CUT-OFF FOR LARGE SUMS OF GRAPHS

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ABSTRACT. If L is the combinatorial Laplacian of a graph, $\exp(-L\,t)$ converges to a matrix with identical coefficients. The speed of convergence is measured by the maximal entropy distance. When the graph is the sum of a large number of components, a cut-off phenomenon may occur: before some instant the distance to equilibrium tends to infinity; after that instant it tends to 0. A sufficient condition for cut-off is given, and the cut-off instant is expressed as a function of the gap and eigenvectors of components. Examples include sums of cliques, stars and lines.

Convergence abrupte pour de grandes sommes de graphes

RÉSUMÉ. Si L est le laplacien combinatoire d'un graphe, $\exp(-L\,t)$ converge vers une matrice dont tous les coefficients sont égaux. La vitesse de convergence est mesurée par la distance d'entropie maximale. Quand le graphe est la somme d'un grand nombre de composantes, un phénomène de convergence abrupte peut survenir : avant un certain instant la distance à l'équilibre tend vers l'infini ; après cet instant elle tend vers 0. Une condition suffisante de convergence abrupte est donnée, et l'instant de convergence est exprimé en fonction du trou spectral et des vecteurs propres des composantes. Les sommes de cliques, d'étoiles et de lignes sont traitées en exemple.

1. Introduction

Many binary operations on graphs result in a graph whose set of vertices is the Cartesian product of the sets of vertices of the graphs to which the operation is applied (see section 2.5 p. 65 of Cvetković et al. [11]). One of the simplest is the sum: if G_1 and G_2 are two graphs, then two couples (x_1, y_1), (x_2, y_2) are adjacent in $G_1 + G_2$ if and only if either $x_1 = x_2$ and y_1, y_2 are adjacent in G_2 or $y_1 = y_2$ and x_1, x_2 are adjacent in G_1. Let $(G_n)_{n \geqslant 1}$ be a sequence of graphs. All are finite, undirected, with no loop or multiple edge, and connected. For $n \geqslant 1$, let

$$S_n = G_1 + \cdots + G_n \ .$$

We are interested here in asymptotic properties of S_n. Sums of identical copies of a given graph sometimes appear in the literature as "Cartesian powers" ([2, 5]). The denomination "sum" that we use following [10, 11], is coherent with spectral properties.

We shall only deal here with the combinatorial Laplacian (see Colin de Verdière [8]): if $G = (V, E)$ is a graph, it is defined as $L = D - A$, where D is the diagonal matrix of degrees and A the adjacency matrix. The matrix $-L$ is the infinitesimal generator of the continuous time random walk on the graph (see for instance Çinlar [7]). If $x \in V$ is a vertex, the distribution at time t of the random walk, starting at x at time 0 is the x-th row of the matrix $\exp(-L\,t)$. As t tends to infinity, it converges to the uniform distribution on V. The maximal entropy distance between rows of $\exp(-L\,t)$ and the uniform distribution (Definition 2.1), measures the speed of convergence. Many other distances could have been chosen, leading to similar results (see [3]). As t tends to infinity, the distance to equilibrium decays

as $ae^{-2\rho t}$, where ρ is the gap (smallest positive eigenvalue of L), and a depends on the eigenvectors associated to the gap-eigenvalues of L (Lemma 2.2).

It is a well-known fact that the Laplacian of $G_1 + G_2$ is the Kronecker sum of the Laplacians of G_1 and G_2 (chap. 12 of Bellman [4]); its spectrum contains all possible sums of eigenvalues of G_1 and G_2. The continous time random walk on $G_1 + G_2$ can be written as a couple whose coordinates are independent copies of the random walks on G_1 and G_2 respectively. The maximal entropy distance to equilibrium for $G_1 + G_2$ is the sum of distances for G_1 and G_2 (Lemma 2.3). As n tends to infinity, the distance to equilibrium for $S_n = G_1 + \cdots + G_n$ may decay quite steeply, exhibiting a so called *cut-off* phenomenon (Definition 2.4): before some instant t_n, the distance is very high, and it abruptly drops down after t_n. In the random walk interpretation, t_n is "the" instant at which the walk reaches its equilibrium. The cut-off phenomenon of steep convergence, first identified by Aldous and Diaconis [1], has been observed on many stochastic processes (see [3, 14] and references therein). Our main result, Theorem 3.1, gives an explicit expression for t_n, and sufficient conditions for cut-off at time t_n for S_n. This result is related to Theorem 3 of [3], obtained in a somewhat different setting. It could be extended to other kinds of symmetric operators, such as weighted Laplacians [6, 9, 12].

