Linear Model Analysis of Observational Data in the Sense of Least –Squares Criterion

J.A.Basabrain[*]

Department of Statistics College of Science for Girls, King Abdulaziz University, Jeddah, Saudi Arabia
*Corresponding author: jbasabrain@yahoo.com

Abstract The present paper is devoted for the following goals: To develop an algorithm for model analysis of observational data in the sense of the least –squares criterion with full error analysis.. By this algorithm one computes, all the solutions with their variances, the variance of the fit, the average square distance between the least square solution and the exact solution, and graphical representation between the row and the fitted data. Mathematica module of the algorithm was established, through five points, its purpose –input - output –needed procedures and the list of the module. By this paper we have been tried to produce an error controlled algorithm of the least squares method for observational data.

Keywords: statistical data analysis -least squares method, mathematica simulations

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1. Introduction

One of the hallmarks of modern astrophysics is the extreme rise in the amount of data available and the prevalence of images and other data in electronic form particularly that available to the public via the Internet. The present situation is in marked contrast to the view given by Kolb and Turner [1] more than 25 years ago who lamented that in cosmology at that time there was a paucity of data. There are now so many people involved with data reduction and analysis that in the last decadal survey there was a call for the formation of a new area of astronomy and astrophysics called *astroinformatics* [3]. Latest information on this rapidly emerging discipline can be found with listings on the Internet through a Google or similar search under that name.

Astronomers and astrophysicists have always shared data and it is even truer today than ever before. The electronic data revolution for astrophysics and astronomy took real hold in the pre-Hubble spacecraft days with the establishment of the NASA/ADC (Astronomical Data Center) when catalogs listing data about a number of stars and other objects were digitized, recorded on CDs, and distributed at national and international meetings for free.

Although the least-squares method is the most powerful techniques that has been devised for the problems of data analysis, it is at the same time exceedingly critical. This is because the least-squares method suffers from the deficiency that, its estimation procedure does not have detecting and controlling techniques for the sensitivity of the solution to the optimization criterion of the variance $\tilde{\sigma}^2$ is minimum. As a result, there may exist a situation in which there are many significantly different solutions that

reduce the variance $\tilde{\sigma}^2$ to an acceptable small value. At this stage we should point out that (1) the accuracy of the estimators and the accuracy of the fitted curve are to distinct problems; and (2) an accurate estimator will always produce small variance, but small variance does not guarantee an accurate estimator. This could be seen from property 3 (Section 3) of the least square solution by noting that the lower bounds for the average square distance between the exact and the least-squares values is $\tilde{\sigma}^2 / \lambda_{min}$ which may be large even if $\tilde{\sigma}^2$ is very small, depending on the magnitude of the minimum eigenvalue, λ_{min}, of the coefficient matrix of the least-squares normal equations.

Unless detecting and controlling the above mentioned situation, it is not possible to make a well-defined diction about the analysis of the observational data. Due to this difficulty and the importance of least squares for treating the nowadays incredible numbers of the available data, the present paper is devoted for the following goals :To develop an algorithm for model analysis of observational data in the sense of the least –squares criterion with error analysis.. By this algorithm one computes, all the solutions with their variances, the variance o the fit, the average square distance between the least square solution an the exact solution an graphical representation between the row and the fitted data. Mathematica module of the algorithm is also given.

2. Observational Data

Let $\{x_k\}; k = 1,2,....,m,$ be a sequences of observational data points assumed free from errors. Corresponding to

each x_k we have a number $\overline{f}_k$ of some function f(x) at x_k which generally will be in error. Denote $f(x_k)$, the true value at x_k, by f_k and define:

$$\delta_k = \overline{f}_k - f_k \ ; \ k = 1,2,....,m \qquad (1)$$

as the observational errors at different data points.

The problem in the analysis of the observational data is to approximate or fit the data $\overline{f}_k$ by some function $\hat{p}(x)$ in such a way that $\hat{p}(x)$ contains or represents most (if not all) the information about f(x) contained in the data and little (if any) of the errors. This is accomplished in practice by selecting a function

$$p(x) = p(x; c_1^{(n)}, c_2^{(n)}, \cdots, c_n^{(n)}), \qquad (2)$$

which depends on the parameters ; $c_1^{(n)}, c_2^{(n)}, \cdots, c_n^{(n)}$. (The superscript n on $c_i^{(n)}$ denotes the fact that they will (generally depend on n). The function p(x) may be linear or non-linear in the parameters $c_i^{(n)}$.

