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An Algorithm for Analytic Continuation

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AN ALGORITHM FOR ANALYTIC CONTINUATION

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1. Introduction

Let an analytic function f of a single complex variable be defined in a neighborhood of a point z_0 by means of its Taylor series at z_0 . In this paper, we wish to discuss a constructive method for the solution of the following problem: Suppose it is known that the function f can be continued analytically into a domain $\mathcal{R}$ of the complex plane. It is desired to compute the value of f at an arbitrary point $b \in \mathcal{R}$.

By a constructive method (or "algorithm") for solving a problem in numerical analysis we mean a sequence of rational functions of the data of the problem which converge to the desired mathematical object.

In a number of special situations classical analysis offers a variety of formulas and methods for solving the problem posed above, such as the Schwarz reflection principle, or the methods of Mittag-Leffler and Borel (see Bieberbach [1955]). The problem is easily solved if the function f is known to satisfy a differential or other functional equation. In some cases the problem may also be solved by classical methods of summability theory (see Hardy [1948]). In a more numerical vein, Euler's series transformation sometimes proves to be an effective means of continuation (van Wijngaarden [1953]). Recently, linear programming techniques have been proposed for the solution of a special continuation problem (Douglas [1960]; Douglas and Gallie [1959]).

The above methods apply only in special (sometimes extremely so) situations. However, the following technique, due to Weierstrass, is generally applicable (for a recent exposition, see Behnke and Sommer [1955], pp. 166-171). We join the points z_0 and b by a rectifiable

are γ lying in $\mathcal{R}$. If $\delta > 0$ denotes the distance of γ from the boundary of $\mathcal{R}$, we select N points $z_1, z_2, \dots, z_N = b$ on γ such that $|z_k - z_{k-1}| < \delta$, $k = 1, 2, \dots, N$. The Taylor series of f at z_0 , having a radius of convergence $\geq \delta$, enables us to calculate the values of f and of all derivatives of f at z_1 . Thus the Taylor series at z_1 is also known, and can be used to calculate the coefficients of the Taylor series at the point z_2 . Proceeding in this manner, we finally obtain the Taylor series at the point z_N , and thus a fortiori the solution of our continuation problem.

Clearly, the above method is not constructive in the sense indicated earlier. The data in this case are the coefficients of the Taylor series at $z = a$. While it is true that the partial sums of the first Taylor series, and its derivatives, are rational functions of these coefficients, their limits generally are not. Yet these limits are required to continue the process. In what follows we shall describe a modification of the above Weierstrassian method of continuation which transforms it into a constructive process.

2. Matrix formulation of Weierstrassian analytic continuation.

Let $a_0 + a_1(z - z_0) + a_2(z - z_0)^2 + \dots$ be the power series defining f near z_0 , and let

$$f(z) = b_0 + b_1(z - z_1) + b_2(z - z_1)^2 + \dots$$

near z_1 . If $|z_1 - z_0|$ is smaller than the radius of convergence of the series at z_0 , we have

$$b_0 = f(z_1) = a_0 + \delta_1 a_1 + \delta_1^2 a_2 + \dots,$$

where $\delta_1 = z_1 - z_0$, and more generally for $k = 0, 1, 2, \dots$

$$\begin{aligned}
 (1) \quad b_k &= \frac{1}{k!} f^{(k)}(z_1) \\
 &= \frac{1}{k!} \left\{ \frac{k!}{0!} a_k + \delta_1 \frac{(k+1)!}{1!} a_{k+1} + \delta_1^2 \frac{(k+2)!}{2!} a_{k+2} + \dots \right\} \\
 &= \binom{k}{0} a_k + \binom{k+1}{1} \delta_1 a_{k+1} + \binom{k+2}{2} \delta_1^2 a_{k+2} + \dots,
 \end{aligned}$$

where $\binom{n}{m}$ denotes a binomial coefficient.

