ON THE INDEPENDENCE NUMBER OF DE BRUIJN GRAPHS

PIETRO MAJER AND MATTEO NOVAGA

Abstract. We derive the asymptotic formula $\alpha(k,q) = \lambda_{k-1}q^k + o(q^k)$, where $\alpha(k,q)$ is the independence number of the de Bruijn graph $B(k,q)$, and λ_{k-1} is a constant arising from a variational problem on the unit $(k-1)$-dimensional cube. When $k = 4$, we show the bounds $91/240 \leq \lambda_3 \leq 11/28$. For odd prime k, we analyse the binary case $q = 2$ via a phase representation on rotation orbits. For $k = 11, 13, 17$ this yields compact orbit-marker certificates for optimal constructions. Combined with a lifting theorem by Lichiardopol, these certificates give exact formulas for $\alpha(11,q)$, $\alpha(13,q)$, and $\alpha(17,q)$ for all $q \geq 2$, extending the known cases $k = 3, 5, 7$.

Contents

1. Introduction

De Bruijn graphs are a classical object in combinatorics, graph theory, and information theory. Their origin goes back to de Bruijn's paper [4], while the Eulerian perspective was developed further by van Aardenne-Ehrenfest and de Bruijn in [1]. Standard references include Fredricksen's survey [7], the necklace construction of Fredricksen and Maiorana [6], Ralston's expository article [10], the survey chapter of Du, Cao, and Hsu on de Bruijn and Kautz digraphs [3], and the recent monograph of Etzion [5].

In this paper we study the independence number of de Bruijn graphs. This problem lies at the intersection of graph theory and coding theory: independent sets in de Bruijn graphs encode collections of words that avoid prescribed overlap patterns, and in several cases they are closely related to comma-free codes. Exact formulas are known only in a limited number of lengths, while the general asymptotic behaviour for fixed word length is governed by the variational constants introduced by Trotter and Winkler [11] and further analysed by the authors in [9].

For integers $k, q \geq 2$, we denote by $B(k,q)$ the de Bruijn digraph with vertex set $[q]^k$, where

$$[q] := \{0, 1, \dots, q-1\},$$

and with directed edges

$$x_1x_2\dots x_k \longrightarrow x_2x_3\dots x_ky, \qquad y \in [q].$$

Thus, for us the first parameter is the word length and the second is the alphabet size. We notice that other conventions can be found in the literature: for instance, the underlying simple graph is denoted $UB(q,k)$ in [8], while the same graph appears as $B(q,k)$ in [2].

We denote by $\alpha(k,q)$ the independence number of the *simple* graph obtained from $B(k,q)$ after deleting self-loops. Two vertices

$$u = x_1x_2\dots x_k, \qquad v = y_1y_2\dots y_k$$

are adjacent in the underlying graph if and only if one of the overlap relations

$$x_2x_3\dots x_k = y_1y_2\dots y_{k-1} \qquad \text{or} \qquad y_2y_3\dots y_k = x_1x_2\dots x_{k-1}$$

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holds. The graph $B(k,q)$ has exactly q looped vertices, namely the constant words

$$0^k,\ 1^k,\ \ldots,\ (q-1)^k.$$

When these self-loops are retained we write $\alpha_{\mathrm{loop}}(k,q)$ for the corresponding independence number. Since only the q constant vertices are affected, one has

$$\alpha_{\mathrm{loop}}(k,q) \le \alpha(k,q) \le \alpha_{\mathrm{loop}}(k,q) + q.$$

In particular, for fixed k the looped and loopless models have the same leading asymptotic coefficient as $q \to \infty$.

The independence problem for de Bruijn graphs has both a continuum asymptotic side and a finite, explicitly certifiable side, and the two viewpoints reinforce each other.

First, we show that for every fixed $k \ge 2$ the leading term of $\alpha(k,q)$, as $q \to \infty$, is given exactly by a variational constant λ_{k-1}. More precisely, as $q \to +\infty$ one has

$$\alpha(k,q) = \lambda_{k-1} q^k + o(q^k).$$

This identifies the asymptotic independence problem on de Bruijn graphs with the variational problem studied in [11, 9].

Second, we focus on the first unresolved case, namely $k = 4$. Here the aim is not an exact formula, but a sharper understanding of the extremal coefficient. We prove explicit bounds on λ_3, combining a soft upper bound from a seven-cycle inequality with a constructive lower bound obtained from an explicit base configuration and an inductive dyadic lift.

Third, we return to exact finite constructions in the binary prime cases $k = 11$, $k = 13$, and $k = 17$. Rotation orbits show that an extremal example with one loop-vertex is determined by one phase choice on each non-trivial orbit. Compatibility between two orbits is encoded by a binary relation on the two phases; it is not, in general, a function only of their difference. The resulting finite constraint problem is computer-verifiable. We record compact orbit-marker certificates for all three cases and deduce exact formulas for the independence number for every alphabet size $q \ge 2$.

The case $k = 4$ sits between several lengths for which the independence number is already understood exactly.

Theorem 1 (see [8, 2])**.** *There holds*

$$\begin{aligned}
&\alpha(2,2) = 2, && \alpha_{\mathrm{loop}}(2,2) = 1,\\
&\alpha(2,3) = 3, && \alpha_{\mathrm{loop}}(2,3) = 2,\\
&\alpha(2,q) = \alpha_{\mathrm{loop}}(2,q) = \left\lfloor \frac{q^2}{4} \right\rfloor && \textit{for every } q \ge 4,\\
&\alpha(3,q) = \frac{q^3 - q}{3} + 1, && \alpha_{\mathrm{loop}}(3,q) = \frac{q^3 - q}{3}.\\
&\alpha(5,q) = \frac{2(q^5 - q)}{5} + 1, && \alpha_{\mathrm{loop}}(5,q) = \frac{2(q^5 - q)}{5},\\
&\alpha(7,q) = \frac{3(q^7 - q)}{7} + 1, && \alpha_{\mathrm{loop}}(7,q) = \frac{3(q^7 - q)}{7}.
\end{aligned}$$

Moreover, if $k \ge 3$ is an odd prime, then for every $q \ge 2$ we have

$$\alpha(k,q) \le \frac{(k-1)(q^k - q)}{2k} + 1, \qquad \alpha_{\mathrm{loop}}(k,q) \le \frac{(k-1)(q^k - q)}{2k}.$$

In Theorems 27, 29, and 31 below, we extend the previous result to the next prime cases $k = 11$, $k = 13$, and $k = 17$, and prove that

$$\alpha(11,q) = \frac{5(q^{11} - q)}{11} + 1, \quad \alpha_{\mathrm{loop}}(11,q) = \frac{5(q^{11} - q)}{11},$$

and

$$\alpha(13,q) = \frac{6(q^{13} - q)}{13} + 1, \quad \alpha_{\mathrm{loop}}(13,q) = \frac{6(q^{13} - q)}{13},$$

while the same method gives

$$\alpha(17,q) = \frac{8(q^{17} - q)}{17} + 1, \quad \alpha_{\mathrm{loop}}(17,q) = \frac{8(q^{17} - q)}{17}.$$

By contrast, no exact formula is presently known for $\alpha(4,q)$. This makes the length 4 case the first genuinely open instance, and one of the main motivations of the present work is to determine explicit bounds for its leading asymptotic coefficient.

For every integer $m \geq 1$ and every measurable set $A \subseteq [0,1]^m$, we now define

$$\Phi_m(A) := \int_{[0,1]^{m+1}} \mathbf{1}_A(x_1,\ldots,x_m)\big(1-\mathbf{1}_A(x_2,\ldots,x_{m+1})\big)\,dx_1\cdots dx_{m+1}, \tag{1}$$

and set

$$\lambda_m := \sup\{\Phi_m(A) : A \subseteq [0,1]^m \text{ measurable}\}. \tag{2}$$

These constants were first introduced in [11], with a different definition, and the variational characterization in (1) was later given in [9]. As stated above, these constants also govern the independence number of de Bruijn graphs for large q: for every fixed $k \geq 2$, the asymptotic coefficient of $\alpha(k,q)$ is exactly λ_{k-1}.

Trotter and Winkler showed in [11] the strict monotonicity of the sequence λ_m, and proved the bounds

$$\frac{m}{2m+2} \leq \lambda_m \leq \frac{m}{2m+1},$$

together with the identities $\lambda_1 = 1/4$, $\lambda_2 = 1/3$ and the inequality $\lambda_5 \geq 27/64$. The authors of this paper showed in [9] that

$$\lambda_m = \frac{m}{2m+2} \qquad \text{for every even } m,$$

and therefore for every odd word length k one obtains the exact asymptotic coefficient

$$\frac{\alpha(k,q)}{q^k} \longrightarrow \lambda_{k-1} = \frac{k-1}{2k}.$$

Moreover, Proposition 8 below yields a refined upper bound for odd k, while preserving the explicit lower bound coming from the elementary construction:

$$\frac{k-1}{2k}q^k - O(q^{k-2}) \leq \alpha(k,q) \leq \frac{k-1}{2k}q^k + O(q^{\delta(k)}),$$

where the parameter $\delta(k)$ is defined in Proposition 8: it equals 1 if k is prime and k/p if k is composite, with p the smallest prime divisor of k. In particular, for odd prime k the error term in the upper bound is of order $O(q)$, consistently with the exact formulas quoted above for $k = 3, 5, 7, 11, 13, 17$.

The even-length case is more delicate. Already for $k = 4$, the general bounds imply only

$$\frac{3}{8} \leq \lambda_3 < \frac{2}{5}.$$

Our second main result improves this interval to

$$\frac{91}{240} \leq \lambda_3 \leq \frac{11}{28},$$

and consequently

$$\frac{91}{240} \leq \lim_{q\to\infty} \frac{\alpha(4,q)}{q^4} = \lambda_3 \leq \frac{11}{28}.$$

Thus, although the exact value of λ_3 remains open, the admissible range becomes substantially narrower.

For the reader's convenience, we summarise the main contributions of the paper.

1) We prove that for every fixed $k \geq 2$ the independence number of the de Bruijn graph satisfies

$$\alpha(k,q) = \lambda_{k-1}q^k + o(q^k),$$

thereby identifying the exact asymptotic coefficient with the continuum variational constant λ_{k-1}.

2) In the case $k = 4$, we establish the explicit bounds

$$\frac{91}{240} \leq \lambda_3 \leq \frac{11}{28}.$$

The upper bound is obtained from a combinatorial inequality on a 7-cycle, while the lower bound comes from an inductive dyadic construction starting from an explicit finite configuration.

3) For binary words of prime length, we represent extremal sets by one phase on each non-trivial rotation orbit and formulate the exact compatibility conditions as a finite binary phase-CSP. Combined with directly verified certificates, this yields exact formulas for $\alpha(11,q)$, $\alpha(13,q)$, and $\alpha(17,q)$ for all $q \geq 2$.

The paper is organised as follows. In Section 2 we reformulate the discrete extremal problem in a way that makes the connection with the variational constants λ_m transparent, and we prove the asymptotic formula for every fixed k. Section 3 is devoted to the case $k = 4$: we first derive the upper bound for λ_3, then construct the dyadic lower bound, and finally translate these bounds into corresponding estimates for $\alpha(4,q)$. To keep the main argument readable, the large explicit $q = 16$ data defining the base configuration are recorded separately in Appendix A, where we record both the explicit data defining the base configuration and the finite verification attached to it. In Section 4 we develop the phase representation for odd prime binary lengths, formulate the exact binary compatibility relations, and use it to record the certified cases $k = 11$, $k = 13$, and $k = 17$. Appendix B records the compact certificates for $k = 11$, $k = 13$, and $k = 17$, and gives a short verifier script.

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2. The asymptotic coefficient

Fix integers $k \ge 2$ and $q \ge 1$. Independent sets in $B(k,q)$ are naturally encoded by subsets of $[q]^{k-1}$.

Definition 2. *For $S \subseteq [q]^{k-1}$, define*

$$\mathcal{I}_{k,q}(S) := \big\{(x_1,\dots,x_k) \in [q]^k : (x_1,\dots,x_{k-1}) \in S,\ (x_2,\dots,x_k) \notin S\big\}.$$

Equivalently, $\mathcal{I}_{k,q}(S)$ consists of the words of length k whose prefix of length $k-1$ belongs to S and whose suffix of length $k-1$ does not. We also set

$$N_{k,q}(S) := |\mathcal{I}_{k,q}(S)|.$$

Proposition 3. *Define*

$$M_{k,q} := \max\big\{N_{k,q}(S) : S \subseteq [q]^{k-1}\big\}.$$

Then

$$M_{k,q} = \alpha_{\mathrm{loop}}(k,q).$$

Moreover,

$$M_{k,q} \le \alpha(k,q) \le M_{k,q} + q,$$

so in particular

$$\alpha(k,q) = M_{k,q} + O(q) \qquad (k \text{ fixed},\ q \to \infty).$$

Proof. Fix $S \subseteq [q]^{k-1}$. $\mathcal{I}_{k,q}(S)$ is an independent set in the graph with loops retained. Let

$$x = (x_1,\dots,x_k) \in \mathcal{I}_{k,q}(S).$$

By definition,

$$(x_1,\dots,x_{k-1}) \in S, \qquad (x_2,\dots,x_k) \notin S.$$

Suppose that a successor

$$y = (x_2,\dots,x_k,t) \qquad (t \in [q])$$

also belonged to $\mathcal{I}_{k,q}(S)$. Then, by the defining condition for $\mathcal{I}_{k,q}(S)$, its prefix $(x_2,\dots,x_k)$ would have to lie in S, a contradiction. Thus x is adjacent to no successor in $\mathcal{I}_{k,q}(S)$. The same argument applied to predecessors shows that no predecessor of x can belong to $\mathcal{I}_{k,q}(S)$ either. Hence no two vertices of $\mathcal{I}_{k,q}(S)$ are adjacent.

