# Hadamard Extensions and the Identification of Mixtures of Product Distributions

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#### Abstract

The Hadamard Extension of a matrix is the matrix consisting of all Hadamard products of subsets of its rows. This construction arises in the context of identifying a mixture of product distributions on binary random variables: full column rank of such extensions is a necessary ingredient of identification algorithms. We provide several results concerning when a Hadamard Extension has full column rank.

#### 1 Introduction

The Hadamard product for row vectors  $u = (u_1, \ldots, u_k)$ ,  $v = (v_1, \ldots, v_k)$  is the mapping  $\odot : \mathbb{R}^k \times \mathbb{R}^k \to \mathbb{R}^k$  given by

$$u \odot v := (u_1 v_1, \dots, u_k v_k)$$

The identity for this product is the all-ones vector 1. We associate with vector v the linear operator  $v_{\odot} = \text{diag}(v)$ , a  $k \times k$  diagonal matrix, so that

$$u \cdot v_{\odot} = v \odot u$$
.

Throughout this paper **m** is a real matrix with row set  $[n] := \{1, ..., n\}$  and column set [k]; write  $\mathbf{m}_i$  for a row and  $\mathbf{m}^j$  for a column.

As a matter of notation, for a matrix Q and nonempty sets R of rows and C of columns, let  $Q|_R^C$  be the restriction of Q to those columns and rows (with either index omitted if all rows or columns are retained).

**Definition 1.** The Hadamard Extension of  $\mathbf{m}$ , written  $\mathbb{H}(\mathbf{m})$ , is the  $2^n \times k$  matrix with rows  $\mathbf{m}_S$  for all  $S \subseteq [n]$ , where, for  $S = \{i_1, \dots, i_\ell\}$ ,  $\mathbf{m}_S = \mathbf{m}_{i_1} \odot \cdots \odot \mathbf{m}_{i_\ell}$ ; equivalently  $\mathbf{m}_S^j = \prod_{i \in S} \mathbf{m}_i^j$ . (In particular  $\mathbf{m}_\emptyset = \mathbb{1}$ .)

This construction has arisen recently in learning theory [3, 8] where it is essential to source identification for a mixture of product distributions on binary random variables. We explain the connection further in Section 5. Motivated by this application, we are interested in the following two questions:

- (1) If  $\mathbb{H}(\mathbf{m})$  has full column rank, must there exist a subset R of the rows, of bounded size, such that  $\mathbb{H}(\mathbf{m}|_R)$  has full column rank?
- (2) In each row of  $\mathbf{m}$ , assign distinct colors to the distinct real values. Is there a condition on the coloring that ensures  $\mathbb{H}(\mathbf{m})$  has full column rank?

In answer to the first question we show in Section 2:

**Theorem 2.** If  $\mathbb{H}(\mathbf{m})$  has full column rank then there is a set R of no more than k-1 of the rows of  $\mathbf{m}$ , such that  $\mathbb{H}(\mathbf{m}|_R)$  has full column rank.

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Considering the more combinatorial second question, observe that if  $\mathbf{m}$  possesses two identical columns then the same is true of  $\mathbb{H}(\mathbf{m})$ , and so it cannot be full rank. Extending this further, suppose there are three columns C in which only one row r has more than one color. Then Rowspace  $\mathbb{H}(\mathbf{m}|^C)$  is spanned by  $\mathbb{1}|^C$  and  $r|^C$ , so again  $\mathbb{H}(\mathbf{m})$  cannot be full rank. Motivated by these necessary conditions, set:

**Definition 3.** For a matrix Q let NAE(Q) be the set of nonconstant rows of Q (NAE="not all equal"); let  $\varepsilon(Q|^C) = |NAE(Q|^C)| - |C|$ ; and let  $\overline{\varepsilon}(Q) = \min_{C \neq \emptyset} \varepsilon(Q|^C)$ . If  $\overline{\varepsilon}(Q) \geq -1$  we say Q satisfies the NAE condition.

In answer to the second question we have the following:

**Theorem 4.** If m satisfies the NAE condition then

- (a) There is a restriction of **m** to some k-1 rows R such that  $\overline{\varepsilon}(\mathbf{m}|_R) = -1$ .
- (b)  $\mathbb{H}(\mathbf{m})$  is full column rank.

