Note on the Round-Off Errors in Iterative Processes

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Summary. This paper discusses round-off errors in iterative processes for solving equations. Let $x_{n+1} = x_n + F(x_n)$ be a scalar iterative converging process; the different values x_n are represented in a computer with a certain precision; when x_n is close to the limit, $F(x_n)$ is small and can perhaps be obtained easily with a higher absolute precision than x_n ; consequently, the addition $x_n + F(x_n)$ will practically involve a rounding operation. Besides some general remarks, it will be shown that for a fixed-point computer an appropriate rounding method can provide a more accurate solution to the problem; analogous results are given in Appendix I for a floating-point computer; Appendix II deals with Aitken's δ^2 process. The author is indebted to A. H. Taub for many suggestions and stimulating discussions.

1. Introduction. Let $G^{(1)}, \dots, G^{(m)}$ be m real functions of the real variables $x^{(1)}, \dots, x^{(m)}$. For any set of m numbers $p^{(1)}, \dots, p^{(m)}$, we shall use the vectorial notations:

$$\mathbf{p} = (p^{(1)}, \dots, p^{(m)});$$

$$|\mathbf{p}| = \sqrt{(p^{(1)})^2 + \dots + (p^{(m)})^2}.$$

We consider the iterative process

$$(1) \quad \mathbf{x}_{n+1} = \mathbf{G}(\mathbf{x}_n), \quad n = 0, 1, \dots$$

and suppose there exist a vector $\mathbf{r}$ and a number b ($0 \leq b < 1$) such that

$$(2) \quad |\mathbf{G}(\mathbf{x}) - \mathbf{r}| \leq b |\mathbf{x} - \mathbf{r}| \quad \text{for all } \mathbf{x};$$

the condition (2) insures the convergence of the $\mathbf{x}_n$'s to $\mathbf{r}$.

We want to realize the process (1) on a fixed-point computer under the two conditions: a) For representing each of the $x_n^{(i)}$, we use only one "word"; we consider the content of the word as an *integer*; b) We may use higher precision for computing the values of the functions $G^{(1)}, \dots, G^{(m)}$ (or the functions $G^{(1)} - x^{(1)}, G^{(2)} - x^{(2)}, \dots, G^{(m)} - x^{(m)}$).

We distinguish two types of errors:

1) *Truncation errors*; even when using double precision, we cannot expect to evaluate the functions $G^{(i)}$ exactly;

2) *Round-off errors*; according to condition a), the value found for $G^{(i)}$ must be rounded to an integer.

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2. Truncation Errors. Let $H^{(1)}(\mathbf{x}), \dots, H^{(m)}(\mathbf{x})$ approximate the functions $G^{(1)}(\mathbf{x}), \dots, G^{(m)}(\mathbf{x})$:

$$H^{(i)}(\mathbf{x}) = G^{(i)}(\mathbf{x}) + \xi^{(i)}(\mathbf{x});$$

$\xi^{(i)}(\mathbf{x})$ is called the truncation error; it is supposed to satisfy the inequality

$$(3) \quad |\xi^{(i)}(\mathbf{x})| \leq a^{(i)}; \quad a^{(i)} = \text{constant}.$$

The iterative process

$$(4) \quad \mathbf{V}_{n+1} = \mathbf{H}(\mathbf{V}_n)$$

is considered as an approximation of (1) and gives some information about $\mathbf{r}$.

THEOREM 1. *For any $\mathbf{V}_0$, the sequence $\mathbf{V}_n$ given by (4) is bounded and all its points of accumulation $\mathbf{V}$ satisfy the inequality*

$$|\mathbf{V} - \mathbf{r}| \leq \frac{|\mathbf{a}|}{1-b}; \quad \mathbf{a} = (a^{(1)}, \dots, a^{(m)}).$$

THEOREM 2. *The process (4) is the best possible in the following sense: for given $\mathbf{a}$ and b , there exist m functions $H^{(i)}(\mathbf{x}), \dots, H^{(m)}(\mathbf{x})$ for which it is impossible to find an algorithm using only $\mathbf{H}$, $\mathbf{a}$, b , providing closer points of accumulation to $\mathbf{r}$ than the algorithm (4).*

