GENDEX: FFD MODULE FOR CONSTRUCTING ORTHOGONAL OR NEAR-ORTHOGONAL FRACTIONAL REPLICATE AND RESPONSE SURFACE TREATMENT DESIGNS

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ABSTRACT

The FFD module of the toolkit Gendex may be used to construct 2-level fractional replicates for $2 \leq m \leq 15$ factors. Resolution III, IV, and V fractional replicates may be created with this module. Response surface designs, RSDs, may also be constructed with this module for $2 \leq m \leq 9$ factors. Variable numbers of center points may be selected. A randomized form of the treatment combinations, the information matrix X'X, and its inverse are given in the output. The plans are orthogonal or near-orthogonal. Several examples are presented to illustrate the use of this module.

Keywords: Fractional replicate, Resolution III, IV, and V, 2-level factor. 3-level factor, Interaction, Design matrix, Main effect plan.

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INTRODUCTION

The FFD module in the toolkit Gendex is a program for constructing orthogonal or near-orthogonal 2-level fractional replicates of a complete factorial design (FFD) and response surface designs (RSDs). The 3-level factor option is only used only to construct RSDs and not FFDs. The FFD program can also augment an existing design with additional factors. A single degree of freedom set of contrasts is used as the input for augmenting a 2-level factor FFD.

For an orthogonal 2-level m-factor FFD in n runs with the design matrix $\mathbf{X}$, the $\mathbf{A} = \mathbf{X}'\mathbf{X}$ matrix takes the form $n\mathbf{I}_p$ and $\mathbf{A}^{-1}$ takes the form $(1/n)\mathbf{I}_p$, where p is the number of parameters. The row of the $\mathbf{X}$ matrix is a p-dimensional row vector $(1, x_1, \ldots x_m, x_1^2, \ldots, x_m^2)$ When $p > n$, $\mathbf{X}'\mathbf{X}$ is still a p p matrix (not n n) and $\mathbf{X}'\mathbf{X}$ is singular. Imposing the conditions $\Sigma_j x_{ij} = \Sigma_j x_{ij}^3 = \Sigma_j x_{ij} x_{uj} = \Sigma_j x_{ij}^2 x_{ij} = \Sigma_j x_{ij}^3 x_{ij} = 0$, $\Sigma_j x_{ij}^2 = b$, $\Sigma_j x_{ij}^2 x_{uj}^2 = c$, and $\Sigma_j x_{ij}^4 = c + d$ $(i, u = 1, \ldots, m;\ i \neq u;\ j = 1, \ldots, n)$ upon a (second order) m-factor RSD in n runs, the A matrix will take the form

$$\left|\begin{array}{lll} n & \mathbf{0}'_r & b\mathbf{1}'_m \\ \mathbf{0}_r & \mathrm{diag}(b,\ldots,c) & \mathbf{0}_{r\times m} \\ b\mathbf{1}_m & \mathbf{0}_{m\times r} & c\mathbf{J}_m + d\mathbf{I}_m \end{array}\right|$$

where $r = m + m(m - 1)/2$, $\mathrm{diag}(b, \ldots, c)$ is a diagonal matrix whose diagonal has m elements having b as the value and $m(m - 1)/2$ elements having c as the value. If $c = b/n$, the design is said to be orthogonal and the $\mathbf{A}^{-1}$ matrix takes the form

$$\left|\begin{array}{lll} (mc+ d)/a & \mathbf{0}'_r & -b/a\mathbf{1}'_m \\ \mathbf{0}_r & \mathrm{diag}(1/b, \ldots, 1/c) & \mathbf{0}_{r\times m} \\ -b/a\mathbf{1}_m & \mathbf{0}_{m\times r} & 1/d\mathbf{I}_m \end{array}\right|$$

where $a = mnc + nd - mb^2$ (John, 1971). Now define $\mathbf{A}^*$ as

$$\mathbf{A}^* = \mathbf{A}\ -\ \left|\begin{array}{ll} \mathbf{0}_{(r+1)(r+1)} & b\mathbf{1}'_m \\ b\mathbf{1}_m & b^2/n\mathbf{J}_m \end{array}\right|$$

The approach used by the FFD module to construct orthogonal or near-orthogonal FFDs or RSDs is to generate a suitable treatment design by allocating -1 or +1 to each of the 2-level factor and -1, 0, or +1 to each 3-level factor and minimize the objective function f; f is defined as the sum of squares of the elements above the main right diagonal of $\mathbf{A}$ in the FFD case and of $\mathbf{A}^*$ in the RSD case. A similar approach was used by Nguyen (1996a, 1996b) to construct supersaturated treatment designs and orthogonal arrays.

