

GEOSEQ2SEQ: INFORMATION GEOMETRIC SEQUENCE-TO-SEQUENCE NETWORKS

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ABSTRACT

The Fisher information metric is an important foundation of information geometry, wherein it allows us to approximate the local geometry of a probability distribution. Recurrent neural networks such as the Sequence-to-Sequence (Seq2Seq) networks that have lately been used to yield state-of-the-art performance on speech translation or image captioning have so far ignored the geometry of the latent embedding, that they iteratively learn. We propose the information geometric Seq2Seq network which abridges the gap between deep recurrent neural networks and information geometry. Specifically, the latent embedding offered by a recurrent network is encoded as a Fisher kernel of a parametric Gaussian Mixture Model, a formalism common in computer vision. We utilise such a network to predict the shortest routes between two nodes of a graph by learning the adjacency matrix using the information geometric Seq2Seq model; our results show that for such a problem the probabilistic representation of the latent embedding supersedes the non-probabilistic embedding by 10-15%.

1 INTRODUCTION

Information geometry situates itself in the intersection of probability theory and differential geometry, wherein it has found utility in understanding the geometry of a wide variety of probability models (Amari & Nagaoka, 2000). By virtue of Cencov’s characterisation theorem, the metric on such probability manifolds is described by a unique kernel known as the Fisher information metric. In statistics, the Fisher information is simply the variance of the score function. In Bayesian statistics, it has found utility in terms of Riemannian Markov Chain Monte Carlo (MCMC) methods (Girolami & Calderhead, 2011) while for computer vision it has resulted in the Fisher kernel encoding (Perronnin & Dance, 2006). Practitioners have also used the geometric make-up of feature vectors obtained from a deep convolutional neural network (dCNN) to rank images (Qian et al., 2017) by encoding them using Fisher kernels. Apart from traditional signal processing methodologies like Kalman filters or Hidden Markov Models, recurrent neural networks that have proved to be beneficial for sequential data haven’t quite utilised the geometry of the latent structure they learn.

There are two paths of an intersection of recurrent networks with Riemann geometry. The first lies in using the natural gradient to optimize loss functions of deep neural networks (Pascanu & Bengio, 2013). This affords invariance to the optimization procedure by breaking the symmetry in parameter space. The other is utilizing the geometry of the latent space to augment classification accuracy. In this paper, we combine a specific sort of recurrent network – the Sequence-to-Sequence (Seq2Seq) model – and utilize the Riemann geometry of the embedded space for boosting the performance of the decoder. We test the algorithm on a combinatorially hard problem called the *shortest route problem*. The problem involves a large graph wherein the shortest route between two nodes in the graph are required. Specifically, we use a meta-heuristic algorithm (a vanilla A^* algorithm) to generate the shortest route between two randomly selected routes. This then serves as the training set for our information geometry based Seq2Seq network.

2 METHODS

In this section, we describe the data-sets, the procedure for generating the routes for training/test datasets, and the employment of information geometric Sequence-to-Sequence networks that forms the novel contribution of this paper.

2.1 DATASETS

The graph is based on the road network of Minnesota¹. Each node represents the intersections of roads while the edges represent the road that connects the two points of intersection. Specifically, the graph we considered has 376 nodes and 455 edges, as we constrained the coordinates of the nodes to be in the range $[-97, -94]$ for the longitude and $[46, 49]$ for the latitude, instead of the full extent of the graph, i.e., a longitude of $[-97, -89]$ and a latitude of $[43, 49]$, with a total number of 2,642 nodes.

2.2 ALGORITHMS

THE A^* META-HEURISTICS

The A^* algorithm is a best-first search algorithm wherein it searches amongst all of the possible paths that yield the smallest cost. This cost function is made up of two parts – particularly, each iteration of the algorithm consists of first evaluating the distance travelled or time expended from the start node to the current node. The second part of the cost function is a heuristic that estimates the cost of the cheapest path from the current node to the goal. Without the heuristic part, this algorithm operationalises the Dijkstra’s algorithm (Dijkstra, 1959). There are many variants of A^* ; in our experiments, we use the vanilla A^* with a heuristic based on the Euclidean distance. Other variants such as Anytime Repairing A^* has been shown to give superior performance (Likhachev et al., 2004).