(As a consequence also  $\mathbb{H}(\mathbf{m}|_R)$  is full column rank.)

Apparently the only well-known example of the NAE condition is when  $\mathbf{m}$  contains k-1 rows which are identical and whose entries are all distinct. Then the vectors  $\mathbf{m}_{\emptyset}, \mathbf{m}_{\{1\}}, \mathbf{m}_{\{1,2\}}, \dots, \mathbf{m}_{\{1,\dots,k-1\}}$  form a nonsingular Vandermonde matrix. This example shows that the bound of k-1 in (a) is best possible.

For another example in which the NAE condition ensures that rank  $\mathbb{H}(\mathbf{m}) = k$ , take the (k-1)-row matrix with  $\mathbf{m}_i^j = 1$  for  $i \leq j$  and  $\mathbf{m}_i^j = 1/2$  for i > j. Here the NAE condition is only minimally satisfied, in that for every  $\ell \leq k$  there are  $\ell$  columns C s.t.  $\varepsilon(\mathbf{m}|^C) = -1$ .

For k > 3 the NAE condition is no longer necessary for  $\mathbb{H}(\mathbf{m})$  to have full column rank. E.g., for  $k = 2^{\ell}$ , the  $\ell \times k$  "Hamming matrix"  $\mathbf{m}_i^j = (-1)^{j_i}$  where j is an  $\ell$ -bit string  $j = (j_1, \ldots, j_{\ell})$ , forms  $\mathbb{H}(\mathbf{m}) =$  the Fourier transform for the group  $(\mathbb{Z}/2)^{\ell}$  (often called a Hadamard matrix), which is invertible. Furthermore, almost all (in the sense of Lebesgue measure)  $\lceil \lg k \rceil \times k$  matrices  $\mathbf{m}$  form a full-rank  $\mathbb{H}(\mathbf{m})$ . (This is because det  $\mathbb{H}(\mathbf{m})$  is a polynomial in the entries of  $\mathbf{m}$ , and the previous example shows the polynomial is nonzero.) Despite this observation, the Vandermonde case, in which k-1 rows are required, is very typical, as it is what arises in  $\mathbb{H}(\mathbf{m})$  for a mixture model of observables  $X_i$  that are iid conditional on a hidden variable.

# 2 Some Theory for Hadamard Products, and a Proof of Theorem 2

For  $v \in \mathbb{R}^k$  and U a subspace, extend the definition  $v_{\odot}$  to

$$v_{\odot}(U) = \{u \cdot v_{\odot} : u \in U\}$$

and introduce the notation

$$v_{\bar{\odot}}(U) = \operatorname{span}\{U \cup v_{\odot}(U)\}.$$

We want to understand which subspaces U are invariant under  $v_{\bar{\odot}}$ . Let v have distinct values  $\lambda_1 > \ldots > \lambda_\ell$  for  $\ell \leq k$ . Let the polynomials  $p_{v,i}$   $(i=1,\ldots,\ell)$  of degree  $\ell-1$  be the Lagrange interpolation polynomials for these values, so  $p_{v,i}(\lambda_j) = \delta_{ij}$  (Kronecker delta). Let B(v) denote the partition of [k] into blocks  $B(v)_{(i)} = \{j: v_j = \lambda_i\}$ . Let  $V_{(i)}$  be the space spanned by the elementary basis vectors in  $B(v)_{(i)}$ , and  $P_{(i)}$  the projection onto  $V_{(i)}$  w.r.t. standard inner product. We have the matrix equation

$$p_{v,i}(v_{\odot}) = P_{(i)}$$
.

The collection of all linear combinations of the matrices  $P_{(i)}$  is a commutative algebra, the B(v) projection algebra, which we denote  $A_{B(v)}$ . The identity of the algebra is  $I = \sum P_{(i)}$ .

**Definition 5.** A subspace of  $\mathbb{R}^k$  respects B(v) if it is spanned by vectors each of which lies in some  $V_{(i)}$ .

For U respecting B(v) write  $U = \operatorname{span}(\bigcup U_{(i)})$  for  $U_{(i)} \subseteq V_{(i)}$ . Let  $D_{(i)} = (U_{(i)})^{\perp} \cap V_{(i)}$ . Then  $(U_{(i)})^{\perp} = D_{(i)} \oplus \bigoplus_{i \neq i} V_{(j)}$ .