Proof: Let $\mathbf{G}(\mathbf{x}) = b\mathbf{x} + \mathbf{a}$,

$$\mathbf{H}(\mathbf{x}) = b\mathbf{x},$$

$$\mathbf{G}'(\mathbf{x}) = b\mathbf{x} - \mathbf{a}.$$

$\mathbf{H}(\mathbf{x})$ is an approximation for both $\mathbf{G}(\mathbf{x})$ and $\mathbf{G}'(\mathbf{x})$ with limits $\mathbf{r} = \frac{\mathbf{a}}{1-b}$ and

$$\mathbf{r}' = \frac{-\mathbf{a}}{1-b}.$$

If any sequence $\mathbf{W}_n$ has a point of accumulation $\mathbf{W}$ such that

$$|\mathbf{W} - \mathbf{r}| < \frac{|\mathbf{a}|}{1-b},$$

then by the triangular inequality,

$$|\mathbf{W} - \mathbf{r}'| > \frac{|\mathbf{a}|}{1-b}$$

and the process (4) provides in this case better information.

3. Round-off Errors. For the computer, the process (1) can be written in the form

$$y_{n+1}^{(i)} = [G^{(i)}(\mathbf{y}_n) + \xi_n^{(i)}]_R;$$

$y_n^{(i)}$ is an integer. $[]_R$ is called a *rounding procedure*. $[x]_R$ is any integer-valued function of x satisfying the inequality:

$$|[x]_R - x| < 1.$$

We consider two particular types of rounding procedures:

- 1) Normal rounding: $[x]_N = [x + 0.5]$;
- 2) Anomalous rounding: $[x]_A$: for $|x| \leq 1$, $|[x]_A| \geq |x|$;
for $|x| \geq 1$, $|[x]_A| \leq |x|$.

THEOREM 3. *Let G and ξ satisfy equations (2) and (3). If*

$$(6) \quad y_{n+1}^{(i)} = [G^{(i)}(y_n) + \xi_n^{(i)}]_N, \quad i = 1, 2 \dots m,$$

then for any y_0 , there exists N such that

$$|y_n - r| \leq \frac{|a|}{1-b} + \frac{\sqrt{m}}{2(1-b)} \quad \text{for } n > N;$$

furthermore, for given a and b , there exists a function G and errors ξ_n for which the bound is attained.

Now, we restrict ourselves to the particular case $m = 1$; i.e., the process (1) becomes scalar. Equations (1), (2), (3), and (5) can be written as:

$$(7) \quad x_{n+1} = G(x_n);$$

$$(8) \quad |G(x) - r| \leq b|x - r|;$$

$$(9) \quad y_{n+1} = [G(y_n) + \xi_n]_R;$$

$$(10) \quad |\xi_n| \leq a;$$

THEOREM 4. *Let $G(x)$ and ξ_n satisfy equations (8) and (10). If*

$$(11) \quad y_{n+1} = y_n + [G(y_n) + \xi_n - y_n]_A,$$

then for any y_0 , there exists N such that

$$|y_{n+1} - r| < \frac{a}{1-b} + 1 \quad \text{for } n > N.$$

Let us compare Theorem 4 with Theorem 3 for $m = 1$. In both cases, the bounds of errors have a common part which can be recognized from Theorems 1 and 2 as provided by the truncation errors. The part due to the round-off errors is independent of b for the anomalous rounding; in particular, if $a = 0$, the error is less than 1 and if the limit r is an integer, it is reached after a finite number of steps. When the convergence is slow, i.e., $b \sim 1$, the errors can be very large for the normal rounding, even if $a = 0$; however, if $b < 0.5$, the normal rounding provides slightly better results than the anomalous rounding.

Remark. The condition (2) insures a first-order convergence for the process (1). If we assume higher convergence, i.e., if

$$|G(x) - r| \leq b|x - r|^p, \quad p > 1,$$

we get results which are quite similar, but generally not simple to formulate. Rather roughly, Theorem 4 becomes: if y_n is computed by (11), then

$$|y_n - r| < B + 1 \quad \text{for } n > N,$$

where B is due to the truncation error.