Main effect treatment designs, resolution III, and main effect plus two factor interaction treatment designs, resolution V, FFDs for 2-level factors may be constructed using the FFD module. Resolution IV designs may also be constructed. Note that a resolution IV design does not confound (alias) main effects and two factor interactions but does confound two factor interactions with other two factor interactions. Resolution V does confound (alias) two with three factor interactions. When a 3-level factor is included, the treatment design created is considered to be a response surface design. This is why the number of times a high level, +1, may be selected and the number of runs at the zero level, center point, may be increased.

STEPS TO OBTAIN A FRACTIONAL REPLICATE

As explained by Federer *et al.* (2001) the Gendex toolkit is installed on an appropriate directory on a PC. Suppose that Gendex has been installed in a folder named Gendex on the C:\ drive. To use the module FFD to construct the desired treatment design, the steps are described below:

1. Click on START/PROGRAMS/MS_DOS PROMPT
2. Change directory to C:\Gendex with the CD\Gendex command, return.
3. In C:\Gendex>, type FFD, return.
4. A screen will appear with the prompt "Choose the number of 3-level factors:". Any number between 0 and 9 may be selected by highlighting the number and clicking on OK.
5. The next prompt will be "Choose the number of 2-level factors:". Any number between 0 and 15 may be selected by highlighting the number and clicking on OK.
6. The next prompt will be "Choose the number of runs:". The lowest number of runs is determined by the number of factors selected. Any number between the lowest number and 128 may be selected as the number of runs, n, by highlighting that number and clicking on OK.
7. The next prompt is "Choose the number of high level +1 for each 3-level factor:". For a fractional replicate, this number is selected for equal numbers of each of the three levels of a factor, that is +1, 0, -1. For a response surface design, the zero level of a 3-level factor occurs more frequently than the +1 or -1 levels; the number of zero levels is selected by choosing the number of times a +1 level appears. The -1 level will appear the same number of times as the +1 level. After selection, click OK.
8. The next prompt is "Choose a resolution:". The choices are III, IV, and V. Resolution III is for linear main effects only; quadratic effects of 3-level factors are not included. Resolution V adds the linear × linear regression interactions and the quadratic effects of the 3-level factors. After selection, click OK.
9. At the next prompt "Enter a random seed:", a number may be entered or not and then clicking on OK.
10. The next prompt requests that one "Enter number of tries:". A number may be entered or left blank. Then, click OK. A number of tries may be entered and this may reduce the time required to obtain the treatment design. This is especially true for large treatment designs.

11. The output for these selections will appear on the screen. Click on Ok to save the output as FFD.HTM or as RSD.HTM in the C:\Gendex directory.
12. A printed output for FFD.HTM (or RSD.HTM) may be obtained by going to START/PROGRAMS/WINDOWS EXPLORER and clicking on C:\Gendex. Highlight the file FFD.HTM. Under FILE, click on PRINT.
13. To obtain an edited copy of FFD.HTM, go to START/PROGRAMS/WINDOWS EXPLORER. Highlight the file FFD.HTM in the Gendex folder. Under FILE, click on OPEN. Under EDIT, click on SELECT ALL and then on COPY . This file may then be PASTED in a word processing file and edited and the edited file saved.

