The Cut-Off Phenomenon in Random Walks on Association Schemes

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1 Introduction

This article is concerned with a critical phenomenon appearing in some probabilistic models. The analysis highly depends on combinatorial and algebraic structure of the models, where association schemes and their Bose-Mesner algebras play a fundamental role.

We begin with a brief description of our problem. Let X be a finite (or countable) set of cardinality $n (\leq \infty)$ and P a stochastic matrix of degree n; $P_{x,y} \geq 0$, $\sum_{y \in X} P_{x,y} = 1$. P induces a random motion on X, in which $P_{x,y}$ gives the transition probability from x to y in one unit time. This motion is called a Markov chain on X with transition (probability) matrix P. Markov chains serve as useful mathematical models to describe random affairs. The transition probability from x to y in k unit times is

$$(P^k)_{x,y} = \sum_{x_1, \cdots, x_{n-1} \in X} P_{x,x_1} \cdots P_{x_{n-1},y}$$
.

Probability distribution π on X is called an invariant probability of the Markov chain if

$$\sum_{z \in X} \pi(z) P_{z,y} = \pi(y) \quad \text{for} \quad \forall y \in X$$
(1)

holds. (1) means that π is kept invariant with respect to time evolution and hence describes an equilibrium state. It is known that, under some mild conditions, a Markov chain on a finite set has a unique invariant probability π and converges to it as time passes:

$$(P^k)_{x,y} \longrightarrow \pi(y)$$
 as $k \to \infty$ for $\forall x, y \in X$. (2)

Let us now consider shuffling of cards as a leading example. In fact, it is an original source of the problem discussed in this article. A model of shuffling n cards is given by a Markov chain on $X = S_n$ (the symmetric group of degree n) where P is determined according to a shuffling rule (riffle, overhand, top to random etc.). A reasonable shuffling rule requires that (2) holds with π being the uniform distribution on S_n (i.e. $\pi(y) = n!^{-1}$). However, (2) is not our goal but a starting point of the discussion. Actually, the central problem concerning us is "how many shuffles are necessary and sufficient to mix up the cards?"

Remarkable works due to Diaconis et al. have shown that mathematically rigorous answers can be given to these sorts of problems. Detailed quantitative analysis reveals a surprising feature of the way of convergence (2) in many interesting models including shuffling of cards. Let us measure closeness to equilibrium of a Markov chain starting at x by the quantity of

$$\|(P^k)_{x,\cdot} - \pi\| = \frac{1}{2} \sum_{y \in X} |(P^k)_{x,y} - \pi(y)| .$$
(3)

In some cases, we can observe an interesting behavior in dependence on time k of (3); namely, (3) stays almost 1 before a specific time k_c , then suddenly decreases near k_c , and finally converges to 0 exponentially fast after k_c . Such a phenomenon is called the *cut-off phenomenon* (after [1]). In shuffling of cards, we conclude that k_c shuffles are necessary and sufficient to mix up the cards. Also in a general Markov chain, k_c can be regarded as a critical time which separates the ordered and the disordered states. Although there exist many articles on the cut-off phenomena until now, we refer only to [3] and [4] here.

Including various types of shuffling of cards, most models in which the cut-off phenomenon has been investigated are formulated as random walks on homogeneous spaces induced by Gel'fand pairs of finite groups or compact Lie groups. Especially, permutation groups and matrix groups occupy a substantial part.

The purpose of this article is to give a precise description of the cut-off phenomenon and to show that we can make those models in which the cut-off phenomena occur in a somewhat systematical manner by using P- and Q-polynomial association schemes. In §2, we introduce random walks on association schemes. §3 is devoted to definition and explanation of the cut-off phenomenon. §4 is the core of this article. In a simple ramdom walk on a Pand Q-polynomial association scheme, we give a criterion for the cut-off phenomenon in terms of several quantities associated with the P- and Q-polynomial association scheme. In §5, we illustrate the cut-off phenomena in several examples by applying the result in §4.

Since this article is a brief report on a certain aspect of the cut-off phenomenon, we omit the details of proofs and processes of computation. The proof of the main result is given in [6]. See also [7]. For a substantial bibliography and more detailed information, see [3] and [4].