4. Proofs.

LEMMA. Let $\mathbf{V}_1 = \mathbf{G}(\mathbf{V}_0) + \xi_0$ under assumptions (2) and (3);

$$\text{a) If } |\mathbf{V}_0 - \mathbf{r}| \leq \frac{|\mathbf{a}|}{1-b}, \text{ then } |\mathbf{V}_1 - \mathbf{r}| \leq \frac{|\mathbf{a}|}{1-b};$$

$$\text{b) If } |\mathbf{V}_0 - \mathbf{r}| > \frac{|\mathbf{a}|}{1-b}, \text{ then } |\mathbf{V}_1 - \mathbf{r}| < |\mathbf{V}_0 - \mathbf{r}|.$$

Proof. Since $\mathbf{V}_1 = \mathbf{G}(\mathbf{V}_0) + \xi_0$:

$$(12) \quad |\mathbf{V}_1 - \mathbf{r}| \leq |\mathbf{G}(\mathbf{V}_0) - \mathbf{r}| + |\xi_0| \leq b |\mathbf{V}_0 - \mathbf{r}| + |\mathbf{a}|;$$

$$\text{a) } |\mathbf{V}_0 - \mathbf{r}| \leq \frac{|\mathbf{a}|}{1-b}; \text{ we have by (12):}$$

$$|\mathbf{V}_1 - \mathbf{r}| \leq |\mathbf{a}| \left\{ \frac{b}{1-b} + 1 \right\} = \frac{|\mathbf{a}|}{1-b}, \text{ q.e.d.}$$

$$\text{b) } |\mathbf{V}_0 - \mathbf{r}| > \frac{|\mathbf{a}|}{1-b}; \text{ we have by (12):}$$

$$|\mathbf{V}_1 - \mathbf{r}| \leq |\mathbf{V}_0 - \mathbf{r}| - (1-b) |\mathbf{V}_0 - \mathbf{r}| + |\mathbf{a}| < |\mathbf{V}_0 - \mathbf{r}| - |\mathbf{a}| + |\mathbf{a}| = |\mathbf{V}_0 - \mathbf{r}|, \text{ q.e.d.}$$

Proof of Theorem 1. First case: There is N such that $|\mathbf{V}_N - \mathbf{r}| \leq \frac{|\mathbf{a}|}{1-b}$; by Lemma a, the same inequality holds for all $n > N$ and the theorem is proved.

Second case: For all $n = 0, 1, 2, \dots$: $|\mathbf{V}_n - \mathbf{r}| > \frac{|\mathbf{a}|}{1-b}$; by Lemma b, the positive sequence $|\mathbf{V}_n - \mathbf{r}|$ is monotone decreasing and converges therefore to a limit l .

Suppose that $l = \frac{|\mathbf{a}|}{1-b} + d$ where $d > 0$; since $b < 1$, there exists $\mathbf{V}_n$ such that $|\mathbf{V}_n - \mathbf{r}| < \frac{|\mathbf{a}|}{1-b} + \frac{d}{b}$; by (12):

$$|\mathbf{V}_{n+1} - \mathbf{r}| < \frac{b}{1-b} |\mathbf{a}| + d + |\mathbf{a}| = \frac{|\mathbf{a}|}{1-b} + d = l,$$

which is a contradiction.

Proof of Theorem 3. Since $|[x]_N - x| \leq 0.5$, we can write the equation (6) in the form

$$y_{n+1}^{(i)} = G^{(i)}(\mathbf{y}_n) + \eta_n^{(i)}, \quad i = 1, 2, \dots, m$$

where

$$|\eta_n^{(i)}| \leq a^{(i)} + 0.5,$$

and therefore

$$|\mathbf{n}_n| \leq |\mathbf{a}| + 0.5 \sqrt{m}.$$

Replacing ξ by $\mathbf{n}$ and $|\mathbf{a}|$ by $|\mathbf{a}| + 0.5\sqrt{m}$, we can apply Theorem 1: for any ϵ , there exists N such that

$$|\mathbf{y}_n - \mathbf{r}| < \frac{|\mathbf{a}| + 0.5\sqrt{m}}{1-b} + \epsilon \quad \text{for } n > N;$$

but since the $y_n^{(i)}$'s are integers, there exists a particular ϵ for which the preceding inequality implies

$$|\mathbf{y}_n - \mathbf{r}| \leq \frac{|\mathbf{a}| + 0.5\sqrt{m}}{1-b} \quad \text{for } n > N,$$

as desired. We have still to show an example valid for every $\mathbf{a}$ and b where the bound of error is attained. Let

$$G^{(i)}(\mathbf{x}) = bx^{(i)} - a^{(i)} - 0.5$$

and suppose that for the particular vector $\mathbf{y}_0 = 0$ we have $\xi_0 = \mathbf{a}$. Then

$$\mathbf{y}_n = 0 \quad \text{and} \quad |\mathbf{y}_n - \mathbf{r}| = \frac{|\mathbf{a}| + \sqrt{m} \cdot 0.5}{1-b} \quad \text{for } n \geq 0.$$

