Approximately Counting Hamilton Cycles in Dense Graphs

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Abstract

We describe a fully polynomial randomized approximation scheme for the problem of determining the number of Hamiltonian cycles in an n-vertex graph with minimum degree $(\frac{1}{2}+\varepsilon)n$, for any fixed $\varepsilon > 0$. We also show that the exact counting problem is #P-complete.

1 Introduction

Combinatorial counting problems have a long history, even from the computational viewpoint. For example, the classical matrix-tree theorem provides a good algorithm for determining the number of trees in a graph. However, it seems that few interesting combinatorial structures possess good counting algorithms. This intuition was made precise by Valiant [17] using the class #P. He showed that many problems for which the decision counterpart is easy were nevertheless complete for this class. Since it is unlikely that #P = P, exact counting is apparently intractable for many natural problems. For example Valiant [16] showed that 0-1 permanent evaluation, and counting the number of bases of a (suitably presented) matroid [17] were #P-complete. Many other problems have since been added to this list, for example volume computation for polyhedra [4], counting linear extensions of a partial order [1] and counting Eulerian orientations of a graph [13].

The hardness of most counting problems has led to an interest in *approximate* counting. The most fruitful approach in this respect has been *randomized approximation*. This

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is based on the idea of a fully polynomial randomized approximation scheme (*fpras*) due to Karp and Luby [11]. Thus if N is the true value, we must determine an estimate $\widehat{N}$ such that for given $\gamma, \delta > 0$

$$\Pr\left(1/(1+\gamma) < \widehat{N}/N < (1+\gamma)\right) > 1 - \delta,$$

in time polynomial in the size of the input, γ^{-1} and $\log(\delta^{-1})$. Examples of problems amenable to this type of approximation are dense 0-1 permanent [2, 8], matchings [8], volume computation [5], counting Eulerian orientations [13], counting linear extensions of a partial order [12] and computing the partition function for the Ising model [9]. The algorithms in the papers cited use a *random walk* to generate an almost uniform random solution to the problem (e.g., a random matching), and then apply multi-stage statistical sampling methods to obtain the desired estimate.

One obvious requirement for such approximate counting to be possible is that the associated decision problem be easy. In fact, it appears from experience that it must be "very easy" in order to have a realistic hope that a randomized approximation scheme can be found.

In this paper, we add another entry to the growing list of randomly approximable counting problems: that of counting the number of Hamiltonian cycles in "dense" graphs. Let $G = (V, E)$ be a graph, where $V = \{v_1, v_2, \ldots, v_n\}$. Denote the degree of vertex v_i by d_i, for $i = 1, 2, \ldots, n$. We will say that G is *dense* if $\min_i d_i \geq (\frac{1}{2} + \varepsilon)n$, where $0 < \varepsilon \leq \frac{1}{2}$ is a fixed constant. Under these circumstances it is known [3] that G must contain a Hamilton cycle. Moreover, the proof of this fact is easily modified to give a simple polynomial-time algorithm for constructing such a Hamilton cycle. This algorithm, which uses edges whose existence is guaranteed by the pigeonhole principle to "patch together" disjoint cycles, provides the required easy decision procedure.

We consider here the more difficult problem of counting the *number* of Hamilton cycles in such graphs. We show in section 4 that this problem is in fact #P-complete, so exact counting is presumably intractable. More positively, our main result in sections 2 and 3, establishes the existence of a *fpras* for this counting problem when $\varepsilon > 0$. We may observe that if the degree condition is relaxed to $\min_i d_i \geq (\frac{1}{2} - \varepsilon_n)n$ with $\varepsilon_n = \Omega(n^{\kappa-1})$ for any fixed $\kappa > 0$, then the question of the existence of any Hamilton cycle becomes NP-Complete,[1] and approximate counting is NP-hard. Thus our results establish quite precisely the difficulty of the counting problem except in the region where ε is close to zero.

The main technical difficulty in our approach lies in obtaining a good upper bound on the ratio of 2-factors to Hamilton cycles in a dense graph. A direct attack — relating the number of 2-factors with k cycles to the number with $k+1$ cycles — appears unworkable. Instead, we introduce a carefully tailored weight function on 2-factors that allows us to argue about the distribution of total weight as a function of the number of cycles. By a rather delicate analysis, we are able to show that the Hamiton cycles carry sufficient weight for our purpose.

