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ON THE GENERALISATIONS OF THE NO-THREE-IN-LINE PROBLEM

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Abstract. The No-Three-in-Line problem asks how many points can be placed on an $n \times n$ integer grid so that no three are collinear. In this paper, we first generalise the problem to an $m \times n$ rectangular grid, establishing a construction method which we prove places the largest possible number of points on the grid for certain constraints on m and n. Then, using probabilistic heuristics, we estimate the maximum number of points that can be placed on the grid. Finally, we extend our analysis to the 3D No-Three-in-Line problem, deriving an asymptotic expression for the total number of collinear triples in an $n \times n \times n$ grid as $n \to \infty$. We demonstrate why the heuristic approach cannot be extended directly to 3D.

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1. Introduction

The No-Three-in-Line problem asks how many points can be placed on integer coordinates in an $n \times n$ grid so that no three points are collinear. For example, points cannot be placed simultaneously on $(1,1)$, $(3,4)$, and $(5,7)$ as the line $y = \frac{3}{2}x - \frac{1}{2}$ passes through all three points.

For an $n \times n$ grid, the trivial upper bound on the number of points that can be placed is $2n$. If more than $2n$ points are placed, there would be 3 or more points on some column or row by the pigeonhole principle, thus violating the rule that no three points can be collinear. By 1998, constructions achieving this bound were known for all $n \leqslant 46$ and a few larger values of n [2] [3]. However, it remains an open question whether $2n$ points can be placed for every n. Guy and Kelly have employed probabilistic arguments to result that the maximum number of points that may be placed approaches $\frac{\pi}{\sqrt{3}}n$ asymptotically as $n \to \infty$ ([4], their original paper, had an arithmetic error; The correction to the result is mentioned in [5]).

The majority of literature on the No-Three-in-Line problem has focused on square grids [9] [4] [10] [5]. In this paper, we investigate two generalisations of the problem, applying the heuristic used in [4] based on counting collinear triples. First, we investigate the problem on an $m \times n$ rectangular grid with m columns and n rows, formulating first a general placement method, then applying similar heuristics to Guy and Kelly's methods in [4] to arrive at probabilistic upper bounds on the number of points which can be placed. We also investigate the problem on an $n \times n \times n$ cubic grid in 3D, developing tools for the analysis of the 3D No-Three-in-Line problem and counting the total number of collinear triples in the 3D grid. We show explicitly the shortcomings of Guy and Kelly's methods as the complexity of

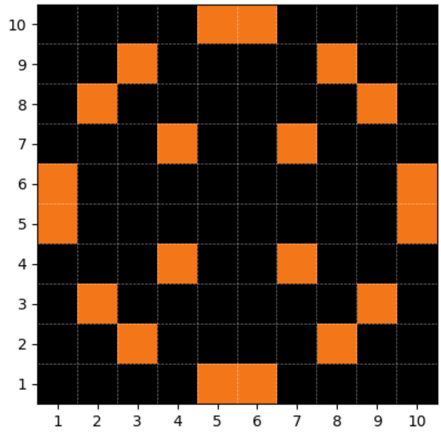

FIGURE 1.1. A symmetric solution for $2n$ points in a 10×10 grid.

the problem increases, and pose an open question for more accurate heuristics to be developed.

1.1. **Problem definition.**

Definition 1.1.1. Define a **collinear triple** to be a set of three points A, B, and C in $\mathbb{Z}^d$ (where d is the dimension of the space which we are considering) which all lie on the same line, i.e. $\exists k \in \mathbb{R} : \overrightarrow{BC} = k\overrightarrow{AB}$. $d = 2$ in Section 2 and $d = 3$ in Section 3.

Definition 1.1.2. Define the **number of collinear triples** in a set $\mathbb{S} \subset \mathbb{Z}^d$ as the number of subsets of size 3 of $\mathbb{S}$ which are collinear triples, i.e.

$$N_{\text{col}}(\mathbb{S}) \stackrel{\text{def}}{=} \text{Number of collinear triples} = |\{x \in \mathcal{P}(\mathbb{S}) : x \text{ is a collinear triple}\}|$$

We say $\mathbb{S}$ has collinear triples if $N_{\text{col}}(\mathbb{S}) > 0$, and $\mathbb{S}$ has no collinear triples if

$$N_{\text{col}}(\mathbb{S}) = 0.$$

Definition 1.1.3. Suppose there is a subset $\mathbb{S}'$ of $\mathbb{Z}^d$. We define a **solution to the No-Three-in-Line problem in** $\mathbb{S}'$ to be a set $\mathbb{U} \subseteq \mathbb{S}'$ with no collinear triples. Define $f(\mathbb{S}')$ to be the maximum cardinality of any solution to the No-Three-in-Line problem in $\mathbb{S}'$, i.e. the maximum number of points that can be placed without forming any collinear triples in $\mathbb{S}'$.