Since our study is the linear model analysis of the observational data, the function p(x) will be selected as linear combinations of the parameters so that it takes the form:

$$p(x) = \sum_{i=1}^{n} c_i^{(n)} \Phi_i(x). \qquad (3)$$

The $\{\Phi_i\}$ may, for example, be the set of monomials, exponentials, trigonometric polynomials, or indeed any arbitrary set of sufficiently defined functional values, provided only that they are *linearly independent* of the m values of x. Normally, n is small compared with the number, m of data points. In fact, the number n is unknown but for the most appropriate approximation to a given data the number n should be :

1-large enough so that the information about f(x) in the data can well be represented by a proper choice of the parameters $c_i^{(n)}$, while at the same time n should be,

2-too small to avoid the fitting of the observed data too closely in the sense that the errors in the observed data are retained in the approximation.

Now the problem is to find the *best* estimate $\hat{p}$ of the function p i.e, to determine particular values $\hat{c}_1^{(n)}, \hat{c}_2^{(n)}, ..., \hat{c}_n^{(n)}$ for the parameters $c_i^{(n)}$ to obtain the best approximation:

$$\hat{p} = p(x, \hat{c}_1^{(n)}, \hat{c}_2^{(n)}, \cdots, \hat{c}_n^{(n)}) \qquad (4)$$

Although there is agreement that the best estimate should give small deviations of the given data from the fitted curve- i.e., that the modulus of the quantity :

$$\varepsilon_k = p\left(x_k, c_1^{(n)}, c_2^{(n)}, ..., c_n^{(n)}\right) - \overline{f}_k \ ; \ k = 1,2,...,m \qquad (5)$$

should be small at each of the m points- there are differences of opinion as to how this to be achieved.

Let ε denote an error vector composed of the m deviations ε_k. Since x_k and $\overline{f}_k$ are regarded as fixed, the vector ε depends only on the parameters $c_1^{(n)}, c_2^{(n)}, ..., c_n^{(n)}$. Each common method for dealing with the competing requirements that ε_k are small, corresponds to the selection of a *norm* $\|\varepsilon\|$ for the vector ε. Some examples of norms in the real m- dimensional space are :

(i)
$$\|\varepsilon\|_1 \equiv \sum_{k=1}^{m} |\varepsilon_k| \qquad (6)$$

(ii)
$$\|\varepsilon\|_2 \equiv \left(\sum_{k=1}^{m} \varepsilon_k^2\right)^{1/2} \qquad (7)$$

(iii)
$$\|\varepsilon\|_\infty \equiv \max_{1 \le k \le m} |\varepsilon_k|. \qquad (8)$$

The norm $\|\bullet\|_1$ is called *Gershgorin norm*, $\|\bullet\|_2$ the *Euclidean norm* and $\|\bullet\|_\infty$ the*maximum norm*or, occasionally, the *uniform norm*. For any choice norm $\|\varepsilon\|$,the best estimate is one satisfying the requirement:

$$\| \varepsilon \| = \text{minimum}. \qquad (9)$$

Assuming one of the above norms, say the Q norm is chosen, then we can determine (by solving certain system of equations) the *estimators* $\hat{c}_i^{(n)}$ of the best estimate $\hat{p}$ of p that satisfies Equation (9), i.e., for the linear model analysis we have the best approximation:

$$\hat{p}(x) = \sum_{i=1}^{n} \hat{c}_i^{(n)} \Phi_i(x), \qquad (10)$$

to be the true function f(x) over $\{x_k\}$ in the sense of the Q norm fitting for the given $\Phi_i(x)$. Our best assumption is that for some unknown value of n, say N, the true function f(x) can be expressed as a finite linear combination of the selected set of functions $\{\Phi_i\}$ in the sense of the Q–norm fitting ;that is, we assume

$$f(x) = \sum_{i=1}^{N} \hat{c}_i^{(n)} \Phi_i(x) \qquad (11)$$

such that the Q norm of

$$\overline{f} - \sum_{i=1}^{n} \hat{c}_i^{(n)} \Phi_i(x_k) \equiv \text{minimum}, \ k = 1,2,\cdots,m; m \succ n \qquad (12)$$

for some n = N and for a given $\Phi_i(x)$. Equation (11),with the condition of Equation (12), are the formulation of the linear model analysis of the observational data in the sense of Q-norm fitting.

