Optimal Properties of Orthogonal Arrays Based on ANOVA High-Dimensional Model Representation *

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Abstract

Global sensitivity indices play important roles in global sensitivity analysis based on ANOVA high-dimensional representation, Wang et al. (2012) showed that orthogonal arrays are A-optimality designs for the estimation of parameter Θ_M , the definition of which can be seen in Section 2. This paper presented several other optimal properties of orthogonal arrays under ANOVA high-dimensional representation, including E-optimality for the estimation of Θ_M and universal optimality for the estimation of β_M , where β_M is the independent parameters of Θ_M . Simulation study showed that randomized orthogonal arrays have less biased and more precise in estimating the confidence intervals comparing with other methods.

Keywords: Matrix image, E-optimality, universal optimality, orthogonal array.

AMS Subject Classification: 62K05.

§1. Introduction

The ANOVA high-dimensional model representation originated from Hoeffding (1948), and was further discussed by Takemura (1983), Efron and Stein (1981) and Stein (1987). That is

$$f(x_1, \dots, x_m) = f_0 + \sum_i f_i(x_i) + \sum_{i < j} f_{ij}(x_i, x_j) + \dots + f_{12\dots m}(x_1, \dots, x_m),$$
(1.1)

where f_0 denotes the mean effect which is a constant. $f_i(x_i)$ gives the effect of the variables x_i independent of the other input variables. $f_{ij}(x_i, x_j)$ describes the interactive effects of the variables x_i and x_j , and so on. Model (1.1) has several interesting properties under the orthogonal condition, $\int f_{i_1...i_s}(x_{i_1}, ..., x_{i_s}) dx_k = 0$, for $k = i_1, ..., i_s$. More details can be found in Sobol (1993).

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Based on this ANOVA model representation, Sobol (1993) proposed global sensitivity index,

$$S_{i_1...i_s} = D_{i_1...i_s}/D,$$

where $D_{i_1...i_s} = \text{Var}(f_{i_1...i_s}(x_{i_1}, \dots, x_{i_s}))$, $D = \sum_i D_i + \sum_{j \leq k} D_{jk} + \dots + D_{12...m}$, to reflect the importance of the input variables and their interactions, and to identify the most important variables and interactions for f. In general, $S_{i_1...i_s} = D_{i_1...i_s}/D$ can be computed numerically and several numerical methods have been investigated by many authors, such as Monte Carlo simulation (Sobol, 2001, 2003; Sobol and Myshetskaya, 2008), quasi-Monte carlo method (Saltelli et al., 2010). However, to most of experimenters, the objective function f often appears as a "black box", that is, a nonparametric model. There has been little study on this subject. Recently, Wang et al. (2011, 2012) discussed the use of design of orthogonal arrays in global sensitivity analysis of nonparametric models, and shows that orthogonal arrays (OAs) are A-optimality designs for the estimation of Θ_M , the definition of which can be seen in Section 2.

This paper shows several optimal properties of orthogonal arrays (OAs) under ANO-VA high-dimensional representation, including E-optimality for the estimation of Θ_M in Section 2 and universal optimality for the estimation of β_M in Section 3, where β_M is the independent parameters of Θ_M . In Section 4, simulation study showed that randomized orthogonal arrays have less biased and more precise in estimating the confidence intervals comparing with other methods, such as MC method and OA method in Wang et al. (2011).

§2. E-optimality for the Estimation of Θ_M

Regard the input variable x_1, \ldots, x_m as control factors, and arrange the experiment according to a design $H = (a_{ij})_{n \times m} = (a_1, \ldots, a_m)$, the jth column of which has p_j levels and $a_{ij} \in \{1, 2, \ldots, p_j\}$. Suppose $Y = (y_1, \ldots, y_n)^T$ is the observation vector with the observation errors $\epsilon_i \sim N(0, \sigma^2)$, hence

$$y_i = f_0 + f_1(x_{i1}) + f_2(x_{i2}) + \dots + f_{12\dots m}(x_{i1}, \dots, x_{im}) + \epsilon_i.$$

Denote

$$\Theta_{i_1...i_s} = \begin{pmatrix} f_{i_1...i_s}(x_{1i_1}, \dots, x_{1i_s}) \\ \vdots \\ f_{i_1...i_s}(x_{ni_1}, \dots, x_{ni_s}) \end{pmatrix}, \qquad \epsilon = \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{pmatrix}.$$

Then the above model can be written as

$$Y = \Theta_0 + \sum_{i} \Theta_i + \sum_{j \le k} \Theta_{jk} + \dots + \Theta_{12\dots m} + \epsilon.$$
 (2.1)

In order to obtain global sensitivity indices, the estimate of $D_{i_1...i_s}$ should be got first. The following two-step approach can be used.