A looped constant vertex cannot occur in $\mathcal{I}_{k,q}(S)$, because a word a^k would require simultaneously $a^{k-1} \in S$ and $a^{k-1} \notin S$. Therefore $\mathcal{I}_{k,q}(S)$ is independent in the looped model, and so

$$\alpha_{\mathrm{loop}}(k,q) \ge |\mathcal{I}_{k,q}(S)| = N_{k,q}(S).$$

Taking the maximum over S yields

$$\alpha_{\mathrm{loop}}(k,q) \ge M_{k,q}.$$

Conversely, let J be an independent set in the graph with loops retained. Define

$$S_J := \big\{(x_1,\dots,x_{k-1}) \in [q]^{k-1} : \exists x_k \in [q] \text{ such that } (x_1,\dots,x_k) \in J\big\}.$$

If $(x_1,\dots,x_k) \in J$, then $(x_1,\dots,x_{k-1}) \in S_J$ by construction. We have $(x_2,\dots,x_k) \notin S_J$, for otherwise there would exist $t \in [q]$ such that $(x_2,\dots,x_k,t) \in J$, and these two vertices would be adjacent, contradicting the independence of J. Therefore every vertex of J belongs to $\mathcal{I}_{k,q}(S_J)$, hence

$$|J| \le |\mathcal{I}_{k,q}(S_J)| = N_{k,q}(S_J) \le M_{k,q}.$$

Taking the maximum over all looped independent sets J gives

$$\alpha_{\mathrm{loop}}(k,q) \le M_{k,q}.$$

Combining the two inequalities proves the identity $M_{k,q} = \alpha_{\mathrm{loop}}(k,q)$.

Finally, passing from the looped graph to the simple graph only affects the q constant vertices a^k. Hence one may gain at most q additional vertices when the loops are deleted, and therefore

$$M_{k,q} = \alpha_{\mathrm{loop}}(k,q) \le \alpha(k,q) \le \alpha_{\mathrm{loop}}(k,q) + q = M_{k,q} + q.$$

□

Thus $M_{k,q}$ is the basic discrete quantity. Once its asymptotics are known, those of $\alpha(k,q)$ follow from the additive error term q.

For $\mathbf{u} = (u_1, \dots, u_{k-2}) \in [q]^{k-2}$, we define

$$I_S(\mathbf{u}) := \#\{a \in [q] : (a, u_1, \dots, u_{k-2}) \in S\},$$
$$O_S(\mathbf{u}) := \#\{b \in [q] : (u_1, \dots, u_{k-2}, b) \in S\}.$$

When $k = 2$, the index set $[q]^0$ is understood as the singleton $\{\emptyset\}$, so $I_S(\emptyset) = O_S(\emptyset) = |S|$.

A direct counting argument gives

$$N_{k,q}(S) = \sum_{\mathbf{u} \in [q]^{k-2}} I_S(\mathbf{u})\big(q - O_S(\mathbf{u})\big). \tag{3}$$

Indeed, for each fixed middle block $\mathbf{u}$, a word counted by $N_{k,q}(S)$ is obtained by choosing a prefix letter a such that $(a, \mathbf{u}) \in S$ and a suffix letter b such that $(\mathbf{u}, b) \notin S$.

For $S \subseteq [q]^{k-1}$ and $(a_1, \dots, a_{k-1}) \in [q]^{k-1}$ we let

$$Q^{(q)}_{a_1 \dots a_{k-1}} := \prod_{j=1}^{k-1} \Big[\frac{a_j}{q}, \frac{a_j + 1}{q}\Big) \subseteq [0,1]^{k-1},$$

and

$$A_S := \bigcup_{(a_1, \dots, a_{k-1}) \in S} Q^{(q)}_{a_1 \dots a_{k-1}} \subseteq [0,1]^{k-1}.$$

Similarly, for $(a_1, \dots, a_k) \in [q]^k$ let

$$Q^{(q)}_{a_1 \dots a_k} := \prod_{j=1}^{k} \Big[\frac{a_j}{q}, \frac{a_j + 1}{q}\Big) \subseteq [0,1]^{k}.$$

Lemma 4. *For every $S \subseteq [q]^{k-1}$ one has*

$$\Phi_{k-1}(A_S) = \Lambda_{k,q}(S) := \frac{N_{k,q}(S)}{q^k}.$$

Proof. Partition $[0,1]^k$ into the q^k cubes $Q^{(q)}_{a_1 \dots a_k}$. On such a cube the integrand in (1), with $m = k-1$, is constant and equals

$$\mathbf{1}_S(a_1, \dots, a_{k-1})\big(1 - \mathbf{1}_S(a_2, \dots, a_k)\big).$$

Since each cube has volume q^{-k}, summing over all cubes gives

$$\Phi_{k-1}(A_S) = q^{-k} \sum_{(a_1, \dots, a_k) \in [q]^k} \mathbf{1}_S(a_1, \dots, a_{k-1})\big(1 - \mathbf{1}_S(a_2, \dots, a_k)\big) = \frac{N_{k,q}(S)}{q^k}.$$

□

Lemma 5. *For all measurable sets $A, B \subseteq [0,1]^{k-1}$,*

$$|\Phi_{k-1}(A) - \Phi_{k-1}(B)| \le 2\,\|\mathbf{1}_A - \mathbf{1}_B\|_{L^1([0,1]^{k-1})} = 2|A \triangle B|.$$

Proof. Write

$$\begin{aligned}
\Phi_{k-1}(A) - \Phi_{k-1}(B) &= \int_{[0,1]^k} \Big(\mathbf{1}_A(x_1, \dots, x_{k-1})(1 - \mathbf{1}_A(x_2, \dots, x_k)) \\
&\qquad - \mathbf{1}_B(x_1, \dots, x_{k-1})(1 - \mathbf{1}_B(x_2, \dots, x_k))\Big)\, dx_1 \cdots dx_k \\
&= \int_{[0,1]^k} \big(\mathbf{1}_A(x_1, \dots, x_{k-1}) - \mathbf{1}_B(x_1, \dots, x_{k-1})\big)\big(1 - \mathbf{1}_A(x_2, \dots, x_k)\big)\, dx \\
&\quad + \int_{[0,1]^k} \mathbf{1}_B(x_1, \dots, x_{k-1})\big(\mathbf{1}_B(x_2, \dots, x_k) - \mathbf{1}_A(x_2, \dots, x_k)\big)\, dx.
\end{aligned}$$

Taking absolute values and using $0 \le \mathbf{1}_A, \mathbf{1}_B \le 1$ gives

$$\begin{aligned}
|\Phi_{k-1}(A) - \Phi_{k-1}(B)| &\le \int_{[0,1]^k} \big|\mathbf{1}_A(x_1, \dots, x_{k-1}) - \mathbf{1}_B(x_1, \dots, x_{k-1})\big|\, dx \\
&\quad + \int_{[0,1]^k} \big|\mathbf{1}_A(x_2, \dots, x_k) - \mathbf{1}_B(x_2, \dots, x_k)\big|\, dx.
\end{aligned}$$

In each integral one variable is free over an interval of length 1, so both terms equal $\|\mathbf{1}_A - \mathbf{1}_B\|_{L^1([0,1]^{k-1})}$. This completes the proof. $\square$

Lemma 6. *For every measurable set $A \subseteq [0,1]^{k-1}$ there exist sets $A_q \subseteq [0,1]^{k-1}$, each of which is a union of q-adic cubes $Q^{(q)}_{a_1\dots a_{k-1}}$, such that*

$$|A_q \triangle A| \longrightarrow 0 \qquad \text{as } q \to \infty.$$

Proof. Let $\mathcal{G}_q$ be the finite sigma-algebra generated by the q-adic partition and put

$$u_q := \mathbb{E}(\mathbf{1}_A \mid \mathcal{G}_q).$$

We first show that $u_q \to \mathbf{1}_A$ in L^1. Given $\varepsilon > 0$, choose $\psi \in C([0,1]^{k-1})$ with $\|\mathbf{1}_A - \psi\|_{L^1} < \varepsilon$. Since conditional expectation is an L^1-contraction,

$$\|u_q - \mathbf{1}_A\|_{L^1} \le 2\varepsilon + \|\mathbb{E}(\psi \mid \mathcal{G}_q) - \psi\|_{L^1}.$$

The last term tends to zero because ψ is uniformly continuous and the diameters of the q-adic cubes tend to zero. Hence $u_q \to \mathbf{1}_A$ in L^1.

For $t \in [0,1]$ let $E_q(t) := \{u_q > t\}$. Each $E_q(t)$ is a union of q-adic cubes, and the layer-cake identity gives

$$\int_0^1 |E_q(t) \triangle A| \, dt = \|u_q - \mathbf{1}_A\|_{L^1}.$$

Choose t_q so that $|E_q(t_q) \triangle A| \le \|u_q - \mathbf{1}_A\|_{L^1}$ and set $A_q := E_q(t_q)$. Then $|A_q \triangle A| \to 0$. $\square$

Theorem 7. *For every fixed $k \ge 2$,*

$$\lim_{q\to\infty} \frac{M_{k,q}}{q^k} = \lambda_{k-1}.$$

Consequently,

$$\alpha(k,q) = \lambda_{k-1} q^k + o(q^k).$$

The same asymptotic formula also holds for $\alpha_{\mathrm{loop}}(k,q)$.

Proof. Fix q and let $S \subseteq [q]^{k-1}$. By Lemma 4,

$$\Phi_{k-1}(A_S) = \frac{N_{k,q}(S)}{q^k}.$$

Since λ_{k-1} is the supremum of Φ_{k-1} over all measurable sets, this gives

$$\frac{M_{k,q}}{q^k} \le \lambda_{k-1} \qquad \text{for every } q,$$

and hence

$$\limsup_{q\to\infty} \frac{M_{k,q}}{q^k} \le \lambda_{k-1}.$$

Conversely, let $\varepsilon > 0$. Choose a measurable set $A \subseteq [0,1]^{k-1}$ such that

$$\Phi_{k-1}(A) > \lambda_{k-1} - \varepsilon.$$

By Lemma 6, choose q-adic sets A_q such that $|A_q \triangle A| \to 0$. Lemma 5 then implies that

$$\Phi_{k-1}(A_q) \to \Phi_{k-1}(A).$$

Each A_q is of the form A_{S_q} for some $S_q \subseteq [q]^{k-1}$, and therefore

$$\frac{M_{k,q}}{q^k} \ge \frac{N_{k,q}(S_q)}{q^k} = \Phi_{k-1}(A_q).$$

For all sufficiently large q,

$$\frac{M_{k,q}}{q^k} \ge \Phi_{k-1}(A_q) > \Phi_{k-1}(A) - \varepsilon > \lambda_{k-1} - 2\varepsilon.$$

Thus

$$\liminf_{q\to\infty} \frac{M_{k,q}}{q^k} \ge \lambda_{k-1} - 2\varepsilon.$$

Since $\varepsilon > 0$ is arbitrary, we conclude that

$$\liminf_{q\to\infty} \frac{M_{k,q}}{q^k} \ge \lambda_{k-1}.$$

Combining this with the limsup bound proves

$$\lim_{q\to\infty}\frac{M_{k,q}}{q^k}=\lambda_{k-1}.$$

Finally, Proposition 3 gives

$$0\le \alpha(k,q)-M_{k,q}\le q,$$

so dividing by q^k and using $M_{k,q}/q^k\to\lambda_{k-1}$ yields

$$\frac{\alpha(k,q)}{q^k}\to\lambda_{k-1}.$$

Since $M_{k,q}=\alpha_{\mathrm{loop}}(k,q)$, the same limit holds directly for $\alpha_{\mathrm{loop}}(k,q)$. This proves the stated asymptotic formulas. □

Proposition 8. *Assume that k is odd and define*

$$\delta(k):=\begin{cases}1, & \text{if } k \text{ is prime},\\ \dfrac{k}{p}, & \text{if } k \text{ is composite, where } p \text{ is the smallest prime divisor of } k.\end{cases}$$

Equivalently, for composite k, the quantity $\delta(k)$ is the largest proper divisor of k.