[1]This is true even if we insist on G being k-connected for any $k = o(n)$.

2 Outline approach

Our approach to constructing an fpras for Hamilton cycles in a dense graph G is via a randomized reduction to sampling and estimating *2-factors* in G. An *almost uniform sampler* for 2-factors in a graph is a randomized algorithm that takes as input a graph G and $\delta > 0$ and outputs a 2-factor Z (a random variable) such that

$$1/(1+\delta)N \leq \Pr(Z = F) \leq (1+\delta)/N,$$

where F is any 2-factor in G and N is the total number of 2-factors. The sampler is said to be *fully polynomial* if it runs in time polynomial in the size of G and $\log \delta^{-1}$. Using known techniques, 2-factors in a dense graph G may be efficiently sampled, and their number estimated.

Theorem 1 *There exist both a fully polynomial randomized approximation scheme and a fully polynomial almost uniform sampler for the set of 2-factors in a dense graph.*

Proof The result follows immediately from Corollary 4.2 of Jerrum and Sinclair [10], as will be clear once the notation used there is explained. In that corollary, $\mathbf{d} = (d_1, \ldots, d_n)$ stands for a degree sequence on $V = \{v_1, v_2, \ldots, v_n\}$, and $X \subseteq V^{(2)}$ for the edge set of an "excluded" graph on vertex set V. The notation $\mathcal{G}(\mathbf{d}, X)$ stands for the set of graphs on vertex set V that have degree sequence $\mathbf{d}$ and avoid all edges in X. Finally, $e(\mathbf{d})$ is the number of edges in any graph with $\mathbf{d}$ as degree sequence, $d_{\max}$ is the largest component of $\mathbf{d}$, and $x_{\max}$ is the largest degree of any vertex in the excluded graph (V, X).

Note that the set of 2-factors in a graph $G = (V, E)$ is equal to $\mathcal{G}(\mathbf{d}, X)$, where $\mathbf{d} = (2, 2, \ldots, 2)$, and $X = V^{(2)} - E$ is the complementary edge set to E. The result now follows from Corollary 4.2 of [10], since, for a dense G and n sufficiently large, $d_{\max} = 2$, $x_{\max} < \frac{1}{2}n - 1$, and $d_{\max}(d_{\max} + x_{\max} - 1) < n = e(\mathbf{d})$. □

Before describing the randomized reduction from Hamiltonian cycles to 2-factors, it is appropriate to recall the algorithmic techniques used to sample from, and estimate the size of $\mathcal{G}(\mathbf{d}, X)$. Using a reduction due to Tutte [15], a graph Γ is constructed whose perfect matchings are in many-one correspondence with elements of $\mathcal{G}(\mathbf{d}, X)$. An algorithm of Jerrum and Sinclair [8], based on the the simulation of a rapidly mixing Markov chain, is then used to sample or estimate the number of perfect matchings in Γ, as required. For this algorithm to be applicable, we require that Γ satisfy a certain condition; it is this condition, translated back through the reduction to the pair $(\mathbf{d}, X)$, that gives rise to the condition $e(\mathbf{d}) < d_{\max}(d_{\max} + x_{\max} - 1)$ in Corollary 4.2 of [10].

Given Theorem 1, the reduction from Hamiltonian cycles to perfect matchings is easy to decribe. We estimate first the number of 2-factors in G, and then the number of Hamilton cycles by standard sampling methods as a proportion of the number of 2-factors. Both counting and sampling phases run in polynomial time, by Theorem 1, provided only that G is dense. For the sampling phase to produce an accurate estimate, it is necessary that the ratio of 2-factors to Hamiltonian cycles in G not be too large. This will be established in section 3.

We remark that it would be sufficient to be able to generate a random Hamilton cycle. We could then proceed alternatively by adding one edge at a time, giving a sequence of $M = O(n^2)$ graphs $G = G_0, G_1, \ldots, G_M = K_n$. We could then estimate the ratio of the number of Hamilton cycles in G_{i-1} to those in G_i for $i = 1, 2, \ldots, M$. The degree conditions can be used to show that each of these ratios is not too small and hence can be estimated efficiently. (This is similar to an idea in [2].)