2 Random Walks on Association Schemes

As a preliminary discussion, let a finite group G act transitively on X from the left side. $X \times X$ is decomposed into G-orbits: $G \setminus X \times X = \{\Lambda_0, \Lambda_1, \dots, \Lambda_d\}$. Let P be a stochastic matrix of degree |X|. P induces a Markov chain on X. In general, random walks are distinguished from other Markov chains by some symmetry (or spatial homogeneity) of the transition matrix P which comes from algebraic structure of the state space X. In the case of a G-space, the symmetry of P means

$$P_{x,y} = P_{gx,gy} \qquad \text{for} \quad x, y \in X, \ g \in G ,$$
(4)

namely that $P_{x,y}$ takes a constant value on each orbit Λ_i . $(X, \{\Lambda_i\}_{i=0}^d)$ possesses structure of an association scheme. Then, (4) holds if and only if P belongs to the Bose-Mesner algebra. We are thus led to the definition of a random walk on an association scheme.

Definition 2.1 Let $\mathcal{X} = (X, \{R_i\}_{i=0}^d)$ be an association scheme, \mathcal{A} its Bose-Mesner albegra, and P a stochastic matrix of degree |X|. A Markov chain on X induced by P is called a random walk on \mathcal{X} (or simply on X) if $P \in \mathcal{A}$.

 $(P^k)_{x,y}$ is the transition probability from x to y after (discrete) time k. We can treat continuous time cases by using semigroup $(e^{t(P-I)})_{t\geq 0}$ instead of $(P^k)_{k\in\mathbb{N}}$, where we are considering an exponentially distributed pausing time at each transition. However we treat only discrete time cases in this article. See [6] and [7].

In what follows, we exclusively deal with *commutative* association schemes. For an association scheme $\mathcal{X} = (X, \{R_i\}_{i=0}^d)$, we use the following notations (which agree with the ones used in [2]).

- I = the identity matrix, J = the matrix whose entries are all 1
- $A_0 (= I), A_1, \dots, A_d$: the adjacency matrices
- $\mathcal{A} = \langle A_0, A_1, \cdots, A_d \rangle$: the Bose-Mesner algebra
- p_{ij}^h : the intersection number, $A_i A_j = \sum_{h=0}^d p_{ij}^h A_h$
- $k_i (= p_{ii'}^0)$: the valency
- $E_0 (= |X|^{-1}J), E_1, \dots, E_d$: the primitive idempotents in \mathcal{A}
- $[p_i(j)]_{j,i=0,1,\dots,d}$: the character table, $A_i = \sum_{j=0}^d p_i(j)E_j$
- m_i : the multiplicity

• q_{ij}^h : the Krein parameter, $(|X|E_i) \circ (|X|E_j) = \sum_{h=0}^d q_{ij}^h (|X|E_h)$ where \circ denotes the Hadamard product.

Under mild conditions, a random walk on \mathcal{X} approaches the equilibrium state which is now the uniform distribution on X. Hence we consider

$$D(k) = \frac{1}{2} \sum_{y \in X} \left| (P^k)_{x,y} - \frac{1}{|X|} \right| = \frac{1}{2} \sum_{y \in X} \left| (P^k - E_0)_{x,y} \right|$$

$$D(k) = \frac{1}{2|X|} \sum_{x \in X} \sum_{y \in X} |(P^k - E_0)_{x,y}|.$$
(5)

Stochastic matrix P in \mathcal{A} is expressed as a convex combination of $k_i^{-1}A_i$'s:

$$P = \sum_{i=0}^{d} \frac{w_i}{k_i} A_i , \qquad w_i \ge 0, \quad \sum_{i=0}^{d} w_i = 1 .$$
 (6)

Then, spectral decomposition of A_i 's and Schwarz' inequality yield the following estimation of D(k).

Proposition 2.2 If P is expressed as (6), we have

$$D(k)^{2} \leq \frac{1}{4} \sum_{j=1}^{d} m_{j} \Big| \sum_{i=0}^{d} w_{i} \frac{p_{i}(j)}{k_{i}} \Big|^{2k} .$$
(7)

In [5], Diaconis and Shahshahani used such an inequality on a finite group to prove the cut-off phenomenon in random transpositions and there they called it the upper bound lemma. (7) plays a decisive role also in our discussion on association schemes.