1. Approximate $D_{i_1...i_s}$ by

$$D_{i_1...i_s}^* = \frac{1}{n} \sum_{i=1}^n [f_{i_1...i_s}(x_{ii_1}, \dots, x_{ii_s})]^2 = \frac{1}{n} (\Theta_{i_1...i_s})^T (\Theta_{i_1...i_s}).$$

2. Estimate $\Theta_{i_1...i_s}$ by a function of observed values $g_{i_1...i_s}(Y)$.

Different choices of H and g may lead to different extent of deviations between the estimated and true values. Thus, it is important to select "good" designs and g(Y) for global sensitivity analysis. Wang et al. (2012) proved that under A-optimality criterion, the choice of orthogonal arrays and $g = A_M Y$ can minimize the distance between $g_{i_1...i_s}(Y)$ and $\Theta_{i_1...i_s}$, where A_M is the matrix image of columns i_1, \ldots, i_s of H, which is developed by Zhang et al. (1999). We give the definition of matrix image and some useful properties in this section.

Definition 2.1 Let SS_M^2 be the treatment sum of squares of column M in the analysis of variance. The matrix image (MI) of column $M = \{i_1, i_2, \dots, i_s\}$, denoted by A_M , is defined to be the $n \times n$ projection matrix A_M if

$$SS_M^2 = Y^T A_M Y.$$

Since SS_M^2 is a quadratic form of Y, there exists a unique symmetric matrix A_M such that $SS_M^2 = Y^T A_M Y$. In particular, denote the sum of squares of main effect of column i as SS_i^2 , then the matrix A_i is called the matrix image of columns i if $SS_i^2 = Y^T A_i Y$. Several important properties can be found for an orthogonal array H with strength s in Zhang et al. (1999), Wang et al. (2012), such as

- 1. The MI of interactions of column M, $A_M = n^{|M|-1} \bigcap_{j:j \in M} A_j$, $\forall |M| \leq s$, where A_j is the MI of column j of H, and |M| is the number of elements in set M, and \bigcirc is the Hadamard product in theory of matrix.
- 2. Compute A_j as follows: $A_j = X_j(X_j^T X_j)X_j^T 1_n 1_n^T/n$, for j = 1, 2, ..., m, where X_j is the incidence matrix of column j, and $1_n = (1, \dots, 1)^T$.
 - 3. The MI of H, A_M , is a projection matrix, and $\operatorname{rk}(A_M) = \prod_{j \in M} (p_j 1)$, for $|M| \leq s$.
 - 4. The MI's of H are orthogonal, $A_M A_N = 0$, for $M \neq N$, $|M \cup N| \leq s$.
 - 5. $A_M \Theta_M = \Theta_M$, for $|M| \le s$.

For convenience of the proof in the later section, we transform model (2.1) into a linear model. Following Wang et al. (2012), we write $N = \prod_{j \in M} p_j$ and denote the $N \times 1$ vector, with elements $f_{i_1...i_s}(x_{i_1},...,x_{i_s})$, arranged in the lexicographic order, by μ_M . Let X_M , having n rows and N columns, be the incidence matrix of columns $i_1,...,i_s$ of H, then

$$\Theta_M = X_M \mu_M. \tag{2.2}$$

For each Θ_M , let β_M be the independent parameters of μ_M . Then there exists a matrix B_M such as

$$\mu_M = B_M \beta_M, \tag{2.3}$$

and $\operatorname{rk}(B_M) = \prod_{j \in M} (p_j - 1)$. From (2.2) and (2.3), we have $\Theta_M = X_M B_M \beta_M$. Let $C_M = X_M B_M$, then $\Theta_M = C_M \beta_M$. Therefore

$$Y = \sum_{M:M\subseteq\{1,2,\dots,m\}} C_M \beta_M + \epsilon = C\beta + \epsilon, \tag{2.4}$$

where $C = (C_0, C_1, \dots, C_{12...m})$ and $\beta = (\beta_0^T, \beta_1^T, \dots, \beta_{12...m}^T)^T$.