PRINTED OUTPUT

The output for a design contains the following:

1. There is a Note: to the effect that m = the number of factors selected, p = the number of parameters to be estimated, and n = the number of runs selected.
2. The number of tries used to obtain the orthogonal or near-orthogonal FFD or RSD.
3. The random seed used for a try, either the one selected or one selected by the program.
4. The number of iterations for each try follows next.
5. The objective function f is defined as the sum of squares of the elements above the main right diagonal of the **A** = **X'X** matrix for a FFD and of the information matrix, **A*** for an RSD.
6. The determinant, det, of **X'X** or **A*** appears next on the output.
7. The std. Det.
8. The value for det indicates how close the obtained design is to the theoretically possible best design. An asterisk, det*, indicates that the best design has been obtained and det has a value of one.
9. The trace V is the sum of the diagonal elements of the inverse of **X'X**.
10. The design for m factor levels in n runs is given under Factor levels.
11. The **A** = **X'X** matrix appears next.
12. This is followed by the inverse of the **X'X** matrix.
13. Time in seconds to create the design.

The solution for the various effects may be obtained by solving the matrix equation $\mathbf{b} = (\mathbf{X'X})^{-1}\mathbf{X'Y}$ where **b** is the vector of p parameters and **Y** is the vector of observations.

EXAMPLE 1. 2-level, m = 3 factors and n = 8 runs

A resolution V treatment design for m = 3 2-level factors, A, B, and C, in n = 8 runs is used as the first example. The design should be all the combinations of a 2^3 factorial. This is what was obtained by the FFD module of the Gendex toolkit. The output is:

FFD 2.0: Construct orthogonal fractional factorial and response surface designs
(C) 2001 Design Computing (URL: http://designcomputing.hypermart.net)

Note: design for m=3, p=7, and n=8.

try #	1
seed	1123
# of iterations	1
f	0
det	2097152.0
std. det	1.0
det*	1.0000
trace V	0.8750

Factor levels:

1	1	1
-1	-1	1
-1	-1	-1
1	1	-1
1	-1	-1
1	-1	1
-1	1	1
-1	1	-1

X'X

8	0	0	0	0	0	0
	8	0	0	0	0	0
		8	0	0	0	0
			8	0	0	0
				8	0	0
					8	0
						8

inverse(X'X)

0.1250	0	0	0	0	0	-0
	0.1250	0	0	0	0	-0
		0.1250	0	0	0	-0
			0.1250	0	0	-0
				0.1250	0	-0
					0.1250	-0
						0.1250

Note: FFD used 0.16 seconds.

The **X** matrix for the above example is

1	1	1	1	1	1	1
1	-1	-1	1	1	-1	-1
1	-1	-1	-1	1	1	1
1	1	1	-1	1	-1	-1
1	1	-1	-1	-1	-1	1

1	1	-1	1	-1	1	-1
1	-1	1	1	-1	-1	1
1	-1	1	-1	-1	1	-1

The first column is for the mean, the second column is for the factor A effect, the third column is for the factor B effect, and the fourth column is for the factor C effect. The fifth column is obtained as the product of the coefficients in the A and B columns for the interaction AB effect; the sixth column is obtained as the product of coefficients in the A and C columns for the AC interaction effect, and the seventh column is obtained as the product of the coefficients in the B and C columns for the BC interaction effect. For the parameter vector **b'** = [mean A B C AB AC BC], the solution for the effects is obtained from the equation $\mathbf{b} = (\mathbf{X'X})^{-1}\mathbf{X'Y}$ where **Y** is the vector of n = 8 observations. This orthogonal fractional replicate of resolution V was obtained at the first iteration of the first try. The determinant is obtained as $8^7 = 2{,}097{,}162$. The det* = 1 indicates that the lower bound has been reached and that this is the best possible design. The value for the determinant is obtained as the m^{th} root of the correlation matrix. Trace V is obtained as 7(0.1250) = 0.8750 from the inverse of **X'X**.

EXAMPLE 2. 3-level, m = 2 factors and n = 9 runs

An example using a 3^2 factorial in 9 runs for the factors A and B and selecting a resolution V design was used to obtain the following output. The FFD program considers this selection to be a RSD instead of a FFD 3^2 factorial.

FFD 2.0: Construct orthogonal fractional factorial and response surface designs
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Note: design for m=2, p=6, and n=9.

try #	1
seed	1123
# of iterations	1
f	0
det	5184.0
std. det	0.00975461
det*	0.4622
trace V	2.1389

Factor levels:

0	1
-1	0
1	-1
0	0
-1	1
1	1
-1	-1
0	-1
1	0

X'X

9	0	0	0	6	6
	6	0	0	0	0
		6	0	0	0
			4	0	0
				6	4
					6

inverse(X'X)

0.5556	0	0	0	-0.3333	-0.3333
	0.1667	0	0	0	-0
		0.1667	0	0	-0
			0.2500	0	-0
				0.5000	-0
					0.5000

Note: FFD used 0.11 seconds.