Paths between two randomly selected nodes are calculated using the A^* algorithm. On an average, the paths are 19 hops long. The average fan-in/fan-out of a randomly selected node is 2.42. We increase the combinatorial difficulty of the shortest route by not constraining the search to the local fan-out neighbourhood, rather the dimension of the search space is $n - 1$ with n representing the number of nodes in the graph.

RECURRENT DEEP NETWORKS

We utilised Sequence-to-Sequence (Seq2Seq, Sutskever et al. (2014)) recurrent neural networks for the shortest route path prediction. Specifically, we use the following variants:

- An LSTM2RNN, where the encoder is modelled by a long short term memory (LSTM, Hochreiter & Schmidhuber (1997)), i.e.

$$\begin{aligned}
 i(t) &= \text{logistic}\left(A_i x(t) + B_i h(t-1) + b_i\right) \\
 j(t) &= \tanh\left(A_j x(t) + B_j h(t-1) + b_j\right) \\
 f(t) &= \text{logistic}\left(A_f x(t) + B_f h(t-1) + b_f\right) \\
 o(t) &= \text{logistic}\left(A_o x(t) + B_o h(t-1) + b_o\right) \\
 c(t) &= f(t) \odot c(t-1) + i(t) \odot j(t) \\
 h(t) &= o(t) \odot \tanh\left(c(t)\right),
 \end{aligned} \tag{1}$$

while the decoder is a vanilla RNN (Goodfellow et al., 2016), i.e.

$$h(t) = \tanh(Ax(t) + Bh(t-1) + b), \tag{2}$$

¹https://www.cs.purdue.edu/homes/dgleich/packages/matlab_bgl

followed by a softmax output layer, i.e.

$$y(t) = \text{logsoftmax}(Ch(t) + c), \quad (3)$$

which gives the probability distribution on the following node, choosing it among the other $n - 1$ nodes.

- A GRU2RNN, where the encoder is modelled by a gated recurrent unit (GRU, [Cho et al. \(2014\)](#)), i.e.

$$\begin{aligned} z(t) &= \text{logistic}\left(A_z x(t) + B_z h(t-1) + b_z\right) \\ r(t) &= \text{logistic}\left(A_r x(t) + B_r h(t-1) + b_r\right) \\ \tilde{h}(t) &= \tanh\left(A_h x(t) + B_h(r(t) \odot h(t-1)) + b_h\right) \\ h(t) &= z(t) \odot h(t-1) + (1 - z(t)) \odot \tilde{h}(t), \end{aligned} \quad (4)$$

while the decoder is again a vanilla RNN with a softmax, as in Equations (2)-(3).

- An LSTM2LSTM, where both the encoder and the decoder are modelled by an LSTM as in Equations (1).
- A GRU2LSTM, where the encoder is a GRU (see Eqn. (4)) and the decoder is an LSTM (see Eqn. (1)).
- *GeoSeq2Seq*, our novel contribution, where the context vector obtained as in one of the previous models is further encoded using either Fisher vectors or vectors of locally aggregated descriptors (see Figure 1), as described in the following section.

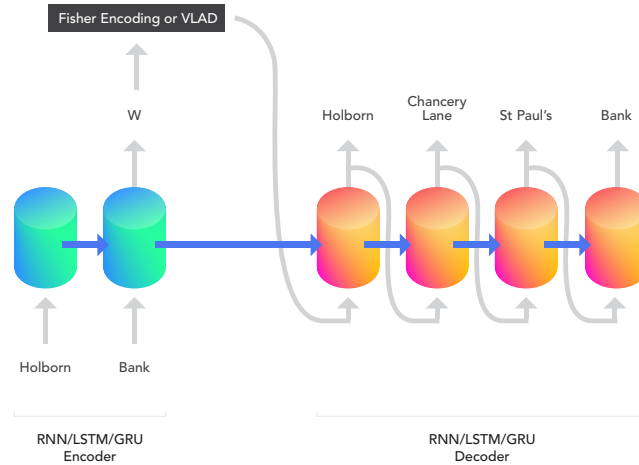


Figure 1: **Information geometric context vectors.** The context vectors (W) that are learnt using the recurrent neural networks are further encoded using either a Fisher vector based encoding or a Vector of Locally Aggregated Descriptors (VLAD) based encoding (see text). Such an encoded context vector is finally fed to a recurrent neural network based decoder.