We can render these formulas more lucid by the use of matrix notation. We denote by $A(z)$ the infinite column vector whose components are the coefficients of the Taylor series at the point z . For instance,

$$A(z_0) = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ \vdots \end{pmatrix}, \quad A(z_1) = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \vdots \end{pmatrix}.$$

We now define an infinite upper triangular matrix $M(z)$ as follows:

$$M(z) = (a_{mn}), \quad m, n = 0, 1, 2, \dots,$$

where

$$a_{mn} = \begin{cases} \binom{n}{m} z^{n-m}, & n \geq m \\ 0, & n < m. \end{cases}$$

Written out in full,

$$M(z) = \begin{pmatrix} 1 & z & z^2 & z^3 & z^4 & \dots \\ & 1 & 2z & 3z^2 & 4z^3 & \\ & & 1 & 3z & 6z^2 & \\ & & & 1 & 4z & \\ & 0 & & & 1 & \\ & & & & & \ddots \end{pmatrix}.$$

The relation (1) now can be combined into the single relation

$$(2) \quad A(z_1) = M(\delta_1) A(z_0).$$

In a similar manner we find, if $|z_k - z_{k-1}|$ is less than the radius of convergence of the Taylor series at z_{k-1} ,

$$(3) \quad A(z_k) = M(\delta_k) A(z_{k-1}), \quad k = 1, 2, \dots, N,$$

where $\delta_k = z_k - z_{k-1}$. Thus the solution of our continuation problem is given by

$$(4) \quad A(z_N) = M(\delta_N) M(\delta_{N-1}) \dots M(\delta_1) A(z_0),$$

with the understanding that the product is to be formed proceeding from the right to the left.

The non-associativity of the product in (4) is shown by the following remark: It is easily seen that the "continuation matrices" $M(z)$ satisfy the addition theorem

$$(5) \quad M(z') M(z'') = M(z' + z'')$$

for arbitrary complex z' and z'' . Since $\delta_N + \delta_{N-1} + \dots + \delta_1 = z_N - z_0$,

the product on the right of (4) thus is formally equivalent to $M(z_N - z_0) A(z_0)$. However, this expression is without analytic content, since it is tantamount to evaluating the Taylor series at z_0 for $z = z_N$, where it diverges in general.

3. Definition of the continuation algorithm

We denote by $M_{m,n}(z)$ the finite matrix consisting of the first m rows and n columns of the matrix $M(z)$. Similarly, we denote by $A_n(z)$ the column vector comprising the first n elements of the vector $A(z)$. By the symbol $A_n^{(k)}$ we denote vectors intended to approximate $A_n(z_k)$.

At first sight, it would seem reasonable to transform the Weierstrassian method of continuation into an algorithm by forming the vectors

$$A_n^{(N)} = M_{n,n}(\delta_N) M_{n,n}(\delta_{N-1}) \cdots M_{n,n}(\delta_1) A_n(z_0),$$

where $n = 1, 2, \dots$. However, since products of finite matrices are always associative, and since the addition theorem (5) also holds for the finite segments $M_{n,n}$, this amounts to nothing more than to forming

$$A_n^{(N)} = M_{n,n}(z_N - z_0) A_n(z_0),$$

which is precisely what we obtain by substituting $z_N - z_0$ into the power series defining f at $z = z_0$. It thus is clear that if we wish to obtain a convergent algorithm, the finite segments of the matrices $M(\delta_k)$ in (4) must be chosen in a more sophisticated manner.

It is fairly obvious that if convergence is to be assured, the vectors $A(z_k)$ must be approximated particularly well if k is small. (The truncation error is propagated forward but not backward.) We can achieve this by replacing the matrices $M(\delta_k)$ by rectangular segments that have q times as many columns as rows, where q is an integer > 1 . We thus are led to defining the approximating vectors $A_n^{(N)}$ in the following manner: For $n = 1, 2, \dots$, let

$$(6) \quad A_n^{(N)} = M_{n, nq}(\delta_N) M_{nq, nq}^{(2)}(\delta_{N-1}) \dots \\ \dots M_{nq, nq}^{(N-1)}(\delta_1) A_{nq}^{(N)}(z_0).$$

These vectors evidently depend on the "magnification ratio" q . For each n , they can be built up recursively as follows:

$$(7) \quad \begin{cases} A_{nq}^{(0)} = A_{nq}^{(N)}(z_0), \\ A_{nq}^{(k)} = M_{nq, nq}^{(N-k)}(\delta_k) A_{nq}^{(k-1)}, \quad k = 1, 2, \dots, N. \end{cases}$$