Note that this plan is not a resolution V fractional replicate but is a RSD. The **X** matrix for the above design is

1	1	1	1	1	1
1	-1	1	-1	1	1
1	0	1	0	0	1
1	-1	0	0	1	0
1	1	0	0	1	0
1	1	-1	-1	1	1
1	0	0	0	0	0
1	-1	-1	1	1	1
1	0	-1	0	0	1

where the first column is the mean effect, the second column the levels of factor A, the third column the levels of factor B, the fourth column is the product of the coefficients of the A and B columns and is the A linear by B linear interaction, The fifth column is obtained by replacing a coefficient in column 2 and with is square, and the sixth column is obtained by placing a +1, i.e., the square of the coefficient, for every 1 in column 3 and 0 otherwise. The vector **b'** = [mean AL BL AL*BL AQ BQ]. AL is the linear contrast of the three levels of factor A, BL is the linear contrast of the three levels of factor B, and AL*BL is the linear by linear interaction of factors A and B. AQ is a parameter to measure lack of fit from linearity (quadratic) for factor A, and BQ is a parameter to measure lack of fit from linearity for factor B. In the **X'X** matrix, the diagonal elements are the sums of squares of the coefficients in the respective columns and the off diagonal elements are the cross products of the coefficients in two columns. For example in column 2, there are six ones squared and summed. The off diagonal elements in **X'X** are the cross products of the coefficients for various pairs of columns.

EXAMPLE 3. RSD for two 3-level factors with one 2-level factor in n = 9 runs

In order to obtain a RSD for two 3-level factors and one 2-level factor and interactions of the 2-level factor with the linear and quadratic contrasts of the two 3-level factors, an input file, FFD.TXT needs to be created in notepad. In this case if resolution V is selected, there will be m = 15 parameters. The steps for creating this RSD follow:

1. Go to START/PROGRAMS/MS_DOS PROMPT.
2. Change directory to C:Gendex with command CD\Gendex.
3. In C:\Gendex>, type the command notebook FFD.TXT.
4. Answer YES to the prompt Create a new File:.
5. In the open file, type in the n = 9 row by 4 column matrix of single degree of freedom contrasts. For this design, the matrix is

-1	1	-1	1
-1	1	0	-2
-1	1	1	1
0	-2	-1	1
0	-2	0	-2
0	-2	1	1
1	1	-1	1
1	1	0	-2
1	1	1	1

6. Save this matrix as FFD.TXT. Return to DOS, and type FFD in C\Gendex>.
7. A prompt that says FFD.TXT has 9 rows and 4 columns. Click YES to include these columns in the new design:
8. The next prompt is Choose the number of 3-level factors: select 0.
9. The next prompt is Choose the number of 2-level factors: select 0.
10. The next prompt is Choose the number of high level (+1) for each 3.level factor: select 3.
11. The next prompt is Choose a resolution: selected V.
12. The next prompt is Enter a random seed: left blank and clicked OK.
13. The next prompt is Enter number of tries: left blank and clicked OK.

The following output was obtained:

FFD 2.0: Construct orthogonal fractional factorial and response surface designs
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Note: design for m=4, p=15, and n=9.

try # 1
seed 1005337549060
# of iterations 0
f 2240
det 0.0
std. det 0.0
det* 0

Factor levels:

-1	1	-1	1
-1	1	0	-2
-1	1	1	1
0	-2	-1	1
0	-2	0	-2
0	-2	1	1
1	1	-1	1
1	1	0	-2
1	1	1	1

X'X

9	0	0	0	0	0	0	0	0	0	0	6	18	6	18
	6	0	0	0	6	0	0	0	0	0	0	0	0	0
		18	0	0	0	0	0	0	0	0	6	-18	0	0
			6	0	0	0	0	0	0	6	0	0	0	0
				18	0	0	0	0	0	0	0	0	6	-18
					6	0	0	0	0	0	0	0	0	0
						4	0	0	0	0	0	0	0	0
							12	0	0	0	0	0	0	0
								12	0	0	0	0	0	0
									36	0	0	0	0	0
										6	0	0	0	0
											6	6	4	12
												54	12	36
													6	6
														54

Note: the first 4 columns of the design are protected columns.
Note: FFD used 0.27 seconds.