For all networks, the input is represented by the [source, destination] tuple (Figure 1), which is encoded in a context vector (W) and subsequently decoded into the final sequence to obtain the shortest path connecting the source to the destination. Moreover, during the test phase, we compute two paths, one from the source to the destination node and the other from the destination to the source node, that form an intersection to result in the shortest path.

INFORMATION GEOMETRY

Classical results from information geometry (Cencov’s characterisation theorem; [Amari & Nagaoka \(2000\)](#)) tell us that, for manifolds based on probability measures, a unique Riemannian metric exists – the Fisher information metric. In statistics, Fisher-information is used to measure the expected value of the observed information. Whilst the Fisher-information becomes the metric (g) for curved probability spaces, the distance between two distributions is provided by the Kullback-Leibler (KL) divergence. It turns out that if the KL-divergence is viewed as a curve on a curved surface, the Fisher-information becomes its curvature. Formally, for a distribution $q(\psi)$ parametrised by θ we have,

$$\begin{aligned}\mathcal{KL}(\theta, \theta') &= \mathbb{E}_\theta \left[\log \frac{q(\psi | \theta)}{q(\psi | \theta')} \right] + \mathbb{E}_{\theta'} \left[\log \frac{q(\psi | \theta')}{q(\psi | \theta)} \right] \\ &= d\theta^T g(\theta) d\theta + \mathcal{O}(d\theta^3) \\ g_{ij}(\theta) &= \int_{-\infty}^{+\infty} q(\psi, \theta) \frac{\partial \ln q(\psi, \theta)}{\partial \theta_i} \frac{\partial \ln q(\psi, \theta)}{\partial \theta_j} d\psi \\ \mathcal{KL}[\theta_0 + \delta\theta : \theta_0] &\doteq \frac{1}{2} g_{ij}(\theta_0) (\delta\theta)^2.\end{aligned}\tag{5}$$

Fisher encoding

We use a Gaussian Mixture Model (GMM) for encoding a probabilistic sequence vocabulary (W) on the training dataset. The context vectors are then represented as Fisher Vectors (FV, [Perronnin & Dance \(2006\)](#)) – derivatives of log-likelihood of the model with respect to its parameters (the score function). Fisher encoding describes how the distribution of features of an individual context differs from the distribution fitted to the feature of all training sequences.

First, a set of D dimension context vector is extracted from a sequence and denoted as $W = (w_1, \dots, w_i, \dots, w_N : w \in \mathbb{R}^D)$. A K component GMM with diagonal covariance is generated ([Simonyan et al., 2013](#); [Cimpoi et al., 2015](#)) on the training set with the parameters $\{\Theta = (\omega_k, \mu_k, \Sigma_k)\}_{k=1}^K$, only the derivatives with respect to the mean $\{\mu_k\}_{k=1}^K$ and variances $\{\Sigma_k\}_{k=1}^K$ are encoded and concatenated to represent a sequence $W(X, \Theta) = \left(\frac{\partial L}{\partial \mu_1}, \dots, \frac{\partial L}{\partial \mu_K}, \frac{\partial L}{\partial \Sigma_1}, \dots, \frac{\partial L}{\partial \Sigma_K} \right)$, where

$$\begin{aligned}L(\Theta) &= \sum_{i=1}^N \log(\pi(w_i)) \\ \pi(w_i) &= \sum_{k=1}^K \omega_k N(w_i; \mu_k, \Sigma_k).\end{aligned}\tag{6}$$

For each component k , mean and covariance deviation on each vector dimension $j = 1, 2, \dots, D$ are

$$\begin{aligned}\frac{\partial L}{\partial \mu_{jk}} &= \frac{1}{N\sqrt{\omega_k}} \sum_{i=1}^N q_{ik} \frac{w_{ji} - \mu_{jk}}{\sigma_{jk}} \\ \frac{\partial L}{\partial \Sigma_{jk}} &= \frac{1}{N\sqrt{2\omega_k}} \sum_{i=1}^N q_{ik} \left[\left(\frac{w_{ji} - \mu_{jk}}{\sigma_{jk}} \right)^2 - 1 \right],\end{aligned}\tag{7}$$

where q_{ik} is the soft assignment weight of feature w_i to the k^{th} Gaussian and defined as

$$q_{ik} = \frac{\exp \left[-\frac{1}{2} (w_i - \mu_k)^T \Sigma_k^{-1} (w_i - \mu_k) \right]}{\sum_{t=1}^K \exp \left[-\frac{1}{2} (w_i - \mu_t)^T \Sigma_t^{-1} (w_i - \mu_t) \right]}.\tag{8}$$