4. Convergence of the algorithm.

Let r_k be the radius of convergence of the Taylor series representing f in a neighborhood of the point z_k . For Weierstrassian analytic continuation it is necessary that $|\delta_k| = |z_k - z_{k-1}| < r_{k-1}$, $k = 1, 2, \dots, N$. Let this condition be met, and let r'_k be any number satisfying $\delta_k < r'_k < r_{k-1}$. By Cauchy's theorem there exists a constant C_k such that

$$|f^{(n)}(z_{k-1})| \leq \frac{n! C_k}{r'_k}, \quad n = 0, 1, 2, \dots$$

Setting $\rho_k = |\delta_k|/r'_k$, this may be written in the form

$$|f^{(n)}(\rho_{k-1})| \leq n! \left(\frac{\rho_k}{|\delta_k|} \right)^n C_k, \quad n = 0, 1, 2, \dots$$

Only a slightly stronger condition is required for the convergence of the algorithm (7).

THEOREM. Let there exist constants C_k and ρ_k , $0 < \rho_k < 1$, such that

$$(8) \quad |f^{(n)}(z)| \leq n! \left(\frac{\rho_k}{|\delta_k|} \right)^n C_k, \quad n = 0, 1, 2, \dots,$$

for all points z on the straight line segment joining z_{k-1} and z_k ($k = 1, 2, \dots, N$). Then there exists a number q_0 such that for all $q > q_0$ the elements of the vectors $A_n^{(N)}$ converge to the corresponding elements of $A(z_N)$ as $n \rightarrow \infty$.

The question as to the infimum of all q_0 for which the theorem is true is left open. An upper bound for this infimum, however, will emerge from the proof.

5. Proof of the Theorem.

Letting

$$R_n^{(k)} = A_n(z_k) - A_n^{(k)}$$

for $k = 1, 2, \dots, N$ and for all values of n for which $A_n^{(k)}$ is defined, our aim is to show that $R_n^{(N)} \rightarrow 0$ as $n \rightarrow \infty$. Our first goal is a recurrence relation for $R_n^{(k)}$. Such a relation is obtained via a recurrence relation for the vectors $A_n(z_k)$.

LEMMA 1. For $k = 1, 2, \dots, N$; $n = 1, 2, \dots$, let

$$D_n^{(k)} = \rho_k^{nq} \begin{pmatrix} \begin{pmatrix} nq \\ 0 \end{pmatrix} \\ \begin{pmatrix} nq \\ 1 \end{pmatrix} \delta_k^{-1} \\ \vdots \\ \begin{pmatrix} nq \\ n-1 \end{pmatrix} \delta_k^{-n+1} \end{pmatrix}$$

Then

$$(9) \quad A_n(z_k) = M_{n,nq}(\delta_k) A_{nq}(z_{k-1}) + \Theta_k D_n^{(k)},$$

where Θ_k denotes a diagonal matrix whose elements are bounded by C_k .

Proof. By Taylor's theorem,

$$\begin{aligned} \frac{1}{m!} f^{(m)}(z_k) &= \frac{1}{m!} f^{(m)}(z_{k-1}) + \frac{1}{m!1!} f^{(m+1)}(z_{k-1}) \delta_k + \\ &\dots + \frac{1}{m!(nq-m-1)!} f^{(nq-1)}(z_{k-1}) \delta_k^{nq-m-1} \\ &+ \frac{1}{m!(nq-m-1)!} \int_{z_{k-1}}^{z_k} (z_k - t)^{nq-m-1} f^{(nq)}(t) dt, \end{aligned}$$

$m = 0, 1, 2, \dots, n-1$. It follows that

$$A_n(z_k) = M_{n,nq}(\delta_k) A_{nq}(z_{k-1})$$

$$+ \int_{z_{k-1}}^{z_k} f^{(nq)}(t) \begin{pmatrix} \frac{1}{0!(nq-1)!} (z_k - t)^{nq-1} \\ \frac{1}{1!(nq-2)!} (z_k - t)^{nq-2} \\ \vdots \\ \frac{1}{(n-1)!(nq-n)!} (z_k - t)^{nq-n} \end{pmatrix} dt.$$

Formula (9) now is obtained by estimating the integral by means of (8).