The **X** matrix used to obtain the above results is:

1	-1	1	-1	1	-1	1	-1	-1	1	-1	1	1	1	1
1	-1	1	0	-2	-1	0	2	0	-2	0	1	1	0	4
1	-1	1	1	1	-1	-1	-1	1	1	1	1	1	1	1
1	0	-2	-1	1	0	0	0	2	-2	-1	0	4	1	1
1	0	-2	0	-2	0	0	0	0	4	0	0	4	0	4
1	0	-2	1	1	0	0	0	-2	-2	1	0	4	1	1
1	1	1	-1	1	1	-1	1	-1	1	-1	1	1	1	1
1	1	1	0	-2	1	0	-2	0	-2	0	1	1	0	4
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

The first four columns are those of FFD.TXT, the input matrix. The coefficients in the last four columns are the squares of the coefficients in columns 2, 3, 4, and 5, respectively. This is a supersaturated RSD in that there are 15 parameters to be estimated and only n = 9 observations. For example, note that columns 2 and 5 and columns 4 aand 11 are identical. The parameter vector **b'** = [mean AL AQ BL BQ AL*AQ AL*BL AL*BQ AQ*BL AQ*BQ BL*BQ C1 C2 C3 C4]. The four columns of the input matrix FFD.TXT are treated as m = 4 factors. To obtain a resolution V, all interactions among these m = 4 "factors" are considered. The meaning of such parameters as AL*AQ and BL*BQ is unclear.

EXAMPLE 4. one 3-level, two 2-level factors, n = 12

Using one 3.level factor and two 2-level factors with resolution V, the following output was obtained for a RSD:

FFD 2.0: Construct orthogonal fractional factorial and response surface designs

Note: design for m=3, p=8, and n=12.

try #	1
seed	1005167557230
# of iterations	1
f	0
det	2.8311552000000004E7
std. det	0.06584362
det*	0.7117
trace V	1.2500

Factor levels:

-1	1	-1
0	-1	1
-1	-1	-1
1	-1	1
1	-1	-1
0	1	-1
-1	1	1
1	1	-1
-1	-1	1
0	-1	-1
0	1	1
1	1	1

X'X

12	0	0	0	0	0	0	8
	8	0	0	0	0	0	0
		12	0	0	0	0	0
			12	0	0	0	0
				8	0	0	0
					8	0	0
						12	0
							8

inverse(X'X)

0.2500	0	0	0	0	0	0	-0.2500
	0.1250	0	0	0	0	0	-0
		0.0833	0	0	0	0	-0

0.0833	0	0	0	-0
	0.1250	0	0	-0
		0.1250	0	-0
			0.0833	-0
				0.3750

Note: FFD used 0.16 seconds.

The **X** matrix for the p = 8 parameters of this design is

1	-1	1	-1	-1	1	-1	1
1	0	-1	1	0	0	-1	0
1	-1	-1	-1	1	1	1	1
1	1	-1	1	-1	1	-1	1
1	1	-1	-1	-1	-1	1	1
1	0	1	-1	0	0	-1	0
1	-1	1	1	-1	-1	1	1
1	1	1	-1	1	-1	-1	1
1	-1	-1	1	1	-1	-1	1
1	0	-1	-1	0	0	1	0
1	0	1	1	0	0	1	0
1	1	1	1	1	1	1	1

To obtain the **X** matrix, add a column of ones the design under factor levels above for the mean effect. Denoting the second column as the linear effect of the A factor at three levels, the third column as the B factor effect with two levels, and the fourth column as the C factor effect with two levels, the fifth column is obtained as the product of the coefficients in columns two and three and is the A linear by B interaction, AL*B. The sixth column is obtained as the product of coefficients in columns two and four and is the A linear by C interaction, AL*C. The seventh column is obtained as the product of the coefficients in columns three and four and is the B by C interaction, B*C. The eighth column is obtained by inserting a +1, i.e., the square of the coefficient, for every ±1 in column 2 and the parameter is denoted as AQ, the quadratic effect of factor A. Then the vector **b'** = [mean AL B C AL*B AL*C B*C AQ].