Proof of Theorem 4. We use the two simple properties of the anomalous rounding procedures:

1) $x - 1 < [x]_A < x + 1$;

2) If $p < x < q$ and $q - p > 1$, then

$$p < p + [x - p]_A < q, \quad \text{provided that } p \text{ is an integer, and}$$

$$p < q + [x - q]_A < q, \quad \text{provided that } q \text{ is an integer.}$$

Since the y_n 's are integers, the theorem results from the three statements:

I If $|y_0 - r| \leq \frac{a}{1-b}$, then $|y_1 - r| < \frac{a}{1-b} + 1$;

II If $\frac{a}{1-b} < |y_0 - r| < \frac{a}{1-b} + 1$, then $|y_1 - r| < \frac{a}{1-b} + 1$;

III If $|y_0 - r| \geq \frac{a}{1-b} + 1$, then $|y_1 - r| < |y_0 - r|$.

Statement I: By Lemma a:

$$r - \frac{a}{1-b} \leq y_0 + G(y_0) + \xi_0 - y_0 \leq r + \frac{a}{1-b};$$

By property 1:

$$r - \frac{a}{1-b} - 1 < y_0 + [G(y_0) + \xi_0 - y_0]_A < r + \frac{a}{1-b} + 1; \quad \text{i.e.,}$$

$$|y_1 - r| < r + \frac{a}{1-b} + 1, \quad \text{q.e.d.}$$

Statement II: We suppose $r + \frac{a}{1-b} < y_0 < r + \frac{a}{1-b} + 1$ (the proof is

analogous, when

$$r - \frac{a}{1-b} - 1 < y_0 < r - \frac{a}{1-b} \Big); \text{ by Lemma } b:$$

$$p \equiv r - \frac{a}{1-b} - 1 < y_0 + G(y_0) + \xi_0 - y_0 < y_0 \equiv q; \text{ since}$$

$$y_0 > r, \quad q - p > 1 \quad \text{and we apply property 2:}$$

$$r - \frac{a}{1-b} - 1 < y_0 + [G(y_0) + \xi_0 - y_0]_A < y_0 < r + \frac{a}{1-b} + 1; \text{ i.e.,}$$

$$|y_1 - r| < r + \frac{a}{1-b} + 1, \quad \text{q.e.d.}$$

Statement III: We suppose $y_0 \geq r + \frac{1}{1-b} + 1$ (the proof is analogous when

$$y_0 \leq r - \frac{a}{1-b} - 1 \Big); \text{ by Lemma } b:$$

$$p \equiv 2r - y_0 < y_0 + G(y_0) + \xi_0 - y_0 < y_0 \equiv q;$$

by property 2, since $q - p > 1$:

$$2r - y_0 < y_0 + [G(y_0) + \xi_0 - y_0]_A < y_0; \text{ i.e.,}$$

$$|y_1 - r| < |y_0 - r|, \quad \text{q.e.d.}$$

APPENDIX I: Iterative Processes with a Floating-Point Computer*

Let r be a real number and $G(x)$ be a function such that

$$(1) \quad |x + G(x) - r| \leq b |x - r| \quad \text{with } 0 \leq b < 1 \quad \text{for any } x;$$

then the sequence

$$(2) \quad x_{n+1} = x_n + G(x_n)$$

converges at least linearly to r for any x_0 .

Suppose we want to realize (2) on a binary floating-point computer, i.e., the numbers are of the form $\alpha \cdot 2^\beta$, where α is an exact binary fraction and β is an integer.

