Cliques in high-dimensional random geometric graphs

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Abstract. Random geometric graphs are good examples of random graphs with a tendency to demonstrate community structure. Vertices of such a graph are represented by points in Euclid space $\mathbb{R}^d$, and edge appearance depends on the distance between the points. Random geometric graphs were extensively explored and many of their basic properties are revealed. However, in the case of growing dimension $d \to \infty$ practically nothing is known; this regime corresponds to the case of data with many features, a case commonly appearing in practice. In this paper, we focus on the cliques of these graphs in the situation when average vertex degree grows significantly slower than the number of vertices n with $n \to \infty$ and $d \to \infty$. We show that under these conditions random geometric graphs do not contain cliques of size 4 a.s. As for the size 3, we will present new bounds on the expected number of triangles in the case $\log^2 n \ll d \ll \log^3 n$ that improve previously known results.

Keywords: random geometric graphs, high dimension, clique number, triangles

1 Introduction

Given the task to describe some complex network, one can use different random graph models for this purpose. The first idea that can come to mind is to use the classical model of Erdős and Rényi (see [1]–[3]) where the edge between any pair of vertices appears independently with equal probability. However, this graph cannot describe important properties of many real networks, for example, a predisposition to create clusters. Another possible way is to use graph models based on geometric properties. These graphs form clusters quite naturally that makes them a popular object for the research. The most studied type of such a graph model is a random geometric graph where the appearance of an edge depends on the distance between given nodes. These graphs are very useful for modeling real social, technological and biological networks. Also, they can be applied in statistics and machine learning tasks since the distance between the nodes represents the correlation between observations in a dataset. We refer to articles [4]–[10] on the applications of random geometric graphs for further reading.

Let us define a random geometric graph $G(n,p,d)$ as follows. Let $X_1,\ldots,X_n$ be independent random vectors uniformly distributed on the $(d-1)$-dimensional sphere $\mathbb{S}^{d-1}\subset\mathbb{R}^d$. In $G(n,p,d)$ distinct vertices $i\in[n]$ and $j\in[n]$ are adjacent if and only if $\langle X_i,X_j\rangle \geq t_{p,d}$ where $t_{p,d}$ defined in such a manner that $\mathbb{P}(\langle X_i,X_j\rangle \geq t_{p,d})=p$. There are a lot of papers studying properties of these graphs. We refer to Penrose [11] for the intensive study; among other papers on this subject we can mark out papers [10], [12]–[16]. However, practically all known results about random geometric graphs are obtained under the condition that the dimension d is fixed. Meanwhile, the case $d\to\infty$ becomes more and more interesting for applications, as, for instance, the number of features in datasets nowadays can be comparable with the number of observations.

Perhaps the first paper treating the case $d\to\infty$ is the article of Devroye, György, Lugosi and Udina [17]. In this paper the clique number was studied in the asymptotic case when $n\to\infty,\ d\gg\log n$ and p is fixed. Authors proved that the clique number of the random geometric graph $G(n,p,d)$ is close to that of the Erdős–Rényi graph $G(n,p)$ in the above mentioned regime.

Our main interest is the investigation of cliques in the asymptotic case when $n\to\infty,\ d\gg\log n$. But instead of *dense* regime when p is fixed we will focus on the *sparse* regime when $p=p(n)=\alpha(n)/n$ where $\lim\limits_{n\to\infty}\alpha(n)/n\to 0$. It is easy to see that the function $\alpha(n)$ denotes the average vertex degree in this case. This mode is practically unexplored and the only paper known to us is the work [18] of Bubeck, Ding, Eldan and Racz. They have obtained a "negative" result: with $d\ll\log^3 n$ the graph $G(n,c/n,d)$ is "different" from the Erdős–Rényi graph $G(n,c/n)$ in the sense that the total variation distance between two random models converges to 1 (here c is a constant). Also they made a conjecture about the "positive" result: with $d/\log^3 n\to\infty$ the graphs $G(n,p,d)$ and $G(n,p)$ are close. In order to obtain the "negative" result, the authors proved that in the case $d\ll\log^3 n$ the average number of triangles in $G(n,p,d)$ grows at least as a poly-logarithmic function of n which is quite different from the expected number of triangles in $G(n,p)$. The difference between these regimes seems quite interesting to us that is why we first concentrate on the case $d=\Theta(\log^m n)$.

