

# From Betti Numbers to Persistence Diagrams:

## A Hybrid Quantum Algorithm for Topological Data Analysis

Dong Liu

*liudong@mit.edu*

### Abstract

Persistence diagrams serve as a core tool in topological data analysis, playing a crucial role in pathological monitoring, drug discovery, and materials design. However, existing quantum topological algorithms, such as the LGZ algorithm, can only efficiently compute summary statistics like Betti numbers, failing to provide persistence diagram information that tracks the lifecycle of individual topological features, severely limiting their practical value. This paper proposes a novel quantum-classical hybrid algorithm that achieves, for the first time, the leap from “quantum computation of Betti numbers” to “quantum acquisition of practical persistence diagrams.” The algorithm leverages the LGZ quantum algorithm as an efficient feature extractor, mining the harmonic form eigenvectors of the combinatorial Laplacian as well as Betti numbers, constructing specialized topological kernel functions to train a quantum support vector machine (QSVM), and learning the mapping from quantum topological features to persistence diagrams. The core contributions of this algorithm are: (1) elevating quantum topological computation from statistical summaries to pattern recognition, greatly expanding its application value; (2) obtaining more practical topological information in the form of persistence diagrams for real-world applications while maintaining the exponential speedup advantage of quantum computation; (3) proposing a novel hybrid paradigm of “classical precision guiding quantum efficiency.” This method provides a feasible pathway for the practical implementation of quantum topological data analysis.

## 1 Introduction

Persistent homology [1, 2], as a core method in topological data analysis [3, 4], reveals the intrinsic structure of data by tracking the evolution of topological features across different scales. Its output—persistence diagrams—represents each topological feature as a point on a two-dimensional plane, with horizontal and vertical coordinates corresponding to the birth and death scales of features, providing crucial information for practical applications such as pathological monitoring, drug discovery, and materials design. However, classical topological algorithms face severe computational bottlenecks. According to the analysis by Lloyd et al. [5], the complexity of classical algorithms for computing  $k$ -dimensional Betti numbers is  $O(n^k)$ , and computing Betti numbers of all dimensions requires at least  $O(2^n \log(1/\delta))$  time, where

$n$  is the number of vertices and  $\delta$  is the precision parameter. This exponential complexity severely limits the application of topological data analysis on large-scale data. The stability of persistence diagrams [6] and their statistical properties [7] have been well established, making them a robust tool for data analysis, but computational bottlenecks remain the primary obstacle to their widespread adoption.

Quantum computing [8] offers revolutionary possibilities for breaking through this bottleneck, with quantum machine learning [9, 10] emerging as a promising paradigm for combining quantum computational advantages with pattern recognition tasks. The LGZ algorithm [5] proposed by Lloyd, Garnerone, and Zanardi in 2016 represents a milestone in this direction. The LGZ algorithm uses quantum phase estimation to compute Betti numbers of all dimensions in  $O(n^5/\delta)$  time, achieving exponential speedup compared to the classical  $O(2^n \log(1/\delta))$  (Lloyd et al., 2016). However, despite the breakthrough in computational efficiency achieved by the LGZ algorithm, its output Betti numbers are merely statistical summaries of topological features, unable to provide lifecycle information of individual features—which is precisely the core driver of practical applications. While Ameneyro et al. [11] extended the LGZ algorithm to compute persistent Betti numbers, it still remains at the statistical level, failing to obtain complete persistence diagram information.

This paper proposes a novel algorithmic pipeline that, for the first time, achieves the acquisition of practical persistence diagrams from quantum topological features. Our core insight is: the LGZ algorithm not only computes Betti numbers, but the harmonic forms of the combinatorial Laplacian produced during its process contain far richer geometric-topological information than Betti numbers. According to Hodge theory [12, 13], these eigenvectors corresponding to zero eigenvalues have a one-to-one correspondence with representatives of homology classes, encoding the specific geometric realization of each topological “hole” (Lloyd et al., 2016). By tracking these eigenvectors and Betti numbers across multiple scales, designing new “topological kernels” that measure differences between different topological structures, and loading them into quantum support vector machines (Rebentrost et al., 2014), we can achieve prediction of more practical topological information in the form of persistence diagrams.