**Lemma 6.** Subspace  $U^{\perp}$  respects B(v) if U does.

*Proof.* In general,  $(\operatorname{span}(W \cup W'))^{\perp} = W^{\perp} \cap W'^{\perp}$ . So  $U^{\perp} = \bigcap (U_{(i)})^{\perp} = \bigoplus D_{(i)}$ .

**Lemma 7.** Subspace U respects B(v) iff  $U = \bigoplus (P_{(i)}U)$ .

Proof. ( $\Leftarrow$ ): Because this gives an explicit representation of U as a direct sum of subspaces each restricted to some  $V_{(i)}$ . ( $\Rightarrow$ ): By definition U is spanned by some collection of subspaces  $V'_{(i)} \subseteq V_{(i)}$ ; since these subspaces are necessarily orthogonal,  $U = \bigoplus V'_{(i)}$ . Moreover, since  $P_{(i)}$  annihilates  $V_{(j)}$ ,  $j \neq i$ , and is the identity on  $V_{(i)}$ , it follows that each  $V'_{(i)} = P_{(i)}U$ .

**Theorem 8.** Subspace U is invariant under  $v_{\bar{0}}$  iff U respects B(v).

*Proof.* ( $\Leftarrow$ ): It suffices to show  $U^{\perp}$  is invariant under  $v_{\bar{\odot}}$ . By the previous lemma, it is equivalent to suppose that  $U^{\perp}$  respects B(v). So let  $d \in U^{\perp}$  and write  $d = \sum d_i, d_i \in D_{(i)}$ . Then  $v \odot d_i = \lambda_i d_i \in D_{(i)}$ . So  $v \odot d = \sum v \odot d_i \in \bigoplus D_{(i)} = U^{\perp}$ .

 $(\Rightarrow)$ : If  $U = v_{\bar{\odot}}(U)$  then these also equal  $v_{\bar{\odot}}(v_{\bar{\odot}}(U))$ , etc., so U is an invariant space of  $A_{B(v)}$ , meaning,  $aU \subseteq U$  for any  $a \in A_{B(v)}$ . In particular for  $a = P_{(i)}$ . So  $U \supseteq \bigoplus (P_{(i)}U)$ . On the other hand, since  $\sum P_{(i)} = I$ ,  $U = (\sum P_{(i)})U \subseteq \bigoplus (P_{(i)}U)$ . So  $U = \bigoplus (P_{(i)}U)$ . Now apply Lemma 7.

The symbol  $\subset$  is reserved for strict inclusion.

**Lemma 9.** If  $S, T \subseteq [n]$  and Rowspace  $\mathbb{H}(\mathbf{m}|_S) \subset \text{Rowspace } \mathbb{H}(\mathbf{m}|_{S \cup T})$ , then there is a row  $t \in T$  such that Rowspace  $\mathbb{H}(\mathbf{m}|_S) \subset \text{Rowspace } \mathbb{H}(\mathbf{m}|_{S \cup \{t\}})$ .

Proof. Without loss of generality S, T are disjoint. Let  $T' \subseteq T$  be a smallest set s.t.  $\exists S' \subseteq S$  s.t.  $\mathbf{m}_{S'} \odot \mathbf{m}_{T'} \notin \mathbb{R}$  Rowspace  $\mathbb{H}(\mathbf{m}_S)$ . Select any  $t \in T'$  and write  $\mathbf{m}_{S'} \odot \mathbf{m}_{T'} = \mathbf{m}_{S'} \odot \mathbf{m}_{T'-\{t\}} \odot \mathbf{m}_t$ . By minimality of T',  $\mathbf{m}_{S'} \odot \mathbf{m}_{T'-\{t\}} \in \mathbb{R}$  Rowspace  $\mathbb{H}(\mathbf{m}_S)$ . But then  $\mathbf{m}_{S'} \odot \mathbf{m}_{T'} \in \mathbb{R}$  Rowspace  $\mathbb{H}(\mathbf{m}_{S \cup \{t\}})$ , so Rowspace  $\mathbb{H}(\mathbf{m}_{|S|}) \subset \mathbb{R}$  Rowspace  $\mathbb{H}(\mathbf{m}_{|S|})$ .