3 Cut-Off Phenomenon

Let us formulate the cut-off phenomenon after Diaconis et al. The definition given here is of a bit general form. The point is that we consider an infinite family of Markov chains and take their *infinite volume limit* in an analogous way to the thermodynamical limit.

Let $\{\mathcal{X}^{(\lambda)} = (X^{(\lambda)}, \{R_i^{(\lambda)}\}_{i=0}^{d^{(\lambda)}})|\lambda \in \Lambda\}$ be a directed family of association schemes parametrized by a directed set Λ . For each $\lambda \in \Lambda$, we consider a random walk on $\mathcal{X}^{(\lambda)}$ with transition matrix $P^{(\lambda)}$ and the quantity $D^{(\lambda)}(k)$ as (5) which describes closeness to equilibrium.

Definition 3.1 Assume that we can take $k_c^{(\lambda)} \in \mathbb{N}$ for each λ satisfying the following conditions:

(i)
$$k_c^{(\lambda)} \longrightarrow \infty \text{ as } \lambda \to \infty$$

(ii)
$$\forall \epsilon > 0, \exists \lambda_{\epsilon} \in \Lambda \text{ and } \exists h_{\epsilon}^{(\lambda)} \text{ such that } h_{\epsilon}^{(\lambda)}/k_{c}^{(\lambda)} \longrightarrow 0 \text{ as } \lambda \to \infty \text{ and, if } \lambda > \lambda_{\epsilon},$$

$$0 \le k \le k_c^{(\lambda)} - h_{\epsilon}^{(\lambda)} \implies D^{(\lambda)}(k) \ge 1 - \epsilon$$
$$k \ge k_c^{(\lambda)} + h_{\epsilon}^{(\lambda)} \implies D^{(\lambda)}(k) \le \epsilon .$$

Then we say that the cut-off phenomenon occurs for this family of random walks and call $k_c^{(\lambda)}$ the critical time (Subscript _c indicates 'critical').

Modification of the definition in a general Markov chain is obvious. We supplement an intuitive explanation. Let $\epsilon > 0$ be fixed very small and the size of the system sufficiently

large (i.e. $\lambda > \lambda_{\epsilon}$). Condition (ii) implies that $D^{(\lambda)}(k)$ stays almost 1 before $k_c^{(\lambda)} - h_{\epsilon}^{(\lambda)}$ while it becomes almost 0 after $k_c^{(\lambda)} + h_{\epsilon}^{(\lambda)}$. Although the picture is ambiguous in time interval $(k_c^{(\lambda)} - h_{\epsilon}^{(\lambda)}, k_c^{(\lambda)} + h_{\epsilon}^{(\lambda)})$, condition (i) and (ii) assure that the interval is negligible in a macroscopic scale.



Under condition (i) of Definition 3.1, let us take $h^{(\lambda)} > 0$ for each $\lambda \in \Lambda$ satisfying $h^{(\lambda)}/k_c^{(\lambda)} \longrightarrow 0$ and set $k^{(\lambda)} = k_c^{(\lambda)} + \theta h^{(\lambda)}$ for $\theta \in \mathbf{R}$. Assume that

 $D^{(\lambda)}(k^{(\lambda)}) \longrightarrow c(\theta) \quad \text{as} \quad \lambda \to \infty$

holds where $c(\theta) : (-\infty, \infty) \longrightarrow [0, 1]$ is a function such that $c(-\infty) = 1$ and $c(\infty) = 0$. Then, for $\forall \epsilon > 0$, taking $\theta_{\epsilon} > 0$ such that

$$c(heta) \left\{ egin{array}{c} \geq 1-\epsilon & ext{if } heta < - heta_\epsilon \ \leq \epsilon & ext{if } heta > heta_\epsilon \end{array}
ight.$$

and setting $h_{\epsilon}^{(\lambda)} = \theta_{\epsilon} h^{(\lambda)}$, we get the situation in Definition 3.1. Diaconis gave a definition of the cut-off phenomenon in this form in [4].

4 Main Result

In general, a random walk is said to be simple if it makes a transition in one unit time to one of the nearest vertices with equal probability. Hence a simple random walk on a symmetric association scheme has transition matrix $k_1^{-1}A_1$.