Just as the sequence representation, the dimension of Fisher vector is $2KD$, K is the number of components in the GMM, and D is the dimension of local context descriptor. After l_2 normalization on Fisher vector, the embedding can be learnt using an arbitrary recurrent neural network based decoder (Perronnin et al., 2010). In our experiments (see Section 3), as a proof of concept, we fixed the number of GMMs to $K = 1$, since more Gaussians would have increased the dimension acted upon by the decoder, making the training computational time prohibitive (for $D = 256$, choosing $K \geq 2$ implies a Fisher vector’s dimension greater than a thousand).

VLAD encoding

In this case, the context vectors are represented as Vector of Locally Aggregated Descriptors (VLAD, Jégou et al. (2010); Arandjelovic & Zisserman (2013)). VLAD is a feature encoding and pooling method, similar to Fisher Vectors. It encodes a set of local feature descriptors extracted from a sequence and denoted as $W = (w_1, \dots, w_n : w \in \mathbb{R}^D)$, using a clustering method such as K-means. Let q_{ik} be the hard assignment of data vectors w_i to the cluster k^{th} cluster, such that $q_{ik} \geq 0$ and $\sum_{k=1}^K q_{ik} = 1$. Furthermore, the assignments of features to dictionary elements must be pre-computed, for example by using KD-trees (Beis & Lowe, 1997; Silpa-Anan & Hartley, 2008). VLAD encodes features W by considering the residuals

$$v_k = \sum_{i=1}^N q_{ik}(w_i - \mu_k), \quad (9)$$

where $\mu_k \in \mathbb{R}^N$ is the k^{th} cluster centre (or mean). Then, these residuals are stacked together to obtain the final context vector.

3 RESULTS

For the graph of Minnesota with $n = 376$ nodes and 455 edges, we generated 3,000 shortest routes between two randomly picked nodes using the A^* algorithm. We used these routes as the training set for the Seq2Seq algorithms using a 67-33% training-test splits; we train the network for 400 epochs, updating the parameters with an Adam optimisation scheme (Kingma & Ba, 2014), with parameters $\beta_1 = 0.9$ and $\beta_2 = 0.999$, starting from a learning rate equal to 10^{-3} . Since Fisher encoding requires a double length for the context vector (it considers means and covariances, see Eqn. (5)), we compared it to a basic Seq2Seq with 256 and 512 hidden units. On the other hand, VLAD encodes only the residual (see Eqn. (9)), therefore we instantiate it with 256 and 512 hidden units.

Moreover, in the decoder, the following node in the predicted sequence is computed choosing among all the other $n - 1$ nodes from a softmax distribution. If we stop the training early, for example after only 40 epochs (see Figure 2), the network cannot reproduce possible paths (see Figure 3 on the left-hand side). On the other hand, if we train the network for more epochs, the training converges after 400 epochs (green dot in Figure 2). Therefore, as shown in Figure 3 (right), if we compute two paths, one starting from the source (magenta dash-dotted line) and the other from the destination (cyan), intersecting them allows us to predict the shortest path (red). This is equal to the one generated by A^* (green). This means that the network is capable of learning the adjacency matrix of the graph.

Then, comparing different approaches, the prediction accuracy on the test data-set is reported in Table 1. As we can see, for what concerns the RNN decoder, doubling the hidden state dimension marginally increases the percentage of shortest paths (1%) and the successful paths, that are not necessarily the shortest (0.2% and 1.6% for GRU and LSTM encoders, respectively). Our proposed information geometry based Fisher encoding achieves an increased accuracy in finding the shortest paths (56% and 60% for LSTM and GRU, respectively). Furthermore, if a VLAD encoding is employed, GRU networks have a higher approximation capability with more than 65% of accuracy on the shortest paths and 83% on the successful cases. Similarly, if the decoder is an LSTM, the accuracies on the shortest paths of simple Seq2Seq models are around 50%, while our *GeoSeq2Seq* models with Fisher encoding we get close to 60% and even above with the VLAD encoding, achieving 65% (and 82% of successful paths) in the case of the LSTM encoder. This means that our probabilistic representation of the latent embedding supersedes the non-probabilistic one by 10-15%.