Now it remains to decide what is the most efficient norm that should be used in the analysis of observational data. This decision constitutes very serious difficultly because:

1- The l norm $\|\boldsymbol{\varepsilon}\|_l$ depends greatly on the distributions of the observational errors δ_k.

2- There is a large variation in the effectiveness of various norms and no single norm is good (or even mediocre).

3- The distributions of the observational errors cannot be determined with any precision.

It is undoubtedly true that the Euclidean norm is the most efficient when δ_k. are normally distributed, and in this case the estimators are the maximum likelihood *estimators*. It is natural therefore, to consider in our study the assumption that δ_k .are normally distributed and analyzed the linear –model representation of the observational data in the sense of the Euclidean norm-i.e., in the *least –squares criterion.*

Before starting the analysis, however, we introduce additional conditions concerning the character of the errors δ_k and assume that $\delta_1, \delta_2, \cdots, \delta_k$ are unbiased (without systematic error),independent and normally distributed with zero mean and variance $\tilde{\sigma}^2$. These conditions indicate that:

$$E(\delta_k) = 0, E(\delta_p \delta_q) = E(\delta_p)E(\delta_q);$$

$$\delta_k \varepsilon N(0, \tilde{\sigma}); \sigma_k^2 = E(\delta_k^2) = \tilde{\sigma}^2$$

E(z) being the expectations of z and $\tilde{\sigma}^2$ the unknown variance.

In the case of weighted observations, Equation (16) is replaced by:

$$\sigma_k^2 = E(\delta_k^2) = \frac{\tilde{\sigma}^2}{\omega_k}, \qquad (13)$$

where ω_k are the weights of the observations ($\omega_k = \omega(x_k)$). Therefore the problem of this section is the application of the least-squares method for the linear model representation of the observational data.

3. Least-squares Approximation

Below is a list of vectors and matrices used in the present section:

Symbol	Order	Element
$\overline{\mathbf{F}}$	$m \times 1$	$\overline{f}_k$
$\mathbf{F}$	$m \times 1$	f_k
$\boldsymbol{\delta}$	$m \times 1$	δ_k
$\hat{\mathbf{C}}$	$n \times 1$	$\hat{c}_i^{(n)}$
$\mathbf{C}$	$n \times 1$	$c_i^{(n)}$
$\boldsymbol{\Phi}$	$n \times m$	$\Phi_{ik} = \Phi_i(x_k)$
$\boldsymbol{\omega}$	$m \times m$	$\omega_{kk} = \omega_k; \omega_{ql} = 0; q \neq l.$

The transpose of a vector or a matrix will be indicated by the superscript 'T'.

3.1. Derivation of the Normal Equations

In matrix notation, the problem of the weighted least-squares approximation is to determine the estimators $\hat{\mathbf{C}}$ such that

$$e_n(\hat{\mathbf{C}}) = \mathbf{v}^T \boldsymbol{\omega} \, \mathbf{v} = \text{minimum}, \qquad (14)$$

where the vector of the residuals $\mathbf{v}$ is defined as

$$\mathbf{v} = \overline{\mathbf{F}} - \boldsymbol{\Phi}^T \hat{\mathbf{C}}. \qquad (15)$$

From Equations (14) and (15) we have ;

$$e_n(\hat{\mathbf{C}}) = (\overline{\mathbf{F}} - \boldsymbol{\Phi}^T \hat{\mathbf{C}})^T \boldsymbol{\omega} \, (\overline{\mathbf{F}} - \boldsymbol{\Phi}^T \hat{\mathbf{C}})$$

$$= (\overline{\mathbf{F}}^T - \hat{\mathbf{C}}^T \boldsymbol{\Phi}) \boldsymbol{\omega} \, (\overline{\mathbf{F}} - \boldsymbol{\Phi}^T \hat{\mathbf{C}})$$

$$= (\overline{\mathbf{F}}^T \boldsymbol{\omega} - \hat{\mathbf{C}}^T \boldsymbol{\Phi}\boldsymbol{\omega}) \, (\overline{\mathbf{F}} - \boldsymbol{\Phi}^T \hat{\mathbf{C}})$$