For each divisor $s\mid k$, let

$$\eta_s(q):=\frac{1}{s}\sum_{d\mid s}\mu(d)\,q^{s/d},$$

the number of cyclic rotation orbits in $[q]^k$ of size s. Then

$$M_{k,q}\le U_k(q):=\frac{1}{2}\sum_{s\mid k}(s-1)\eta_s(q),$$

and therefore

$$M_{k,q}\le\frac{k-1}{2k}q^k+O(q^{\delta(k)}).$$

Moreover,

$$M_{k,q}\ge\frac{k-1}{2k}q^k-O(q^{k-2}).$$

Consequently,

$$\frac{k-1}{2k}q^k-O(q^{k-2})\le M_{k,q}\le\frac{k-1}{2k}q^k+O(q^{\delta(k)}),$$

and, by Proposition 3,

$$\frac{k-1}{2k}q^k-O(q^{k-2})\le \alpha(k,q)\le\frac{k-1}{2k}q^k+O(q^{\delta(k)}).$$

In particular, if k is odd prime, then

$$M_{k,q}\le\frac{k-1}{2k}(q^k-q),\qquad \alpha(k,q)\le\frac{k-1}{2k}q^k+O(q).$$

Proof. We first prove the upper bound for $M_{k,q}=\alpha_{\mathrm{loop}}(k,q)$.

Let $\sigma:[q]^k\to[q]^k$ be the cyclic shift

$$\sigma(x_1,\dots,x_k):=(x_2,\dots,x_k,x_1).$$

For $x\in[q]^k$, let

$$\mathcal{O}(x):=\{x,\sigma x,\dots,\sigma^{s-1}x\},\qquad s:=|\mathcal{O}(x)|.$$

Since $\sigma^k=\mathrm{id}$, every orbit size s divides k. The graph induced by $\mathcal{O}(x)$ contains the cyclic edges

$$x\to\sigma x\to\cdots\to\sigma^{s-1}x\to x.$$

If $s=1$, the unique vertex is looped and contributes nothing to a looped independent set. If $s>1$, then s is odd because $s\mid k$, and every independent set in the induced graph is in particular independent in this odd cycle. It therefore contains at most

$$\left\lfloor\frac{s}{2}\right\rfloor=\frac{s-1}{2}$$

vertices. No assertion that the orbit induces only these cyclic edges is needed here.

Therefore every looped independent set $J \subseteq [q]^k$ satisfies

$$|J| \le \sum_{s|k} \frac{s-1}{2}\, \eta_s(q) = U_k(q),$$

where $\eta_s(q)$ denotes the number of σ-orbits of size s. Taking the maximum over all looped independent sets gives

$$M_{k,q} \le U_k(q).$$

It remains to identify $\eta_s(q)$. A σ-orbit of size s is the same thing as a word of length k whose minimal period is s, modulo cyclic rotation. Such a word is obtained by repeating k/s times a primitive word of length s. The number of primitive words of length s is

$$\sum_{d|s} \mu(d)\, q^{s/d},$$

and dividing by s gives

$$\eta_s(q) = \frac{1}{s} \sum_{d|s} \mu(d)\, q^{s/d}.$$

Now isolate the contribution of $s = k$:

$$U_k(q) = \frac{k-1}{2}\eta_k(q) + \frac{1}{2} \sum_{\substack{s|k \\ s<k}} (s-1)\eta_s(q).$$

Since

$$\eta_k(q) = \frac{1}{k} \sum_{d|k} \mu(d)\, q^{k/d} = \frac{1}{k} q^k + O(q^{\delta(k)}),$$

and every proper divisor $s < k$ satisfies $s \le \delta(k)$, we obtain

$$U_k(q) = \frac{k-1}{2k} q^k + O(q^{\delta(k)}).$$

This proves

$$M_{k,q} \le \frac{k-1}{2k} q^k + O(q^{\delta(k)}).$$

For the lower bound, define

$$S^{\mathrm{ev}}_{k,q} \subseteq [q]^{k-1}$$

be the set of $(u_1, \dots, u_{k-1})$ such that the first occurrence of the maximum value among $u_1, \dots, u_{k-1}$ is in an even position. We claim that a word

$$x = (x_1, \dots, x_k) \in [q]^k$$

belongs to $\mathcal{I}_{k,q}(S^{\mathrm{ev}}_{k,q})$ if and only if the first occurrence of the maximum value among $x_1, \dots, x_k$ is in an even position $t \in \{2, 4, \dots, k-1\}$.

Indeed, if the first global maximum occurs at such a position t, then in the prefix $(x_1, \dots, x_{k-1})$ the first occurrence of the maximum is also at position t, whereas in the suffix $(x_2, \dots, x_k)$ it occurs at position $t-1$; hence the prefix lies in $S^{\mathrm{ev}}_{k,q}$ and the suffix does not. Conversely, if $x \in \mathcal{I}_{k,q}(S^{\mathrm{ev}}_{k,q})$, then the first occurrence of the maximum in the prefix is even and in the suffix is odd, so the first global maximum cannot occur at position 1 or k and must therefore occur at an even position $t \in \{2, 4, \dots, k-1\}$.

Fix such an even position t and let $M \in \{0, \dots, q-1\}$ be the maximum value. Then the first $t-1$ coordinates may be chosen arbitrarily in $\{0, \dots, M-1\}$, the coordinate x_t must equal M, and the remaining $k-t$ coordinates may be chosen arbitrarily in $\{0, \dots, M\}$. Hence the number of such words is

$$M^{t-1}(M+1)^{k-t}.$$

Summing over all admissible t and M yields

$$N_{k,q}(S^{\mathrm{ev}}_{k,q}) = \sum_{\substack{2 \le t \le k-1 \\ t \text{ even}}} \sum_{M=0}^{q-1} M^{t-1}(M+1)^{k-t}.$$

Expanding each summand,

$$M^{t-1}(M+1)^{k-t} = M^{k-1} + (k-t)M^{k-2} + O(M^{k-3}),$$

where the implied constant depends only on k. Since there are $(k-1)/2$ admissible values of t, and

$$\sum_{\substack{2\le t\le k-1\\ t \text{ even}}}(k-t)=\sum_{j=1}^{(k-1)/2}(k-2j)=\frac{(k-1)^2}{4},$$

we get

$$N_{k,q}(S^{\mathrm{ev}}_{k,q})=\frac{k-1}{2}\sum_{M=0}^{q-1}M^{k-1}+\frac{(k-1)^2}{4}\sum_{M=0}^{q-1}M^{k-2}+O(q^{k-2}).$$

By Faulhaber's formula,

$$\sum_{M=0}^{q-1}M^{k-1}=\frac{q^k}{k}-\frac{1}{2}q^{k-1}+O(q^{k-2}),\qquad \sum_{M=0}^{q-1}M^{k-2}=\frac{q^{k-1}}{k-1}-\frac{1}{2}q^{k-2}+O(q^{k-3}).$$

Substituting these expansions gives

$$N_{k,q}(S^{\mathrm{ev}}_{k,q})=\frac{k-1}{2k}q^k+\left(-\frac{k-1}{4}+\frac{k-1}{4}\right)q^{k-1}+O(q^{k-2})=\frac{k-1}{2k}q^k+O(q^{k-2}).$$

Therefore

$$M_{k,q}\ge N_{k,q}(S^{\mathrm{ev}}_{k,q})=\frac{k-1}{2k}q^k-O(q^{k-2}).$$

Finally, Proposition 3 yields

$$M_{k,q}\le\alpha(k,q)\le M_{k,q}+q.$$

Since $\delta(k)\ge 1$, the upper bound for $M_{k,q}$ implies

$$\alpha(k,q)\le\frac{k-1}{2k}q^k+O(q^{\delta(k)}),$$

and the lower bound for $M_{k,q}$ gives

$$\alpha(k,q)\ge\frac{k-1}{2k}q^k-O(q^{k-2}).$$

This completes the proof. □

3. Asymptotic bounds for $k=4$

For the rest of this section we fix $k=4$. Accordingly, for every integer $q\ge 1$ and every set $S\subseteq[q]^3$ we write

$$N_q(S):=N_{4,q}(S),\qquad \Lambda_q(S):=\Lambda_{4,q}(S),\qquad \Phi:=\Phi_3.$$

Our goal is to prove explicit upper and lower bounds for λ_3, and hence for the asymptotic independence ratio of $B(4,q)$.

3.1. **Upper bound via a seven-cycle inequality.**

The upper bound in this section is independent of the dyadic construction and works simultaneously in the discrete and continuum settings.

For a finite set $S\subseteq[q]^3$ write

$$\rho_q(S):=\frac{|S|}{q^3}.$$

Lemma 9. *For every binary 7-tuple $y=(y_i)_{i\in\mathbb{Z}/7\mathbb{Z}}\in\{0,1\}^{\mathbb{Z}/7\mathbb{Z}}$ one has*

$$\sum_{i\in\mathbb{Z}/7\mathbb{Z}}y_i\bigl(1-y_{i+1}\bigr)\le 1+\sum_{i\in\mathbb{Z}/7\mathbb{Z}}y_i\bigl(1-y_{i+3}\bigr).$$

Proof. Let

$$B:=\{i\in\mathbb{Z}/7\mathbb{Z}:y_i=1\}.$$

For $s\in\{1,3\}$ define

$$R_s(B):=\#\{i\in B:i+s\notin B\}.$$

Then the stated inequality is exactly

$$R_1(B)\le R_3(B)+1.$$

For every $s\in\{1,3\}$ we have $R_s(B)=R_s(B^c)$: indeed, for the permutation $i\mapsto i+s$ of $\mathbb{Z}/7\mathbb{Z}$, the number of transitions $1\to 0$ equals the number of transitions $0\to 1$. Hence we may replace B by its complement and assume

$$|B|\le 3.$$

If $B = \varnothing$, then $R_1(B) = R_3(B) = 0$ and there is nothing to prove. Assume now that $B \neq \varnothing$. Since $i \mapsto i + 3$ is a single 7-cycle, some element of B must exit B under the step $+3$, so $R_3(B) \geq 1$. Therefore the claim is immediate whenever $R_1(B) \leq 2$. It remains only to consider the case

$$R_1(B) = 3.$$

Because $|B| \leq 3$, this forces $|B| = 3$, and the three elements of B are pairwise nonadjacent in the usual cycle on $\mathbb{Z}/7\mathbb{Z}$.

Assume for contradiction that $R_3(B) = 1$. Along the cyclic order generated by repeated addition of 3, the indicator of B changes from 1 to 0 exactly once, so B must be a single contiguous block in that $+3$-cycle. Since $|B| = 3$, there exists $t \in \mathbb{Z}/7\mathbb{Z}$ such that

$$B = \{t, t+3, t+6\}.$$

But t and $t + 6 = t - 1$ are adjacent in the usual cycle, contradicting $R_1(B) = 3$. Hence $R_3(B) \geq 2$, and therefore

$$R_1(B) = 3 \leq 2 + 1 \leq R_3(B) + 1.$$

This completes the proof. $\square$

Proposition 10. *For every integer $q \geq 1$ and every set $S \subseteq [q]^3$,*

$$\Lambda_q(S) \leq \rho_q(S)\big(1 - \rho_q(S)\big) + \frac{1}{7} \leq \frac{11}{28}.$$

Equivalently,

$$N_q(S) \leq \left(\frac{11}{28}\right) q^4.$$

Proof. For each $i \in \mathbb{Z}/7\mathbb{Z}$, define

$$C_i := \big\{x = (x_0, \ldots, x_6) \in [q]^7 : (x_i, x_{i+1}, x_{i+2}) \in S\big\},$$

with indices read modulo 7. For a fixed $x \in [q]^7$, set

$$y_i := \mathbf{1}_{C_i}(x) \in \{0, 1\}.$$

Applying Lemma 9 to the binary 7-tuple $(y_i)_{i \in \mathbb{Z}/7\mathbb{Z}}$ gives

$$\sum_{i \in \mathbb{Z}/7\mathbb{Z}} y_i(1 - y_{i+1}) \leq 1 + \sum_{i \in \mathbb{Z}/7\mathbb{Z}} y_i(1 - y_{i+3}).$$

Since this inequality holds pointwise for every $x \in [q]^7$, summing over all x yields

$$\sum_{i \in \mathbb{Z}/7\mathbb{Z}} |C_i \setminus C_{i+1}| \leq q^7 + \sum_{i \in \mathbb{Z}/7\mathbb{Z}} |C_i \setminus C_{i+3}|. \tag{4}$$

We evaluate the two sides of (4). By cyclic symmetry, the cardinalities do not depend on i.

For $C_i \setminus C_{i+1}$, the condition $x \in C_i \setminus C_{i+1}$ is equivalent to

$$(x_i, x_{i+1}, x_{i+2}) \in S, \qquad (x_{i+1}, x_{i+2}, x_{i+3}) \notin S,$$

while the remaining three coordinates are arbitrary. Therefore

$$|C_i \setminus C_{i+1}| = q^3 N_q(S) = q^7 \Lambda_q(S).$$

Hence the left-hand side of (4) is $7q^7 \Lambda_q(S)$.