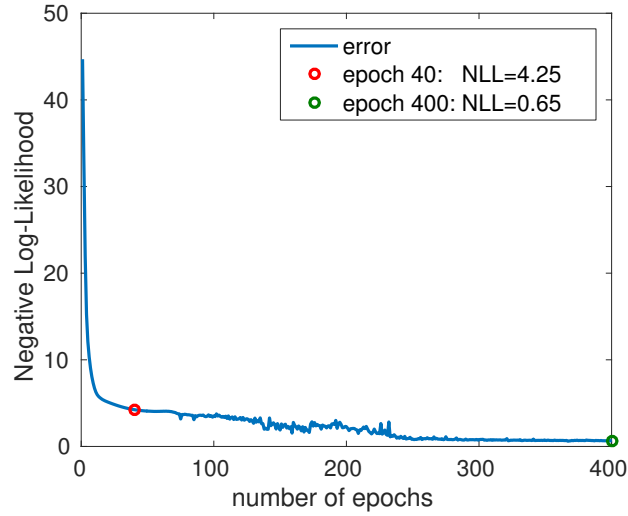


Figure 2: **Training error.** We illustrate the negative log-likelihood loss function during the training phase. The adjacency matrix is iteratively learnt during such a training phase. We highlight the situation after 40 epochs (red dot) and at the end of the training (after 400 epochs, green dot) when the back-propagation through time algorithm has converged. The paths are shown in Figure 3.

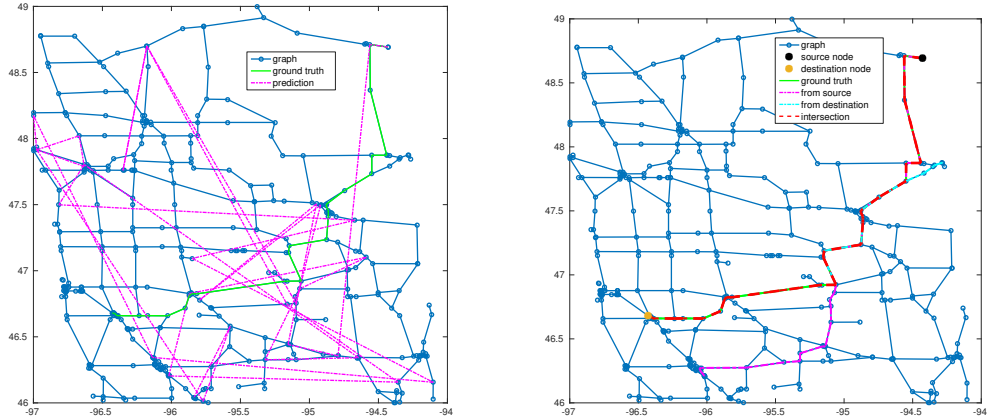


Figure 3: **Predicted path.** Here, we show an example of a prediction of shortest path on the Minnesota dataset (blue graph). The A^* shortest path between the source (black dot) and destination (yellow dot) nodes is represented in green. On the left-hand side, we show the prediction (magenta) after only 40 epochs of training (Figure 2). On the right-hand side, instead, we show the prediction at the end of the training: we compute two paths, one starting from the source (magenta) and the other from the destination (cyan), and finally, we intersect them to compute the predicted shortest path (red). The ‘flying-object syndrome’ only occurs during the earlier phase of training.

4 DISCUSSION

This paper proposes the *GeoSeq2Seq*, an information geometric Seq2Seq architecture that utilises an information geometric embedding of the context vector. The RNN is tasked with learning the adjacency matrix of the graph such that at each decision step the search space becomes $n - 1$, where n is the total number of nodes in the graph. Unlike algorithms like *q-routing* (Boyan & Littman, 1994) that constrains the search space to contain only the connected neighbours, our instantiation of the Seq2Seq operates under a larger search space. Indeed, the accuracy of our algorithm is expected to increase where we use neighbourhood information from the adjacency matrix. In summary, such a recurrent network shows increased fidelity for approximating the shortest route produced by a meta-heuristic algorithm.