The probability transition matrix of the *discrete time* random walk on a graph G is $P = I - \frac{1}{d}L$, where I is the identity matrix, d the maximal degree and L the Laplacian. If P_1 and P_2 are the transition matrices of the discrete time random walks on two graphs G_1 and G_2, then the Kronecker *product $P_1 \otimes P_2$* is the transition matrix of the discrete time random walk on the Cartesian *product* of G_1 and G_2. Thus a similar study could be carried out by replacing continuous time by discrete time, Kronecker sums of matrices by Kronecker products and Cartesian sums of graphs by Cartesian products: see [15] for the correspondence between discrete and continuous time.

In Section 2, notations and preliminary results are exposed. Section 3 contains the statement and proof of Theorem 3.1. The particular cases of sums of cliques, stars and lines are discussed.

2. Entropy distance to equilibrium

Let $G = (V, E)$ be a graph with k vertices. Denote by L its combinatorial Laplacian. Let $x, y \in V$ be two vertices. The coefficient of the matrix $\exp(-Lt)$ indexed by x, y is the probability for the continuous time random walk on the graph, starting on vertex x at time 0, to be found on vertex y at time t. It will be denoted by $p_{x,y}(t)$. As t tends to infinity, the random walk converges in distribution to the uniform law on V. In other words, the matrix $\exp(-Lt)$ converges to the matrix whose coefficients are all equal to $1/k$. We choose to measure the distance from $\exp(-Lt)$ to its limit by the maximal entropy (or Kullback) distance between rows of $\exp(-Lt)$ and the uniform distribution on vertices.

DEFINITION 2.1. — *We call* maximal entropy distance *of the graph G the function d defined for $t > 0$ by:*

$$d(t) = \max_{x \in V} -\frac{1}{k} \sum_{y \in V} \log(k p_{x,y}(t)) \ .$$

The maximal entropy distance decays as $e^{-2\rho t}$, where ρ is the gap (smallest positive eigenvalue). The equivalent can be expressed in terms of the eigenvectors associated to eigenvalues equal to the gap. Let $\lambda_1 = 0 < \lambda_2 \leqslant \cdots \leqslant \lambda_k$ be the eigenvalues of L. Denote by $v_1, \ldots, v_k$ eigenvectors such that $Lv_i = \lambda_i v_i$ and $(v_1, \ldots, v_k)$ is an orthonormal basis for the Euclidean norm. As usual, v_1 is the constant vector whose coordinates are all equal to $k^{-1/2}$.

LEMMA 2.2. —

$$\lim_{t \to +\infty} \frac{d(t)}{ae^{-2\rho t}} = 1 \ ,$$

with

$$a = \frac{k}{2} \max_{x \in V} \sum_{i: \lambda_i = \rho} v_i(x)^2 .$$

Note that a is bounded above by $k/2$ and below by $1/2$.

Proof. — Using the eigenvectors,

$$\begin{aligned} p_{x,y}(t) &= \sum_{i=1}^{k} v_i(x)v_i(y) e^{-\lambda_i t} , \\ &= \frac{1}{k} + \sum_{i=2}^{k} v_i(x)v_i(y) e^{-\lambda_i t} . \end{aligned}$$

Thus

$$\begin{aligned} \log(k p_{x,y}(t)) &= \log \left(1 + k \sum_{i=2}^{k} v_i(x)v_i(y) e^{-\lambda_i t} \right) , \\ &= k \left(\sum_{i=2}^{k} v_i(x)v_i(y) e^{-\lambda_i t} \right) \\ &\quad - \frac{k^2}{2} \left(\sum_{i=2}^{k} v_i(x)v_i(y) e^{-\lambda_i t} \right)^2 + o(e^{-2\rho t}) . \end{aligned}$$