A number will be called *normalized* if 1) $0.5 \leq |\alpha| < 1$; 2) α is an exact binary fraction representable by N bits and the sign; 3) $\beta \geq -p$ (N and p are fixed numbers); furthermore there exists a *real zero*, representable for example by $\alpha = 0$, $\beta = -p$; for greater simplicity, this zero will also be included in the class of normalized numbers.

We assume that in the realization of (2) on the computer, both x_n and $G(x_n)$ are represented by normalized numbers; of course $G(x)$ cannot be computed exactly in general; so we assume that value effectively computed, $\tilde{G}(x)$, satisfies the relation:

$$(3) \quad \tilde{G}(x) = (1 + \eta)G(x) + \zeta; \quad |\eta| \leq d, |\zeta| \leq a;$$

* A detailed discussion of the results of this appendix will be found in reference [4].

where η and ζ are functions of x , but d and a are fixed numbers.

The effective process is given by the operation

$$(4) \quad Y_{n+1} = [Y_n + \tilde{G}(Y_n)]_R$$

where Y_n and Y_{n+1} are normalized numbers; since $Y_n + \tilde{G}(Y_n)$ cannot be generally represented by a normalized number, it must be rounded as indicated by $[\]_R$.

We concentrate our attention on the rounding procedure in (4) and consider two types of rounding procedures:

1) *Normal rounding*. $Y_{n+1} = [Y_n + \tilde{G}(Y_n)]_N$; Y_{n+1} is a normalized number such that

$$|Y_{n+1} - (Y_n + \tilde{G}(Y_n))| = \text{minimum};$$

when two different normalized numbers satisfy the above relation, either of them can be chosen as Y_{n+1} .

2) *Anomalous rounding*. $Y_{n+1} = [Y_n + \tilde{G}(Y_n)]_A$; if $\tilde{G}(Y_n) \geq 0$ let

Z be the smallest normalized number such that $Z \geq Y_n + \tilde{G}(Y_n)$,

W be the greatest normalized number such that $W \leq Y_n + \tilde{G}(Y_n)$;

if $\tilde{G}(Y_n) \leq 0$ let

Z be the greatest normalized number such that $Z \leq Y_n + \tilde{G}(Y_n)$,

W be the smallest normalized number such that $W \geq Y_n + \tilde{G}(Y_n)$;

then

$$\begin{aligned} [Y_n + \tilde{G}(Y_n)]_A &= W \quad \text{if } W \neq Y_n \\ [Y_n + \tilde{G}(Y_n)]_A &= Z \quad \text{if } W = Y_n. \end{aligned}$$

THEOREM. a) For any Y_0 , by using normal rounding in (4), there exists a finite number M such that

$$|Y_n - r| \leq B_N \equiv \frac{2^{-N} |r| + a(1 + 2^{-N})}{2 + 2^{-N} - (1 + d)(1 + b)(1 + 2^{-N})} \quad \text{for } n > M.$$

b) For any Y_0 , by using anomalous rounding in (4), there exists a finite number M such that

$$|Y_n - r| < B_A \equiv |r| 2^{-N+1} + 2^{-p-1} + \frac{a(1 + 2^{-N+1})}{2 - (1 + d)(1 + b)} \quad \text{for } n > M.$$

If B_N or B_A is negative, it must be replaced by $+\infty$.

In order to compare these results, first suppose $a = 0$. Then B_A is independent of b and d and furthermore remains very small; in case of slow convergence, i.e., when $b \cong 1$, B_N can become very large. The increase of magnitude of the bounds when $a > 0$ is almost the same for B_A and B_N for reasonable cases, so that the anomalous rounding can be considered safer than the normal rounding.

Remarks. 1) The relations of normal and anomalous rounding procedures are very similar in fixed-point and in floating-point arithmetics;

2) The bounds B_A and B_N are reached only in trivial cases; however, examples show that they remain realistic in every case.

APPENDIX II: Round-off Errors in Aitken's δ^2 Process*

Let $G(x)$ be a real continuous function of the real variable x such that the sequence x_n defined by

$$(1) \quad x_{n+1} = G(x_n)$$

converges to the limit $x = r$.