The main contribution of this paper consists of three results in the sparse regime. First one, presented in Section 3, states that the clique number of $G(n,\alpha(n)/n,d)$ does not exceed 3 almost surely under the condition $d\gg\log^{1+\epsilon} n$. The second one gives bounds on the expected number of triangles in the case $d\gg\log^3 n$ and shows that it grows as the function $\alpha(n)$. This result is given by Theorem 6 in Section 4. Finally, in Theorem 7 (Section 4) we will present new lower and upper bounds on the expected number of triangles in the case $\log^2 n\ll d\ll\log^3 n$. This lower bound improves the result of the paper [18] since it grows faster than any poly-logarithmic function (let us remind that the lower bound from [18] is poly-logarithmic in n). Let us also notice that the first two results more likely confirm the conjecture of Bubeck et al. about the similarity of $G(n,\alpha(n)/n,d)$ and $G(n,\alpha(n)/n)$ when $d\gg\log^3 n$. As for the opposite case $d\ll\log^3 n$, it seems that random geometric graphs show more disposition for clustering than was discovered in the paper [18].

In the present version of the work we just outline the proofs of our main results. The detailed proofs will be given in an extended journal version.

2 Auxiliary results

We start with citing the results of the paper [17]. Though this paper is devoted to the dense regime, the next two theorems do not require the condition $p = \text{const}$ and are applicable in our situation. Let us denote by $N_k = N_k(n, d, p)$ the number of cliques of size k. Obviously, $\mathbb{E}[N_k] = \binom{n}{k}\mathbb{P}\{X_1, \dots, X_k \text{ form a clique}\}$. The following two results establish lower and upper bounds on $\mathbb{E}[N_k]$.

Theorem 1 (Devroye, György, Lugosi, Udina, 2011). *Introduce*

$$\tilde{p} = \tilde{p}(p) = 1 - \Phi(2t_{p,d}\sqrt{d} + 1)$$

and let $\delta_n \in (0, 2/3]$ *and fix* $k \geq 3$. *Assume*

$$d > \frac{8(k+1)^2 \ln \frac{1}{\tilde{p}}}{\delta_n^2} \left(k \ln \frac{4}{\tilde{p}} + \ln \frac{k-1}{2} \right).$$

Define $\alpha > 0$ *as*

$$\alpha^2 = 1 + \sqrt{\frac{8k}{d} \ln \frac{4}{\tilde{p}}}.$$

Then

$$\mathbb{E}[N_k(n, d, p)] \geq \frac{4}{5} \binom{n}{k} \left(1 - \tilde{\Phi}_k(d, p) \right)^{\binom{k}{2}},$$

where $\tilde{\Phi}_k(d, p) = \Phi \left(\frac{\alpha t_{p,d}\sqrt{d} + \delta_n}{\sqrt{1 - \frac{2(k+1)^2 \ln(1/\tilde{p})}{d}}} \right)$

Theorem 2 (Devroye, György, Lugosi, Udina, 2011). *Let* $k \geq 2$ *be a positive integer, let* $\delta_n > 0$ *and define*

$$\hat{p} = \hat{p}(p) = 1 - \Phi(t_{p,d}\sqrt{d}).$$

Assume

$$d \geq \frac{8(k+1)^2 \ln \frac{1}{\hat{p}}}{\delta_n^2} \left(k \ln \frac{4}{\hat{p}} + \ln \frac{k-1}{2} \right).$$

Furthermore, for $p < 1/2$, *define* $\beta = 2\sqrt{\ln(4/\hat{p})}$ *and for* $\beta\sqrt{k/d} < 1$ *let* $\alpha = \sqrt{1 - \beta\sqrt{k/d}}$. *Then for any* $0 < \delta_n < \alpha t_{p,d}\sqrt{d}$ *we have*

$$\mathbb{E}[N_k(n, d, p)] \leq e^{1/\sqrt{2}} \binom{n}{k} \left(1 - \Phi(\alpha t_{p,d}\sqrt{d} - \delta_n) \right)^{\binom{k}{2}}.$$