The method of using random 2-factors to generate random Hamilton cycles was previously used by Frieze and Suen [6] in the context of *random digraphs*. It is interesting that the same method should be successful here also. It raises the intriguing possibility of using existing approaches to other random graph problems to guide the design of new randomized algorithms for restricted versions of the corresponding deterministic problem.

3 Many 2-factors are Hamiltonian

Let n be a natural number and α a positive constant. Let $k_0 = \max\{\lfloor \alpha \ln n \rfloor, 1\}$, and for $1 \le k \le n$, define $g(k) = n^\alpha k!(\alpha \ln n)^{-k}$, and

$$f(k) = \begin{cases} g(k), & \text{if } k \le k_0; \\ g(k_0), & \text{otherwise.} \end{cases}$$

Lemma 1 *Let f be the function defined above. Then*

1. *f is non-increasing and satisfies*

$$\min\{f(k-1), f(k-2)\} = f(k-1) \ge (\alpha \ln n) k^{-1} f(k);$$

2. *$f(k) \ge 1$, for all k.*

Proof Observe that g is unimodal, and that k_0 is the value of k minimizing $g(k)$; it follows that f is non-increasing. When $k \le k_0$, we have $f(k-1) = g(k-1) = (\alpha \ln n)k^{-1} g(k) = (\alpha \ln n)k^{-1} f(k)$; otherwise, $f(k-1) = g(k_0) = f(k) \ge (\alpha \ln n)k^{-1} f(k)$. In either case, the inequality in part 1 of the lemma holds.

Part 2 of the lemma follows from the chain of inequalities

$$\frac{1}{f(k)} \le \frac{1}{g(k_0)} \le \frac{(\alpha \ln n)^{k_0}}{n^\alpha k_0!} \le n^{-\alpha} \sum_{k=0}^{\infty} \frac{(\alpha \ln n)^k}{k!} = n^{-\alpha} \exp(\alpha \ln n) = 1.$$

$\Box$

Lemma 2 *Suppose ε is constant greater than 0. Let G be an undirected graph of order n and minimum degree $(\frac{1}{2} + \varepsilon)n$. Then the number of 2-factors in G exceeds the number of Hamiltonian cycles by at most a polynomial (in n) factor, the degree of the polynomial depending only on ε.*

Proof For $1 \le k \le \lfloor n/3 \rfloor$, let Φ_k be the set of all 2-factors in G containing exactly k cycles, and let $\Phi = \cup_k \Phi_k$ be the set of all 2-factors. Define

$$\Psi = \{(F, F') : F \in \Phi_k, F' \in \Phi_{k'}, k' < k, \text{ and } F \oplus F' \cong C_6\},$$

where $\oplus$ denotes symmetric difference, and C_6 is the cycle on 6 vertices. Observe that (Φ, Ψ) is an acyclic directed graph; let us agree to call its component parts *nodes* and *arcs* to avoid confusion with the vertices and edges of G. Observe also that if $(F, F') \in \Psi$ is an arc, then F' can be obtained from F by deleting three edges and adding three others, and that this operation can decrease the number of cycles by at most two. Thus every arc $(F, F') \in \Psi$ is directed from a node F in some Φ_k to a node F' in Φ_{k-1} or Φ_{k-2}.

Our proof strategy is to define a positive weight function on the edge set Ψ such that the total weight of arcs leaving each node (2-factor) $F \in \Phi \setminus \Phi_1$ is at least one greater than the total weight of arcs entering F. This will imply that the total weight of arcs entering Φ_1 is an upper bound on the number of non-Hamiltonian 2-factors in G, and that the maximum total weight of arcs entering a single node in Φ_1 is an upper bound on the ratio $|\Phi \setminus \Phi_1|/|\Phi_1|$.

The weight function $w : \Psi \to \mathbb{R}^+$ we employ is defined as follows. For any arc (F, F') with $F' \in \Phi_k$: if the 2-factor F' is obtained from F by coalescing two cycles of lengths l_1 and l_2 into a single cycle of length $l_1 + l_2$, then $w(F, F') = (l_1^{-1} + l_2^{-1}) f(k)$; if F' results from coalescing three cycles of length l_1, l_2, and l_3 into a single one of length $l_1 + l_2 + l_3$, then $w(F, F') = (l_1^{-1} + l_2^{-1} + l_3^{-1}) f(k)$.