Method	Shortest	Successful
LSTM2RNN (256)	47%	69.5%
LSTM2RNN (512)	48%	71.1%
GRU2RNN (256)	48.3%	73.1%
GRU2RNN (512)	49%	73.3%
LSTM2RNN with FV	56%	76.4%
GRU2RNN with FV	60.1%	79%
LSTM2RNN with VLAD (256)	59.3%	76.8%
LSTM2RNN with VLAD (512)	60.1%	76.2%
GRU2RNN with VLAD (256)	64%	79.9%
GRU2RNN with VLAD (512)	65.7%	83%
LSTM2LSTM (256)	50.3%	72.7%
LSTM2LSTM (512)	54%	73.3%
GRU2LSTM (256)	48%	69.5%
GRU2LSTM (512)	48.2%	73.5%
LSTM2LSTM with FV	57.9%	78.8%
GRU2LSTM with FV	59%	79.3%
LSTM2LSTM with VLAD (256)	62.4%	79.8%
LSTM2LSTM with VLAD (512)	65.2%	82.1%
GRU2LSTM with VLAD (256)	63%	80.6%
GRU2LSTM with VLAD (512)	63.7%	81.6%

Table 1: **Results on the Minnesota graph.** Percentage of shortest path and successful paths (that are not necessarily shortest) are shown for a wide-variety of Seq2Seq models, with context vector dimension equal to either 256 or 512. All scores are relative to an A^* algorithm, that achieves a shortest path score of 100%.

Apart from encoding, context vector stacking using dual encoders have been proven to be beneficial (Bay & Sengupta, 2017b). Utilising homotopy based continuation has been a different line of work where the emphasis lies in smoothing the loss function of the recurrent network by convolving it with a Gaussian kernel (Bay & Sengupta, 2017a). All of these strategies have shown to improve the temporal memory of the recurrent network. This line of work is distinct from architecture engineering, that has placed emphasis on constructing exquisite memory mechanism for the recurrent networks. For example, Neural Turing Machines (Graves et al., 2014) are augmented recurrent networks that have a (differentiable) external memory that can be selectively read or written to, enabling the network to store the latent structure of the sequence. Attention networks, on the other hand, enable the recurrent networks to attend to snippets of their inputs (*cf.* in conversational modelling Vinyals & Le (2015)). Nevertheless, for the long-term dependencies that shortest paths in large graphs inherit, these methods are small steps towards alleviating the central problem of controlling spectral radius in recurrent neural networks.

The 4-5% gain in accuracy for VLAD in contrast to Fisher encoding is a bit surprising. As a matter of fact, Fisher encoding should be more precise since it takes covariances into account. We notice that the covariances matrix (i.e. a diagonal matrix) has a high condition number ($\approx 10^3$), this means it can propagate small variations into bigger errors. In particular, we obtain a condition number equal to 2.69e3 and 1.70e3 for the LSTM and GRU encoders, respectively. We believe it is for this reason that the GRU encoder leads to a better accuracy than the LSTM encoder, as shown in Table 1.

The use of Riemann geometry to encode context (feature) vector has a long history in computer vision (Srivastava & Turaga, 2015), our work demonstrates yet another way to embed the curved geometry of the context vector for decoding. The Riemannian metric for a recurrent network can be evaluated in two ways – one where we describe the probability distribution over the entire sequence

and another where we describe a conditional distribution at time i conditioned on time $i - 1$. We anticipate that the latter is more suited to a dynamic scenario (where the structure of the graph may be slowly changing) while the former is more suitable for static graphs. Analytically, averaging over time and assuming ergodicity, both metrics should be fairly close to one another, nonetheless, it is only with further experiments we can demonstrate the value of one over the other.

In this paper, we have constrained the use of the Riemannian metric on the encoding end, one can follow a similar treatise for the decoder. Together with architecture engineering (Graves et al., 2014), natural gradient-based optimization (Pascanu & Bengio, 2013), homotopy continuation (Bay & Sengupta, 2017a) and ensembling of recurrent encoders (Bay & Sengupta, 2017b), we posit that understanding the information geometry of recurrent networks can take us a step closer to finessing the temporal footprint of a sequence learning network.

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