The following two lemmas play an important role in Wang et al. (2012):

Lemma 2.1 For the linear model

$$Y = C\beta + \epsilon$$
.

where Y is a $n \times 1$ observation vector, C is a $n \times p$ design matrix, β is a $p \times 1$ parameter vector, ϵ is a $n \times 1$ random error vector and $\mathsf{E}(\epsilon) = 0$, β is estimable if and only if C has full column rank.

Lemma 2.2 Assume that H is a feasible design (H satisfies that for any $\Theta_M(H)$, $M \subset \Omega$, there exists a matrix B such that $\mathsf{E}(BY) = \Theta_M(H)$, $\mathsf{rk}(C_M) = \alpha(M)$ and the best linear unbiased estimate of $\Theta_M(H)$ is $\widehat{\Theta}_M(H)$, then

$$\operatorname{tr}(\operatorname{Var}(\widehat{\Theta}_M(H))) \ge \sigma^2 \prod_{j \in M} (p_j - 1).$$

By properties of MI's of orthogonal arrays with strength s and the above lemmas, we have

Theorem 2.1 Let $\widehat{\Theta}_M(H) = A_M Y$. If H is an orthogonal array with strength m, then

$$\mathsf{E}(\widehat{\Theta}_M(H)) = \mathsf{E}(A_M Y) = \Theta_M$$

and

$$\operatorname{tr}(\operatorname{\sf Var}\left(A_MY
ight)) = \sigma^2 \prod_{j \in M} (p_j - 1)$$

for $M \subseteq \{1, \ldots, m\}$.

From Lemma 2.2 and Theorem 2.1, we have

Orthogonal arrays with strength m are the best experimental plans for the estimation of Θ_M under the A-optimality criterion.

We now consider the E-optimality of orthogonal arrays in the remaining of this section.

Orthogonal arrays with strength m are the best experimental plans for the estimation of Θ_M under the E-optimality criterion.

Proof That is to prove

$$\lambda_{\max}(\operatorname{Var}(A_M Y)) = \min_{H} \lambda_{\max}(\operatorname{Var}(\widehat{\Theta}_M(H))), \tag{2.5}$$

where $\lambda_{\max}(A)$ denotes the maximum eigenvalue of matrix A. From the proof of Lemma 2.2, we obtain $\text{Var}(\widehat{\Theta}_M(H)) \geq \sigma^2 C_M (C_M^T C_M)^{-1} C_M^T$. Let $P_{C_M} = C_M (C_M^T C_M)^{-1} C_M^T$. Then P_{C_M} is a projection matrix and $\lambda_{\max}(P_{C_M}) = 1$. By Theorem 2.2, we have $\text{Var}(A_M Y)$ $=\sigma^2 A_M$. From property 1 of MI's of orthogonal arrays with strength m, A_M is also a projection matrix. So $\lambda_{\max}(A_M) = 1$, for $|M| \leq s$. Thus (2.5) holds.

Since parameters in Θ_M are correlated with each other, thus for any feasible design H, $\det(\Theta_M(H)) = 0$. Therefore, there is no sense to discuss the Doptimality.

§3. Universal Optimality for the Estimation of eta_M

The notion of universal optimality, due to Kiefer (1975), helps in unifying the various optimality criteria. Let Z denote the class of positive definite matrices of order $\alpha(M)$ $\prod_{i} (p_j - 1)$, and for a positive integer v, let J_v denote the $v \times v$ matrix with all elements unity. consider the class Φ of real-valued functions $\phi(x)$, such that

1. $\phi(x)$ is convex; that is, for every $x_1, x_2 \in Z$, and real $a(0 \le a \le 1)$,

$$a\phi(x_1) + (1-a)\phi(x_2) \ge \phi(ax_1 + (1-a)x_2);$$

2. $\phi(c_1I_{\alpha(M)}+c_2J_{\alpha(M)}) \geq \phi(cI_{\alpha(M)})$ whenever $c \geq c_1+c_2$, where c_1,c_2 and c are scalars;

3. $\phi(x)$ is permutation invariant; that is, $\phi(rxr^T) = \phi(x)$, for every x and every permutation matrix r of order $\alpha(M)$.