Let $F \in \Phi_k$ be a 2-factor with $k > 1$ cycles $\gamma_1, \gamma_2, \ldots, \gamma_k$, of lengths $n_1, n_2, \ldots, n_k$. We proceed to bound from below the total weight of arcs leaving F. Imagine that the cycles $\gamma_1, \gamma_2, \ldots, \gamma_k$ are oriented in some way, so that we can speak of each oriented edge (u, u') in some cycle γ_i as being "forward" or "backward". Since we are interested in obtaining a *lower* bound, it is enough to consider only arcs (F, F') from F of a certain kind: namely, those for which the 6-cycle $\gamma = F \oplus F'$ is of the form $\gamma = (x, x', y, y', z, z')$, where (x, x') is a forward cycle edge, (y, y') is a forward edge in a cycle distinct from the first, and (z, z') is a backward cycle edge. The edge (z, z') may be in the same cycle as either (x, x') or (y, y'), or in a third cycle. Observe that (x', y), (y', z) and (z', x) must necessarily be non-cycle edges (with respect to F). It is routine to check that any cycle $\gamma = (x, x', y, y', z, z')$ satisfying the above constraints does correspond to a valid arc from F. The fact that (z, z') is oriented in the opposite sense to (x, x') and (y, y') plays a crucial role in ensuring that the number of cycles decreases in the passage to F' when there are only two cycles involved.

First, we estimate the number of cycles γ for which (x, x') is contained in a particular cycle γ_i of F. We might say that γ is *rooted* at γ_i. Assume, for a moment, that the vertices x, x', y, y' have already been chosen. There are at least $(\frac{1}{2} + \varepsilon)n - 6$ ways to extend the path (x, x', y, y'), first to z and then to z', which are consistent with the rules given above; let Z' be the set of all vertices z' so reachable. Denote by $G(x)$ the set of vertices adjacent to x. The number of ways of completing the path (x, x', y, y') to a valid 6-cycle is at least

$$|G(x)| + |Z'| - n \ge (\tfrac{1}{2} + \varepsilon)n + [(\tfrac{1}{2} + \varepsilon)n - 6] - n = 2\varepsilon n - 6 \ge \varepsilon n,$$

for n sufficiently large. A lower bound on the number of 6-cycles γ rooted at γ_i now follows easily: there are n_i choices for (x, x'); then at least $(\frac{1}{2}+\varepsilon)n - n_i$ choices for (y, y'); and finally — as we have just argued — at least εn ways to complete the cycle. Thus the total number of 6-cycles rooted at γ_i is at least $\varepsilon n n_i[(\frac{1}{2}+\varepsilon)n - n_i]$.

We are now poised to bound the total weight of arcs leaving F. Each arc (F, F') defined by a cycle γ rooted at γ_i has weight at least $n_i^{-1}\min\{f(k-1), f(k-2)\}$, which, by Lemma 1, is bounded below by $(\alpha \ln n)(kn_i)^{-1} f(k)$. Thus the total weight of arcs leaving F is bounded as follows:

$$\begin{aligned}
\sum_{F':(F,F')\in\Psi} w(F, F') &\geq \sum_{i=1}^{k} \varepsilon n n_i[(\tfrac{1}{2}+\varepsilon)n - n_i] \times \frac{(\alpha \ln n) f(k)}{k n_i} && (1)\\
&= \varepsilon n^2[(\tfrac{1}{2}+\varepsilon)k - 1] \times \frac{(\alpha \ln n) f(k)}{k} \\
&\geq \varepsilon^2 \alpha\, f(k) n^2 \ln n \\
&\geq 4 f(k) n^2 \ln n, && (2)
\end{aligned}$$

for a suitable choice of α, where we have used the fact that $k \geq 2$. Note that the presence of a unique backward edge, namely (z, z'), ensures that each cycle γ has a distinguishable root, and hence that the arcs (F, F') were not overcounted in summation (1).