Theorem 2 is now a consequence of Lemma 9.

It follows from Theorem 2 that we can check whether rank  $\mathbb{H}(\mathbf{m}) = k$  in time  $O(n)^k$  by computing rank  $\mathbb{H}(\mathbf{m}|_S)$  for each  $S \in \binom{[n]}{k-1}$ .

# 3 Combinatorics of the NAE Condition: Proof of Theorem 4 (a)

Recall we are to show: 4 (a): If  $\overline{\varepsilon}(\mathbf{m}) \geq -1$  then  $\mathbf{m}$  has a restriction to some k-1 rows on which  $\overline{\varepsilon} = -1$ .

Proof. We induct on k. The (vacuous) base-case is k=1. For k>1, we induct on n, with base-case n=k-1. Supposing the Theorem fails for k, k>1, let  $\mathbf{m}$  be a k-column counterexample with least n. Necessarily every row is in NAE( $\mathbf{m}$ ), and  $n>k-1\geq 1$ . We will show  $\mathbf{m}$  has a restriction  $\mathbf{m}'$  to n-1 rows, for which  $\overline{\varepsilon}(\mathbf{m}')\geq -1$ ; this will imply a contradiction because, by minimality of  $\mathbf{m}$ ,  $\mathbf{m}'$  has a restriction to k-1 rows on which  $\overline{\varepsilon}=-1$ . If  $\overline{\varepsilon}(\mathbf{m})\geq 0$  then we can remove any single row of  $\mathbf{m}$  and still satisfy  $\overline{\varepsilon}\geq -1$ .

Otherwise,  $\bar{\varepsilon}(\mathbf{m}) = -1$ , so there is a nonempty S such that  $|\text{NAE}(\mathbf{m}|^S)| = |S| - 1$ ; choose a largest such S. It cannot be that S = [k] (as then n = k - 1). Arrange the rows  $\text{NAE}(\mathbf{m}|^S)$  as the bottom |S| - 1 rows of the matrix. As discussed earlier, for the NAE condition one may regard the distinct real values in each row of  $\mathbf{m}$  simply as distinct colors; relabel the colors in each row above  $\text{NAE}(\mathbf{m}|^S)$  so the color above S is called "white." (There need be no consistency among the real numbers called white in different rows.) See Figure 1.

Due to the maximality of |S|, there is no white rectangle on  $\ell$  columns and  $n - |S| - \ell + 1$  rows inside  $\mathbf{m}|_{[n]-\mathrm{NAE}(\mathbf{m}|^S)}^{[k]-S}$  for any  $\ell \geq 1$ . That is to say, if we form a bipartite graph on right vertices corresponding to the columns [k] - S, and left vertices corresponding to the rows  $[n] - \mathrm{NAE}(\mathbf{m}|^S)$ , with non-white cells being edges, then any subset of the right vertices of size  $\ell \geq 1$  has at least  $\ell + 1$  neighbors within the left vertices.

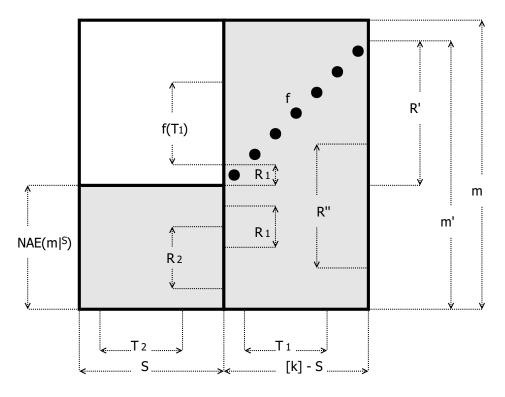


Figure 1: Argument for Theorem 4 (a). Upper-left region is white. Entries (t, f(t)) are not white.

By the induction on k (since  $S \neq \emptyset$ ), for the set of columns [k] - S there is a set R'' of k - |S| - 1 rows such that  $\overline{\varepsilon}(\mathbf{m}|_{R''}^{[k]-S}) = -1$ . Together with the rows of NAE( $\mathbf{m}|^S$ ) this amounts to at most k-2 rows, so since  $n \geq k$ , we can find two rows outside this union; delete either one of them, leaving a matrix  $\mathbf{m}'$  with n-1 rows. This matrix has the rows NAE( $\mathbf{m}|^S$ ) at the bottom, and n-|S| remaining rows which we call R'. The lemma will follow by showing that  $\overline{\varepsilon}(\mathbf{m}') \geq -1$ .