Let Q_H denotes the information matrix for β_M under plan H and model (2.4),

Definition 3.1 A universally optimality plan is one that for each $\phi(0) \in \Phi$, minimizes $\phi(Q_H)$ over $H \in D_n^*$, where D_n^* denotes the *n*-run plans which are capable of keeping β_M estimable under (2.4).

Universal optimality is more power than the specific optimality criteria. Consideration of the functions

$$\phi(G) = \log(\det(G^{-1})), \qquad \phi(G) = \operatorname{tr}(G^{-1}), \qquad \phi(G) = \lambda_{\max}(G^{-1}),$$

which are all members of Φ , shows that a universally optimal plan is also D-, A- and E- optimal. The following Theorem from Dey and Mukerjee (1999) demonstrate that orthogonal arrays is the universally optimal plans for the estimation of β_M with orders less than m/2, where m denotes the strength of the OA.

Theorem 3.1 Let H_0 be represented by an n-run orthogonal array with strength m, where $2 \le m \le l$, l is the column number of H_0 . Then H_0 is a universally optimal plan for every choice of β_M , such that $|M| \le m/2$.

This was first proved by Cheng (1980) for the gage m=2 and later extended by Mukerjee (1982) to the case of general m. It covers many of the earlier findings in Kounias (1977) who worked with 2^n factorials and specific optimality criteria. Under model (2.4), l=m, then Theorem 3.2 can be strengthened. We now present the main result of this section, which shows H_0 is a universally optimal plan for every choice of β_M with orders less than m, that is $|M| \leq m$. The following lemma will be useful in the subsequent development (The proof can be found in Dey and Mukerjee (1999), Lemma 2.5.2, P_{22}):

Lemma 3.1 Let there exist a plan H_0 such that the information matrix $G_{H_0} = I_{\alpha(M)}$. Then H_0 is a universally optimal plan for estimating β_M .

Theorem 3.2 Let H_0 be represented by an n-run orthogonal array with strength m, where m = l, l is the column number of H_0 . Then H_0 is a universally optimal plan for every choice of β_M with orders less than m under model (2.4).

Proof Following Dey and Mukerjee (1999), we rewrite

$$\mathsf{E}(Y) = (X_{1d} \ \vdots \ X_{1d}) \left(\begin{array}{c} \beta^{(1)} \\ \beta^{(2)} \end{array} \right), \qquad D(Y) = \sigma^2 I_n,$$

where parameter $\beta^{(1)}$ denotes the interest ones in the above model (2.4) and X_{1d} = $X_d(P^1)^T$, $X_{2d} = X_d(P^2)^T$. X_d is the design matrix and $(P^1)^T = (\cdots P^M \cdots)$. P^M is the orthogonal contrast coefficients of effect β_M . By linear model theory, we have

$$G_d = X_{1d}^T X_{1d} - X_{1d}^T X_{2d} (X_{2d}^T X_{2d})^T X_{2d}^T X_{1d}.$$

Hence by Lemma 2.6.1 in Dey and Mukerjee (1999), for orthogonal arrays,

$$X_M^T X_M = I_{\alpha(M)},$$
 for each $M \subseteq \{1, \dots, m\},$ $X_M^T X_N = 0,$ for each $M, N \subseteq \{1, \dots, m\}, M \neq N.$

If the interest parameter is β_M , we obtain $G_d = I_{\alpha(M)}$, Hence by Lemma 3.1, orthogonal arrays with strength m is universal optimality for the estimation of β_M , such that $M \in$ $\{1,\ldots,m\},\,|M|\leq m.$

ξ4. Simulation Study

To test the performance of the proposed estimators by matrix image, Wang suggested that orthogonal arrays which have a much smaller sample size comparing with MC-method and Q-MC method for the estimation of Θ_M . However, as Wang et al. (2011) indicated, the estimates for the significant sensitivity indices by the OA method have much smaller lengths of confidence intervals but a larger degree of bias than those of the Q-MC method and MC method.