We now turn to the corresponding upper bound on the total weight of arcs $(F', F) \in \Psi$ *entering* F. It is straightforward to verify that the cycle $\gamma = (x, x', y, y', z, z') = F \oplus F'$ must contain three edges — (x, x'), (y, y'), and (z, z') — from a single cycle γ_i of F, and three non-cycle edges (x', y), (y', z), and (z', x). (The labeling of vertices in γ is not canonical: each cycle appears in six labeled guises.) Removing these three edges from γ_i leaves a triple of simple paths of lengths (say) $a-1$, $b-1$, and $c-1$: these lengths correspond (respectively) to the segments joining edge (x, x') to (y, y'), edge (y, y') to (z, z'), and edge (z, z') to (x, x'). Note that each triple (a, b, c) is consistent with up to $16n_i$ choices for the edges (x, x'), (y, y'), and (z, z'). (This maximum will be attained when cycle γ_i is contained in a clique of G.) Five cases should be distinguished.

1. For $8n_i$ of the $16n_i$ choices, $\gamma_i \oplus \gamma$ is a single cycle;
2. for $2n_i$ choices, $\gamma_i \oplus \gamma$ is a pair of cycles of lengths a and $b+c$;
3. for $2n_i$ choices, $\gamma_i \oplus \gamma$ is a pair of cycles of lengths b and $a+c$;
4. for $2n_i$ choices, $\gamma_i \oplus \gamma$ is a pair of cycles of lengths c and $a+b$;
5. for $2n_i$ choices, $\gamma_i \oplus \gamma$ is a triple of cycles of lengths a, b, and c.

The first case does not yield an arc (F', F), since the number of cycles does not decrease when passing from $F' = F \oplus \gamma$ to F; but the other four cases do have to be reckoned with.

Allowing for the previously noted overcounting of cycles γ, the total weight of arcs entering F can be bounded above as follows:

$$\begin{aligned}
\sum_{F':(F',F)\in\Psi} w(F',F) &\leq \frac{1}{6}\sum_{i=1}^{k} 2n_i f(k) \sum_{\substack{a,b,c\geq 1\\ a+b+c=n_i}} \left[\left(\frac{1}{a}+\frac{1}{b}+\frac{1}{c}\right)\right.\\
&\qquad \left. +\left(\frac{1}{a}+\frac{1}{b+c}\right)+\left(\frac{1}{b}+\frac{1}{a+c}\right)+\left(\frac{1}{c}+\frac{1}{a+b}\right)\right]\\
&= \sum_{i=1}^{k} n_i f(k) \sum_{\substack{a,b,c\geq 1\\ a+b+c=n_i}} \left[\frac{2}{a}+\frac{1}{b+c}\right]\\
&\leq \sum_{i=1}^{k} n_i f(k) n \sum_{a=1}^{n_i-1} \left[\frac{2}{a}+\frac{1}{n_i-a}\right]\\
&\leq 3f(k)n^2 H_n, \qquad (3)
\end{aligned}$$

where $H_n = \sum_{i=1}^{n} i^{-1} \leq \ln n + 1$ is the nth harmonic number [7, eq. (6.60)]. Combining inequalities (2) and (3), we have

$$\begin{aligned}
\sum_{F':(F,F')\in\Psi} w(F,F') - \sum_{F':(F',F)\in\Psi} w(F',F) &\geq 4f(k)n^2\ln n - 3f(k)n^2 H_n\\
&\geq f(k)n^2(\ln n - 3)\\
&\geq n^2(\ln n - 3),
\end{aligned}$$

where the final inequality is by Lemma 1. Thus the total weight of arcs leaving F exceeds the total weight of arcs entering by at least 1, provided $n \geq 21$. The number of non-Hamiltonian 2-factors $|\Phi \setminus \Phi_1|$ is bounded above by the total weight of arcs entering Φ_1, which in turn is bounded — see inequality (3) — by $|\Phi_1| \times 3f(1)n^2 H_n = |\Phi_1| \times O(n^{2+\alpha})$. This establishes the lemma. □

4 Exact counting is #P-complete

Let #HC (resp. #HP) be the problem of counting the number of Hamiltonian cycles (resp. paths) in an undirected graph. It is known [17, 14] that #HC is #P-complete, and it follows, by an easy reduction, that #HP is also #P-complete.