In  $\mathbf{m}'$ , the induced bipartite graph on right vertices [k] - S and left vertices R' has the property that any right subset of size  $\ell \ge 1$  has a neighborhood of size at least  $\ell$  in R'. Applying Hall's Marriage Theorem, there is an injective  $f: [k] - S \to R'$  employing only edges of the graph.

Now consider any set of columns T,  $T = T_1 \cup T_2$ ,  $T_1 \subseteq [k] - S$ ,  $T_2 \subseteq S$ . We need to show that  $\varepsilon(\mathbf{m}|^T) \ge -1$ . Let  $R_1 = \text{NAE}(\mathbf{m}|^{T_1}) \cap R''$ ,  $R_2 = \text{NAE}(\mathbf{m}|^{T_2}) \subseteq \text{NAE}(\mathbf{m}|^S)$ , and note that  $|R_1| \ge |T_1| - 1$ ,  $|R_2| \ge |T_2| - 1$ . If  $T_2 = \emptyset$  we simply use  $R_1$ . Likewise if  $T_1 = \emptyset$ , we use  $R_2$ .

If both  $T_1$  and  $T_2$  are nonempty,  $\text{NAE}(\mathbf{m}|^{T_2}) \subseteq \text{NAE}(\mathbf{m}|^S)$ , and  $|\text{NAE}(\mathbf{m}|^{T_2})| \ge |T_2| - 1$ . Now use the matching f. The set of rows  $f(T_1)$  lies in R' and is therefore disjoint from  $\text{NAE}(\mathbf{m}|^{T_2})$ . Moreover since  $T_2 \ne \emptyset$ , every entry (t,j) for  $t \in T_2, j \in R'$  is white. On the other hand due to the construction of f, for every  $t \in T_1$  the entry (t,f(t)) is non-white. Therefore every row in  $f(T_1)$  is in  $\text{NAE}(\mathbf{m}|^{T_1 \cup T_2})$ . So  $|\text{NAE}(\mathbf{m}|^{T_1 \cup T_2})| \ge |T_2| - 1 + |T_1|$ . Thus  $\overline{\varepsilon}(\mathbf{m}') \ge -1$ .

# 4 From NAE to Rank: Proof of Theorem 4 (b)

Recall we are to show: 4 (b):  $\mathbb{H}(\mathbf{m})$  has full column rank if  $\overline{\varepsilon}(\mathbf{m}) > -1$ .

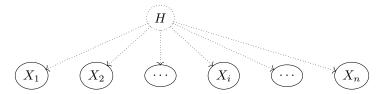
*Proof.* The case k = 1 is trivial. Now suppose  $k \ge 2$  and that Theorem 4 (b) holds for all k' < k. Any constant rows of **m** affect neither the hypothesis nor the conclusion, so remove them, leaving **m** with at least k - 1 rows. Now pick any set, C, of k - 1 columns of **m**. By Theorem 4 (a) there are some k - 2 rows of **m**, call them R', on which  $\overline{\varepsilon}(\mathbf{m}|_{R'}^C) = -1$ . Let v be a row of **m** outside R'. Call the rows of **m** apart from v, R''. Since R'' contains

R', by induction dim Rowspace  $\mathbb{H}(\mathbf{m}|_{R''}^C) = k - 1$ . Therefore  $U := \text{Rowspace } \mathbb{H}(\mathbf{m}|_{R''}) \subseteq \mathbb{R}^k$  is of dimension at least k - 1. We claim now that dim U = k.