We consider randomized orthogonal array (R-OA) sampling designs to improve the confidence intervals. Owen (1992, 1994) and Tang (1993) independently proposed the use of randomized orthogonal arrays in computer experiment sampling designs. A class of randomized orthogonal array sampling designs proposed by Owen (1992) is as follows: Let $D \in OA(n, m, q, t)$, where d_{ij} denotes the (i, j)th element of D, and

- 1. π_1, \ldots, π_d be random permutation of $\{0, \ldots, q-1\}$, each uniformly distributed on all the q! possible permutations.
 - 2. $\epsilon_{i,j}$ be (0,1) independent uniform random variables.

We randomize the symbols of D by applying the permutation π_j to the jth column of D, j = 1, ..., m. This gives us another orthogonal array D^* , such that its (i, j)th element satisfies $d_{i,j}^* = \pi_j(d_{i,j})$. Orthogonal array-based sample of size n is defined to be $\{d_1^*, \ldots, d_m^*\}$ where for $i = 1, \ldots, n, d_i^* = (d_{i,1}^*, \ldots, d_{i,m}^*)$, where $d_{i,j}^* = \pi_j(d_{i,j}) + \alpha\epsilon$ and α is a scaler. The following model (Morris et al., 2006; Wang et al., 2011) are restudied here

by R-OAs.

$$f(x_1, ..., x_m) = \beta_0 + \sum_{i=1}^m \beta_i z_i + \sum_{i \le j} \beta_{ij} z_i z_j + \dots + \beta_{12...m} z_1 \cdots z_m,$$

where x_i s are uniformly distributed between 0 and 1, and $z_i = x_i - 0.5$, i = 1, ..., m. Then we have

$$f_0 = \beta_0, \ f_i(x_i) = \beta_i z_i, \ \cdots, \ f_{12...m} = \beta_{1...m} z_1 z_2 \ldots z_m.$$

Hence

$$D_i = \mathsf{Var}\left(f_i(x_i)\right) = \beta_i^2/12, \ D_{ij} = \mathsf{Var}\left(f_{ij}(x_i, x_j)\right) = \beta_{ij}^2/12^2, \ \cdots, \ D_{12...m} = \beta_{12...m}^2/12^m$$

$$D = \sum_{i} \beta_{i}^{2}/12 + \sum_{j \leq k} \beta_{jk}^{2}/12^{2} + \dots + \beta_{12...m}^{2}/12^{m}. \qquad S_{M} = \frac{D_{M}}{D}, \quad M \subseteq \{1, 2, \dots, m\}.$$

We consider the situation that the sum of the first sensitivity indices is close to 1. Let case 1: m=4, $\beta_0=10$, $\beta_1=4$, $\beta_2=0.3$, $\beta_3=-5$, $\beta_4=2$, $\beta_{12}=0.2$, $\beta_{13}=1.5$, $\beta_{23}=0.2$, $\beta_{123}=0.1$ and all other β_M s equal zero. In this case, $S_1+S_2+S_3+S_4=0.995$. Wang et al. (2011) studied this situation by the complete orthogonal array with two levels OA(64,6,4,3) in their step 2. Table 1 give the results of the three methods, that is, MC method, OA method in Wang et al. (2011) and randomized OA method with $\alpha=1/100$, respectively.

Table 1 90% confidence intervals for the three methods (case 1)

\overline{M}	True value	MC (N = 4000)	OA(N = 64, Wang et al., 2011)	R-OA(N=64)
{3}	0.5521	(0.5425, 0.5620)	(0.5501, 0.5506)	(0.5501, 0.5551)
{1}	0.3533	(0.3439, 0.3621)	(0.3521, 0.3636)	(0.3515, 0.3558)
$\{4\}$	0.0883	(0.0828, 0.0914)	(0.0744, 0.0983)	(0.0871, 0.0897)
$\{1,3\}$	0.0041	(0.0007, 0.0071)	(0.0016, 0.0072)	(0.0028, 0.0034)
{2}	0.0019	(0.0008, 0.0029)	(0.0013, 0.0027)	(0.0017, 0.0022)