The algorithmic pipeline adopts the design philosophy of “classical precision guiding quantum efficiency,” specifically designed for particular application scenarios such as colon lesion detection. In these scenarios, the possible topological patterns are finite and enumerable, making it feasible to construct a complete training set. In the training phase, we use classical algorithms to compute persistence diagrams as labels for a limited set of representative data, while running the LGZ quantum algorithm to extract topological features. Through the new topological kernel functions and the quantum support vector machine framework of Rebentrost et al. (2014), we learn the mapping from relatively simple topological features to persistence diagrams. In the prediction phase, the algorithmic pipeline achieves complete quantization: new data only requires LGZ algorithm feature extraction and QSVM classification, without any

classical persistent homology computation.

This design elevates quantum computation for topology from a purely statistical tool to a practical pattern recognition system. Through the quantum support vector machine framework, we successfully transform summary Betti numbers into structural persistence diagram information, obtaining the topological information truly needed by practical applications while maintaining quantum speedup advantages. This marks a crucial step toward the practical implementation of quantum topological data analysis.

## 2 Harmonic Form Feature Extraction

The first key module of our algorithm is extracting features rich in geometric-topological information from quantum states. For a given point cloud dataset  $D$  in a specific scenario, we first construct corresponding Vietoris-Rips complexes at a series of scales  $\epsilon_1 < \epsilon_2 < \dots < \epsilon_T$  (where  $T$  is the number of scales). At each scale  $\epsilon_j$ , for each dimension  $k \in \{0, 1, \dots, K\}$  (where  $K$  is the maximum dimension), we run the LGZ quantum algorithm to compute the combinatorial Laplacian  $\Delta_k$  [5].

The combinatorial Laplacian is defined as  $\Delta_k = \partial_k^\dagger \partial_k + \partial_{k+1} \partial_{k+1}^\dagger$ , where  $\partial_k$  is the boundary operator. The spectral properties of such Laplacians on simplicial complexes [12, 14] provide deep insights into the topological structure of the underlying space. The LGZ algorithm obtains the spectral decomposition of  $\Delta_k$  by constructing the Dirac operator  $B_k$  (a Hermitian matrix embedding the boundary operator) and utilizing quantum phase estimation. Specifically, the algorithm first constructs a uniform superposition state of  $k$ -simplices through Grover search [15], with time complexity  $O(n^2 \sqrt{z_k})$ , where  $z_k$  is the proportion of  $k$ -simplices in the complex. Then it applies quantum phase estimation to decompose the Dirac operator, extracting all eigenvalues and corresponding eigenvectors, with complexity  $O(n^5/\delta)$  [5].

These harmonic form eigenvectors carry profound topological-geometric significance. According to the Hodge decomposition theorem [13], the kernel space (zero eigenspace) of the combinatorial Laplacian is isomorphic to the  $k$ -dimensional homology group. Each zero eigenvector corresponds to an independent  $k$ -dimensional homology class, encoding the specific geometric realization of a  $k$ -dimensional ‘‘hole’’ in the simplicial complex. For example, in the one-dimensional case, each zero eigenvector corresponds to an independent one-dimensional loop; in the two-dimensional case, it corresponds to a two-dimensional cavity. Through quantum phase estimation, we can not only count these features (i.e., Betti numbers  $b_k = \dim(\ker \Delta_k)$ ), but also obtain their explicit quantum state representations.

To handle the inconsistency in simplicial complex sizes across different datasets, we adopt an eigenvector pooling strategy. Suppose at scale  $\epsilon_j$ , the zero eigenspace of  $\Delta_k$  is spanned by  $b_k(\epsilon_j)$  orthogonal eigenvectors  $\{|v_i^k(\epsilon_j)\rangle\}_{i=1}^{b_k(\epsilon_j)}$ . We construct a normalized quantum superposition state:

$$|\psi_k(\epsilon_j)\rangle = \frac{1}{\sqrt{b_k(\epsilon_j)}} \sum_{i=1}^{b_k(\epsilon_j)} |v_i^k(\epsilon_j)\rangle. \quad (1)$$

This superposition state encodes the collective geometric information of all  $k$ -dimensional holes while maintaining a fixed quantum state dimension, providing a unified interface for subsequent kernel function calculations.