To apply these two theorems we need a lemma that establishes the growth rate of $t_{p,d}$ which is crucial for asymptotic analysis in the sparse regime (see, for example, the proof of Theorem 5). Since p is the normalized surface area of a spherical cap of angle $\arccos t_{p,d}$ (the example for a circle is given by the figure 1 below), from convex geometry we learn that (see [20]):

$$\frac{1}{6t_{p,d}\sqrt{d}}(1-t_{p,d}^2)^{\frac{d-1}{2}} \le p \le \frac{1}{2t_{p,d}\sqrt{d}}(1-t_{p,d}^2)^{\frac{d-1}{2}}. \tag{1}$$

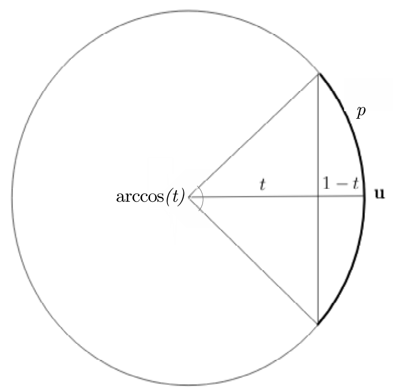

Fig. 1. A spherical cap of height $1-t$

These inequalities already give that $t_{p,d}\sqrt{d} \sim \sqrt{\log(1/p)}$. The bound from the below lemma can now be obtained by applying the asymptotics of the Lambert function $W(x)$ (that is the unique solution of the equation $ze^z = x$ for $x > 0$) to (1).

Lemma 1. *Let p be the probability of an edge between two vertices and suppose $d \gg \log^2 n$. Then*

$$\sqrt{2\log(1/p) + \log\log(1/p) + \log 2} \le t_{p,d}\sqrt{d} \le$$
$$\le \sqrt{2\log(1/p) + \log\log(12/p) + \log(288 + 288e^{-1})}.$$

Also, we need to present the result from the paper [18] that gives a lower bound on the expected number of triangles.

Theorem 3 (Bubeck, Ding, Eldan, Rácz, 2016). *There exists a universal constant $C > 0$ such that whenever $p < 1/4$ we have that*

$$\mathbb{E}[N_3(n,d,p)] \ge p^3\binom{n}{3}\left(1 + C\frac{\left(\log\frac{1}{p}\right)^{3/2}}{\sqrt{d}}\right).$$

Note that if $p = \alpha(n)/n$ with $\alpha(n) \ll n$ and $d \ll \log^3 n$ the expected number of triangles grows like a poly-logarithmic function that is totally different from Erdős–Rényi graph $G(n, \alpha(n)/n)$ where the average number of triangles grows as $c^3(n)$ with $n \to \infty$. This result will be improved by our new theorem in Section 4. In order to make this improvement we present the result from convex geometry providing the expression for the surface area of the intersection of two spherical caps in $\mathbb{R}^d$ of angles θ_1 and θ_2 with the angle θ_ν between axes defining these caps. Let us denote this surface area by $A_d(\theta_1, \theta_2, \theta_\nu)$. The paper [19] gives the exact formula for this quantity in terms of an incomplete beta function.

Theorem 4 (Lee and Kim, 2011). *Let us suppose that* $\theta_\nu \in [0, \pi/2)$ *and* $\theta_1, \theta_2 \in [0, \theta_\nu]$. *Then*

$$A_d(\theta_1, \theta_2, \theta_\nu) = \frac{\pi^{(n-1)/2}}{\Gamma\left(\frac{n-1}{2}\right)} \left\{ \int_{\theta_{min}}^{\theta_2} \sin^{d-2}(\phi) I_{1-\left(\frac{\tan(\theta_{min})}{\tan(\phi)}\right)^2} \left(\frac{n-1}{2}, \frac{1}{2}\right) d\phi + \right.$$
$$\left. + \int_{\theta_\nu - \theta_{min}}^{\theta_1} \sin^{d-2}(\phi) I_{1-\left(\frac{\tan(\theta_\nu - \theta_{min})}{\tan(\phi)}\right)^2} \left(\frac{n-1}{2}, \frac{1}{2}\right) d\phi \right\} :=$$
$$:= J_n^{\theta_{min}, \theta_2} + J_n^{\theta_\nu - \theta_{min}, \theta_1}$$

where θ_{min} *is defined as follows*

$$\theta_{min} = \arctan\left(\frac{\cos(\theta_1)}{\cos(\theta_2)\sin(\theta_\nu)} - \frac{1}{\tan(\theta_\nu)}\right)$$

and $I_x(a, b)$ *stands for the regularized incomplete beta function that is*

$$I_x(a, b) = \frac{\mathrm{B}(x, a, b)}{\mathrm{B}(a, b)} = \frac{\int_0^x t^{a-1}(1-t)^{b-1} dt}{\int_0^1 t^{a-1}(1-t)^{b-1} dt}.$$