Subtracting (7) from (9) we now find

$$R_n^{(k)} = M_{n,nq}(\delta_k) R_{nq}^{(k-1)} + \Theta_k D_n^{(k)},$$

where n runs through all multiples of q^{N-k} . A standard argument in the theory of difference equations now shows that

$$R_n^{(N)} = \sum_{k=1}^N \prod_n^{(k)} \Theta_k D_{nq^{N-k}}^{(k)},$$

where $\prod_n^{(N)} = I$, and for $k = 1, 2, \dots, N-1$

$$\prod_n^{(k)} = M_{n,nq}(\delta_N) M_{nq,nq^2}(\delta_{N-1}) \cdots M_{nq^{N-k-1},nq^{N-k}}(\delta_{k+1}).$$

We shall denote by $\hat{A}$ the vector or matrix whose elements are the absolute values of the elements of A , and use a notation such as $A < B$ to indicate the corresponding inequality between corresponding elements. We then have, in view of Lemma 1,

$$(10) \quad R_n^{(N)} \leq \sum_{k=1}^N C_k \prod_n^{(k)} \hat{D}_{nq^{N-k}}^{(k)},$$

where $\tilde{\prod}_n^{(N)} = I$, and for $k = 1, 2, \dots, N-1$

$$\tilde{\prod}_n^{(k)} = \hat{M}_{n,nq}(\delta_N) \cdots \hat{M}_{nq^{N-k-1},nq^{N-k}}(\delta_{k+1}).$$

The resulting products of matrices in (10) can be further estimated by a reduction formula based on the following result.

LEMMA 2. Let

$$(11) \quad q_k > 1 + |\delta_k \delta_{k+1}^{-1}|,$$

$k = 1, 2, \dots, N-1$. There exist constants K_k not depending on q or

n such that for all $q \geq q_k$ and all sufficiently large n

$$(12) \quad \hat{M}_{n,nq}(\delta_{k+1}) \hat{D}_{nq}^{(k)} \leq K_k Z_k^{nq} \hat{D}_n^{(k+1)},$$

where

$$(13) \quad Z_k = \frac{q^q}{(q-1)^{q-1}} \rho_k^q \rho_{k+1}^{-1} |\delta_{k+1} \delta_k^{-1}|.$$

A value for K_k will be given below.

Proof. For brevity we set $|\delta_k| = a$, $|\delta_{k+1}| = b$. Denoting by c_m the m^{th} element of the vector

$$\hat{M}_{n,nq}(\delta_k) \hat{D}_{nq}^{(k)},$$

we have

$$(14) \quad c_m = \rho_k^{q^2 n} a^{-m} S,$$

where

$$S = \binom{m}{m} \binom{nq^2}{m} + \binom{m+1}{m} \binom{nq^2}{m+1} \left(\frac{b}{a}\right) + \dots \\ + \binom{nq-1}{m} \binom{nq^2}{nq-1} \left(\frac{b}{a}\right)^{nq-1-m}.$$

It turns out that the dominant term in the sum S is the last term.

Factoring out this term, we have

$$(15) \quad S = \binom{nq-1}{m} \binom{nq^2}{nq-1} \left(\frac{b}{a}\right)^{nq-1-m} S_1,$$

where

$$S_1 = 1 + \frac{nq-m-1}{nq^2-nq+2} \frac{a}{b} + \frac{(nq-m-1)(nq-m-2)}{(nq^2-nq+2)(nq^2-nq+3)} \left(\frac{a}{b}\right)^2 + \dots$$

The sum S_1 terminates. Since $0 \leq m < n$, it is clearly bounded by the geometric sum $1 + X + X^2 + \dots$, terminated after the same number of terms, where

$$X = \frac{nq - 1}{nq^2 - nq + 2} \frac{a}{b}.$$

Now

$$\frac{nq - 1}{nq^2 - nq + 2} = \frac{nq - 1}{q(nq - 1) + q - nq + 2} \leq \frac{1}{q - 1},$$

hence, if $q \geq q_k$,

$$X \leq \frac{1}{q - 1} \frac{a}{b} \leq \frac{1}{q_k - 1} \frac{a}{b} < 1.$$

Summing the geometric series, we thus have

$$(16) \quad S_1 \leq \frac{b}{a} K_k,$$

where

$$K_k = \frac{a(q_k - 1)}{b(q_k - 1) - a}.$$

Since $q \geq 2$, $m < n$, we have

$$(17) \quad \binom{nq - 1}{m} \binom{nq^2}{nq - 1} \leq \binom{nq}{m} \binom{nq^2}{nq}.$$