### 3 Multi-scale Persistence Feature Construction

Harmonic forms at a single scale are insufficient to capture the persistence information of topological features. The core value of persistence diagrams lies in tracking the lifecycle of each topological feature across multiple scales. Inspired by the work of Ameneiro et al. [11], we design a multi-level feature extraction strategy to capture topological evolution information from different perspectives.

The first layer of features is the harmonic form evolution sequence. For each dimension  $k$ , we extract the quantum superposition state sequence  $\{|\psi_k(\epsilon_1)\rangle, |\psi_k(\epsilon_2)\rangle, \dots, |\psi_k(\epsilon_T)\rangle\}$  across all scales. This sequence encodes the geometric evolution process of  $k$ -dimensional topological features as scale changes. When a new  $k$ -dimensional hole appears at scale  $\epsilon_i$ , the dimension of the zero eigenspace increases by one, and the corresponding superposition state contains new eigenvector components. When a hole is filled at scale  $\epsilon_j$ , the corresponding eigenvector disappears from the zero eigenspace, and the structure of the superposition state changes accordingly.

The second layer of features is Betti numbers. We record the Betti numbers  $\beta_k(\epsilon_j) = \dim(\ker \Delta_k)$  for each dimension at each scale. Betti numbers provide global statistical information about the quantity of topological features, serving as an important complement to harmonic form features. Jump points in Betti numbers correspond to the occurrence of topological events, while plateau periods to some extent reflect the relative stability of topological structure.

The third layer of features is the persistence measure. We compute the inner product between quantum superposition states at adjacent scales:

$$\mathcal{P}_k(j, j+1) = |\langle \psi_k(\epsilon_j) | \psi_k(\epsilon_{j+1}) \rangle|^2. \quad (2)$$

This quantity directly measures the stability of topological structure, which is closely related to the bottleneck and Wasserstein distances commonly used to compare persistence diagrams [16]. When the inner product is close to 1, it indicates that the  $k$ -dimensional topological structure remains stable between these two scales; when the inner product decreases significantly, it suggests the birth or death of topological features. This measure has a direct correspondence with the distance from points to the diagonal in persistence diagrams (i.e., the persistence of features).

Topological theory tells us that there exist intrinsic connections between topological features,

such as holes, of different dimensions. For example, the formation of  $k$ -dimensional holes often depends on the disappearance of  $(k - 1)$ -dimensional structures. This dependency means that the category of  $k$ -dimensional persistence diagrams may be influenced by features of other dimensions. Consider a simple example: the topological structure of a torus involves  $H_1$  (two loops) and  $H_2$  (one cavity) features, while a sphere mainly involves  $H_2$  (one cavity) features. If we only use the Betti curve of  $H_2$ , we might not be able to distinguish between a torus and a sphere, as both have similar performance in  $H_2$  ( $\beta_2 = 1$ ), but combining the Betti curve of  $H_1$  (torus  $\beta_1 = 2$ , sphere  $\beta_1 = 0$ ) allows easy distinction. Therefore, using Betti curves of more dimensions can provide more comprehensive topological information, helping the model capture these cross-dimensional patterns, thereby improving the accuracy of persistence diagram prediction.

## 4 Mixed Topological Kernel Function Design

The design of kernel functions is key to connecting quantum feature extraction and support vector machine classification, and also an important criterion for measuring differences. Topological kernels have been successfully applied in various machine learning tasks [17, 18], demonstrating the effectiveness of incorporating topological features into kernel-based learning. We design kernel functions specifically suitable for topological data. For two datasets  $D_i$  and  $D_j$ , the mixed topological kernel function is defined as:

$$k_{\text{topo}}(D_i, D_j) = \lambda_1 k_{\text{harmonic}}(D_i, D_j) + \lambda_2 k_{\text{betti}}(D_i, D_j) + \lambda_3 k_{\text{persist}}(D_i, D_j), \quad (3)$$

where  $\lambda_1, \lambda_2, \lambda_3$  are weight parameters determined through cross-validation.

The harmonic kernel  $k_{\text{harmonic}}$  measures the similarity of harmonic forms between two datasets:

$$k_{\text{harmonic}}(D_i, D_j) = \sum_{k=0}^K \sum_{t=1}^T |\langle \psi_k^{(i)}(\epsilon_t) | \psi_k^{(j)}(\epsilon_t) \rangle|^2. \quad (4)$$

This kernel function directly compares the geometric realization of topological features. According to the inner product properties of quantum states, it can be efficiently computed on a quantum computer through swap test, with complexity  $O(\log N)$ , where  $N$  is the feature dimension [19].