that is

$$e_n(\hat{\mathbf{C}}) = \overline{\mathbf{F}}^T \boldsymbol{\omega} \overline{\mathbf{F}} - \hat{\mathbf{C}}^T \boldsymbol{\Phi}\boldsymbol{\omega}\overline{\mathbf{F}} - \overline{\mathbf{F}}^T \boldsymbol{\omega}\boldsymbol{\Phi}^T \hat{\mathbf{C}} + \hat{\mathbf{C}}^T \boldsymbol{\Phi}\boldsymbol{\omega}\boldsymbol{\Phi}^T \hat{\mathbf{C}}. \quad (16)$$

Since $\overline{\mathbf{F}}^T \boldsymbol{\omega}\boldsymbol{\Phi}^T \hat{\mathbf{C}}$ is scalar then,

$$\overline{\mathbf{F}}^T \boldsymbol{\omega}\boldsymbol{\Phi}^T \hat{\mathbf{C}} = (\overline{\mathbf{F}}^T \boldsymbol{\omega}\boldsymbol{\Phi}^T \hat{\mathbf{C}})^T = [(\boldsymbol{\Phi}^T \hat{\mathbf{C}})^T . (\overline{\mathbf{F}}^T \boldsymbol{\omega})^T]$$

that is:

$$\overline{\mathbf{F}}^T \boldsymbol{\omega}\boldsymbol{\Phi}^T \hat{\mathbf{C}} = \hat{\mathbf{C}}^T \boldsymbol{\Phi}\boldsymbol{\omega}^T \overline{\mathbf{F}}, \qquad (17)$$

since

$$\boldsymbol{\omega}^T = \boldsymbol{\omega}, \qquad (18)$$

then

$$\overline{\mathbf{F}}^T \boldsymbol{\omega}\boldsymbol{\Phi}^T \hat{\mathbf{C}} = \hat{\mathbf{C}}^T \boldsymbol{\Phi}\boldsymbol{\omega}\overline{\mathbf{F}} \qquad (19)$$

From Equations (16) and (19) we get ;

$$e_n(\hat{\mathbf{C}}) = \overline{\mathbf{F}}^T \boldsymbol{\omega}\overline{\mathbf{F}} - 2\hat{\mathbf{C}}^T \boldsymbol{\Phi}\boldsymbol{\omega}\overline{\mathbf{F}} + \hat{\mathbf{C}}^T \boldsymbol{\Phi}\boldsymbol{\omega}\boldsymbol{\Phi}^T \hat{\mathbf{C}}. \qquad (20)$$

Equation (20) could be written as:

$$e_n(\hat{\mathbf{C}}) = \text{constant} - 2\hat{\mathbf{C}}^T \mathbf{b} + \hat{\mathbf{C}}^T \mathbf{G} \, \hat{\mathbf{C}}. \qquad (21)$$

$$\left. \begin{aligned} \text{constant} &\equiv \overline{\mathbf{F}}^T \boldsymbol{\omega}\overline{\mathbf{F}} \\ \mathbf{b} &\equiv \boldsymbol{\Phi}\boldsymbol{\omega}\overline{\mathbf{F}} \\ \mathbf{G} &\equiv \boldsymbol{\Phi}\boldsymbol{\omega}\boldsymbol{\Phi}^T \end{aligned} \right\} \qquad (22)$$

The necessary conditions for the minimum are

$$\frac{\partial e_n(\hat{\mathbf{C}})}{\partial \hat{\mathbf{C}}} = \mathbf{0}.$$