$$f(\mathbb{S}') = \max_{\mathbb{U} \in \mathcal{P}(\mathbb{S}') : N_{\text{col}}(\mathbb{U}) = 0} |\mathbb{U}|$$

We will investigate the No-Three-in-Line problem on two sets $\mathbb{S}'$:

Definition 1.1.4. Define the rectangular lattice $\mathbb{L}_{mn}$ as the set of all points on the $\mathbb{Z}^2$ satisfying the following condition, where $m, n \in \mathbb{Z}^+$.

$$\mathbb{L}_{mn} = \{(x, y) \in \mathbb{Z}^2 : 1 \leqslant x \leqslant m, 1 \leqslant y \leqslant n\} \tag{1.1}$$

Definition 1.1.5. Define the cubic lattice $\mathbb{T}_n$ as the set of all points in $\mathbb{Z}^3$ satisfying the following condition, where $n \in \mathbb{Z}^+$.

$$\mathbb{T}_n = \{(x, y, z) \in \mathbb{Z}^3 : 1 \leqslant x \leqslant n, 1 \leqslant y \leqslant n, 1 \leqslant z \leqslant n\} \tag{1.2}$$

Points in $\mathbb{L}_{mn}$ and $\mathbb{T}_n$ are referred to as *lattice points* in what follows.

1.2. **Main results.**

In Section 2, we investigate the No-Three-in-Line problem in $\mathbb{L}_{mn}$. Without loss of generality, we assume $m \leqslant n$; We prove that the trivial maximum on the number of points placed is $2m$ in Theorem 2.1.1. Then, by using probabilistic arguments, we arrive at the following conjectures, which are the main results of our paper.

Conjecture 1. For large m and n, solutions reaching the trivial maximum are only expected for $n > \dfrac{12}{\pi^2}m$.

Conjecture 2. In the range $m \leqslant n \leqslant \dfrac{12}{\pi^2}m$, $f(\mathbb{L}_{mn})$ has an upper bound of

$$\frac{\pi}{\sqrt{3}}\sqrt{mn} + O\left(\frac{\sqrt{mn}}{\ln mn}\right).$$

In Section 3, we investigate the No-Three-in-Line problem in $\mathbb{T}_n$. The complexity of the problem is increased greatly compared to the 2D case. For large n, we prove that

$$N_{\text{col}}(\mathbb{T}_n) = \frac{30191 - 16320\zeta(3) - 640\pi^2}{19200\,\zeta(3)}n^6 + O(n^5 \ln n) \approx 0.18444n^6 + O\left(n^5 \ln n\right)$$

Moreover, we propose the following conjecture.

Conjecture 3. If some function $g(n)$ is of order $O(n)$, the chance that a randomly chosen subset $\mathbb{S} \subset \mathbb{T}_n$ with $|\mathbb{S}| = g(n)$ has no collinear triples is well approximated by the following formula as $n \to \infty$:

$$P_{\text{no collinear}} = \left(1 - \frac{N_{\text{col}}}{\binom{n^3}{3}}\right)^{\binom{g(n)}{3}}$$

2. No-Three-in-Line problem on a rectangle

2.1. Non-probabilistic properties of the $m \times n$ grid.

For brevity, we define $f_{mn} \overset{\text{def}}{=} f(\mathbb{L}_{mn})$, and the No-Three-in-Line problem shall refer exclusively to the No-Three-in-Line problem in $\mathbb{L}_{mn}$ throughout Section 2.

Proposition 2.1.1. f_{mn} is a weakly monotonically increasing function of both m and n.

Proof. Let $\mathbb{S}$ be a solution on an $m \times n$ grid with $|\mathbb{S}| = f_{mn}$. At least f_{mn} points can be placed on an $(m+1) \times n$ or $m \times (n+1)$ grid, by placing points only in a $m \times n$ subset of the grid in the exact same way as in $\mathbb{S}$, since $\mathbb{S} \subseteq \mathbb{L}_{mn}$, and we have $\mathbb{L}_{mn} \subset \mathbb{L}_{(m+1)n}$ and $\mathbb{L}_{mn} \subset \mathbb{L}_{m(n+1)}$. By induction, the number of points that can be placed must be a weakly monotonically increasing function of both m and n. ■

2.1.1. *Upper and lower bounds on size of solutions to the $m \times n$ No-Three-in-Line problem.*

Theorem 2.1.1. $f_{mn} \leqslant 2\min(m,n)$

Proof. By the pigeonhole principle, if more than $2\min(m,n)$ points are placed on the grid, there must be 3 points on the same row or column, therefore forming a collinear triple. This establishes an important upper bound for f_{mn}. ■

Definition 2.1.1. Define a **maximal solution** to be a solution to the No-Three-in-Line problem with $2\min(m,n)$ points.