For $C_i \setminus C_{i+3}$, the condition $x \in C_i \setminus C_{i+3}$ is equivalent to

$$(x_i, x_{i+1}, x_{i+2}) \in S, \qquad (x_{i+3}, x_{i+4}, x_{i+5}) \notin S,$$

with x_{i+6} arbitrary. Here the two displayed constraints involve disjoint coordinate triples, namely (x_i, x_{i+1}, x_{i+2}) and $(x_{i+3}, x_{i+4}, x_{i+5})$, while x_{i+6} is free. Thus

$$|C_i \setminus C_{i+3}| = |S| \, (q^3 - |S|) \, q = \rho_q(S)\big(1 - \rho_q(S)\big) q^7.$$

Hence the right-hand side of (4) is

$$q^7 + 7\rho_q(S)\big(1 - \rho_q(S)\big) q^7.$$

Substituting into (4) and dividing by $7q^7$, we obtain

$$\Lambda_q(S) \leq \rho_q(S)\big(1 - \rho_q(S)\big) + \frac{1}{7}.$$

Since $\rho_q(S)(1-\rho_q(S)) \le 1/4$, it follows that

$$\Lambda_q(S) \le \frac{1}{4} + \frac{1}{7} = \frac{11}{28}.$$

Multiplying by q^4 gives the equivalent bound for $N_q(S)$. □

Corollary 11. *One has*

$$\lambda_3 \le \frac{11}{28}.$$

Proof. This is the measure-theoretic analogue of Proposition 10. Let $A \subseteq [0,1]^3$ be measurable, and write $|A| := \mathcal{L}^3(A)$. For each $i \in \mathbb{Z}/7\mathbb{Z}$, define

$$C_i := \{x = (x_0, \dots, x_6) \in [0,1]^7 : (x_i, x_{i+1}, x_{i+2}) \in A\},$$

with indices read modulo 7. For a fixed $x \in [0,1]^7$, set

$$y_i := \mathbf{1}_{C_i}(x) \in \{0,1\}.$$

Applying Lemma 9 to the binary 7-tuple $(y_i)_{i\in\mathbb{Z}/7\mathbb{Z}}$ gives

$$\sum_{i\in\mathbb{Z}/7\mathbb{Z}} y_i(1-y_{i+1}) \le 1 + \sum_{i\in\mathbb{Z}/7\mathbb{Z}} y_i(1-y_{i+3}).$$

Integrating over $[0,1]^7$ yields

$$\sum_{i\in\mathbb{Z}/7\mathbb{Z}} \mathcal{L}^7(C_i \setminus C_{i+1}) \le 1 + \sum_{i\in\mathbb{Z}/7\mathbb{Z}} \mathcal{L}^7(C_i \setminus C_{i+3}). \tag{5}$$

Again, by cyclic symmetry the measures do not depend on i. For $C_i \setminus C_{i+1}$,

$$\mathcal{L}^7(C_i \setminus C_{i+1}) = \int_{[0,1]^7} \mathbf{1}_A(x_i, x_{i+1}, x_{i+2})\big(1 - \mathbf{1}_A(x_{i+1}, x_{i+2}, x_{i+3})\big)\, dx.$$

The integrand depends only on the four coordinates $(x_i, x_{i+1}, x_{i+2}, x_{i+3})$; after integrating out the remaining three free variables and relabelling $(u, v, w, z) = (x_i, x_{i+1}, x_{i+2}, x_{i+3})$, we obtain

$$\mathcal{L}^7(C_i \setminus C_{i+1}) = \int_{[0,1]^4} \mathbf{1}_A(u,v,w)\big(1 - \mathbf{1}_A(v,w,z)\big)\, du dv dw dz = \Phi(A).$$

Hence the left-hand side of (5) is $7\Phi(A)$.

For $C_i \setminus C_{i+3}$,

$$\mathcal{L}^7(C_i \setminus C_{i+3}) = \int_{[0,1]^7} \mathbf{1}_A(x_i, x_{i+1}, x_{i+2})\big(1 - \mathbf{1}_A(x_{i+3}, x_{i+4}, x_{i+5})\big)\, dx.$$

The two factors depend on disjoint triples of coordinates, while x_{i+6} is free. By Fubini,

$$\mathcal{L}^7(C_i \setminus C_{i+3}) = \left(\int_{[0,1]^3} \mathbf{1}_A\right)\left(\int_{[0,1]^3} (1 - \mathbf{1}_A)\right) = |A|(1-|A|).$$

Therefore the right-hand side of (5) is

$$1 + 7|A|(1-|A|).$$

Substituting into (5), we find

$$\Phi(A) \le |A|(1-|A|) + \frac{1}{7} \le \frac{1}{4} + \frac{1}{7} = \frac{11}{28}.$$

Taking the supremum over measurable $A \subseteq [0,1]^3$ proves the claim. □

3.2. **Lower bound via a seven-site gadget.** We now construct an explicit dyadic family of sets that yields the lower bound $\lambda_3 \ge 91/240$.

Given $S \subseteq [q]^3$, its *dyadic lift* $L_q(S) \subseteq [2q]^3$ is defined by

$$(r, s, t) \in L_q(S) \iff \big(\lfloor r/2 \rfloor, \lfloor s/2 \rfloor, \lfloor t/2 \rfloor\big) \in S.$$

Lemma 12. *For every $q \ge 1$ and every $S \subseteq [q]^3$,*

$$N_{2q}(L_q(S)) = 16\, N_q(S).$$

Proof. A quadruple $(\alpha, \beta, \gamma, \delta) \in [q]^4$ contributes to $N_q(S)$ if and only if

$$(\alpha, \beta, \gamma) \in S, \qquad (\beta, \gamma, \delta) \notin S.$$

A quadruple $(r, s, t, u) \in [2q]^4$ contributes to $N_{2q}(L_q(S))$ if and only if its floor image

$$(\lfloor r/2 \rfloor, \lfloor s/2 \rfloor, \lfloor t/2 \rfloor, \lfloor u/2 \rfloor)$$

contributes to $N_q(S)$; membership and non-membership are preserved under the floor map by definition of the lift. Each contributing quadruple in $[q]^4$ has exactly $2^4 = 16$ lifts to $[2q]^4$. Hence

$$N_{2q}(L_q(S)) = 16\, N_q(S).$$

□

The next ingredient is a local seven-site modification that increases the count by exactly one while preserving the local hypothesis needed for iteration.

Let $a, b \in [q]$ with $a \neq b$. We say that $H_q(a, b; S)$ holds if

(i) $(a, a, a) \in S, \quad (b, b, a) \in S, \quad (b, a, a) \notin S, \quad (b, b, b) \notin S,$
(ii) $I_S(a, a) + O_S(a, a) = q,$
(iii) $I_S(b, b) + O_S(b, b) = q,$
(iv) $I_S(b, b) + O_S(b, a) = q - 1,$
(v) $I_S(b, a) + O_S(a, a) = q + 1.$

Assume now that $H_q(a, b; S)$ holds, and set $X := L_q(S) \subseteq [2q]^3$. We define seven distinguished sites in $[2q]^3$:

$$\begin{aligned} \text{Additions:} \quad & P_1 = (2b, 2b, 2b+1), \quad P_2 = (2b+1, 2b, 2b+1), \quad P_3 = (2b+1, 2a+1, 2a), \\ \text{Removals:} \quad & M_1 = (2a+1, 2a, 2a), \quad M_2 = (2a+1, 2a, 2a+1), \\ & M_3 = (2b, 2b+1, 2a), \quad M_4 = (2b, 2b+1, 2a+1). \end{aligned}$$

All seven sites are pairwise distinct because $a \neq b$. Moreover, the membership part of $H_q(a, b; S)$ implies that

– the microcell above (b, b, b) is absent from X, so $P_1, P_2 \notin X$;
– the microcell above (b, a, a) is absent from X, so $P_3 \notin X$;
– the microcell above (a, a, a) is present in X, so $M_1, M_2 \in X$;
– the microcell above (b, b, a) is present in X, so $M_3, M_4 \in X$;

hence the operation is

$$T := \big(X \cup \{P_1, P_2, P_3\}\big) \setminus \{M_1, M_2, M_3, M_4\}.$$

Lemma 13. *Under the assumptions above, we have*

$$N_{2q}(T) = 16\, N_q(S) + 1.$$

Proof. By Lemma 12,

$$N_{2q}(X) = 16 N_q(S).$$

We compute the increment

$$\Delta N := N_{2q}(T) - N_{2q}(X)$$

using the degree formula (3). For $(u, v) \in [2q]^2$, set

$$\Delta I(u, v) := I_T(u, v) - I_X(u, v), \qquad \Delta O(u, v) := O_T(u, v) - O_X(u, v).$$

Expanding

$$(I_X + \Delta I)\big(2q - (O_X + \Delta O)\big) - I_X(2q - O_X)$$

inside the sum (3) gives

$$\Delta N = \sum_{u,v} \Big[\Delta I(u, v)\big(2q - O_X(u, v)\big) - I_X(u, v)\Delta O(u, v) - \Delta I(u, v)\Delta O(u, v)\Big].$$

Only finitely many ordered pairs (u, v) are affected. For each such pair we also record its coarse image $(\lfloor u/2 \rfloor, \lfloor v/2 \rfloor)$. Since $X = L_q(S)$, we have

$$I_X(u, v) = 2 I_S(\lfloor u/2 \rfloor, \lfloor v/2 \rfloor), \qquad O_X(u, v) = 2 O_S(\lfloor u/2 \rfloor, \lfloor v/2 \rfloor).$$

We first localise the effect of the seven toggled triples on the ordered pairs (u, v), and then rewrite the increment ΔN through a small collection of scalar balance quantities. A direct inspection yields the following variation table:

(u, v)	$(\lfloor u/2 \rfloor, \lfloor v/2 \rfloor)$	ΔO	ΔI
$(2b, 2b)$	(b, b)	$+1$	0
$(2b+1, 2b)$	(b, b)	$+1$	0
$(2b+1, 2a+1)$	(b, a)	$+1$	-1
$(2a+1, 2a)$	(a, a)	-2	$+1$
$(2a, 2a)$	(a, a)	0	-1
$(2a, 2a+1)$	(a, a)	0	-1
$(2b, 2b+1)$	(b, b)	-2	$+2$
$(2b+1, 2a)$	(b, a)	0	-1

No other ordered pair is affected, hence every other pair contributes 0.

For brevity write

$$I_{aa} := I_S(a, a), \quad O_{aa} := O_S(a, a), \quad I_{bb} := I_S(b, b),$$
$$O_{bb} := O_S(b, b), \quad I_{ba} := I_S(b, a), \quad O_{ba} := O_S(b, a).$$

Using the table, the eight non-zero contributions to ΔN are:

$$\begin{aligned}
(2b, 2b) &: \quad -2I_{bb}, \\
(2b+1, 2b) &: \quad -2I_{bb}, \\
(2b+1, 2a+1) &: \quad -2q + 2O_{ba} - 2I_{ba} + 1, \\
(2a+1, 2a) &: \quad 2q - 2O_{aa} + 4I_{aa} + 2, \\
(2a, 2a) &: \quad -2q + 2O_{aa}, \\
(2a, 2a+1) &: \quad -2q + 2O_{aa}, \\
(2b, 2b+1) &: \quad 4q - 4O_{bb} + 4I_{bb} + 4, \\
(2b+1, 2a) &: \quad -2q + 2O_{ba}.
\end{aligned}$$

Summing them gives

$$\Delta N = -2I_{ba} + 4I_{aa} + 2O_{aa} + 4O_{ba} - 4O_{bb} - 2q + 7.$$

Now invoke the four degree relations contained in $H_q(a, b; S)$:

$$I_{aa} + O_{aa} = q, \qquad I_{bb} + O_{bb} = q, \qquad I_{bb} + O_{ba} = q - 1, \qquad I_{ba} + O_{aa} = q + 1.$$

From these we obtain

$$O_{aa} = q + 1 - I_{ba}, \qquad I_{aa} = I_{ba} - 1, \qquad O_{ba} = q - 1 - I_{bb}, \qquad O_{bb} = q - I_{bb}.$$

Substituting into the formula for ΔN,

$$\begin{aligned}
\Delta N &= -2I_{ba} + 4(I_{ba} - 1) + 2(q + 1 - I_{ba}) + 4(q - 1 - I_{bb}) - 4(q - I_{bb}) - 2q + 7 \\
&= 1.
\end{aligned}$$

Therefore

$$N_{2q}(T) = N_{2q}(X) + 1 = 16N_q(S) + 1,$$

as claimed. □

3.2.1. *Propagation of the local hypothesis.* For $u = (u_1, u_2, u_3) \in [q]^3$, write

$$B(u) := \{(2u_1 + \varepsilon_1, 2u_2 + \varepsilon_2, 2u_3 + \varepsilon_3) : \varepsilon_1, \varepsilon_2, \varepsilon_3 \in \{0, 1\}\} \subseteq [2q]^3.$$

We call $B(u)$ the *microcell above* u.

Proposition 14. *Let $S \subseteq [q]^3$, and let $a, b \in [q]$ with $a \neq b$. Assume that $H_q(a, b; S)$ holds. Let*

$$X := L_q(S) \subseteq [2q]^3,$$

and let $T \subseteq [2q]^3$ be obtained from X by the seven-site gadget above. Define

$$a' := 2a + 1, \qquad b' := 2b + 1.$$

Then

$$H_{2q}(a', b'; T)$$

holds.

Proof. All seven toggled sites lie in the four microcells above (a,a,a), (b,b,a), (b,a,a), and (b,b,b). We verify the four membership conditions and the four degree-balance conditions for the new pair $(a',b') = (2a+1, 2b+1)$.