For P-polynomial association scheme $\mathcal{X} = (X, \{R_i\}_{i=0}^d)$, we use the notations in [2]:

$$k = k_1$$
 (valency), $m = m_1$ (multiplicity), $\theta_i = p_1(j)$.

Then, we have

$$-k \leq heta_d < heta_{d-1} < \cdots < heta_1 < heta_0 = k$$
 .

Let $\{\mathcal{X}^{(\lambda)}|\lambda \in \Lambda\}$ be a directed family of P- and Q-polynomial association schemes with $\mathcal{X}^{(\lambda)}$ being of class $d^{(\lambda)}$. We consider a simple random walk on each $\mathcal{X}^{(\lambda)}$ starting at a single point. Superscript $^{(\lambda)}$ indicates an associated quantity of $\mathcal{X}^{(\lambda)}$ such as $k^{(\lambda)}, m^{(\lambda)}, m^{(\lambda)}_j, \theta^{(\lambda)}_j, D^{(\lambda)}(k)$ etc. Now we can state our main result which gives a criterion for the cut-off phenomenon in simple random walks on P- and Q-polynomial association schemes.

Theorem 4.1 (1) Let us assume

$$|\theta_{d^{(\lambda)}}^{(\lambda)}| \le \theta_1^{(\lambda)} \qquad (\forall \lambda \in \Lambda)$$
(U0)

and that $\exists \alpha > 0, \ \exists \phi : \mathbf{N} \longrightarrow \mathbf{R}, \ \exists \psi : \mathbf{N} \longrightarrow \mathbf{R}_+$ (all being independent of λ) satisfying:

$$\frac{\log |\theta_j^{(\lambda)}/k^{(\lambda)}|}{\log(\theta_1^{(\lambda)}/k^{(\lambda)})} \ge \psi(j) \qquad (j = 1, \cdots, d^{(\lambda)})$$
(U1)

$$\log m^{(\lambda)} - \frac{\log(\theta_1^{(\lambda)}/k^{(\lambda)})}{\log|\theta_j^{(\lambda)}/k^{(\lambda)}|} \log m_j^{(\lambda)} \ge \phi(j) \qquad (j = 1, \cdots, d^{(\lambda)})$$
(U2)

$$\liminf_{j \to \infty} \phi(j) > \alpha \tag{U3}$$

$$\sum_{j=1}^{\infty} e^{-\alpha \psi(j)} < \infty .$$
 (U4)

Then, at time

$$k = \left[\frac{\log m^{(\lambda)} + r}{-2\log(\theta_1^{(\lambda)}/k^{(\lambda)})}\right] + 1 , \qquad r > 0$$

 $([\cdot]$ denoting the integral part of a positive number), we get

 $D^{(\lambda)}(k) \le K e^{-r/2}$

where K is a constant independent of λ and r.

(2) Let us assume

$$\theta_2^{(\lambda)} > 0 \quad (\forall \lambda \in \Lambda) \quad \text{and} \quad \{k^{(\lambda)}/\theta_1^{(\lambda)} | \lambda \in \Lambda\} \text{ is bounded above}$$
(L0)

$$m^{(\lambda)} \longrightarrow \infty \quad \text{as} \quad \lambda \to \infty$$
 (L1)

$$\frac{\log(\theta_2^{(\lambda)}/k^{(\lambda)})}{2\log(\theta_1^{(\lambda)}/k^{(\lambda)})} = 1 + \frac{o(1)}{\log m^{(\lambda)}} \quad \text{as} \quad \lambda \to \infty$$
(L2)

 $\exists \lambda_1 \in \Lambda \text{ and } \exists \rho : \Lambda \longrightarrow [1, \infty) \text{ such that}$

$$\begin{array}{ll} (q_{11}^{1(\lambda)})^2 \leq m^{(\lambda)} \rho^{(\lambda)} & \text{for } \forall \lambda > \lambda_1 \\ \log \rho^{(\lambda)} / \log m^{(\lambda)} \longrightarrow 0 & \text{as } \lambda \to \infty \end{array} .$$
 (L3)

Then, at time

$$k = \left[\frac{\log m^{(\lambda)} - \log \rho^{(\lambda)} - r}{-2\log(\theta_1^{(\lambda)}/k^{(\lambda)})}\right], \quad \log \rho^{(\lambda)} \le r \le \log m^{(\lambda)} - \log \rho^{(\lambda)},$$

we get $\forall \epsilon > 0, \exists \lambda_{\epsilon} \in \Lambda$ such that $\lambda > \lambda_{\epsilon} \Longrightarrow D^{(\lambda)}(k) \ge 1 - \epsilon$.