3 Clique number in the sparse regime

As was mentioned above, our main interest is the clique number. Theorems 1 and 2 allow to say that when p is constant and $d \gg \log^7 n$ the clique number grows similarly to the clique number of the Erdős–Rényi graph which is $2\log_{1/p} n - 2\log_{1/p}\log_{1/p} n + O(1)$. We will show that in the sparse regime, when $p = \alpha(n)/n$, if $d/\log^{1+\epsilon} n \to \infty$ then there is no clique of size 4 in $G(n, p, d)$ a. s.

Theorem 5. *Let us suppose that* $k \geq 4, p = \dfrac{\alpha(n)}{n}$ *with* $\alpha(n) \ll n^{1/6}$ *and* $d \gg \log^{1+\epsilon} n$ *for some* $\epsilon > 0$. *Then*

$$\mathbb{P}[N_k(n, d, p) \geq 1] \to 0, \quad n \to \infty.$$

To prove this theorem, we need to apply Theorem 2. First of all, it is easy to verify that the conditions of Theorem 2 are satisfied in our situation when $p = \alpha(n)/n$ and $d \gg \log^{1+\epsilon} n$. Next, we need to bound the most important term $1 - \Phi(\alpha t_{p,d}\sqrt{d} - \delta_n)$. It can be shown with asymptotic analysis and the result of Lemma 1 that

$$1 - \Phi(\alpha t_{p,d}\sqrt{d} - \delta_n) \leq Cpn^{\gamma} = \frac{C\alpha(n)}{n^{1-\gamma}} \leq \frac{C}{n^{5/6-\gamma}} \text{ for any } \gamma > 0, \qquad (2)$$

where $C > 0$ is absolute constant. If k is fixed and $n \to \infty$ then $\binom{n}{k} \sim \frac{n^k}{k!}$. It is easy to verify that

$$(5/6 - \gamma)k(k-1)/2 > k$$

for $k \geq 4$ and $\gamma < 1/6$. Denote constant $C_2 = C_1^{\binom{k}{2}}/6 > 0$ and get that

$$\mathbb{E}[N_k(n,d,p)] \leq e^{1/\sqrt{2}} \binom{n}{k} \left(1 - \Phi(\alpha t_{p,d}\sqrt{d} - \delta_n)\right)^{\binom{k}{2}} \leq$$
$$\leq C_2 n^k n^{-(5/6-\gamma)\frac{k(k-1)}{2}} \to 0, \quad n \to \infty.$$

It only remains to mention that

$$\mathbb{P}[N_k \geq 1] \leq \mathbb{E}[N_k(n,d,p)] \to 0, \quad n \to \infty.$$

4 Number of triangles in the sparse regime

As was observed in the previous section, $G(n,p,d)$ does not contain any complete subgraph larger than a triangle in the sparse regime. The natural question is how many triangles are in $G(n,p,d)$. The next two results give some notion about the expected number of triangles. First result deals with the case $d \gg \log^3 n$ and in this case the average number of triangles grows as the function $\alpha(n)$ that defines the probability $p(n) = \alpha(n)/n$.

Theorem 6. *Let us suppose that $p = \alpha(n)/n$ with $\alpha(n) \ll n$ and $d \gg \log^3 n$. Then for n sufficiently large the expected number of triangles can be bounded from above as follows:*

$$\frac{2}{15}(2\pi)^{-3/2}c^3(n)(1+o(1)) \leq \mathbb{E}[N_3(n,d,p)] \leq \frac{3}{2}(2\pi)^{-3/2}e^{9/\sqrt{2}}c^3(n), \quad n \to \infty.$$

The idea of the proof is quite similar to the proof of Theorem 5 but it uses both Theorems 1 and 2. Besides, we need more accurate asymptotic analysis as now a rough bound like in (2) is not sufficient for the application of Theorems 1 and 2.

