq 0$, the function goes from $-\infty$ to the value corresponding to $\lambda = 0$. A necessary and sufficient condition in order that there is a root in this interval is that

$$y_1^2/m_1 + \cdots + y_p^2/m_p + 1 \geqq 0.$$

This is a hyperboloid, whose center is at the origin, and whose boundary has two sheets which are symmetric with respect to the hyperplane $y_p = 0$, which is totally contained in it. In matrix notation the above inequality may be written

$$\mathbf{y}'\mathbf{U}\mathbf{M}^{-1}\mathbf{U}'\mathbf{y} + 1 \geqq 0,$$

and going back to the old variables, (5.1) follows immediately.

THEOREM 2. *If the confidence region for the linear relation is the hyperboloid* (5.1), *then a necessary and sufficient condition in order that a hyperplane be rejected by the F-test, is that it is not covered by the region* (5.1).

PROOF. According to the definition of the region R, the hyperboloid is the region covered by all hyperplanes which are not rejected by the test. Conversely, assume now that the hyperplane $A + \mathbf{Bx} = 0$ is entirely contained in (5.1). Let d be the minimum distance from the boundary of (5.1) to the hyperplane $A + \mathbf{Bx} = 0$, measured in the direction perpendicular to the hyperplane. Let $\mathbf{x}_0$ be the point on the boundary of (5.1) whose distance to that hyperplane is precisely d. Then the normal to the boundary of R at $\mathbf{x}_0$ is perpendicular to $A + \mathbf{Bx} = 0$, and therefore

$$\mathbf{B} = \rho(\mathbf{x}_0 - \mathbf{x}.)'\mathbf{M}^{-1}. \tag{5.5}$$

Since $\mathbf{x}_0$ is on the boundary of R, we have

$$\rho^{-1}\mathbf{B}(\mathbf{x}_0 - \mathbf{x}.) + 1 = 0.$$

Multiplying (5.5) on the right by $\mathbf{MB}'$ we have

$$\mathbf{BMB}' = \rho(\mathbf{x}_0 - \mathbf{x}.)'\mathbf{B}',$$

and, eliminating ρ from the last two equations,

$$[\mathbf{B}(\mathbf{x}_0 - \mathbf{x}.)]^2 + \mathbf{BMB}' = 0.$$

Since $\mathbf{x}_0$ is the point on the boundary of R whose distance from the hyperplane $A + \mathbf{Bx} = 0$ is the minimum distance d from that boundary to the hyperplane, and $\mathbf{x}.$ is the center of the hyperboloid, we have

$$(A + \mathbf{Bx}.)^2 \leqq [\mathbf{B}(\mathbf{x}_0 - \mathbf{x}.)]^2,$$

and therefore, (4.8) holds, that is, the hyperplane $A + \mathbf{Bx} = 0$ is not rejected by the test.

THEOREM 3.

(i) *If the proper values of* $\mathbf{S}^{-\frac{1}{2}}(\mathbf{SP})\mathbf{S}^{-\frac{1}{2}}$ *are all greater than* qF, *then the confidence region for the linear relation is empty.*

(ii) *If the proper values of* $\mathbf{S}^{-\frac{1}{2}}(\mathbf{SP})\mathbf{S}^{-\frac{1}{2}}$ *are all greater than* qF, *with the only exception of one which is equal to* qF, *or one which is smaller than* qF, *then the confidence region is, respectively, the maximum likelihood hyperplane or the hyperboloid* (5.1).

(iii) *If two or more of the proper values of* $\mathbf{S}^{-\frac{1}{2}}(\mathbf{SP})\mathbf{S}^{-\frac{1}{2}}$ *are equal or smaller than* qF, *then the confidence region is all the space.*

PROOF. If $l_1, \cdots, l_p$ are the proper values of the matrix $\mathbf{S}^{-\frac{1}{2}}(\mathbf{SP})\mathbf{S}^{-\frac{1}{2}}$, then the proper values of

$$\mathbf{M}^* = \mathbf{S}^{-\frac{1}{2}}\mathbf{M}\mathbf{S}^{-\frac{1}{2}} = [\mathbf{S}^{-\frac{1}{2}}(\mathbf{SP})\mathbf{S}^{-\frac{1}{2}} - qF\mathbf{I}]/n$$

are, obviously,

$$m_h^* = (l_h - qF)/n. \tag{5.6}$$

Since, by the law of inertia (see for instance [3], p. 297), the matrices $\mathbf{M}$ and $\mathbf{M}^*$ have the same number of positive and negative proper values, the theorem follows immediately from (5.6) and the previous theorem.