1. Membership conditions.

Because $(a,a,a) \in S$, the whole microcell above (a,a,a) lies in X, hence

$$(a',a',a') = (2a+1, 2a+1, 2a+1) \in X.$$

This site is not toggled, so $(a',a',a') \in T$.

Because $(b,b,a) \in S$, the whole microcell above (b,b,a) lies in X, hence

$$(b',b',a') = (2b+1, 2b+1, 2a+1) \in X \subseteq T,$$

again because this site is not toggled.

Because $(b,a,a) \notin S$, the whole microcell above (b,a,a) is absent from X, so

$$(b',a',a') = (2b+1, 2a+1, 2a+1) \notin X.$$

Among the three additions, only $P_3 = (2b+1, 2a+1, 2a)$ lies in that microcell, so (b',a',a') is still absent from T.

Because $(b,b,b) \notin S$, the whole microcell above (b,b,b) is absent from X, in particular

$$(b',b',b') = (2b+1, 2b+1, 2b+1) \notin X.$$

The gadget adds only P_1 and P_2 in that microcell, so $(b',b',b') \notin T$.

Thus the membership part of $H_{2q}(a',b';T)$ holds.

2. The identity $I_T(a',a') + O_T(a',a') = 2q$.

No toggled site has initial pair (a',a'), and no toggled site has terminal pair (a',a'). Therefore

$$I_T(a',a') = I_X(a',a') = 2I_S(a,a), \qquad O_T(a',a') = O_X(a',a') = 2O_S(a,a).$$

Using $I_S(a,a) + O_S(a,a) = q$, we obtain

$$I_T(a',a') + O_T(a',a') = 2q.$$

3. The identity $I_T(b',b') + O_T(b',b') = 2q$.

Exactly the same argument gives

$$I_T(b',b') = 2I_S(b,b), \qquad O_T(b',b') = 2O_S(b,b),$$

so from $I_S(b,b) + O_S(b,b) = q$ we get

$$I_T(b',b') + O_T(b',b') = 2q.$$

4. The identity $I_T(b',b') + O_T(b',a') = 2q - 1$.

We already know that $I_T(b',b') = 2I_S(b,b)$. Moreover, $O_T(b',a')$ counts triples of T whose first two coordinates are $(b',a') = (2b+1, 2a+1)$. In the lift X, this count is $2O_S(b,a)$. The gadget adds exactly one such triple, namely

$$P_3 = (2b+1, 2a+1, 2a),$$

and removes none with the same initial pair. Hence

$$O_T(b',a') = 2O_S(b,a) + 1.$$

Using $I_S(b,b) + O_S(b,a) = q - 1$, we conclude that

$$I_T(b',b') + O_T(b',a') = 2I_S(b,b) + 2O_S(b,a) + 1 = 2q - 1.$$

5. The identity $I_T(b',a') + O_T(a',a') = 2q + 1$.

We already know that $O_T(a',a') = 2O_S(a,a)$. On the other hand, $I_T(b',a')$ counts triples of T whose last two coordinates are $(b',a') = (2b+1, 2a+1)$. In the lift X, this count is $2I_S(b,a)$. The gadget removes exactly one such triple, namely

$$M_4 = (2b, 2b+1, 2a+1),$$

and adds none with the same terminal pair. Therefore

$$I_T(b',a') = 2I_S(b,a) - 1.$$

Using $I_S(b,a) + O_S(a,a) = q + 1$, we obtain

$$I_T(b',a') + O_T(a',a') = 2I_S(b,a) - 1 + 2O_S(a,a) = 2q + 1.$$

All four membership conditions and all four degree-balance conditions hold, so $H_{2q}(a',b';T)$ follows. $\square$

3.2.2. *The explicit base configuration at scale $q = 16$.* The lower-bound construction requires one explicit seed configuration $S_{16} \subseteq [16]^3$ satisfying a local compatibility hypothesis and having a sufficiently large value of N_{16}. The full specification of S_{16} is finite but bulky: it is described by ten fibres and a 16×16 fibre table. Since these data play a purely foundational role in the induction, we place the complete definition in Appendix A.1 and keep only the summary needed for the argument here.

More precisely, Appendix A.1 defines ten fibres

$$\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}, \mathcal{E}, \mathcal{F}, \mathcal{G}, \mathcal{H}, \mathcal{I}, \mathcal{J} \subseteq [16]$$

and a fibre table $(T_{a,b})_{(a,b)\in[16]^2}$ with values among these ten sets. The seed configuration is then

$$(a, b, c) \in S_{16} \quad \Longleftrightarrow \quad c \in T_{a,b}.$$

The choice $q = 16 = 2^4$ is the natural base scale for the construction: the propagation step is dyadic, so once a single admissible seed is available at one power of two, it propagates canonically to all larger dyadic scales. We have not attempted to optimise the smallest possible seed size; rather, $q = 16$ is the first scale at which we found a convenient explicit configuration with enough room to enforce the local hypothesis and achieve the target density.

The next lemma records exactly the two facts from this explicit dataset that are needed later: the base count and the local hypothesis required by the dyadic propagation. Their complete finite verification is given in Appendix A.

Lemma 15. *Let $S_{16} \subseteq [16]^3$ be the explicit set defined in Appendix A.1. Then:*

(1)
$$N_{16}(S_{16}) = 24849.$$

(2) *The local hypothesis $H_{16}(8, 14; S_{16})$ holds. Equivalently,*

$$\begin{aligned}
&(8,8,8) \in S_{16}, \qquad (14,14,8) \in S_{16}, \qquad (14,8,8) \notin S_{16}, \qquad (14,14,14) \notin S_{16},\\
&I_{S_{16}}(8,8) + O_{S_{16}}(8,8) = 16,\\
&I_{S_{16}}(14,14) + O_{S_{16}}(14,14) = 16,\\
&I_{S_{16}}(14,14) + O_{S_{16}}(14,8) = 15,\\
&I_{S_{16}}(14,8) + O_{S_{16}}(8,8) = 17.
\end{aligned}$$

Proof. The full finite verification is recorded in Appendix A. In brief, the four membership assertions are read directly from the fibre table, the four degree identities are obtained by counting the occurrences of the values 8 and 14 in the corresponding rows and columns, and the counting identity

$$N_{16}(S_{16}) = \sum_{u,v=0}^{15} I_{S_{16}}(u,v)\big(16 - O_{S_{16}}(u,v)\big)$$

is then evaluated from the complete incoming- and outgoing-degree matrices. The resulting row sums add up to 24849. □

3.2.3. *Inductive construction and the resulting lower bound.*

Proposition 16. *Set $q_m := 2^m$ for $m \geq 4$. Define*

$$S_{q_4} := S_{16}, \qquad a_4 := 8, \qquad b_4 := 14,$$

and recursively, for $m \geq 4$, let $S_{q_{m+1}} \subseteq [q_{m+1}]^3$ be obtained from S_{q_m} by first taking the dyadic lift and then applying the seven-site gadget with parameters (a_m, b_m). Set

$$a_{m+1} := 2a_m + 1, \qquad b_{m+1} := 2b_m + 1.$$

Then for every $m \geq 4$:

(1) *$H_{q_m}(a_m, b_m; S_{q_m})$ holds;*

(2)
$$N_{q_{m+1}}(S_{q_{m+1}}) = 16\, N_{q_m}(S_{q_m}) + 1;$$

(3)
$$N_{q_m}(S_{q_m}) = \frac{91}{240}\, q_m^4 - \frac{1}{15}.$$

Proof. The base lemma gives $H_{16}(8,14;S_{16})$, so the claim in (1) holds for $m=4$. If $H_{q_m}(a_m,b_m;S_{q_m})$ holds, then Proposition 14 gives

$$H_{q_{m+1}}(a_{m+1},b_{m+1};S_{q_{m+1}}),$$

which proves (1) for all $m\geq 4$ by induction.

Under the same inductive hypothesis, Lemma 13 yields

$$N_{q_{m+1}}(S_{q_{m+1}})=16\,N_{q_m}(S_{q_m})+1,$$

which is (2).

To solve the recurrence, use the initial value $N_{16}(S_{16})=24849$. Iterating (2) gives

$$N_{q_m}(S_{q_m})=16^{m-4}\cdot 24849+\sum_{j=0}^{m-5}16^j=16^{m-4}\cdot 24849+\frac{16^{m-4}-1}{15}.$$

Since $q_m=2^m$, so that $16^{m-4}=q_m^4/16^4=q_m^4/65536$, and since

$$\frac{24849}{65536}+\frac{1}{15\cdot 65536}=\frac{91}{240},$$

we obtain

$$N_{q_m}(S_{q_m})=\frac{91}{240}\,q_m^4-\frac{1}{15}.$$

This proves (3). □

Corollary 17.

$$\frac{3}{8}<\frac{91}{240}\leq\lambda_3\leq\frac{11}{28}<\frac{2}{5}.$$

Proof. For each $m\geq 4$, let $A_m:=A_{S_{q_m}}\subseteq[0,1]^3$ be the q_m-adic set associated with S_{q_m}. By Proposition 16 and the correspondence lemma,

$$\Phi(A_m)=\Lambda_{q_m}(S_{q_m})=\frac{N_{q_m}(S_{q_m})}{q_m^4}=\frac{91}{240}-\frac{1}{15q_m^4}.$$

Letting $m\to\infty$ gives

$$\lambda_3\geq\frac{91}{240}.$$

The upper bound $\lambda_3\leq 11/28$ is Corollary 11. The strict inequalities with $3/8$ and $2/5$ are immediate. □

3.3. **The independence number of $B(4,q)$.** We now combine Proposition 3, the asymptotic result of Section 2, and the explicit bounds for λ_3 established above.

Theorem 18. *As $q\to\infty$,*

$$\alpha(4,q)=\lambda_3q^4+o(q^4),$$

with

$$\frac{91}{240}\leq\lambda_3\leq\frac{11}{28}.$$

In particular,

$$\frac{91}{240}\leq\lim_{q\to\infty}\frac{\alpha(4,q)}{q^4}=\lambda_3\leq\frac{11}{28}.$$

The same limit statement holds for $\alpha_{\mathrm{loop}}(4,q)$.

Proof. The asymptotic formula is exactly Theorem 7 specialised to $k=4$. The upper bound for λ_3 is Corollary 11, and the lower bound is Corollary 17. Substituting these bounds into Theorem 7 yields the claim. □

Along the dyadic subsequence $q=2^m$, Proposition 16 gives the sharper explicit bound

$$N_{2^m}(S_{2^m})=\frac{91}{240}\,2^{4m}-\frac{1}{15}.$$

Therefore

$$\alpha_{\mathrm{loop}}(4,2^m)\geq\frac{91}{240}\,2^{4m}-\frac{1}{15},\qquad \alpha(4,2^m)\geq\frac{91}{240}\,2^{4m}-\frac{1}{15}.$$

The universal upper bound from Proposition 10 reads

$$\alpha_{\mathrm{loop}}(4,q)\leq\frac{11}{28}q^4,\qquad \alpha(4,q)\leq\frac{11}{28}q^4+q.$$

Remark 19 (Road map of the $k = 4$ lower bound)**.** *The lower bound has four logically distinct layers. One starts from the explicit seed S_{16}, verifies finitely that it has the required local structure and that $N_{16}(S_{16}) = 24849$, propagates this information to all dyadic scales by the lift-plus-gadget construction, and finally passes from dyadic discrete sets to the continuum variational problem through the correspondence established in Section 2. This separation is useful for refereeing: only the first layer is finite bookkeeping, while the later steps are conceptual and remain unchanged once the base seed has been verified.*

4. Exact formulas for $k = 11, 13, 17$

In this section we specialise to the binary graph underlying $B(k, 2)$, where k is an odd prime. We write words as

$$x = x_0x_1 \dots x_{k-1} \in \{0, 1\}^k,$$

and let

$$\rho(x_0x_1 \dots x_{k-1}) := x_1x_2 \dots x_{k-1}x_0$$

be the cyclic left rotation. Throughout this section, orbit indices are understood modulo k. We also write 0^k and 1^k for the two constant words. This is the only place in the paper where we switch to 0-based coordinate indexing, in order to align the notation with the cyclic rotation action.

Two results of Lichiardopol are the external input for what follows. First, Propositions 4.2 and 4.3(b) of [8], specialised to the odd prime binary case, give

$$\alpha(k, 2) \le 1 + \frac{k-1}{2k}(2^k - 2). \tag{6}$$

Second, by [8, Theorem 4.4], if the bound (6) is attained by an independent set containing exactly one loop-vertex, then for every alphabet size $q \ge 2$ one has

$$\alpha(k, q) = \frac{(k-1)(q^k - q)}{2k} + 1, \qquad \alpha_{\text{loop}}(k, q) = \frac{(k-1)(q^k - q)}{2k}. \tag{7}$$

Thus the binary problem controls the exact formulas for all $q \ge 2$.

4.1. Rotation orbits and the phase constraint system.

For $x \in \{0, 1\}^k$, let

$$C(x) := \{\rho^i(x) : i \in \mathbb{Z}/k\mathbb{Z}\}$$

be its rotation orbit.