Consequently, from Equation (21) we get

$$-2\mathbf{b} + 2\mathbf{G}\hat{\mathbf{C}} = \mathbf{0}, \qquad (23)$$

therefore

$$\mathbf{G}\hat{\mathbf{C}} = \mathbf{b} \qquad (24)$$

where the general elements are given by

$$g_{ij} = \sum_{k=1}^{m} \omega_k \Phi_{ik} \Phi_{jk} \qquad (25)$$

and

$$b_i = \sum_{k=1}^{m} \omega_k \Phi_{ik} \overline{f}_k. \qquad (26)$$

Equations (24) are called the *normal equations* of the weighted least-squares approximations for the linear – model representations of the observational data. These equations represent a set of n *linear equations* in n unknowns $\hat{c}_i^{(n)}; i = 1, 2, \cdots, n$. The coefficient matrix **G** is symmetric and is positive definite (i.e., all eigen values $\lambda_i; i = 1, 2, \cdots, n$ are positive) if all the fundamental functions $\Phi_i(x)$ are linearly independent for the arguments x_k; that is, if the rows of **Φ** are linearly independent. It should be noted that the normal Equations (24) represent a relation between two exact quantities in the sense that if the matrix **G** and the right-hand side **b** represent the observational data exactly, then there is a vector $\hat{\mathbf{C}}$ which satisfies exactly the least –squares criterion. Of course, in practice such an exact situation no longer exists. In the following section, some important properties of $\hat{\mathbf{C}}$ (in the sense described above) will be given.

3.2. Some Properties of $\hat{C}$

According to the conditions of Equations (13) and (17) it was proved [1] the following properties of $\hat{\mathbf{C}}$:

Property 1

1- *The estimators $\hat{c}$ by the method of least-squares gives the minimum of* e_n

Property 2

2- *The estimators $\hat{\mathbf{C}}$ by the parameters **C**, obtained by the method of least-squares are unbiased; i.e.*

$$E(\hat{\mathbf{C}}) = \mathbf{C}.$$

Property 3

3- *The variance –covariance matrix $Var(\hat{\mathbf{C}})$ of the unbiased estimators $\hat{c}$ is given by*

$$Var(\hat{\mathbf{C}}) = \tilde{\sigma}^2 \mathbf{G}^{-1}.$$

Property 4

4- *The average squared distance between $\hat{\mathbf{C}}$ and **C** is*

$$E(L^2) = \tilde{\sigma}^2 \sum_{i=1}^{n} \frac{1}{\lambda_i}$$

Property 5

5- *The average squared Euclidean norm of $\hat{\mathbf{C}}$ is*

$$E(\hat{\mathbf{C}}^T \hat{\mathbf{C}}) = \mathbf{C}^T \mathbf{C} + \tilde{\sigma}^2 \sum_{i=1}^{n} \frac{1}{\lambda_i}$$

Also it should be noted that:

®If H(u) is a function of a measured quantity u, then the standard error $\tilde{\sigma}_H$ then

$$\tilde{\sigma}_H = \frac{dH}{du}\tilde{\sigma}_u \qquad (27)$$

where $\tilde{\sigma}_u$ is the standard error of u

® If the precision is measured by the probable error e, then

$$e = 0.6745\ \tilde{\sigma}. \qquad (28)$$

4. Mathematica Simulation

4.1. Mathematica Module: Linear Model

● **Purpose**

To fit observational data (x,y)(say) to the linear model $y = \sum c_i \Phi_i(x)$ in the sense of least-squares criterion with its error analysis.

● **Input**

x1 : List of the independet varibles of the data.

y1 : List of the dependet varibles of the data.

f : List of the basic functions used for the linear model representation of the data.

I1 ,I2 ,I3 : Positive numbers each $\varepsilon[0,1]$ used to disply color drawing according to the built in function **Backgroung** $\rightarrow$ **RGBColor[I1, I2, I3]** .

ind : A charcter indecating the name of the independent variable, (x for example).

dep: A charcter indecating the name of the dependent variable, (y for example).

● **Output**

The c's coefficients and their probable errors.

The probable error of the fit.

The average square distance between the exact and the least squares solutions.