So far, the presented results more likely confirm the similarity between the random geometric graph $G(n,p,d)$ and the Erdős–Rényi graph $G(n,p)$. However, from paper [18] one can learn that these graphs are completely different in sparse regime if only $d \ll \log^3 n$. This can be easily deduced from the result of the Theorem 3 that states that the expected number of triangles of a random geometric graph grows significantly faster (as a poly-logarithmic function of n) than one of the corresponding Erdős–Rényi graph. It turns out that this bound can be improved as the next result states.

Theorem 7. *Let $p = \alpha(n)/n$ with $\alpha(n) \ll n$ be the probability that two given vertices are connected with an edge and let $d \gg \log^2 n$. Then there exist constants $C_l > 0$ and $C_u > 0$ such that*

$$C_l c^3(n) t_{p,d}^2 e^{t_{p,d}^3 d}(1+o(1)) \le \mathbb{E}[N_3(n,d,p)] \le C_u c^3(n) e^{t_{p,d}^3 d}(1+o(1)).$$

The concept of the proof goes as follows. Let us introduce some additional notation. Denote by $E_{i,j}$ the event $\{\langle X_i, X_j\rangle \ge t_{p,d}\}$ and by $E_{i,j}(x)$ the event $\{\langle X_i, X_j\rangle = x\}$. Obviously it is enough to calculate $\mathbb{P}(E_{1,2}E_{1,3}E_{2,3})$ in order to obtain the expected number of triangles. In what follows we use a conditioning on the zero-probability event $E_{i,j}(x)$. It should be understood as conditioning on the event $\{x-\epsilon \le \langle X_i, X_j\rangle \le x+\epsilon\}$ with $\epsilon \to 0$. Using this notation we can rewrite

$$\begin{aligned}
\mathbb{P}[E_{1,2}E_{1,3}E_{2,3}] &= \int_{t_{p,d}}^{1} \mathbb{P}\left[E_{2,3}E_{1,3}|E_{1,2}(x)\right] f_d(x) = \\
&= \int_{t_{p,d}}^{2t_{p,d}} \mathbb{P}\left[E_{2,3}E_{1,3}|E_{1,2}(x)\right] f_d(x)dx + \int_{2t_{p,d}}^{1} \mathbb{P}\left[E_{2,3}E_{1,3}|E_{1,2}(x)\right] f_d(x)\big)dx := \\
&:= T_1 + T_2,
\end{aligned} \tag{3}$$

where $f_d(x)$ is the density of a coordinate of uniform random point on $\mathbb{S}^{d-1}$ (see [18]) that is

$$f_d(x) = \frac{\Gamma(d/2)}{\Gamma((d-1)/2)\sqrt{\pi}}(1-x^2)^{(d-3)/2}, \quad x \in [-1,1].$$

Here is the general plan of the proof. We treat the terms T_1 and T_2 separately and we start with T_1. The probability $\mathbb{P}\left[E_{2,3}E_{1,3}|E_{1,2}(x)\right]$ can be expressed with the normalized surface area of the intersections of two spherical caps. First, we need to bound this quantity, using Theorem 4. After that we can calculate T_1 in terms of CDF of the standard normal distribution and estimate its asymptotics. As for T_2, it is enough to show that $T_2 = o(T_1)$ as $n \to \infty$.

Let us now discuss the result of this theorem. First of all, as we know from lemma 1, $t_{p,d}^3 d \sim C\frac{\log^{3/2} n}{\sqrt{d}}$. The exponent $\exp\left(\frac{\log^{3/2} n}{\sqrt{d}}\right)$ grows faster than any poly-logarithmic function of n that means that the obtained result is better than lemma 3 and our bound has significantly faster mode of growing. Unfortunately, the upper bound is still $1/t_{p,d}^2$ times larger then the lower bound though this margin is significantly smaller than the "main" term of the bounds $e^{t_{p,d}^3 d}$. This exponent is still growing slower than any power of n, but we believe that if $d \sim C \log n$ the number of triangles is linear (or almost linear) in n.

What can we say about the concentration? Unfortunately, the variance of $N_3(n, d, p)$ does not go to 0 as $n \to \infty$. The next proposition states the variance of the number of triangles can be bounded from below by $\mathbb{E}[N_3(n, d, p)]$. Within the proof we are using practically the same technique as one that presented in paper [18].