REMARK. Consider the new random vectors $\mathbf{x}_i^* = \mathbf{S}^{-\frac{1}{2}}\mathbf{x}_i$. The centroid of the points $\mathbf{x}_i^*$ with weights n_i is obviously equal to $\mathbf{x}_.^* = \mathbf{S}^{-\frac{1}{2}}\mathbf{x}_.$, and the central moment matrix of the system of points $\mathbf{x}_i^*$ with weights n_i is

$$\sum n_i(\mathbf{x}_i^* - \mathbf{x}_.^*)(\mathbf{x}_i^* - \mathbf{x}_.^*)' = \mathbf{S}^{-\frac{1}{2}}(\mathbf{SP})\mathbf{S}^{-\frac{1}{2}}.$$

The points $\mathbf{x}_i^*$ converge in probability to the points $\xi_i^* = \Sigma^{-\frac{1}{2}}\xi_i$, which lie on the hyperplane $\alpha + \beta\Sigma^{\frac{1}{2}}\mathbf{x} = 0$. If the points ξ_i^* are well spread over this hyperplane, that is, if they do not cluster around a flat of smaller dimension, (a necessary condition for this is that $q \geqq p$) then the ellipsoid of inertia of the points $\mathbf{x}_i^*$ with weights n_i will usually have one small axis and $p - 1$ large ones, that is, the matrix $\mathbf{S}^{-\frac{1}{2}}(\mathbf{SP})\mathbf{S}^{-\frac{1}{2}}$ will have one small proper value and $p - 1$ large ones, so that, for usual values of F, there will be one proper value smaller than qF and $p - 1$ proper values greater than it, and, by the last theorem, the confidence region will be a hyperboloid.

6. Homogeneous linear relation. We shall consider now the homogeneous case in which it is known that the true hyperplane goes through the origin; then $\alpha = 0$ and the linear relation is simply $\beta\mathbf{x} = 0$. Consider the hypothesis H that $\beta = \mathbf{B}$, i.e., that the linear relation is $\mathbf{Bx} = 0$, where $\mathbf{B}$ is a given row vector. A test of this hypothesis can be derived from (4.6) by simply replacing A by 0. In other words, we shall not reject the hypothesis H if

$$\mathbf{B}(\mathbf{SP})\mathbf{B}'/\mathbf{BSB}' \leqq qF, \tag{6.1}$$

where we define now the sums of products for treatments matrix $(\mathbf{SP})$ not by (4.7) but simply by

$$(\mathbf{SP}) = \sum n_i\mathbf{x}_i\mathbf{x}_i'. \tag{6.2}$$

The confidence region for the linear relation will be the set of all points $\mathbf{x}$ which belong to hyperplanes not rejected by the test. Then, $\mathbf{x}$ will belong to the confidence region if the minimum of $\mathbf{BMB}'$ for all $\mathbf{B}$'s subject to the conditions

$$\mathbf{Bx} = 0 \tag{6.3}$$

$$\mathbf{BB}' = 1 \tag{6.4}$$

is negative. By differentiation we have, if λ and μ are Lagrange multipliers,

$$\mathbf{B}(\mathbf{M} - \lambda\mathbf{I}) + \mu\mathbf{x}' = \mathbf{0}. \tag{6.5}$$

If we consider (6.3) and (6.5) as a linear system of equations in the variables $\mathbf{B}$, μ the condition for compatibility is that

$$\begin{vmatrix} 0 & \mathbf{x}' \\ \mathbf{x} & \mathbf{M} - \lambda \mathbf{I} \end{vmatrix} = 0 \tag{6.6}$$

If we multiply (6.5) on the right by $\mathbf{B}'$, we have $\lambda = \mathbf{BMB}'$. Therefore, the region R is the set of all points $\mathbf{x}$ such that (6.6) has a non-positive root λ. Let $\mathbf{U}$ be, as before, an orthogonal matrix such that $\mathbf{UMU}'$ is a diagonal matrix. Consider the change of variables $\mathbf{y} = \mathbf{Ux}$. Then, if $m_1, \cdots, m_p$ are the proper values of $\mathbf{M}$, the region R is the set of all points $\mathbf{y}$ for which the determinant

$$\begin{vmatrix} 0 & y_1 & y_2 & \cdots & y_p \\ y_1 & m_1 - \lambda & 0 & \cdots & 0 \\ y_2 & 0 & m_2 - \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ y_p & 0 & 0 & \cdots & m_p - \lambda \end{vmatrix}$$

vanishes for some non-positive λ. Results similar to those of the previous section can then be derived using the same methods, the only difference being that instead of a hyperboloid (5.1) we have now a hypercone

$$\mathbf{x}\mathbf{M}^{-1}\mathbf{x}' \geqq 0. \tag{6.7}$$

Thus, for instance, the following theorem holds.

THEOREM.

(i) *If the proper values* $l_1, \cdots, l_p$ *of the matrix* $\mathbf{S}^{-\frac{1}{2}}(\mathbf{SP})\mathbf{S}^{-\frac{1}{2}}$ *are all greater than* qF*, then the confidence region is empty.*

(ii) *If the proper values* l_h *are all greater than* qF*, with the only exception of one which is equal to or smaller than* qF*, the confidence region is, respectively, the maximum likelihood hyperplane or the hypercone* (6.7).

(iii) *If two or more of the proper values* l_h *are equal to or smaller than* qF*, then the confidence region is all the space.*

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