Graphical representations

● **Needed procedures**

None

● **List of the Module**

```
LinearModel [x1_List,y1_List,I1_,I2_,I3_,ind_,dep_] :=
Module[{str, stt, n, m, b, eO, ma, mai, qf, pro, dcs, ei,qv, es, sx, sy, sx2, sy2,sxy, rc}

( str=Min[x1];stt=Max[x1];n=Length[f];m= Length[xl];

Print[ StyleForm["Liner Least –Squares  Fit by the Model: ",FontWeight->"Bold",

FontSize->12],

StyleForm{dep, ” ",fontWeight->"Bold",FontSize-> 12],

StyleForm{=, ” ",FontWeight->"Bold",FontSize-> 12],

StyleForm{" ∑ᵢ₌₁ⁿ ci Φi,Where ",fontWeight->"Bold",FontSize-> 12],

StyleForm[f[[i]]/ξ-> ind//TraditionalForm, FontWeight->"Bold",FontSize->12]], {i,1,n}],

C [l_,k_] := f [[ l ]] /. ξ -> xl [{ k }] ;

B = Table [ Sum [ C [ i, k ] * yl[[k]], {k, m}], {i, 1,n}]; e0=Sum[y1[[k]] ^2, {k, m}];

ma= Table[Which[i<=j,g[I,j] = ∑ₖ₌₁ᵐ c[ i , k] * c[j, k],i > j ,

g{i,j]=g[j,i]] ,{i,1,n}, {j,1,n}] ; mai=Inverse[ma];  cs=mai.b; qf=Expand[cs.ma.cs];

sigma=Sqrt(e0-qf)/ (m-n)]; pro=0.6745  * sigma;dcs=pro * Table[sqrt[mai[[i,i]]], {i,1,n}];

ei=Eigenvalues[N[ma]]; qv=sigma ^2 * Sum[1./ei[[j]], {j,n}]; es=qv+Sum[cs[[k]]^2,{k,n}];

funFit= ∑ᵢ₌₁ⁿ cs [[ i ]] * f[[i]];sx=Apply[plus,x1];sy= Apply[plus,y1] ; sx2 Apply[plus, x1^2];

sy2= Apply[Plus,y1^2]; sxy= Apply[plus, x1*y1];
```

```
Print[   StyleForm["(2) The Solutions and their probable Errors" ,FontWeight-›"Bold",

FontSize-› Do[Print[StyleForm["="ci,FontWeight-›"Bold",FontSize-›l2],

StyleForm["=",FontWeight-›"Bold", FontSize-› 12],

StyleForm[cs[[i]],FontWeight-›"Bold", FontSize->l2],StyleForm["±" ,FontWeight-›"Bold",FontSize

    StyleForm[dcs[[i]],FontWeight-›"Bold", FontSize-›l2]],{i,l,n}],

Print[ StyleForm["(3) The Probable Error of the Fit is" ,FontWeight->"Bold", FontSize->l2]];

Print[ StyleForm[" "e,FontWeight-› Bold", FontSize->12],

StyleForm["=", FontWeight-›"Bold", FontSize-›12],


StyleForm[pro,fontWeight-›"Bold", FontSize-›12]];

Print[ StyleForm["(4) The Average Squared Distance Between ĉ and c is" ,

  FontWeight-›"Bold",fontSize-› 12]];

Print[StyleForm[" "Q, FontWeight-›"Bo1d",FontSize-›

12], StyleForm["=",FontWeight-›"Bold",FontSize-›12],

StyleForm[qv,FontWeight-›"Bold",FontSize-›12]] ;

Print[ styleForm["(5) Graphical Representations" ,FontWeight-›"Bold,FontSize-›12]];

Print[ StyleForm[" 5-a GraphoftheRawData" ,FontWeight->"Bold",FontSize-›12]];

datacorr=Table[{x1[[i]],yl[[i]]}, {i,1,m}];dataPlot=ListPlot[datacorr, PlotStyle-› PointSize[O.

Background→RGBColor[I1, I2,I3],AxesLabel→ {"x","y"}];

 Print[ StyleForm["  5-b GraphoftheRaw and the Fitted Data " ,

   FontWeight-› "Bold",FontSize->l2]];

fitPlot=Plot[funFit/. ξ-› ʋ , {ʋ, str, stt}, Plotable →"v",DisplayFunction -›

   Identity];

 Show[{dataPlot, fitPlot}, DisplayFunction -› $DisplayFunction]; ) ]
```

We applied this module for many problems for galactic structure, the results are very satisfactory and will be published soon in astronomical journals

In concluding the present paper, an algorithm for model analysis of observational data was deloped in the sense of the least –squares criterion with full error analysis.. By

this algorithm one computes, all the solutions with their variances, the variance of the fit, the average square distance between the least square solution and the exact solution, and graphical representation between the row and the fitted data. Mathematica module of the algorithm was established, through five points, its purpose –input - output - needed procedures and the list of the module. By this paper we have been tried to produce an error controlled algorithm of the least squares method for observational data.

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