Proposition 1. *For n large enough and for any p*

$$\text{Var}\left[N_3(n, d, p)\right] \geq \mathbb{E}[N_3(n, d, p)].$$

The proof is quite simple. Let us denote by $T(i, j, k)$ the indicator that distinct vertices i, j, k form a triangle in $G(n, d, p)$. Then the number of triangles can be written as follows:

$$N_3(n, d, p) = \sum_{[i,j,k] \subset \binom{[n]}{3}} T(i, j, k).$$

Expanding this, we have that

$$\mathbb{E}\left[(N_3(n, d, p))^2\right] = \binom{n}{3}\binom{n-3}{3}\mathbb{E}\left[T(1, 2, 3)T(4, 5, 6)\right] +$$
$$+ 5\binom{n}{5}\mathbb{E}\left[T(1, 2, 3)T(1, 4, 5)\right] + 6\binom{n}{4}\mathbb{E}\left[T(1, 2, 3)T(1, 2, 4)\right] + \binom{n}{3}\mathbb{E}\left[T^2(1, 2, 3)\right].$$

Since $T(1, 2, 3)$ and $T(4, 5, 6)$ are independent, we may conclude that

$$\binom{n}{3}\binom{n-3}{3}\mathbb{E}\left[T(1, 2, 3)T(4, 5, 6)\right] \leq \binom{n}{3}^2 \left(\mathbb{E}[T(1, 2, 3)]\right)^2 = \left(\mathbb{E}[N_3(n, d, p)]\right)^2,$$

and therefore,

$$\text{Var}\left[N_3(n, d, p)\right] \geq \binom{n}{3}\mathbb{E}\left[T^2(1, 2, 3)\right] = \binom{n}{3}\mathbb{E}\left[T(1, 2, 3)\right] =$$
$$= \binom{n}{3}\mathbb{P}[\{X_1, X_2, X_3\} \text{ form a triangle}] = \mathbb{E}[N_3(n, d, p)].$$

Let us also mention that with the standard technique (see, e. g., [11, ch. 2]) it is not hard to prove that the number of triangles has a Poisson distribution $Pois(\lambda)$, where $\lambda = E[N_3(n, d, p)]$. But, since we do not know the exact value of the expected number of triangles, we ignore the exact value of λ, that is why we are not so interested in this result.

5 Conclusion

As one can easily see from the results above, the threshold $d \sim \log^3 n$ is absolutely crucial in the sparse regime. Apparently, it seems that if $d \gg \log^3 n$ the graphs $G(n,p,d)$ and $G(n,p)$ are practically identical. In this case it looks quite reasonable to try to get a result about small distance between the two random models as in the paper [18]. However, the technique of this paper applied in the dense regime cannot be easily extended to the sparse regime. Any result describing the total variation between $G(n,p,d)$ and $G(n,p)$ in this regime would be very interesting.

Another natural question is what happens in the case of slow-growing d. It is known that in the dense regime the clique number is almost linear in n if $d \ll \log n$ (see [17]). We have no idea what happens to the clique number near this "second" threshold in the sparse regime.

As for triangles (and, as consequence, for the clustering coefficient), we still need at least to get a sharp bound on the expected number. We are convinced that the upper bound in Theorem 7 cannot be improved and the statement holds true with $\log n \ll d \ll \log^2 n$.

For sure, there are a lot of graph properties that remain unexplored for $d \to \infty$ such as the connectivity, the existence of giant component, chromatic and independence numbers. But even for fixed d the results describing these properties require quite complex methods, so we do not expect immediate breakthroughs in this direction.

For conclusion, let us mention some possible practical implications of the present work. Firstly, cliques might be very useful for clustering algorithms in real networks with a geometrical structure. Secondly, we think that some ideas of the paper can help to determine if network has an underlying geometry and (if answer to the previous question is positive) to estimate the dimension of this geometry. The latter is important because if it is known that the nodes of a network are embedded in some space then one can hope to make a lower-dimensional representation of a network structure or to use some properties of a geometric structure (e.g., two distant nodes cannot have a common neighbour). Finally, the results obtained above can be helpful for the investigation of possible correlations between observations in datasets with many features.

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