Theorem 2.1.2. f_{mn} is at least equal to $\dfrac{3}{2}\min(m,n) - o(\min(m,n))$ for large $\min(m,n)$.

Proof. A construction which can achieve $\dfrac{3}{2}n - o(n)$ points in an $n \times n$ grid is given by [10]. Without loss of generality, we shall assume $m < n$ so that $\min(m,n) = m$. Since $\dfrac{3}{2}m - o(m)$ points can be placed on a $m \times m$ grid, it follows from Proposition 2.1.1 that it must be possible to place $\dfrac{3}{2}m - o(m)$ points on a $m \times n$ grid as well. This establishes a lower bound on f_{mn}. ■

2.1.2. *Constraints on m and n for maximal solutions to be guaranteed.*
This proof follows a similar construction to the one in [10].

Definition 2.1.2. Given a prime number p and an integer $k \not\equiv 0 \pmod p$, define the p-hyperbola $H(k,p)$ to be the set of all points in the plane of integer coordinates (x,y) satisfying $xy \equiv k \pmod p$.

Definition 2.1.3. Two points (x_1, y_1) and $(x_2, y_2) \in \mathbb{Z}^2$ are said to be congruent if

$$x_1 \equiv x_2 \pmod p \text{ and } y_1 \equiv y_2 \pmod p$$

Proposition 2.1.2. There are at most two distinct residue classes $\pmod p$ of x that satisfy the equation

$$ax^2 + bx + c \equiv 0 \pmod p, (a,b,c) \in \mathbb{Z}_p^3, a \not\equiv 0 \pmod p \tag{2.1}$$

Proof. Suppose there are 3 distinct residue classes $x \equiv s_1, s_2, s_3 \pmod p$ satisfying the equation. Subtracting, we get

$$a(s_1^2 - s_2^2) + b(s_1 - s_2) \equiv 0 \pmod p$$
$$(a(s_1 + s_2) + b)(s_1 - s_2) \equiv 0 \pmod p$$

We know that $s_1 \not\equiv s_2 \pmod p$, so

$$a(s_1 + s_2) + b \equiv 0 \pmod p$$

Similarly,

$$a(s_2 + s_3) + b \equiv 0 \pmod p$$

However, $s_1 + s_2 \equiv s_2 + s_3 \equiv -ba^{-1} \pmod p$ where the inverse of a always exists since p is prime. Therefore, $s_1 \equiv s_3 \pmod p$, and a contradiction arises. ■

Proposition 2.1.3. If three points in $H(k, p)$ lie on a straight line, two of them must be congruent.

Proof. Suppose the three points pass through the same straight line

$$L : ax + by + c = 0$$

Since the line passes through two integer points, we may set $(a, b, c) \in \mathbb{Z}$, where a and b are coprime. (If $\gcd(a, b) \neq 1$, we can simply divide the whole equation by it.) Hence, all integer points on L satisfy

$$ax + by + c \equiv 0 \pmod p \tag{2.2}$$

Since a and b are coprime, at least one of them is indivisible by p. We assume $a \not\equiv 0 \pmod p$; The case for b proceeds analogously.
First, multiply Equation 2.2 by x on both sides, and replace xy with k:

$$ax^2 + cx + bk \equiv 0 \pmod p$$

By Proposition 2.1.2, there are at most two residue classes of $x \pmod p$ satisfying the equation. Each corresponds to a unique $y \equiv kx^{-1} \pmod p$, where the inverse of x exists as $xy \equiv k \pmod p \implies x \not\equiv 0 \pmod p$. Thus, there are at most two non-congruent points that lie both on a straight line and are in $H(k, p)$. ■

Definition 2.1.4. Denote the smallest prime number larger than m by $\lceil m \rceil_p$.

Definition 2.1.5. Define the set $\mathbb{P}$ as the section of the p-hyperbola $H\left(-1, \lceil m \rceil_p\right)$ that lies within the rectangular lattice $\mathbb{L}_{\lceil m \rceil_p n}$, i.e.

$$\mathbb{P} \stackrel{\text{def}}{=} \mathbb{L}_{\lceil m \rceil_p n} \cap H\left(-1, \lceil m \rceil_p\right) \tag{2.3}$$

Proposition 2.1.4. Define $\mathbb{Y} \stackrel{\text{def}}{=} [1, \lceil m \rceil_p - 1]$ and $\mathbb{X}$ to be the set of all x-coordinates of points in $\mathbb{P}$ with the y-coordinate in the range of $\mathbb{Y}$, i.e.
$\mathbb{X} = \{x : (x, y) \in \mathbb{P} \text{ and } y \in \mathbb{Y}\}$. Then, there is a bijection between $\mathbb{X}$ and $\mathbb{Y}$, i.e. Each y-coordinate in $\mathbb{Y}$ corresponds to one unique x-coordinate.