Theorem 2 *#HC is #P-complete, even when restricted to graphs G of minimum degree at least $(1-\varepsilon)n$, where n is the number of vertices in G, and $\varepsilon > 0$.*

Proof We present a Turing reduction from #HP to #HC such that all the target instances of #HC satisfy the required minimum degree condition. Let $G = (V, E)$ be a undirected graph of order n with vertex set V and edge set E, considered as an instance of #HP. A typical target instance of #HC is a graph G_t constructed from G by forming the disjoint union of G with the complete graph K_t on $t \geq n$ vertices, and connecting every vertex in G with every vertex in K_t.

Assume $t \geq 3$. For $1 \leq k \leq n$, denote by P_k the set of all covers of G by k vertex-disjoint oriented paths, where paths of length 0 are allowed. Each oriented Hamilton cycle H in G_t induces an element of $\cup_k P_k$ by restriction to G. Conversely, each element of P_k may be extended in precisely $(t-1)!\binom{t}{k}k! = t!\binom{t-1}{k-1}(k-1)!$ ways to an oriented Hamiltonian cycle in G_t: the vertices in K_t may be visited in $(t-1)!$ cyclic orders; there are $\binom{t}{k}$ ways to choose k gaps in that order during which excursions to G can be made, and $k!$ ways to match those gaps to the k oriented paths covering G. Thus the number c_t of oriented Hamiltonian cycles in G_t can be expressed as the sum

$$c_t = \sum_{k=1}^{n} t!\binom{t-1}{k-1}(k-1)!|P_k|.$$

Note that c_t may be evaluated by one call to an oracle for #HC, since the number of oriented Hamilton cycles is twice the number of unoriented cycles. Using n such calls we may evaluate c_t for $t = t_0 + j$ and $j = 1, 2, \ldots, n$, where $t_0 = \lceil \varepsilon^{-1} n \rceil$ is chosen sufficiently large that every graph G_t with $t > t_0$ satisfies the minimum degree constraint. Recovering the values $\{(k-1)!|P_k| : 1 \leq k \leq n\}$ from $\{c_{t_0+j}/(t_0+j)! : 1 \leq j \leq n\}$ amounts to inverting the matrix

$$A = (A_{jk}) = \left(\binom{t_0 + j - 1}{k-1} : 1 \leq j, k \leq n\right),$$

which may be expressed as the product $A = LU$ of a lower triangular matrix $L = (L_{jh})$ and upper triangular matrix $U = (U_{hk})$ defined as follows:

$$L_{jh} = \binom{j-1}{h-1} \quad \text{and} \quad U_{hk} = \binom{t_0}{k-h}.$$

The equality $A = LU$ is a direct consequence of the "Vandermonde convolution" formula [7, eq. (5.22)]

$$\sum_{h=1}^{n} \binom{j-1}{h-1}\binom{t_0}{k-h} = \binom{t_0 + j - 1}{k-1}.$$

Both L and U have unit diagonals and are hence non-singular: indeed their inverses have the following simple explicit forms, as can be verified by direct multiplication using standard identities involving sums of products of binomial coefficients [7, eqs (5.24), (5.25)]:

$$(L^{-1})_{hk} = (-1)^{h+k}\binom{h-1}{k-1} \quad \text{and} \quad (U^{-1})_{jh} = (-1)^{j+h}\binom{t_0 + h - j - 1}{t_0 - 1}.$$

Since $A^{-1} = U^{-1}L^{-1}$, the values $\{|P_k| : 1 \leq k \leq n\}$ may be computed in polynomial time using two matrix multiplications involving integers of $O(n \log n)$ bits. Observe that $\frac{1}{2}|P_1|$ gives the number of (unoriented) Hamiltonian paths in G. □

5 Concluding remarks

We remark that it is not difficult to adapt the above methods to the corresponding *directed* case. Here we will have both minimum indegree and outdegree at each vertex guaranteed to be at least $(\frac{1}{2}+\varepsilon)n$. Also we may similarly count the number of connected k-factors in G for any $k = o(n)$. (Hamilton cycles are, of course, connected 2-factors.)

We leave open the following questions. First, is it possible to count approximately as $\varepsilon \to 0$ in any fashion? Secondly, is there a random walk on Hamilton cycles and (in some sense) "near-Hamilton-cycles" which is rapidly mixing? In other words, can we avoid the Tutte construction and the need for 2-factors with many cycles?

Finally, are there other interesting counting problems which are tractable on such dense graphs?

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