So,

$$\begin{aligned} -\frac{1}{k} \sum_{y \in V} \log(k p_{x,y}(t)) &= -\sum_{y \in V} \sum_{i=2}^{k} v_i(x)v_i(y) e^{-\lambda_i t} \\ &\quad + \frac{k}{2} \sum_{y \in V} \left(\sum_{i=2}^{k} v_i(x)v_i(y) e^{-\lambda_i t} \right)^2 + o(e^{-2\rho t}) . \end{aligned}$$

The fact that $v_1, \ldots, v_n$ are orthonormal simplifies the sums appearing in the last expression. Since for $i = 2, \ldots, n$, v_i is orthogonal to v_1, the sum $\sum_{y \in V} v_i(y)$ of its coordinates is null, so the first term vanishes. Furthermore,

$$\begin{aligned} &\sum_{y \in V} \left(\sum_{i=2}^{k} v_i(x)v_i(y) e^{-t\lambda_i} \right)^2 \\ &= \sum_{y \in V} \left(\sum_{i=2}^{k} v_i^2(x)v_i^2(y) e^{-2\lambda_i t} + 2 \sum_{i<j=2}^{n} v_i(x)v_j(x)v_i(y)v_j(y) e^{-(\lambda_i + \lambda_j)t} \right) \\ &= \sum_{i=2}^{k} v_i^2(x) e^{-2\lambda_i t} , \end{aligned}$$

where the last simplification is due to the identities

$$\sum_{y \in V} v_i^2(y) = 1 \quad \text{and} \quad \sum_{y \in V} v_i(y)v_j(y) = 0 .$$

Hence,

$$-\frac{1}{k} \sum_{y \in V} \log(k p_{x,y}(t)) = \frac{k\, e^{-2\rho t}}{2} \sum_{i: \lambda_i = \rho} v_i^2(x) + o(e^{-2\rho t}) .$$

Since the eigenvector v_i is non-null, $v_i(x)$ cannot vanish for every $x \in V$. (For a given $x \in V$, it may however happen that $v_i(x) = 0$ for all i such that $\lambda_i = \rho$.) This implies that the order of $d(t)$ is exactly $e^{-2\rho t}$ and not smaller.   □

We will consider three examples of graphs with k vertices: the clique, the star and the line, respectively denoted by K_k, T_k and L_k. The spectral decomposition of their Laplacian is easy to compute. Colin de Verdière [8] mentions that the spectrum of the line graph is the first ever published, by Lagrange in 1867. We summarize below the values of ρ and a for K_k, T_k and L_k.

Graph	ρ	a
Clique K_k	k	$(k-1)/2$
Star T_k	1	$k(k-2)/(2(k-1))$
Line L_k	$2(1-\cos(\pi/k))$	$\cos^2(\pi/(2k))$

The entropy distance is particularly well adapted to sums of graphs.

LEMMA 2.3. — *Let G_1, G_2 be two graphs. Let d_1 and d_2 be the maximal entropy distances of G_1 and G_2 respectively. The maximal entropy distance of $G_1 + G_2$ is $d_1 + d_2$.*

Proof. — That the Kullback distance between tensor products is the sum of Kullback distances between components is a well-known fact (see for instance Lemma 3.3.10 p. 100 in [13]). It can be easily checked using Definition 2.1. Let $x = (x_1, x_2)$ and $y = (y_1, y_2)$ be two vertices of $G_1 + G_2$. One has

$$p_{x,y}(t) = p_{x_1,y_1}(t)\, p_{x_2,y_2}(t) \ ,$$

Thus,

$$-\frac{1}{k_1 k_2} \sum_{y=(y_1,y_2)} \log(k_1 k_2 p_{x,y}(t)) = \sum_{i=1}^{2} -\frac{1}{k_i} \sum_{y_i \in V_i} \log(k_i p_{x_i,y_i}(t)) \ .$$

Hence the result, by taking the maximum over all vertices (x_1, x_2).   □

Here is the definition of cut-off for a sequence of graphs.

DEFINITION 2.4. — *For $n = 1, 2, \ldots$, let H_n be a graph and d_n be the maximal entropy distance of H_n. Let (t_n) be a sequence of positive reals, tending to $+\infty$. The sequence of graphs (H_n) has a cut-off at (t_n) if for $c > 0$:*

$$c < 1 \implies \lim_{n \to \infty} d_n(ct_n) = +\infty$$
$$c > 1 \implies \lim_{n \to \infty} d_n(ct_n) = 0 \ .$$

This definition matches the usual definition for cut-off of stochastic processes (see [3] and references therein).