Suppose to the contrary that  $\dim U = k-1$ . If  $v_{\odot}(U) \subseteq U$  then as proven earlier in Theorem 8, U respects B(v). Since v is nonconstant, B(v) is a partition of [k] into  $\ell \geq 2$  nonempty blocks  $B(v)_{(i)}$ , and  $U = \bigoplus_{i=1}^{\ell} U_{(i)}$  with  $U_{(i)} = P_{(i)}U_{(i)}$ . So there is some  $i_0$  for which  $U_{(i_0)} \subset V_{(i_0)}$ ; specifically,  $U_{(i)} = V_{(i)}$  for all  $i \neq i_0$ , and  $\dim U_{(i_0)} = \dim V_{(i_0)} - 1$ . Since  $|B(v)_{(i_0)}| < k$ , we know by induction that the rows of  $\mathbb{H}(\mathbf{m})$  span  $V_{(i_0)}$ . Thus in fact  $U = \mathbb{R}^k$ . (Further detail for the last step: let  $w \in \mathbb{R}^k$ . Since the rows of  $\mathbb{H}(\mathbf{m})$  span  $V_{(i_0)}$ , there is a  $w' \in \operatorname{Rowspace} \mathbb{H}(\mathbf{m})$  s.t.  $P_{(i_0)}w' = P_{(i_0)}w$ . Moreover since  $U_{(i)} = V_{(i)}$  for all  $i \neq i_0$ , there is a  $w'' \in U$  s.t.  $w'' = (I - P_{(i_0)})(w - w')$ . Then  $w' + w'' \in \operatorname{Rowspace} \mathbb{H}(\mathbf{m})$ , and w' + w'' = w.)

#### 5 Motivation

Consider observable random variables  $X_1, \ldots, X_n$  that are statistically independent conditional on H, a hidden random variable H supported on  $\{1, \ldots, k\}$ . (See causal diagram.)



The most fundamental case is that the  $X_i$  are binary. Then we denote  $\mathbf{m}_i^j = \Pr(X_i = 1 | H = j)$ . The model parameters are  $\mathbf{m}$  along with a probability distribution (the *mixture* distribution)  $\pi = (\pi_1, \dots, \pi_k)$  on H.

Finite mixture models were pioneered in the late 1800s in [13, 14]. The problem of learning such distributions has drawn a great deal of attention. For surveys see, e.g., [5, 17, 11, 12]. For some algorithmic papers on discrete  $X_i$ , see [9, 4, 7, 2, 6, 1, 15, 10, 3, 8]. The source identification problem is that of computing  $(\mathbf{m}, \pi)$  from the joint statistics of the  $X_i$ . Put another way, the problem is to invert the multilinear moment map

$$\mu : (\mathbf{m}, \pi) \to \mathbb{R}^{2^{[n]}}$$

$$\mu(\mathbf{m}, \pi)_S = \Pr(X_S = 1) \quad \text{where } S \subseteq [n], \ X_S = \prod_{i \in S} X_i$$

$$= \mathbf{m}_S \cdot \pi^\top$$

The last line shows the significance of  $\mathbb{H}(\mathbf{m})$  to mixture model identification, since  $\mathbf{m}_S^j = \Pr(X_S = 1 | H = j)$ .

Connection to rank  $\mathbb{H}(\mathbf{m})$ . In general  $\mu$  is not injective (even allowing for permutation among the values of H). For instance it is clearly not injective if  $\mathbf{m}$  has two identical columns (unless  $\pi$  places no weight on those). More generally, and assuming all  $\pi_j > 0$ , it cannot be injective unless  $\mathbb{H}(\mathbf{m})$  has full column rank.

One sufficient condition for injectivity, due to [16], is that there be 2k-1 "separated" observables  $X_i$ ;  $X_i$  is separated if all  $\mathbf{m}_i^j$  are distinct, or in our terminology, if no color recurs in  $\mathbf{m}_i$ . (Further [8], one can lower bound the distance between  $\mu(\mathbf{m}, \pi)$  and any  $\mu(\mathbf{m}', \pi')$  in terms of  $\min_{i,j} |\mathbf{m}_i^j - \mathbf{m}_i^{j'}|$  and the distance between  $(\mathbf{m}, \pi)$  and  $(\mathbf{m}', \pi')$ .)

A weaker sufficient condition for injectivity of  $\mu$ , due to [8], is that for every  $i \in [n]$  there exist two disjoint sets  $A, B \subseteq [n] - \{i\}$  such that  $\mathbb{H}(\mathbf{m}|_A)$  and  $\mathbb{H}(\mathbf{m}|_B)$  have full column rank. (It is not known whether two disjoint such A, B are strictly necessary, but the implied  $n \leq 2k - 1$  is in general best possible [15].)

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