 (2^{\sharp}) Let us assume (L0) – (L2) and, instead of (L3),

 $\exists \beta > 0 \quad \text{and} \quad \exists \lambda_1 \in \Lambda \quad \text{such that} \quad \forall \lambda > \lambda_1, \ (q_{11}^{1(\lambda)})^2 \le \beta m^{(\lambda)} \ .$ (L3[#])

Then, at time

$$k = \left[\frac{\log m^{(\lambda)} - r}{-2\log(\theta_1^{(\lambda)}/k^{(\lambda)})}\right], \quad 0 \le r \le \log m^{(\lambda)},$$

we get $\forall \epsilon > 0, \exists r_{\epsilon} > 0 \text{ and } \exists \lambda_{\epsilon} \in \Lambda \text{ such that}$

$$\begin{array}{ccc} \lambda > \lambda_{\epsilon} & \Longrightarrow & \log m^{(\lambda)} > r_{\epsilon} \\ \lambda > \lambda_{\epsilon}, \ \log m^{(\lambda)} \ge r > r_{\epsilon} & \Longrightarrow & D^{(\lambda)}(k) \ge 1 - \epsilon \end{array}$$

Corollary The cut-off phenomenon occurs in the simple random walks on P- and Q-polynomial assocaition schemes which satisfy (U0) - (U4) and (L0) - (L3). Furthermore, if (L3) is replaced by $(L3^{\sharp})$ and a spectral gap condition

$$\exists \delta > 0 \quad \text{and} \quad \exists \lambda_0 \in \Lambda \quad \text{such that} \quad \lambda > \lambda_0 \implies 1 - \frac{\theta_1^{(\lambda)}}{k^{(\lambda)}} \geq \delta$$

holds, then the cut-off phenomenon becomes sharper in that the width $h_{\epsilon}^{(\lambda)}$ in Definition 3.1 can be taken to be bounded with respect to λ .

Although the conditions in Theorem 4.1 may be rather complicated, we should note that they can be checked if the following quantities of P- and Q-polynomial association schemes are known:

$$\begin{cases} \theta_0(=k), \theta_1, \cdots, \theta_d &: \text{ the 1st column of the character table} \\ m_0(=1), m_1, \cdots, m_d &: \text{ the multiplicities} \\ q_{11}^1 &: a \text{ Krein parameter.} \end{cases}$$
(8)

The proof of Theorem 4.1 (given in [6]) is based on harmonic analysis on association schemes. Crucial for our analysis is the fact that quantities (8) are explicitly computable by using the Askey-Wilson polynomials.

5 Examples

We mention several concrete P- and Q-polynomial association schemes on which the cut-off phenomena can be observed in simple random walks. [2] contains all the required

1. Hamming scheme H(d, n)

Let $X = F^d$ where |F| = n and $R_i = \{(x, y) \in X \times X | d(x, y) = i\}$ where $d(x, y) = |\{j|x_j \neq y_j\}|$ for $x = (x_j), y = (y_j)$. The case of n = 2 is the classical Ehrenfests' urn model. Here we allow both d and n to get unbounded. We have

$$heta_j = (n-1)d - nj, \quad m_j = (n-1)^j \binom{d}{j}, \quad q_{11}^1 = n-2 \; .$$

The cut-off phenomenon occurs in the simple random walks on H(d, n) if

$$n \ge 3$$
 and $\limsup_{(d,n)\to\infty} \frac{\log n}{\log d} \le 1$.

The critical time is asymptotically

$$k_c \sim \frac{d}{2} \left(1 - \frac{1}{n}\right) (\log n + \log d)$$

When n = 2, the simple random walk becomes periodic. Slightly modifying the transition matrix (e.g. $P = (d+1)^{-1}(A_0 + A_1)$), we can observe the cut-off phenomenon.