Our first example is the sum of copies of a given graph. Let G be a graph, and d be its maximal entropy distance. For $n = 1, 2, \ldots$, let G_n be isomorphic to G. The maximal entropy distance of the sum $S_n = G_1 + \cdots + G_n$ is nd. It follows from Lemma 2.2 that the sequence (S_n) has a cut-off at $\log(n)/(2\rho)$, where ρ is the gap of G. Actually in this example, the convergence takes place in a window of time of order 1, since for all $u \in \mathbb{R}$:

$$\lim_{n \to \infty} n\, d\left(\frac{\log(n)}{2\rho} + u\right) = a\, e^{-2\rho u} \ .$$

In the next section we will discuss the cut-off phenomenon for sums of possibly distinct graphs.

3. Cut-off for a sum of graphs

Let $(G_n)_{n \geqslant 1}$ be a sequence of graphs. For $n \geqslant 1$, let k_n be the number of vertices of G_n, let d_n be the maximal entropy distance of G_n, and let ρ_n and a_n be, as in Lemma 2.2, such that

$$(3.1) \qquad \lim_{t \to \infty} \frac{d_n(t)}{a_n e^{-2\rho_n t}} = 1 \ .$$

Let S_n be the sum $G_1 + \cdots + G_n$. By Lemma 2.3, the maximal entropy distance of S_n is

$$D_n = d_1 + \cdots + d_n \ .$$

The cut-off instant t_n will be defined as a function of the ρ_i's and a_i's.

Let $(\rho_{(1,n)}, a_{(1,n)}), \ldots, (\rho_{(n,n)}, a_{(n,n)})$ be the values of $(\rho_1, a_1), \ldots, (\rho_n, a_n)$ once the ρ_i's have been ranked in non-decreasing order:

$$0 < \rho_{(1,n)} \leqslant \cdots \leqslant \rho_{(n,n)} \ .$$

For $n \geqslant 1$ and $i = 1, \ldots, n$, let $A_{(i,n)}$ be the cumulated sum

$$A_{(i,n)} = a_{(1,n)} + \cdots + a_{(i,n)} \ .$$

The cut-off instant is

$$(3.2) \qquad t_n = \max \left\{ \frac{\log A_{(i,n)}}{2\rho_{(i,n)}} \ ; \ i = 1, \ldots, n \right\} \ .$$

Our main result gives conditions under which a cut-off occurs at (t_n).

THEOREM 3.1. — *Assume that:*

(1) *the convergence in* (3.1) *is uniform in* n,

(2)

$$(3.3) \qquad \lim_{n \to \infty} \rho_{(1,n)} t_n = +\infty \ ,$$

(3) *there exists a constant* α *such that* $0 < \alpha < 1$ *and for* n *large enough,*

$$(3.4) \qquad \forall i = 2, \ldots, n \ , \quad a_{(i,n)} \leqslant \alpha A_{(i-1,n)} \ .$$

Then (S_n) *has a cut-off at* (t_n), *defined by* (3.2).

Proof. — By the first hypothesis, there exists t_0 such that for $t \geqslant t_0$ and for all n,

$$\frac{1}{2} a_n e^{-2\rho_n t} \leqslant d_n(t) \leqslant 2 a_n e^{-2\rho_n t} \ .$$

Let σ_n denote the sum of equivalents:

$$(3.5) \qquad \sigma_n = \sum_{i=1}^{n} a_i e^{-2\rho_i c t_n} = \sum_{i=1}^{n} a_{(i,n)} e^{-2\rho_{(i,n)} c t_n} \ .$$

It suffices to prove that σ_n tends to $+\infty$ for $c < 1$, to 0 for $c > 1$. We first check the former. Let i_n^* be the smallest integer such that

$$t_n = \frac{\log A_{(i_n^*,n)}}{2\rho_{(i_n^*,n)}} \ .$$

One has:

$$
\begin{aligned}
\sigma_n \ &\geqslant \ \sum_{i=1}^{i_n^*} a_{(i,n)} e^{-2\rho_{(i,n)} c t_n} \\[2mm]
&\geqslant \ A_{(i_n^*,n)} e^{-2\rho_{(i_n^*,n)} c t_n} \\[2mm]
&= \ e^{2(1-c)\rho_{(i_n^*,n)} t_n} \\[2mm]
&\geqslant \ e^{2(1-c)\rho_{(1,n)} t_n}
\end{aligned}
$$

For $0 < c < 1$, the result follows by (3.3).