EXAMPLE 5. 3-level RSD, m = 3 factors and n = 15 runs

For this RSD, m =3 3-level factors, n = 15 runs, and p = 10 parameters, the number of levels for the +1 level of a factor was set as n1 = 4. This zero level will occur 7 times. The resolution V option was selected to obtain the following output:

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Note: design for m=3, p=10, and n=15.

try # 1
seed 1005227291180

# of iterations	3
f	9.2133
det	1.5071616000000002E7
std. det	2.6136488E-5
det*	0.3481
trace V	2.5574

try #	2
seed	1164588796
# of iterations	5
f	9.2133
det	1.5071616000000002E7
std. det	2.6136488E-5
det*	0.3481
trace V	2.5574

try #	3
seed	177443470
# of iterations	6
f	0.2133 (R)
det	2.5165824E7
std. det	4.364139E-5
det*	0.3664
trace V	2.2708

Factor levels:

0	1	-1
0	0	0
-1	0	-1
1	0	-1
-1	0	1
0	-1	-1
1	0	1
0	0	0
1	-1	0
1	1	0
0	1	1
-1	-1	0
0	0	0
0	-1	1
-1	1	0

X'X

15	0	0	0	0	0	0	8	8	8
	8	0	0	0	0	0	0	0	0
		8	0	0	0	0	0	0	0
			8	0	0	0	0	0	0
				4	0	0	0	0	0
					4	0	0	0	0
						4	0	0	0
							8	4	4
								8	4
									8

inverse(X'X)

0.3333	0	0	0	0	0	0	-0.1667	-0.1667	-0.1667
	0.1250	0	0	0	0	0	-0	-0	-0
		0.1250	0	0	0	0	-0	-0	-0
			0.1250	0	0	0	-0	-0	-0
				0.2500	0	0	-0	-0	-0
					0.2500	0	-0	-0	-0
						0.2500	-0	-0	-0
							0.2708	0.0208	0.0208
								0.2708	0.0208
									0.2708

Note: FFD used 0.38 seconds.

The X matrix for the above design is

1	0	1	-1	0	0	-1	0	1	1
1	0	0	0	0	0	0	0	0	0
1	-1	0	-1	0	1	0	1	0	1
1	1	0	-1	0	-1	0	1	0	1
1	-1	0	1	0	-1	0	1	0	1
1	0	-1	-1	0	0	1	0	1	1
1	1	0	1	0	1	0	1	0	1
1	0	0	0	0	0	0	0	0	0
1	1	-1	0	-1	0	0	1	1	0
1	1	1	0	1	0	0	1	1	0
1	0	1	1	0	0	1	0	1	1
1	-1	-1	0	1	0	0	1	1	0
1	0	0	0	0	0	0	0	0	0
1	0	-1	1	0	0	-1	0	1	1
1	-1	1	0	-1	0	0	1	1	0

A vector of ones is the first column of X for the mean effect. The second, third, and fourth columns of X are the items under Factor levels for the linear effects of factors A, B, and C. The fifth column is the product of the coefficients of columns 2 and 3 and is the A linear by B linear interaction effect AL*BL. The sixth column is the product of the coefficients in columns 2 and 4 and is the A linear by C linear interaction effect AL*CL. The seventh column is obtained as the product of the coefficients in columns 3 and 4 and is the B linear by C linear interaction effect BL*CL. The eighth column is obtained by placing a +1 for every ±1 in column 2, parameter AQ, and zero otherwise. The ninth column is obtained by placing a +1 for every ±1 in column 3, parameter BQ, and zero otherwise. The last column is obtained by placing a +1 for every ±1 in column 4, parameter CQ, and zero otherwise. Then the vector **b'** = [mean AL BL CL AL*BL AL*CL BL*CL AQ BQ CQ].

COMMENTS

This module is very useful for constructing 2-level resolutions III and V fractional replicates and response surface designs. The treatment designs are optimal or near optimal. This module eliminates the need for tables of these designs.

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