The m^{th} element of $\hat{D}_n^{(k+1)}$ being given by

$$d_m = \rho_{k+1}^{nq} \binom{nq}{m} b^{-m},$$

we thus have from (14), (15), (16) and (17)

$$(18) \quad c_m \leq \rho_k^{nq^2} \rho_{k+1}^{-nq} \left(\frac{b}{a}\right)^{nq} \binom{nq^2}{nq} K_k d_m.$$

Estimating the factorials by means of Stirling's formula, we have

$$\binom{nq^2}{nq} = \frac{(nq^2)!}{(nq)!(n(q^2 - q))!} \sim \frac{1}{\sqrt{2\pi(q-1)n}} \left[\frac{q^q}{(q-1)^{q-1}} \right]^{nq},$$

and thus, in view of the presence of $\sqrt{n}$ in the denominator,

$$(19) \quad \binom{nq^2}{nq} < \left[\frac{q^q}{(q-1)^{q-1}} \right]^{nq}$$

for all large n . It thus follows from (18) and (19) that

$$c_m \leq \left[\frac{q^q}{(q-1)^{q-1}} \rho_k^q \rho_{k+1}^{q-1} \frac{b}{a} \right]^{nq} K_{k+m}^d,$$

which is the desired result.

It follows from (12) that

$$\prod_n^{(k)} \hat{D}_{nq^{N-k}}^{(k)} \leq K_k Z_k^{nq^{N-k}} \prod_n^{(k+1)} \hat{D}_{nq^{N-k-1}}^{(k+1)},$$

and thus, using induction,

$$(20) \quad \prod_n^{(k)} \hat{D}_{nq^{N-k}}^{(k)} \leq K_k K_{k+1} \cdots K_{N-1} Z_k^{nq^{N-k}} Z_{k+1}^{nq^{N-k-1}} \cdots Z_{N-1}^{nq} \hat{D}_n^{(N)}.$$

We shall estimate $\hat{D}_n^{(N)}$ by a bound very similar to that of Lemma 2.

LEMMA 3. Let

$$(21) \quad q_N > 1 + |\delta_N|.$$

There exists a constant K_N , independent of n or q , such that the elements of $\hat{D}_n^{(N)}$ are bounded by $K_N Z_N^n$ for all $q \geq q_N$ and

all large n , where

$$(22) \quad Z_N = \frac{q^q}{(q-1)^{q-1}} \rho_N^q |\delta_N|^{-1}.$$

Proof. We bound the elements of the vector $\hat{D}_n^{(N)}$ by the sum of the absolute values of all elements. This sum can be formed by multiplying $\hat{D}_n^{(N)}$ by the matrix $M_{1,n}(1)$. An application of the method of proof of Lemma 2 now yields the bound of Lemma 3, where

$$K_N = \frac{(q_N - 1) |\delta_N|}{q_N - 1 - |\delta_N|}.$$

In view of (10), (20), and Lemma 3 we find that every element of $R_n^{(N)}$ is bounded by

$$(23) \quad \sum_{k=1}^N C'_k \left[Z_k^{q^{N-k}} Z_{k+1}^{q^{N-k-1}} \cdots Z_N \right]^n,$$

where

$$C'_k = C_k K_k K_{k+1} \cdots K_N,$$

and where the numbers Z_k are defined by (13) and (22). The proof of the theorem now is an easy consequence of the following fact:

LEMMA 4. For $k = 1, 2, \dots, N$,

$$(24) \quad \lim_{q \rightarrow \infty} Z_k = 0.$$

Proof. If we set $\rho_{k+1} = |\delta_{k+1}| = 1$, we have

$$Z_k = \left(1 - \frac{1}{q}\right)^{-q} (q-1) \rho_k^q \cdot c_k$$

for $k = 1, 2, \dots, N$, where

$$(25) \quad c_k = \rho_{k+1}^{-1} |\delta_k^{-1} \delta_{k+1}|.$$

Relation (24) now follows trivially from the well-known result

$$\lim_{q \rightarrow \infty} (1 - \frac{1}{q})^{-q} = e$$

and from the fact that, by virtue of $|\rho_k| < 1$,

$$\lim_{q \rightarrow \infty} (q - 1) \rho_k^q = 0.$$

In view of Lemma 4 there certainly exists q^* such that $|Z_k| < 1$ for $q \geq q^*$, $k = 1, 2, \dots, N$. If $q \geq q_0$, where $q_0 = \max(q^*, q_1, q_2, \dots, q_N)$, then all elements of $R_n^{(N)}$ are bounded by the expression (23), which tends to zero as $n \rightarrow \infty$. This completes the proof of the theorem.

6. Choice of the enlargement ratio

Once the continuation points $z_1, z_2, \dots, z_N$, and with them the numbers ρ_k and δ_k ($k = 1, 2, \dots, N$), are fixed, the enlargement ratio q has to satisfy the following conditions: In order to satisfy (11) and (21) we must have

$$(A) \quad q > 1 + \left| \frac{\delta_k}{\delta_{k+1}} \right|, \quad k = 1, 2, \dots, N$$

($\delta_{N+1} = 1$), and in order to make $|Z_k| < 1$, we must require

$$(B) \quad \frac{q^q}{(q - 1)^{q-1}} \rho_k^q c_k < 1,$$

where c_k is given by (25), or approximately

$$(26) \quad (q-1)\rho_k^q < e^{-1}c_k^{-1}, \quad k = 1, 2, \dots, N.$$

Condition (26) shows that unless ρ_k is small, q may have to be taken quite large. Small values of ρ_k , on the other hand, force us to make N , the number of continuation steps, large. Thus in any case the continuation matrices $M_{n,qn}$ are likely to be large. As an example, we consider the problem of continuing the function $\log z$ around the unit circle, starting from $z = 1$. Choosing the continuation points

$$z_k = e^{ik\varphi}, \quad \text{where} \quad \varphi = \frac{\pi}{6},$$

we find

$$\rho_k = \rho = 2 \tan \frac{\varphi}{2} = 0.535898.$$

Since all $|\delta_k|$ are the same in the present case, condition (A) is satisfied for $q > 2$, and condition (B) simplifies to

$$(q-1)\rho^{q-1} < e^{-1}.$$

This is satisfied for $q \geq 5$, but not for $q = 4$. Since $N = 12$ in the present problem, even the very first matrix used in the algorithm (7) has $5^{12} = 244,140,625$ columns.

7. Numerical examples

The algorithm (7) has been carried out numerically in some very simple examples. The author is indebted to Mr. Thomas A. Bray of the Boeing Scientific Research Laboratories for his expert assistance in the planning of these computations. We wish to report briefly on the results of two such computations.

(I) The power series

$$f(z) = 1 - z + z^2 - z^3 + \dots$$

has been continued using the points $z_k = 0.35k$, $k = 0, 1, 2, 3$. An enlargement ratio $q = 3$ was used. The following table lists the first components of the vectors $A_n^{(k)}$, and of the exact vectors $A(z_k)$.

$n \backslash k$	1	2	3
1	0.740740741	0.588239567	0.492237049
2	0.740740741	0.588235294	0.487767430
3	0.740740741	0.588235294	0.487805203
4	0.740740741	0.588235294	0.487804475
$A(z_k)$	0.740740741	0.588235294	0.487804878

The values in the last column approximate the function at a point where the original power series does not converge.

(II) The power series

$$f(z) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2} z^n = \int_0^z t^{-1} \log(1+t) dt$$

was continued using the points $z_k = 0.3k$, $k = 0, 1, 2, 3, 4$. Again working with $q = 3$, the following values of the first components of $A_k^{(n)}$ were

found:

$n \backslash k$	1	2	3	4
1	0.280074	0.528107	0.752163	0.956771
2	0.280074	0.528107	0.752163	0.957406
3	0.280074	0.528107	0.752163	0.957405

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