The Betti kernel  $k_{\text{betti}}$  is based on the similarity of Betti numbers across multiple dimensions and scales, vectorizing Betti numbers as  $\vec{v}_{\text{betti}} \in \mathbb{R}^{T \times (K+1)}$ , with the kernel function defined as:

$$k_{\text{betti}}(D_i, D_j) = \langle \vec{v}_{\text{betti}}^{(i)} | \vec{v}_{\text{betti}}^{(j)} \rangle. \quad (5)$$

This linear kernel captures the evolution patterns of topological statistics, helping to identify

topological differences between different datasets.

The persistence kernel  $k_{\text{persist}}$  measures the similarity of topological feature stability between two datasets. We compute the inner product sequence between adjacent scales for each dataset, forming the persistence feature vector  $\vec{v}_{\text{persist}}$ , then define it in the form of a Gaussian kernel:

$$k_{\text{persist}}(D_i, D_j) = \exp\left(-\gamma\|\vec{v}_{\text{persist}}^{(i)} - \vec{v}_{\text{persist}}^{(j)}\|^2\right), \quad (6)$$

where  $\gamma$  is the bandwidth parameter. This Gaussian kernel is sensitive to small differences in scale persistence patterns, helping to distinguish topological features with different lifecycle patterns.

## 5 Quantum Support Vector Machine Training

The core task of the training phase is to construct a quantum support vector machine model that learns the mapping from quantum topological features extracted by the LGZ algorithm to persistence diagrams. We adopt the quantum least-squares support vector machine (LS-SVM) framework proposed by Rebentrost et al. [19].

The training dataset  $\mathcal{S} = \{(\mathbf{X}_i, y_i)\}_{i=1}^M$  is constructed for specific application scenarios, such as colon lesion detection. Features  $\mathbf{X}_i$  are extracted through the LGZ algorithm, containing harmonic form superposition states, Betti numbers, and persistence measures. Labels  $y_i \in \{1, 2, \dots, L\}$  are obtained through classical persistent homology computation (note that to reduce complexity, we can use heuristic classical algorithms here), representing  $L$  different persistence diagrams. The algebraic structure of persistence diagrams [20] allows us to naturally categorize them into discrete classes for supervised learning. Since we focus on specific scenarios, the number of categories  $L$  is usually limited, so the number of classical persistent homology computations needed to obtain this training set is also limited. However, since the scenario is specific, this is sufficient to ensure that the training set can cover all typical topological patterns in that scenario.

The kernel matrix  $K \in \mathbb{R}^{M \times M}$  with elements  $K_{ij} = k_{\text{topo}}(\mathbf{X}_i, \mathbf{X}_j)$  is computed through the mixed topological kernel function. On a quantum computer, the kernel matrix is represented through the density matrix  $\hat{K} = K/\text{tr}(K)$ . According to the analysis by Rebentrost et al. [19], non-sparse kernel matrices can be exponentiated through swap operator techniques:

$$e^{-i\hat{K}\Delta t} \rho e^{i\hat{K}\Delta t} \approx \text{tr}_1\{e^{-iS\Delta t}(\hat{K} \otimes \rho)e^{iS\Delta t}\}, \quad (7)$$

where  $S = \sum_{m,n} |m\rangle\langle n| \otimes |n\rangle\langle m|$  is the swap operator, with implementation complexity  $O(\log M\Delta t)$ .

For multi-class problems, we adopt the one-vs-rest strategy to train  $L$  binary classifiers. The  $\ell$ -th classifier solves the linear system:

$$\mathbf{F}^{(\ell)} \begin{pmatrix} b^{(\ell)} \\ \vec{\alpha}^{(\ell)} \end{pmatrix} = \begin{pmatrix} 0 \\ \vec{y}^{(\ell)} \end{pmatrix}, \quad (8)$$

where  $\mathbf{F}^{(\ell)} = \begin{pmatrix} 0 & \vec{1}^T \\ \vec{1} & K + \gamma^{-1}I \end{pmatrix}$  is the augmented matrix,  $\gamma$  is the regularization parameter,  $y_i^{(\ell)} = +1$  if the original label  $y_i = \ell$ , otherwise  $y_i^{(\ell)} = -1$ .