By Aitken's δ^2 process, we define another sequence:

$$(2) \quad \begin{cases} V_{3n+1} = G(V_{3n}) \\ V_{3n+2} = G(V_{3n+1}) \\ V_{3n+2} = \frac{V_{3n} V_{3n+2} - V_{3n+1}^2}{V_{3n} + V_{3n+2} - 2V_{3n+1}} \end{cases}$$

Let us suppose we want to realize process (2) on a *fixed-point computer* with the following conditions: a) We use only one "word" for representing the V_i 's; we may consider the content of the word as an *integer*; b) We may use higher precision for computing $G(V_i)$.

We cannot expect to compute $G(V_i)$ without error; furthermore, if we are using higher precision, the result must be rounded to an integer.

Definition. A *rounding procedure* denoted by $[x]_R$ is any integer-valued function of the real variable x satisfying the inequality:

$$| [x]_R - x | < 1.$$

We shall use the following particular rounding procedures:

1) $[x]^\nearrow$: *rounding away from zero*; it is defined by the inequality

$$| [x]^\nearrow | \geq | x |;$$

2) $[x]^\swarrow$: *rounding toward zero*; it is defined by the inequality

$$| [x]^\swarrow | \leq | x |.$$

Example. Let $G(x) = 7/8 x$ and $V_0 = 8$; by (2), we have

$$V_1 = 7$$

$$V_2 = 6,125$$

$$V_3 = 0.$$

If we want to represent the V_i 's only by integers and if we use the normal rounding procedure, we shall find:

$$\bar{V}_1 = 7$$

$$\bar{V}_2 = 6$$

$$\bar{V}_3 = \infty.$$

* For the proof see reference [3], part II.

This situation can be improved by using the following integer process:

$$(3) \quad \begin{cases} W_{3n+1} = W_{3n} + [G(W_{3n}) + \xi_{3n} - W_{3n}]^{\nearrow} \\ W_{3n+2} = W_{3n} + [G(W_{3n+1}) + \xi_{3n+1} - W_{3n}]^{\nwarrow} \\ W_{3n+3} = W_{3n} + \left[\frac{(W_{3n} - W_{3n+1})^2}{2W_{3n+1} - W_{3n} - W_{3n+2}} \right]. \end{cases}$$

ξ_{3n} and ξ_{3n+1} are the errors of computation of $G(W_{3n})$ and $G(W_{3n+1})$; since the numerator and the denominator are integers, it is possible with the help of the remainder to compute W_{3n+3} without any error; if the numerator and the denominator are simultaneously equal to zero, then $W_{3n} = W_{3n+1} = W_{3n+2}$ and we set $W_{3n+3} = W_{3n}$.

THEOREM 1. *We suppose there exist numbers $0 \leq b < 1$, $0 \leq c < 1$, $\delta \geq 0$ such that:*

$$1) \quad |x_1 - r| \leq b |x_0 - r|$$

for any x_0 and x_1 satisfying the relation (1);

$$2) \quad |V_3 - r| \leq c |V_0 - r|$$

for any V_0 and V_3 satisfying the relations (2);

$$3) \quad |G(x) - G(y)| \leq \delta |x - y|$$

for any x and y ;

4) the errors ξ_{3n} and ξ_{3n+1} in (3) satisfy the inequality

$$|\xi_j| \leq a \leq d = \frac{1}{4} \frac{(1-b)^2(1-c)}{(1+c)(1+\delta)};$$

then, for any W_0 there exists a finite number N such that

$$|W_{3n} - r| < 1 + \frac{a}{1-b} \quad \text{for } n > N.$$

THEOREM 2. *We make the assumptions:*

1) *The convergence of process (1) is alternating, i.e., for any x*

$$0 \leq r - G(x) < x - r \quad \text{if } x - r > 0,$$

$$0 \leq G(x) - r < r - x \quad \text{if } x - r < 0,$$

$$G(x) = r \quad \text{if } x = r;$$

2) *The errors ξ_{3n} and ξ_{3n+1} in (3) satisfy the inequality*

$$|\xi_j| \leq a \leq \frac{1}{3},$$

where a is a fixed number; then, for any W_0 there exists a finite number N such that

$$|W_{3n} - r| \leq 1 + a \quad \text{for } n > N.$$

Remark. Assumption (1) of Theorem 2 is sufficient for providing the conver-

gence of the V_n 's satisfying the equations (2) for any V_0 . It is easy to prove the inequality:

$$|V_{3n} - r| < \frac{|V_0 - r|}{3^n}.$$

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