Lemma 20. *If $x \in \{0, 1\}^k$ is non-constant, then $|C(x)| = k$.*

Proof. If $\rho^r(x) = x$ for some $r \in \mathbb{Z}/k\mathbb{Z}$, then x has cyclic period r. Since k is prime, every non-zero class in $\mathbb{Z}/k\mathbb{Z}$ generates the whole group, so a non-trivial period would force all coordinates of x to coincide. Hence a non-constant word has no non-trivial stabiliser under rotation, and its orbit has cardinality k. □

Lemma 21. *Let $x \in \{0, 1\}^k$ be non-constant, and write $x^{(i)} := \rho^i(x)$ for $i \in \mathbb{Z}/k\mathbb{Z}$. Then the subgraph induced by $C(x)$ in the simple graph underlying $B(k, 2)$ is the cycle graph C_k. Equivalently,*

$$x^{(i)} \sim x^{(j)} \qquad \Longleftrightarrow \qquad j - i \equiv \pm 1 \pmod k.$$

Proof. The implications for consecutive rotations are immediate: for every i, $x^{(i)}$ and $x^{(i+1)}$ overlap in their common block of length $k - 1$.

Conversely, suppose first that the suffix of length $k - 1$ of $x^{(i)}$ equals the prefix of length $k - 1$ of $x^{(j)}$. With all subscripts read modulo k, this says

$$x_{i+1+r} = x_{j+r}, \qquad r = 0, \dots, k-2.$$

Set $d := j - i - 1$. Equivalently,

$$x_s = x_{s+d} \qquad \text{for every } s \ne i.$$

If $d \ne 0$, translation by d is a single k-cycle on $\mathbb{Z}/k\mathbb{Z}$ because k is prime. Removing the one edge that starts at i leaves a path through all k residues, and the displayed equalities force all coordinates of x to be equal. This contradicts the assumption that x is non-constant. Hence $d = 0$, so $j - i \equiv 1 \pmod k$.

If instead the prefix of length $k - 1$ of $x^{(i)}$ equals the suffix of length $k - 1$ of $x^{(j)}$, the same argument, with $d := j - i + 1$, gives $j - i \equiv -1 \pmod k$. Thus no other adjacency occurs inside the orbit. □

Let

$$J_k := \{1, 3, 5, \dots, k-2\} \subseteq \mathbb{Z}/k\mathbb{Z}.$$

For a non-trivial rotation orbit $C = (x^{(i)})_{i \in \mathbb{Z}/k\mathbb{Z}}$ and a phase $t \in \mathbb{Z}/k\mathbb{Z}$, define

$$A_t(C) := \{x^{(t+r)} : r \in J_k\}.$$

Lemma 22. *For every non-trivial rotation orbit C and every $t \in \mathbb{Z}/k\mathbb{Z}$, the set $A_t(C)$ is independent and has cardinality $(k-1)/2$.*

Proof. By Lemma 21, the only edges inside C join consecutive residues modulo k. The translate $J_k + t$ contains no two consecutive residues, hence $A_t(C)$ is independent. Its cardinality is $|J_k| = (k-1)/2$. □

Proposition 23. *Let $S \subseteq \{0,1\}^k$ be an independent set such that*

$$|S| = 1 + \frac{k-1}{2k}(2^k - 2)$$

and such that S contains exactly one loop-vertex. Then for every non-trivial rotation orbit C one has

$$|S \cap C| = \frac{k-1}{2},$$

and there exists a unique phase $t_C \in \mathbb{Z}/k\mathbb{Z}$ such that

$$S \cap C = A_{t_C}(C).$$

Proof. The $2^k - 2$ non-constant words split into

$$N_k := \frac{2^k - 2}{k}$$

non-trivial rotation orbits by Lemma 20. Since S contains exactly one loop-vertex and has cardinality

$$1 + \frac{k-1}{2} N_k,$$

its non-constant part has size exactly $\frac{k-1}{2} N_k$. By Lemma 21, each non-trivial orbit induces a copy of C_k, so it contributes at most $(k-1)/2$ vertices to S. Therefore every non-trivial orbit must attain this maximum. The k maximum independent sets of C_k are exactly the translates of the alternating pattern J_k. Hence there exists a unique phase $t_C \in \mathbb{Z}/k\mathbb{Z}$ such that $S \cap C = A_{t_C}(C)$. □

Remark 24 (Simultaneous rotation does not preserve adjacency)**.** *For arbitrary words, de Bruijn adjacency is not invariant under simultaneous cyclic rotation. For example, for every $k \geq 3$ let*

$$x = 0^{k-1}1, \qquad y = 0^{k-2}11.$$

Then $x \sim y$, whereas

$$\rho(x) = 0^{k-2}10, \qquad \rho(y) = 0^{k-3}110$$

are not adjacent. Consequently, compatibility between two distinct rotation orbits cannot in general be encoded only by the difference of their phase parameters.

To formulate the exact compatibility constraints, fix an indexing $C = (x^{(i)})_{i \in \mathbb{Z}/k\mathbb{Z}}$ for every non-trivial rotation orbit. For two distinct indexed orbits $C = (x^{(i)})$ and $C' = (y^{(j)})$, define the adjacency relation

$$E(C, C') := \{(i,j) \in (\mathbb{Z}/k\mathbb{Z})^2 : x^{(i)} \sim y^{(j)}\}$$

and the corresponding forbidden phase-pair relation

$$\mathfrak{F}(C, C') := \{(i - a, j - b) : (i,j) \in E(C, C'),\ a, b \in J_k\} \subseteq (\mathbb{Z}/k\mathbb{Z})^2.$$

If $\ell \in \{0^k, 1^k\}$ is the chosen loop-vertex, define also

$$E(\ell, C) := \{i \in \mathbb{Z}/k\mathbb{Z} : \ell \sim x^{(i)}\}$$

and

$$\mathfrak{F}(\ell, C) := \{i - a : i \in E(\ell, C),\ a \in J_k\} \subseteq \mathbb{Z}/k\mathbb{Z}.$$

Thus a phase t_C is compatible with ℓ precisely when $t_C \notin \mathfrak{F}(\ell, C)$.

Theorem 25. *Fix $\ell \in \{0^k, 1^k\}$. For each non-trivial rotation orbit C, choose a phase $t_C \in \mathbb{Z}/k\mathbb{Z}$ and set*

$$S_\ell(\{t_C\}) := \{\ell\} \cup \bigcup_C A_{t_C}(C),$$

where the union runs over all non-trivial rotation orbits. Then $S_\ell(\{t_C\})$ is independent if and only if the following two conditions hold:

(i) *for every non-trivial orbit C,*

$$t_C \notin \mathfrak{F}(\ell, C);$$

(ii) *for every pair of distinct non-trivial orbits C, C',*

$$(t_C, t_{C'}) \notin \mathfrak{F}(C, C').$$

Whenever these conditions are satisfied,

$$|S_\ell(\{t_C\})| = 1 + \frac{k-1}{2k}(2^k - 2).$$

Conversely, every independent set of this cardinality with exactly one loop-vertex arises in this way.

Proof. By Lemma 22, each $A_{t_C}(C)$ is independent inside its own orbit. A cross-conflict between $A_{t_C}(C)$ and $A_{t_{C'}}(C')$ occurs if and only if there exist $a, b \in J_k$ such that

$$x^{(t_C+a)} \sim y^{(t_{C'}+b)}.$$

By the definition of $E(C, C')$, this is equivalent to

$$(t_C + a, t_{C'} + b) \in E(C, C'),$$

and hence, by the definition of $\mathfrak{F}(C, C')$, to

$$(t_C, t_{C'}) \in \mathfrak{F}(C, C').$$

This proves the exact equivalence in condition (ii). Likewise, ℓ is adjacent to a vertex of $A_{t_C}(C)$ if and only if $t_C \in \mathfrak{F}(\ell, C)$, which gives condition (i). The cardinality formula follows from Lemma 22, and the converse is Proposition 23. □

Remark 26. *The phase representation converts the search for an extremal binary example with one prescribed loop-vertex into a finite binary CSP with one variable $t_C \in \mathbb{Z}/k\mathbb{Z}$ per non-trivial orbit and one binary forbidden relation $\mathfrak{F}(C, C')$ for each interacting pair of orbits. It is not, in general, a difference-CSP. The constraint graph is sparse for two elementary reasons. First, if $x \sim y$ in the simple graph underlying $B(k, 2)$, then $|\mathrm{wt}(x) - \mathrm{wt}(y)| \le 1$, so only adjacent Hamming-weight layers can interact. Second, each binary word has at most four de Bruijn neighbours, and therefore the orbit-conflict graph has maximum degree at most $4k$.*

4.2. **Certificates and the cases $k = 11, 13, 17$.** For the prime cases $k = 11$, $k = 13$, and $k = 17$, we use a single *compact orbit-marker certificate*: it records one marked word for each non-trivial rotation orbit. From this data one reconstructs the entire candidate independent set. The three compact certificates and the verifier script are given in Appendix B.

The role of the certificates is entirely finite and explicit. Starting from the compact orbit-marker file, one decodes each listed decimal marker as a length-k binary word and treats it as the first selected vertex after the unique double gap in its rotation orbit, selects every second rotation from it, takes the union together with 0^k, checks the target cardinality, verifies independence directly by testing the at most four de Bruijn neighbours of each selected vertex, and confirms that 1^k is absent. Thus the computer-assisted part of Theorems 27, 29, and 31 is a verification statement, not a search statement. For reproducibility, Appendix B records the compact certificate format, the three compact certificates, and the verifier script. The verifier uses only the Python standard library; no external solver, random search, or hidden preprocessing is required.

Theorem 27. *One has*

$$\alpha(11, 2) = 931.$$

More precisely, there exists an independent set in the simple graph underlying $B(11, 2)$ of cardinality 931 that contains 0^{11} and excludes 1^{11}.

Proof. There are

$$N_{11} = \frac{2^{11} - 2}{11} = 186$$

non-trivial rotation orbits, so the binary upper bound (6) gives

$$\alpha(11, 2) \le 1 + \frac{10}{22}(2^{11} - 2) = 1 + 5 \cdot 186 = 931.$$

The certificate for $k = 11$ records one decimal marker for each of the 186 non-trivial rotation orbits. Applying the verification protocol described above reconstructs an independent set of cardinality 931 containing 0^{11} and excluding 1^{11}. Therefore the upper bound is attained, and $\alpha(11, 2) = 931$. □

Corollary 28. *For every $q \ge 2$,*

$$\alpha(11, q) = \frac{5(q^{11} - q)}{11} + 1, \qquad \alpha_{\mathrm{loop}}(11, q) = \frac{5(q^{11} - q)}{11}.$$

Proof. The verified binary extremal set in Theorem 27 contains exactly one loop-vertex. The formulas follow from the lifting statement (7). □

Theorem 29. *One has*

$$\alpha(13,2) = 3781.$$

More precisely, there exists an independent set in the simple graph underlying $B(13,2)$ *of cardinality* 3781 *that contains* 0^{13} *and excludes* 1^{13}*.*

Proof. There are

$$N_{13} = \frac{2^{13}-2}{13} = 630$$

non-trivial rotation orbits, so the binary upper bound (6) gives

$$\alpha(13,2) \le 1 + \frac{12}{26}(2^{13}-2) = 1 + 6\cdot 630 = 3781.$$

The certificate for $k = 13$ records one decimal marker for each of the 630 non-trivial rotation orbits. Applying the verification protocol described above reconstructs an independent set of cardinality 3781 containing 0^{13} and excluding 1^{13}. Therefore the upper bound is sharp, and $\alpha(13,2) = 3781$. □

Corollary 30. *For every* $q \ge 2$*,*

$$\alpha(13,q) = \frac{6(q^{13}-q)}{13} + 1, \qquad \alpha_{\mathrm{loop}}(13,q) = \frac{6(q^{13}-q)}{13}.$$

Proof. The verified binary extremal set in Theorem 29 contains exactly one loop-vertex. The formulas follow from the lifting statement (7). □

Theorem 31. *One has*

$$\alpha(17,2) = 61681.$$

More precisely, there exists an independent set in the simple graph underlying $B(17,2)$ *of cardinality* 61681 *that contains* 0^{17} *and excludes* 1^{17}*.*

Proof. There are

$$N_{17} = \frac{2^{17}-2}{17} = 7710$$

non-trivial rotation orbits, so the binary upper bound (6) gives

$$\alpha(17,2) \le 1 + \frac{16}{34}(2^{17}-2) = 1 + 8\cdot 7710 = 61681.$$

The certificate for $k = 17$ records one decimal marker for each of the 7710 non-trivial rotation orbits. Applying the verification protocol described above reconstructs an independent set of cardinality 61681 containing 0^{17} and excluding 1^{17}. Therefore the upper bound is attained, and $\alpha(17,2) = 61681$. □

Corollary 32. *For every* $q \ge 2$*,*

$$\alpha(17,q) = \frac{8(q^{17}-q)}{17} + 1, \qquad \alpha_{\mathrm{loop}}(17,q) = \frac{8(q^{17}-q)}{17}.$$

Proof. The verified binary extremal set in Theorem 31 contains exactly one loop-vertex. The formulas follow from the lifting statement (7). □

Appendix A. Data and verification for $k = 4$, $q = 16$

This appendix incorporates the complete finite component of the lower-bound construction for $k = 4$ at the base scale $q = 16$. In parallel with Appendix B, we present the seed in a compact, uniform form: first the defining data, then the verification protocol and script, and finally the derived degree and contribution tables used in the computation of $N_{16}(S_{16})$.