Quantum matrix inversion is implemented through the HHL algorithm [21]. The algorithm first decomposes the label vector  $|\vec{y}^{(\ell)}\rangle$  into the eigenspace of  $\mathbf{F}^{(\ell)}$  through quantum phase estimation, then performs controlled rotation on each eigenvalue  $\lambda_j$  to implement  $\lambda_j^{-1}$ , and finally obtains the solution vector  $|b^{(\ell)}, \vec{\alpha}^{(\ell)}\rangle$  through inverse phase estimation. According to the analysis by Rebentrost et al. [19], the time complexity for training a single classifier is  $O(\log(M)\kappa_{\text{eff}}^3/\epsilon^3)$ , where  $\kappa_{\text{eff}}$  is the effective condition number (obtained by truncating small eigenvalues) and  $\epsilon$  is the precision parameter. The total complexity for training all  $L$  classifiers is  $O(L \log(M)\kappa_{\text{eff}}^3/\epsilon^3)$ .

## 6 Quantum Support Vector Machine Prediction

The prediction phase demonstrates the core advantage of our algorithm: for a new dataset  $D_{\text{new}}$ , persistence diagrams are predicted through a pure quantum pipeline with speed advantages, completely avoiding classical persistent homology computation.

First, we run the LGZ algorithm to extract features. At  $T$  scales, for each dimension  $k$ , we compute the spectral decomposition of the combinatorial Laplacian. According to the analysis by Lloyd et al. [5], constructing the simplicial superposition state requires  $O(n^2)$  operations, and quantum phase estimation requires  $O(n^3/\delta)$  operations (for an  $n$ -sparse Dirac operator), so the complexity for extracting features of all dimensions at a single scale is  $O(n^5/\delta)$ . For all  $T$  scales, the total complexity is  $O(Tn^5/\delta)$ .

The extracted features include harmonic form superposition states  $|\psi_k^{\text{new}}(\epsilon_t)\rangle$ , Betti numbers  $\beta_k^{\text{new}}(\epsilon_t)$ , and persistence measures  $\mathcal{P}_k^{\text{new}}(t, t+1)$ , forming the feature vector  $\mathbf{X}_{\text{new}}$ .

Next, we perform classification decision. For the  $\ell$ -th classifier, the decision function is:

$$f^{(\ell)}(D_{\text{new}}) = b^{(\ell)} + \sum_{i=1}^M \alpha_i^{(\ell)} y_i^{(\ell)} k_{\text{topo}}(\mathbf{X}_i, \mathbf{X}_{\text{new}}). \quad (9)$$

On a quantum computer, we utilize quantum parallelism to compute all kernel function values simultaneously. We prepare the superposition state of training data:

$$|\Psi_{\text{train}}\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^M |i\rangle |\mathbf{X}_i\rangle. \quad (10)$$

Through quantum interference, we compute  $\langle \mathbf{X}_{\text{new}} | \mathbf{X}_i \rangle$ , then use amplitude encoding to encode

the weights  $\alpha_i^{(\ell)} y_i^{(\ell)}$  into quantum states. According to the analysis by Rebentrost et al. [19], the decision function value can be estimated with complexity  $O(\log(M)/\epsilon^2)$  through quantum amplitude estimation.

The final prediction is determined by comparing the outputs of all classifiers:

$$\hat{y}_{\text{new}} = \arg \max_{\ell \in \{1, \dots, L\}} f^{(\ell)}(D_{\text{new}}). \quad (11)$$

The total prediction complexity is  $O(Tn^5/\delta + L \log(M)/\epsilon^2)$ , where the first term comes from LGZ feature extraction and the second from QSVM classification. This completely avoids classical persistent homology computation. For scenarios where optimized classical algorithms require  $O(n^3)$ , our method provides significant theoretical acceleration potential.

## 7 Algorithm Analysis

### 7.1 Complexity Analysis

We conduct a rigorous analysis of computational complexity for the complete simplicial complex scenario. Consider a dataset containing  $n$  vertices, whose complete simplicial complex contains all  $2^n$  possible simplices.