Let now c be larger than 1. For all $l = 1, \ldots, n-1$, one has:

$$\sigma_n \quad \leqslant \quad A_{(l,n)} e^{-2\rho_{(1,n)} c t_n} + \sum_{i=l+1}^{n} a_{(i,n)} e^{-2\rho_{(i,n)} c t_n}$$

$$\leqslant \quad A_{(l,n)} e^{-2\rho_{(1,n)} c t_n} + \sum_{i=l+1}^{n} a_{(i,n)} A_{(i,n)}^{-c} .$$

In the last inequality, the sum is a Riemann sum for the (decreasing) function $x \mapsto x^{-c}$. Hence:

$$\sigma_n \quad \leqslant \quad A_{(l,n)} e^{-2\rho_{(1,n)} c t_n} + \int_{A_{(l,n)}}^{A_{(n,n)}} x^{-c}\, dx$$

$$(3.6) \qquad\qquad \leqslant \quad A_{(l,n)} e^{-2\rho_{(1,n)} c t_n} + \frac{1}{c-1} A_{(l,n)}^{1-c} .$$

If $i_n^* = 1$, then applying (3.6) for $l = 1$ yields

$$(3.7) \qquad\qquad \sigma_n \leqslant e^{-2\rho_{(1,n)}(1-c)t_n} \left(1 + \frac{1}{c-1} \right) .$$

Otherwise,

$$A_{(1,n)} < e^{2\rho_{(1,n)} t_n} \leqslant e^{2\rho_{(i_n^*,n)} t_n} = A_{(i_n^*,n)} .$$

Let $l_n > 1$ be such that

$$A_{(l_n-1,n)} < e^{2\rho_{(1,n)} t_n} \leqslant A_{(l_n,n)} = A_{(l_n-1,n)} + a_{(l_n,n)} .$$

Applying (3.6) to $l = l_n - 1$ yields

$$\sigma_n \quad \leqslant \quad e^{2\rho_{(1,n)}(1-c)t_n} + \frac{1}{c-1} \left(e^{2\rho_{(1,n)} t_n} - a_{(l_n,n)} \right)^{1-c}$$

$$= \quad e^{2(1-c)\rho_{(1,n)} t_n} \left(1 + \frac{1}{c-1} \left(1 - a_{(l_n,n)} e^{-2\rho_{(1,n)} t_n} \right)^{1-c} \right)$$

$$(3.8) \qquad\qquad \leqslant \quad e^{2(1-c)\rho_{(1,n)} t_n} \left(1 + \frac{1}{c-1} (1-\alpha)^{1-c} \right) ,$$

using the definition of l_n and condition (3.4) for the last inequality. Since $\rho_{(1,n)} t_n$ tends to infinity, the result follows from (3.7) and (3.8). $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Observe that $\rho_{(1,n)}$ is the gap of the graph S_n. The cut-off time t_n can be seen as a mixing time for the continuous time random walk on S_n. In the proof above, the hypothesis (3.3) is crucial. This condition has recently appeared in a number of different contexts as a sufficient condition for cut-off (see [3] and references therein).

As a first example, assume that the number of vertices of G_n remains bounded. Since the sequence (k_n) only takes a finite number of different values, so do the sequences (ρ_n) and (a_n), and also the sequence of differences between the third smallest eigenvalue of the Laplacian of G_n and ρ_n: they all remain bounded, and bounded away from 0. As a consequence, the three hypotheses of Theorem 3.1 are satisfied.

We will give more examples in the three particular cases where the components are cliques, stars or lines. In what follows, $(k_n)_{n \geqslant 1}$ is a sequence of integers, each no lesser than 2. For $k \geqslant 2$, we denote by $N_k(n)$ the number of values equal to k among $k_1, \ldots, k_n$.