A.1. **Seed data.**

A.1.1. *Named fibres.* We define ten fibres as subsets of [16]:

$$\begin{aligned}
&\mathcal{A} := \varnothing,\\
&\mathcal{B} := \{0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15\},\\
&\mathcal{C} := \{6,7\},\\
&\mathcal{D} := \{2,3,6,7\},\\
&\mathcal{E} := \{2,3,6,7,12,13\},\\
&\mathcal{F} := \{2,3,6,7,8,9,12,13\},\\
&\mathcal{G} := \{2,3,4,5,6,7,8,9,12,13,14,15\},\\
&\mathcal{H} := \{2,3,6,7,8,9,12,13,14,15\},\\
&\mathcal{I} := \{2,3,6,7,9,12,13\},\\
&\mathcal{J} := \{2,3,6,7,8,9,12,13,14\}.
\end{aligned}$$

A.1.2. *Fibre table.* Define $S_{16} \subseteq [16]^3$ by

$$(a,b,c) \in S_{16} \quad \Longleftrightarrow \quad c \in T_{a,b},$$

where the fibre $T_{a,b}$ is selected from the following 16×16 label matrix:

$T_{a,b}$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$
1	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$
2	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$
3	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$
4	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{C}$	$\mathcal{C}$	$\mathcal{H}$	$\mathcal{H}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{D}$
5	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{C}$	$\mathcal{C}$	$\mathcal{H}$	$\mathcal{H}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{D}$
6	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$
7	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$
8	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{C}$	$\mathcal{C}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{F}$	$\mathcal{E}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{B}$	$\mathcal{B}$
9	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{C}$	$\mathcal{C}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{B}$	$\mathcal{B}$
10	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$
11	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{A}$
12	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{C}$	$\mathcal{C}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$
13	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{C}$	$\mathcal{C}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{F}$	$\mathcal{F}$	$\mathcal{B}$	$\mathcal{B}$
14	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{C}$	$\mathcal{C}$	$\mathcal{H}$	$\mathcal{H}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{I}$	$\mathcal{E}$	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{F}$	$\mathcal{J}$
15	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{C}$	$\mathcal{C}$	$\mathcal{H}$	$\mathcal{H}$	$\mathcal{A}$	$\mathcal{A}$	$\mathcal{E}$	$\mathcal{E}$	$\mathcal{G}$	$\mathcal{G}$	$\mathcal{D}$	$\mathcal{D}$	$\mathcal{E}$	$\mathcal{J}$

A.1.3. *Fibre cardinalities.* We recall the ten fibres used to define $S_{16} \subseteq [16]^3$:

$$\begin{aligned}
&\mathcal{A} := \varnothing, && |\mathcal{A}| = 0,\\
&\mathcal{B} := [16], && |\mathcal{B}| = 16,\\
&\mathcal{C} := \{6,7\}, && |\mathcal{C}| = 2,\\
&\mathcal{D} := \{2,3,6,7\}, && |\mathcal{D}| = 4,\\
&\mathcal{E} := \{2,3,6,7,12,13\}, && |\mathcal{E}| = 6,\\
&\mathcal{F} := \{2,3,6,7,8,9,12,13\}, && |\mathcal{F}| = 8,\\
&\mathcal{G} := \{2,3,4,5,6,7,8,9,12,13,14,15\}, && |\mathcal{G}| = 12,\\
&\mathcal{H} := \{2,3,6,7,8,9,12,13,14,15\}, && |\mathcal{H}| = 10,\\
&\mathcal{I} := \{2,3,6,7,9,12,13\}, && |\mathcal{I}| = 7,\\
&\mathcal{J} := \{2,3,6,7,8,9,12,13,14\}, && |\mathcal{J}| = 9.
\end{aligned}$$

Thus, for every pair $(a,b) \in [16]^2$, the outgoing degree is simply

$$O_{S_{16}}(a,b) = |T_{a,b}|.$$

This compact description is the complete defining data for the seed: all subsequent verifications are reconstructed from these ten named fibres and the 16×16 label matrix.

A.2. **Verification protocol.** The finite verification has three components: first one checks the local hypothesis $H_{16}(8,14;S_{16})$; next one computes the incoming and outgoing degree matrices; finally one evaluates the contribution matrix and the resulting count $N_{16}(S_{16})$. We begin with the local hypothesis. By inspection of the fibre table,

$$\begin{aligned}
T_{8,8} &= \mathcal{F} = \{2,3,6,7,8,9,12,13\},\\
T_{14,14} &= \mathcal{F} = \{2,3,6,7,8,9,12,13\},\\
T_{14,8} &= \mathcal{I} = \{2,3,6,7,9,12,13\}.
\end{aligned}$$

Therefore

$$(8,8,8) \in S_{16}, \qquad (14,14,8) \in S_{16}, \qquad (14,8,8) \notin S_{16}, \qquad (14,14,14) \notin S_{16}.$$

Moreover,

$$O_{S_{16}}(8,8) = |\mathcal{F}| = 8, \qquad O_{S_{16}}(14,14) = |\mathcal{F}| = 8, \qquad O_{S_{16}}(14,8) = |\mathcal{I}| = 7.$$

To compute the relevant incoming degrees, recall that

$$I_{S_{16}}(u,v) = \#\{x \in [16] : (x,u,v) \in S_{16}\} = \#\{x \in [16] : v \in T_{x,u}\}.$$

Hence:

- $I_{S_{16}}(8,8)$ is the number of rows x such that $8 \in T_{x,8}$. Reading the eighth column of the fibre table, this happens for
$$x \in \{2,3,6,7,8,9,12,13\},$$
so $I_{S_{16}}(8,8) = 8$.
- $I_{S_{16}}(14,14)$ is the number of rows x such that $14 \in T_{x,14}$. Reading the fourteenth column of the fibre table, this happens for
$$x \in \{2,3,6,7,8,9,12,13\},$$
so $I_{S_{16}}(14,14) = 8$.
- $I_{S_{16}}(14,8)$ is the number of rows x such that $8 \in T_{x,14}$. Reading the fourteenth column of the fibre table and checking where the value 8 occurs, this happens for
$$x \in \{2,3,6,7,8,9,12,13,14\},$$
so $I_{S_{16}}(14,8) = 9$.

Consequently,

$$\begin{aligned}
I_{S_{16}}(8,8) + O_{S_{16}}(8,8) &= 8+8 = 16,\\
I_{S_{16}}(14,14) + O_{S_{16}}(14,14) &= 8+8 = 16,\\
I_{S_{16}}(14,14) + O_{S_{16}}(14,8) &= 8+7 = 15,\\
I_{S_{16}}(14,8) + O_{S_{16}}(8,8) &= 9+8 = 17.
\end{aligned}$$

This proves the full local hypothesis $H_{16}(8,14;S_{16})$.

The script in the next subsection implements the same checks directly from the defining fibre table and also computes the matrices used later in this appendix.

A.3. **Verifier script.** To make the finite verification of the seed S_{16} independently checkable, we record here a short Python script that reconstructs the fibre table, computes the incoming and outgoing degree matrices, verifies the local hypothesis $H_{16}(8,14;S_{16})$, and evaluates the count

$$N_{16}(S_{16}) = \#\{(a,b,c,d) \in [16]^4 : (a,b,c) \in S_{16},\ (b,c,d) \notin S_{16}\}.$$

When run exactly as printed below, the script outputs

$$O(8,8) = 8,\ I(8,8) = 8,\ O(14,14) = 8,\ I(14,14) = 8,\ O(14,8) = 7,\ I(14,8) = 9,$$

and finally

$$H_{16}(8,14;S_{16}) \text{ holds}, \qquad N_{16}(S_{16}) = 24849.$$

```
Q = 16

fibres = {
    "A": set(),
    "B": set(range(16)),
    "C": {6, 7},
    "D": {2, 3, 6, 7},
    "E": {2, 3, 6, 7, 12, 13},
    "F": {2, 3, 6, 7, 8, 9, 12, 13},
    "G": {2, 3, 4, 5, 6, 7, 8, 9, 12, 13, 14, 15},
    "H": {2, 3, 6, 7, 8, 9, 12, 13, 14, 15},
    "I": {2, 3, 6, 7, 9, 12, 13},
    "J": {2, 3, 6, 7, 8, 9, 12, 13, 14},
}

labels = [
```

```
    ["G","G","A","A","A","A","A","A","A","A","G","G","A","A","A","A"],
    ["G","G","A","A","A","A","A","A","A","A","G","G","A","A","A","A"],
    ["B","B","F","F","B","B","A","A","F","F","B","B","F","F","B","B"],
    ["B","B","F","F","B","B","A","A","F","F","B","B","F","F","B","B"],
    ["G","G","C","C","H","H","A","A","D","D","G","G","D","D","D","D"],
    ["G","G","C","C","H","H","A","A","D","D","G","G","D","D","D","D"],
    ["B","B","F","F","B","B","F","F","F","F","B","B","F","F","B","B"],
    ["B","B","F","F","B","B","F","F","F","F","B","B","F","F","B","B"],
    ["B","B","C","C","B","B","A","A","F","E","B","B","D","D","B","B"],
    ["B","B","C","C","B","B","A","A","F","F","B","B","D","D","B","B"],
    ["G","G","A","A","A","A","A","A","A","A","G","G","A","A","A","A"],
    ["G","G","A","A","A","A","A","A","A","A","G","G","A","A","A","A"],
    ["B","B","C","C","B","B","A","A","F","F","B","B","F","F","B","B"],
    ["B","B","C","C","B","B","A","A","F","F","B","B","F","F","B","B"],
    ["G","G","C","C","H","H","A","A","I","E","G","G","D","D","F","J"],
    ["G","G","C","C","H","H","A","A","E","E","G","G","D","D","E","J"],
]

T = [[fibres[name] for name in row] for row in labels]

# Outgoing and incoming degree matrices.
O = [[len(T[a][b]) for b in range(Q)] for a in range(Q)]
I = [[sum(1 for x in range(Q) if v in T[x][u]) for v in range(Q)] for u in range(Q)]

# Local hypothesis H_16(8,14; S_16).
assert 8 in T[8][8]
assert 8 in T[14][14]
assert 8 not in T[14][8]
assert 14 not in T[14][14]
assert I[8][8] + O[8][8] == 16
assert I[14][14] + O[14][14] == 16
assert I[14][14] + O[14][8] == 15
assert I[14][8] + O[8][8] == 17

print(f"O(8,8)={O[8][8]},␣I(8,8)={I[8][8]}")
print(f"O(14,14)={O[14][14]},␣I(14,14)={I[14][14]}")
print(f"O(14,8)={O[14][8]},␣I(14,8)={I[14][8]}")
print("H_16(8,14;S_16)␣holds")

# Count N_16(S_16).
N = 0
for a in range(Q):
    for b in range(Q):
        for c in T[a][b]:
            for d in range(Q):
                if d not in T[b][c]:
                    N += 1

print(f"N_16(S_16)={N}")
assert N == 24849
```

A.4. **Derived degree tables.** For convenience we record the matrices

$$O_{16}(u,v) := O_{S_{16}}(u,v), \qquad I_{16}(u,v) := I_{S_{16}}(u,v), \qquad u,v \in [16].$$

They are listed row by row below.

Table 1: The outgoing-degree matrix $O_{16}(u,v) = |T_{u,v}|$.

$u\backslash v$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	12	12	0	0	0	0	0	0	0	0	12	12	0	0	0	0
1	12	12	0	0	0	0	0	0	0	0	12	12	0	0	0	0

Table 1 – continued from previous page

$u\backslash v$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
2	16	16	8	8	16	16	0	0	8	8	16	16	8	8	16	16
3	16	16	8	8	16	16	0	0	8	8	16	16	8	8	16	16
4	12	12	2	2	10	10	0	0	4	4	12	12	4	4	4	4
5	12	12	2	2	10	10	0	0	4	4	12	12	4	4	4	4
6	16	16	8	8	16	16	8	8	8	8	16	16	8	8	16	16
7	16	16	8	8	16	16	8	8	8	8	16	16	8	8	16	16
8	16	16	2	2	16	16	0	0	8	6	16	16	4	4	16	16
9	16	16	2	2	16	16	0	0	8	8	16	16	4	4	16	16
10	12	12	0	0	0	0	0	0	0	0	12	12	0	0	0	0
11	12	12	0	0	0	0	0	0	0	0	12	12	0	0	0	0
12	16	16	2	2	16	16	0	0	8	8	16	16	8	8	16	16
13	16	16	2	2	16	16	0	0	8	8	16	16	8	8	16	16
14	12	12	2	2	10	10	0	0	7	6	12	12	4	4	8	9
15	12	12	2	2	10	10	0	0	6	6	12	12	4	4	6	9

Table 2: The incoming-degree matrix $I_{16}(u,v) = \#\{x \in [16] : (x,u,v) \in S_{16}\}$.