Under the classical computational paradigm, persistent homology algorithms need to construct boundary matrices and perform matrix reduction to obtain persistent pairings. The standard algorithm has complexity  $O(m^3)$ , where  $m$  is the number of simplices, thus the complexity for a complete simplicial complex reaches  $O(2^{3n})$ . Even with optimization techniques such as twist optimization, the complexity remains  $O(2^{2n})$ . Lloyd et al. [5] proved that the classical complexity for computing Betti numbers of all dimensions alone (without persistent pairing information) requires  $O(2^n \log(1/\delta))$  (Lloyd et al., 2016).

In contrast, our proposed quantum algorithm achieves significant complexity reduction in the prediction phase. Although the training phase requires computing classical persistence diagrams for  $M$  samples, incurring a one-time cost of  $O(M \cdot 2^{2n})$ , the trained model can be reused, and this one-time cost can be replaced with heuristic algorithms to reduce complexity. For prediction on new data, the algorithm only needs to perform LGZ feature extraction and QSVM classification, with total complexity  $O(Tn^5/\delta + L \log(M)/\epsilon^2)$ , where  $T$  is the number of scales,  $L$  is the number of categories, and  $\delta$  and  $\epsilon$  are the precision parameters for LGZ and QSVM respectively.

The significance of this complexity improvement is profound. For medium-scale data with  $n = 30$ , the classical method requires approximately  $2^{60} \approx 10^{18}$  operations, while our quantum method only requires approximately  $30^5 \cdot T \approx 10^7$  operations (assuming  $T = 20$ ). This reduction from double exponential to polynomial makes real-time persistence diagram prediction, which was previously infeasible, now possible. It is worth emphasizing that the LGZ algorithm not

only provides computational acceleration but also extracts harmonic forms containing geometric information that Betti numbers cannot capture, which is crucial for accurate persistence diagram prediction.

## 7.2 Applicability Analysis

The effectiveness of the algorithm depends on the finiteness of topological patterns in specific application scenarios. In medical image analysis [22, 23], the topological patterns of normal and diseased tissues are relatively fixed; in materials science, the molecular topological structures of specific types of materials are enumerable; in network analysis, the topological features of domain-specific networks are limited. These scenarios all satisfy our basic assumptions, making it feasible to construct complete training sets.

It should be noted that the quantum advantage of the LGZ algorithm is mainly reflected in processing dense data or scenarios requiring consideration of all possible simplices. For sparse data common in practice, optimized classical algorithms [24], such as Ripser, may be more practical at medium scales. However, as data scales grow and quantum hardware develops, the advantages of quantum algorithms will gradually become apparent.

## 8 Discussion

This work achieves the first-ever prediction from quantum topological features to persistence diagrams, marking a crucial transition of quantum topological data analysis from a pure computational tool to a practical system. By deeply mining the harmonic forms and Betti numbers of the LGZ quantum algorithm, combined with quantum support vector machine learning [19, 9], we successfully elevate statistical Betti numbers to structural persistence diagram information, solving the long-standing practical bottleneck of quantum topological algorithms.

The core innovation of the algorithm lies in recognizing that the intermediate results of the LGZ algorithm—harmonic form eigenvectors—contain information far richer than Betti numbers. These eigenvectors not only tell us how many holes there are (Betti numbers) but also encode the specific geometric realization of each hole. Through multi-scale tracking and machine learning, we can infer persistence diagram patterns from this geometric information. This method successfully combines the efficiency advantages of quantum computing with the information needs of practical applications.

The algorithm has significant advantages in specific application scenarios. In pathological monitoring, drug discovery, materials design, and other specific contexts, the topological patterns of tissue samples are relatively limited, and a well-trained model can quickly screen the topological structures of large numbers of samples.

Current limitations are mainly reflected in two aspects. First, the algorithm outputs only relatively approximate persistence diagrams, not absolutely precise ones. Second, the full real-

ization of quantum advantages requires processing truly large-scale or high-dimensional data; for medium-scale sparse data, optimized classical algorithms may be more practical.

Looking forward, as quantum computing hardware matures, this algorithm is expected to play a key role in applications such as real-time topological analysis and large-scale screening. Particularly in scenarios requiring processing of exponential simplicial spaces, the advantages of this quantum algorithm will be fully realized. This work provides a feasible pathway for the practical implementation of quantum topological data analysis, promising to advance the field toward real-world applications.

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