Sums of cliques

The maximal entropy distance d of the clique K_k is:

$$(3.9) \qquad d(t) = -\frac{k-1}{k}\log(1 - e^{-kt}) - \frac{1}{k}\log\left(1 + \frac{k-1}{k}e^{-kt}\right) \, .$$

Using elementary calculus, one can show that the ratio

$$\frac{d(t)}{((k-1)/2)e^{-kt}}$$

tends to 1 as t tends to infinity, uniformly in k. So the first hypothesis of Theorem 3.1 is satisfied.

Observe that for all k,

$$t_n \geqslant \frac{\log(N_k(n)(k-1)/2)}{2k} \, ,$$

Assume that $N_k(n)$ is unbounded for some integer k (the value k is repeated an infinity of times in the sequence (k_n)). Then t_n tends to infinity as well as $\rho_{(1,n)}t_n$, and the second hypothesis also holds. There remains to check the third hypothesis, which imposes to control the jumps of the $A_{(i,n)}$'s.

Assume now that each integer k occurs only a finite number of times b_k in the sequence k_n.

$$b_k = \sum_{n=1}^{+\infty} \mathbb{I}_{k_n = k} \, .$$

Then t_n tends to infinity iff

$$\lim_{k \to \infty} \frac{\log(2b_2 + \cdots + kb_k)}{k} = +\infty \, ,$$

which imposes that b_k should grow faster than exponentially in k.

We will check that if b_k grows at most exponentially in k, then there is no cut-off. The radius of convergence of the series $\sum b_k z^k$ is no larger than 1. Suppose it is equal to e^{-2t_0} for some positive t_0. Consider the series

$$\sum_{k=2}^{\infty} b_k \frac{k-1}{2} e^{-2kt}$$

It diverges for $t < t_0$ and it converges for $t > t_0$. Therefore

$$\sum_{k=2}^{\infty} N_k(n) \frac{k-1}{2} e^{-2kt}$$

tends to $+\infty$ for $t < t_0$, to a finite value for $t > t_0$. So does $D_n(t)$, and there is no cut-off. If the radius of convergence is 1, then $D_n(t)$ remains bounded for all positive t.

Sums of stars

The maximal entropy distance of the star T_k is:

$$(3.10) \qquad d(t) = -\frac{k-2}{k}\log\left(1 - \frac{k}{k-1}e^{-t} + \frac{1}{k-1}e^{-kt}\right) - \frac{1}{k}\log\left(1 + \frac{k(k-2)}{k-1}e^{-t} + \frac{1}{k-1}e^{-kt}\right) \, .$$

This time the convergence is not uniform in k and the first hypothesis of Theorem 3.1 holds only if (k_n) is bounded. If it is unbounded, there may still be a cut-off for (S_n). It may be at the instant t_n defined by (3.2), or elsewhere. For instance, if $k_n = n + 1$, there is a cutoff at $(\log n)$, as expected. But if $k_n = 2^n$, there is a cutoff at $n/(\log 2)$, and not $n/(2\log 2)$ as (3.2) would lead to think.

Sums of lines

Let $G_n = L_{k_n}$. Recall that $\rho_n = 2(1 - \cos(\pi/k_n))$ and $a_n = \cos^2(\pi/(2k_n))$. If (k_n) is unbounded, then the gap $\rho_{(1,n)}$ tends to zero and the convergence in (3.1) is not uniform. However, in this particular case, there exists a positive constant b such that for all n,

$$a_n e^{-2\rho_n t}(1 - be^{-\rho_n t}) \leqslant d_n(t) \leqslant a_n e^{-2\rho_n t}(1 + be^{-\rho_n t}) \, .$$

Using the definition (3.5) of σ_n, one has:

$$(1 - be^{-\rho_{(1,n)}ct_n})\,\sigma_n \leqslant D_n(ct_n) \leqslant (1 + be^{-\rho_{(1,n)}ct_n})\,\sigma_n \ .$$

So $D_n(ct_n)$ can be replaced by σ_n provided $\rho_{(1,n)}t_n$ tends to infinity. Since $1/2 < a_n < 1$, the third hypothesis of Theorem 3.1 is satisfied. Therefore (3.3) alone is a sufficient condition of cut-off for a sum of lines. If (k_n) grows at most polynomially in n, then (3.3) holds. But if (k_n) grows exponentially in n, then $\rho_{(1,n)}t_n$ remains bounded.

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