2. Johnson scheme J(v, d)

Let $X = \{x \subset S | |x| = d\}$ where |S| = v and $R_i = \{(x, y) \in X \times X | d(x, y) = i\}$ where $d(x, y) = d - |x \cap y|$. This is the Bernoulli-Laplace diffusion model. We can set $2d \leq v$. We have

$$\theta_j = d(v-d) - j(v-j+1), \quad m_j = \binom{v}{j} - \binom{v}{j-1},$$

$$q_{11}^1 = v \left\{ 1 - \frac{v(v-d-1)(d-1)}{(v-2)(v-d)d} \right\} - 2.$$

The cut-off phenomenon occurs in the simple random walks on J(v, d) if

$$2d \le v$$
 and $\limsup_{d \to \infty} \frac{\log v}{2\log d} \le 1$.

The critical time is asymptotically

$$k_c \sim \frac{d}{2} \left(1 - \frac{d}{v}\right) \log v \; .$$

3. Association scheme of bilinear forms

Let q be fixed as the order of finite field GF(q) and $[\cdot]_q$ denote Gauss' q-integer:

$$[l]_q = \frac{q^l - 1}{q - 1}, \quad [l]!_q = [l]_q [l - 1]_q \cdots [1]_q, \quad \begin{bmatrix} l \\ i \end{bmatrix}_q = \frac{[l]!_q}{[i]!_q [l - i]!_q}.$$

Let X be the totality of $d \times n$ matrices over GF(q) and $R_i = \{(x, y) \in X \times X | d(x, y) = i\}$ where $d(x, y) = \operatorname{rank}(x - y)$. We can set $d \leq n$. This is a kind of generalization of H(d, n). We have

$$\theta_j = (q^n - 1)[d]_q - q^{d+n-j}[j]_q, \quad m_j = (q^n - 1)(q^n - q) \cdots (q^n - q^{j-1}) \begin{bmatrix} d \\ j \end{bmatrix}_q,$$
$$q_{11}^1 = q^n + q^d - q - 2.$$

The cut-off phenomenon occurs in the simple random walks if

$$d \le n$$
 and $\lim_{d \to \infty} \frac{n}{d} = 1$.

The critical time is asymptotically $k_c \sim d$.

4. q-analogue of Johnson scheme $J_q(v, d)$

Let $X = \{x \in V | \dim x = d\}$ where V is a vector space over GF(q) with $\dim V = v$ and $R_i = \{(x, y) \in X \times X | d(x, y) = i\}$ where $d(x, y) = d - \dim(x \cap y)$. We can set $2d \leq v$. We have

$$\begin{aligned} \theta_j &= q[d]_q[v-d]_q - [j]_q[v-j+1]_q, \quad m_j = \begin{bmatrix} v \\ j \end{bmatrix}_q - \begin{bmatrix} v \\ j-1 \end{bmatrix}_q, \\ q_{11}^1 &= [v]_q \Big(1 - \frac{[v]_q[v-d-1]_q[d-1]_q}{[v-2]_q[v-d]_q[d]_q} \Big) - 2 . \end{aligned}$$

(Compare with J(v, d).) The cut-off phenomenon occurs in the simple random walks on $J_q(v, d)$ if

$$2d \le v$$
 and $\lim_{d \to \infty} \frac{v}{d} = 2$.

The critical time is asymptotically $k_c \sim d$.

5. Association scheme of quadratic forms

Let X be the totality of symmetric matrices of degree n-1 over $GF(p^f)$ where p is a prime number $\neq 2$ and $R_i = \{(x, y) \in X \times X | \operatorname{rank}(x-y) = 2i-1 \text{ or } 2i\}$ $(i = 0, 1, \dots, [n/2] = d)$. This model has special interest in that it does not come from a Gel'fand pair. Fix $q = p^{2f}$. We have

$$\theta_{j} = \frac{1}{q-1} (1 + q^{n-j-1/2} - q^{(n-1)/2} - q^{n/2})$$

$$m_{j} = q^{j(n-j-1/2)} \prod_{i=1}^{j} \frac{(1 - q^{i-1-n/2})(1 - q^{i-(n+1)/2})}{1 - q^{-i}}$$

$$q_{11}^{1} = \frac{q^{n/2}}{q-1} (q + q^{1/2} - q^{-1/2} - 1 + q^{-n/2} - q^{-(n-3)/2}) - 1$$

The cut-off phenomenon occurs in the simple random walks with critical time $k_c \sim n/2$.

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