$u\backslash v$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	8	8	16	16	16	16	16	16	16	16	8	8	16	16	16	16
1	8	8	16	16	16	16	16	16	16	16	8	8	16	16	16	16
2	0	0	4	4	0	0	12	12	4	4	0	0	4	4	0	0
3	0	0	4	4	0	0	12	12	4	4	0	0	4	4	0	0
4	8	8	12	12	8	8	12	12	12	12	8	8	12	12	12	12
5	8	8	12	12	8	8	12	12	12	12	8	8	12	12	12	12
6	0	0	2	2	0	0	2	2	2	2	0	0	2	2	0	0
7	0	0	2	2	0	0	2	2	2	2	0	0	2	2	0	0
8	0	0	12	12	0	0	12	12	8	9	0	0	10	10	0	0
9	0	0	12	12	0	0	12	12	7	7	0	0	10	10	0	0
10	8	8	16	16	16	16	16	16	16	16	8	8	16	16	16	16
11	8	8	16	16	16	16	16	16	16	16	8	8	16	16	16	16
12	0	0	12	12	0	0	12	12	6	6	0	0	6	6	0	0
13	0	0	12	12	0	0	12	12	6	6	0	0	6	6	0	0
14	8	8	12	12	8	8	12	12	9	9	8	8	10	10	8	8
15	8	8	12	12	8	8	12	12	10	10	8	8	10	10	10	8

A.5. **Contribution table and the computation of $N_{16}(S_{16})$.** The counting identity used in the proof of the base lemma is

$$N_{16}(S_{16}) = \sum_{u,v=0}^{15} I_{16}(u,v)\big(16 - O_{16}(u,v)\big).$$

Define the entrywise contribution matrix

$$C_{16}(u,v) := I_{16}(u,v)\big(16 - O_{16}(u,v)\big).$$

Using Tables 1 and 2, one obtains the following matrix.

Table 3: The contribution matrix $C_{16}(u,v) = I_{16}(u,v)(16 - O_{16}(u,v))$.

$u\backslash v$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	32	32	256	256	256	256	256	256	256	256	32	32	256	256	256	256
1	32	32	256	256	256	256	256	256	256	256	32	32	256	256	256	256
2	0	0	32	32	0	0	192	192	32	32	0	0	32	32	0	0
3	0	0	32	32	0	0	192	192	32	32	0	0	32	32	0	0
4	32	32	168	168	48	48	192	192	144	144	32	32	144	144	144	144
5	32	32	168	168	48	48	192	192	144	144	32	32	144	144	144	144
6	0	0	16	16	0	0	16	16	16	16	0	0	16	16	0	0
7	0	0	16	16	0	0	16	16	16	16	0	0	16	16	0	0
8	0	0	168	168	0	0	192	192	64	90	0	0	120	120	0	0
9	0	0	168	168	0	0	192	192	56	56	0	0	120	120	0	0
10	32	32	256	256	256	256	256	256	256	256	32	32	256	256	256	256
11	32	32	256	256	256	256	256	256	256	256	32	32	256	256	256	256
12	0	0	168	168	0	0	192	192	48	48	0	0	48	48	0	0
13	0	0	168	168	0	0	192	192	48	48	0	0	48	48	0	0
14	32	32	168	168	48	48	192	192	81	90	32	32	120	120	64	56
15	32	32	168	168	48	48	192	192	100	100	32	32	120	120	100	56

Summing each row of C_{16} gives

$$\begin{aligned}(r_0, \dots, r_{15}) = (&3200, 3200, 576, 576, 1808, 1808, 128, 128,\\ &1114, 1072, 3200, 3200, 912, 912, 1475, 1540).\end{aligned}$$

Finally,

$$\begin{aligned} N_{16}(S_{16}) &= 3200 + 3200 + 576 + 576 + 1808 + 1808 + 128 + 128 \\ &\qquad + 1114 + 1072 + 3200 + 3200 + 912 + 912 + 1475 + 1540 \\ &= 24849. \end{aligned}$$

Appendix B. Data and verification for $k = 11, 13, 17$

This appendix incorporates the computer-assisted component of Theorems 27, 29, and 31. In parallel with Appendix A, we present first the defining data format, then the verification protocol and verifier script, and finally the compact certificate data for $k = 11$, $k = 13$, and $k = 17$.

B.1. **Compact orbit-marker certificate data for $k = 11, 13, 17$.** For a fixed prime length $k \in \{11, 13, 17\}$, the certificate is a plain-text file with:

- a one-line header specifying k, the target cardinality, the mandatory included vertex 0^k, and the mandatory excluded vertex 1^k;
- one decimal marker for each non-trivial rotation orbit; the marker n denotes the length-k binary word with standard base-2 value n;
- line breaks are purely for compactness; the data below use at most thirteen decimal markers per line.

The marker convention removes the explicit phase from the earlier orbit-phase format. If $k = 2m + 1$ and w is the binary word decoded from a listed marker on its orbit, then the selected vertices from that orbit are

$$w, \rho^2(w), \rho^4(w), \dots, \rho^{2m-2}(w).$$

Equivalently, in the cyclic order of the orbit the marker w is the first selected vertex after the unique double gap. Thus every listed marker determines the same alternating maximum independent set on its orbit as a suitable phase t_C, but without recording t_C separately.

B.2. **Verification protocol.** The verification procedure is finite and explicit:

(1) parse the certificate header and the list of decimal markers;
(2) decode every marker as a length-k word, check that it is non-constant, and check that the decoded words belong to distinct non-trivial rotation orbits of size k;
(3) reconstruct the selected vertices on each orbit by taking every second rotation from the marker;
(4) add the mandatory loop-vertex 0^k and verify that the total size is the target size;
(5) verify directly that no selected vertex is adjacent to another selected vertex in the underlying simple de Bruijn graph;
(6) verify that 1^k is not selected.

The following script implements exactly this protocol.

B.3. **Verifier script.**

```
#!/usr/bin/env python3
from __future__ import annotations

import re
import sys
from pathlib import Path

HEADER_RE = re.compile(
    r'#\s*CERTIFICATE\s+k=(\d+)\s+target_size=(\d+)\s+include=([01]+)\s+exclude=([01]+)'
)
INT_RE = re.compile(r'^[0-9]+$')


def rotate(word: str, shift: int = 1) -> str:
    shift %= len(word)
    return word[shift:] + word[:shift]


def parse_certificate(path: Path):
    lines = path.read_text().splitlines()
    if not lines:
        raise ValueError('empty certificate file')
    m = HEADER_RE.fullmatch(lines[0].strip())
    if not m:
        raise ValueError('invalid header in certificate file')
    k = int(m.group(1))
    target = int(m.group(2))
    include_word = m.group(3)
    exclude_word = m.group(4)
    if len(include_word) != k or len(exclude_word) != k:
        raise ValueError('header words have the wrong length')

    markers = []
    seen_values = set()
    for line in lines[1:]:
        line = line.strip()
        if not line or line.startswith('#'):
            continue
        for token in line.split():
```

```
            if not INT_RE.fullmatch(token):
                raise ValueError(f'invalid decimal marker: {token}')
            value = int(token, 10)
            if value < 0 or value >= 2**k:
                raise ValueError(f'decimal marker out of range for k={k}: {token}')
            if value in seen_values:
                raise ValueError(f'duplicate decimal marker value: {token}')
            seen_values.add(value)
            markers.append(format(value, f'0{k}b'))
    return k, target, include_word, exclude_word, markers


def canonical_rotation(word: str) -> str:
    return min(rotate(word, i) for i in range(len(word)))


def orbit_from_word(word: str):
    seen = []
    cur = word
    while cur not in seen:
        seen.append(cur)
        cur = rotate(cur, 1)
    return seen


def neighbors(word: str):
    left = word[1:]
    right = word[:-1]
    out = {left + bit for bit in '01'}
    out.update({bit + right for bit in '01'})
    out.discard(word)
    return out


def verify(path: Path) -> int:
    k, target, include_word, exclude_word, markers = parse_certificate(path)
    constants = {'0' * k, '1' * k}
    if include_word not in constants or exclude_word not in constants:
        raise ValueError('the included and excluded header words must be constant')
    if include_word == exclude_word:
        raise ValueError('the included and excluded header words must be distinct')
    if (2**k - 2) % k != 0:
        raise ValueError('the certificate format requires the prime-length orbit count')
    expected_orbits = (2**k - 2) // k
    if len(markers) != expected_orbits:
        raise ValueError(
            f'expected {expected_orbits} orbit markers, found {len(markers)}'
        )

    orbit_reps_seen = set()
    selected = {include_word}
    m = (k - 1) // 2

    for marker in markers:
        if marker == '0' * k or marker == '1' * k:
            raise ValueError(f'constant marker is not allowed: {marker}')
        orbit = orbit_from_word(marker)
        if len(orbit) != k:
            raise ValueError(f'nontrivial orbit has wrong size for {marker}')
        rep = canonical_rotation(marker)
        if rep in orbit_reps_seen:
            raise ValueError(f'duplicate rotation orbit: {marker}')
        orbit_reps_seen.add(rep)
        for a in range(m):
            selected.add(rotate(marker, 2 * a))

    if exclude_word in selected:
        raise ValueError(f'excluded word {exclude_word} was selected')
    if len(selected) != target:
        raise ValueError(f'wrong size: expected {target}, found {len(selected)}')

    selected_set = set(selected)
    for word in selected:
        for nb in neighbors(word):
            if nb in selected_set:
                raise ValueError(f'adjacent selected vertices found: {word} ~ {nb}')

    print(f'OK: k={k}, selected={len(selected)}, nontrivial_orbits={len(markers)}')
    return 0


if __name__ == '__main__':
    if len(sys.argv) != 2:
        print(f'usage: {Path(sys.argv[0]).name} CERTIFICATE.txt', file=sys.stderr)
        sys.exit(2)
    sys.exit(verify(Path(sys.argv[1])))
```

B.4. Certificate for $k = 11$.

```
# CERTIFICATE k=11 target_size=931 include=00000000000 exclude=11111111111
# format: one decimal marker per non-trivial rotation orbit (up to thirteen per line)
# decoding: n represents the length-k binary word with standard base-2 value n
2 6 10 14 288 352 26 1920 1032 1033 42 46 50
864 58 62 264 1120 296 78 1312 1410 360 1922 98 102
1050 1051 1824 1888 122 2016 776 1058 1800 265 706 1062 79
266 778 1066 1802 267 779 1070 1803 1121 202 206 1313 1414
872 1926 226 230 234 238 242 246 250 254 290 354 282
482 294 298 302 1224 866 314 318 1122 1320 1336 1162 1378
1384 1930 1634 362 366 1826 1890 1512 2018 1123 1608 355 410
483 794 1306 1818 283 795 1307 1819 1832 1848 1166 1379 1896
1934 1635 490 494 1992 1891 506 2040 586 590 1610 602 1611
818 1178 1830 1614 489 1615 1202 1321 1340 1226 1194 1834 1738
1198 1994 1203 1626 730 1627 1842 1210 1838 1970 1214 2034 411
1230 1996 1337 1642 1385 1946 874 878 1646 1513 1947 1852 1338
1850 1742 1339 1998 491 1341 495 1274 1854 507 1278 2035 1386
1962 1390 1898 1530 1387 1754 1391 1966 1978 2010 2042 1755 1902
2011 1531 1982 2046
```

B.5. Certificate for $k = 13$.

```
# CERTIFICATE k=13 target_size=3781 include=0000000000000 exclude=1111111111111
# format: one decimal marker per non-trivial rotation orbit (up to thirteen per line)
# decoding: n represents the length-k binary word with standard base-2 value n
2 6144 10 14 1152 6146 26 6147 1026 1216 5122 7170 1027
27 5123 7936 66 6152 74 78 5248 6154 1440 6155 392 51
4122 7174 7296 59 488 63 130 6160 138 142 146 6162 154
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8047 7662 8174 7663 6127 8190
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B.6. Certificate for $k = 17$.

```
# CERTIFICATE k=17 target_size=61681 include=00000000000000000 exclude=11111111111111111
# format: one decimal marker per non-trivial rotation orbit (up to thirteen per line)
# decoding: n represents the length-k binary word with standard base-2 value n
2 1536 10 14 4608 22528 26624 122880 65544 65545 65546 65547 50
54 65550 65551 67584 24578 75776 78 83968 88064 92160 96256 98 102
106 110 116736 120832 124928 129024 130 134 138 142 146 150 154
122884 162 166 170 174 65580 65581 186 190 194 24582 202 206
210 214 218 96257 65592 65593 65594 114702 65596 65597 65598 114703 1032
6146 4256 270 18434 22530 26626 30722 4640 1176 298 4832 51202 55298
314 318 67586 24586 21120 334 83970 88066 92162 96258 354 22912 5792
5856 116738 120834 124930 129026 1544 6147 394 398 18435 22531 410 30723
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Dipartimento di Matematica, Università di Pisa, Largo Bruno Pontecorvo 5, 56127 Pisa, Italy
Email address: `pietro.majer@unipi.it`

Dipartimento di Matematica, Università di Pisa, Largo Bruno Pontecorvo 5, 56127 Pisa, Italy
Email address: `matteo.novaga@unipi.it`