Table 1 shows the 90% confidence intervals for the significant sensitivity indices obtained by replicating the experiments (MC, OA approach and R-OA method) 20 times. The left point and the right point of each interval are the 5th and 95th percentiles of the estimate, respectively. As it indicated, the 90% confidence intervals estimated by MC method contain the true value but have a larger size. For example, the 90% confidence interval for {3} is (0.5425, 0.5620) by MC method, which is large than the other two methods. The 90% confidence interval for {3} is (0.5501, 0.5506) by OA method and

(0.5501, 0.5551) by randomized OAs. However, for OA method, they have much smaller confidence intervals but they seem to have a degree of bias. By R-OA method, confidence intervals get a better balance, which are less biased comparing with OA method and much more smaller comparing with MC method.

Now we consider the situation that high-order sensitivity indices are significant. Let case 2: m = 4, $\beta_0 = 10$, $\beta_1 = 1.8$, $\beta_2 = 1.5$, $\beta_3 = -2$, $\beta_4 = 2.5$, $\beta_{12} = 7.5$, $\beta_{13} = 8.5$, $\beta_{23} = 7$, $\beta_{123} = 1.5$ and all other β_{M} s equal zero. In this case, $S_1 + S_2 + S_3 + S_4 = 0.515$. Wang et al. (2011) also studied this situation by the complete orthogonal array with two levels OA(64, 6, 4, 3) in their step 2. Table 2 lists the results of the three methods, that is, MC method, OA method in Wang et al. (2011) and randomized OA method with $\alpha = 1/5$, respectively. It also shows that the confidence intervals estimated by MC method contain the true value but have a larger size. For OA method, they have much smaller confidence intervals but they are all biased. However, confidence intervals estimated by R-OA method get a better balance, which are less biased comparing with OA method and much more smaller comparing with MC method.

Table 2 90% confidence intervals for the three methods (case 2)

\overline{M}	True value	MC(N = 4000)	OA $(N = 64, Wang et al., 2011)$	R-OA (N = 64)
{4}	0.2046	(0.1851, 0.2247)	(0.1547, 0.1698)	(0.1676, 0.2581)
$\{1,3\}$	0.1971	(0.1235, 0.2908)	(0.2240, 0.2484)	(0.1238, 0.1978)
$\{1,2\}$	0.1535	(0.1169, 0.2173)	(0.1899, 0.1934)	(0.0895, 0.1647)
$\{2,3\}$	0.1337	(0.0747, 0.1869)	(0.1654, 0.1684)	(0.0812, 0.1363)
{3}	0.1309	(0.0388, 0.1988)	(0.0973, 0.1001)	(0.1028, 0.1827)
{1}	0.1060	(0.0662, 0.1489)	(0.0788, 0.0802)	(0.0815, 0.1488)
{2}	0.0736	(-0.0076, 0.1397)	(0.0547, 0.0557)	(0.0475, 0.1063)

§5. Concluding

In this paper, we have presented several optimal properties of orthogonal arrays for the estimation of Θ_M under model (2.1), such as E-optimality, which combined with Aoptimality in Wang et al. (2012) generalized the results of Cheng (1980) and Mukerjee (1982). Wang et al. (2011, 2012) used $\widehat{\Theta}_M(H) = A_M Y$ to estimate the global sensitivity indices when the objective function is a nonparametric model and proved to be accurate for small indices. By the generalized ANOVA model in Dey and Mukerjee (1999), we demonstrated that orthogonal arrays is universal optimality for the estimation of β_M under model (2.4). In simulation study, we proposed to use the randomized OAs in estimating the parameter and to estimate confidence intervals, which have less biased comparing with OA method and smaller size comparing with MC method.

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基于ANOVA高维模型的正交设计的优良性

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全局敏感性指标在全局敏感性分析中占有重要的地位, Wang等(2012)证明了正交设计在估计参数 β_M 时具有A最优,本文论证了正交设计在估计参数时的一些其他最优性质,包括估计参数 β_M 的E最优和估计参数 Θ_M 的一致最优性.在模拟论证中,我们提出了用随机化正交表来替代一般的正交表,并得到了较好的性质,如减少了偏差并且提高了精度.

关键词: 矩阵象, E最优, 一致最优, 正交设计.

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