Proof. Suppose $a \in [1, 2\lceil m \rceil_p - 1] \ / \ \{\lceil m \rceil_p\}$. Since multiplication by a nonzero number (mod $\lceil m \rceil_p$) is invertible, we see that $\mathbb{P}$ consists of $2\lceil m \rceil_p - 2$ points, corresponding to

$$y = a \qquad\qquad x \equiv -a^{-1} \pmod{\lceil m \rceil_p}$$

This establishes a bijection between $x \in \mathbb{Z}^*_{\lceil m \rceil_p}$ and $y \in \mathbb{Z}^*_{\lceil m \rceil_p}$, where $\mathbb{Z}^*_{\lceil m \rceil_p}$ is the multiplicative group (mod $\lceil m \rceil_p$).
Noting that $x \in [1, \lceil m \rceil_p - 1]$ since $\mathbb{P} \subset L_{\lceil m \rceil_p n}$, we see that there is only one possible x-coordinate for each residue class (mod $\lceil m \rceil_p$); The same is true of the y-coordinate in the interval we are considering. Therefore a bijection $x \in \mathbb{Z}^*_{\lceil m \rceil_p} \leftrightarrow y \in \mathbb{Z}^*_{\lceil m \rceil_p}$ implies a bijection $x \in \mathbb{X} \leftrightarrow y \in \mathbb{Y}$. ■

Proposition 2.1.5. $\mathbb{P}$ is a solution to the No-Three-in-Line problem in $\mathbb{L}_{\lceil m \rceil_p n}$.

Proof. Suppose there are three collinear points in $\mathbb{L}_{\lceil m \rceil_p n}$. According to Proposition 2.1.3, two of them must be congruent (mod $\lceil m \rceil_p$). The only pairs of congruent points that are in $\mathbb{L}_{n \lceil m \rceil_p}$ are of the form (a, b) and $(a, b + \lceil m \rceil_p)$. Therefore, the only way the points can be collinear is if they lie on the same column. We showed in Proposition 2.1.4 that there is at most one point on each column in the interval $y \in [1, \lceil m \rceil_p - 1]$, and the same applies to $y \in [\lceil m \rceil_p + 1, 2\lceil m \rceil_p - 1]$. Thus, there are at most two points on each column, leading to a contradiction.

■

Definition 2.1.6. Define $\mathbb{P}' \overset{\text{def}}{=} \mathbb{L}_{mn} \cap H(-1, \lceil m \rceil_p)$, i.e. $\mathbb{P}$ truncated to the range $x \in [1, m]$.

Theorem 2.1.3. For any rectangular grid with $n \geqslant 2\lceil m \rceil_p - 1$, $f_{mn} = 2m$, i.e. maximal solutions are guaranteed.

Proof. As noted in Proposition 2.1.4, there is a bijection from $y \in [1, \lceil m \rceil_p - 1]$ to $x \in [1, \lceil m \rceil_p - 1]$. It follows that there must be a surjection from $y \in [1, \lceil m \rceil_p - 1]$ to $x \in [1, m]$, since $m \leqslant \lceil m \rceil_p - 1$. Hence, there must be m points in $\mathbb{P}'$ for $y \in [1, \lceil m \rceil_p - 1]$. Repeating for $y \in [\lceil m \rceil_p + 1, 2\lceil m \rceil_p - 1]$, we see that $|\mathbb{P}'| = 2m$. Also, as proved in Proposition 2.1.5, $\mathbb{P}$ has no collinear triples; It follows that, since $\mathbb{P}' \subset \mathbb{P}$, $\mathbb{P}$ also has no collinear triples and therefore is a solution to the No-Three-in-Line problem, and the proposition is proved.
The theorem implies that maximal solutions are guaranteed for

$$n > 2(m + O(m^\theta)) - 1 = 2m + O(m^\theta) = (2 + o(1))m,$$

where $\theta \leqslant 0.525$ is the upper bound on the order of magnitude of the prime gap at m [1]. Since m must be larger than or equal to the prime number preceding $\lceil m \rceil_p$, it follows that $\lceil m \rceil_p - m$ is at most the size of the prime gap at $\lceil m \rceil_p$. The size of the prime gap is at most of order $O(\lceil m \rceil_p^{\ \theta}) = O(m^\theta)$.

■

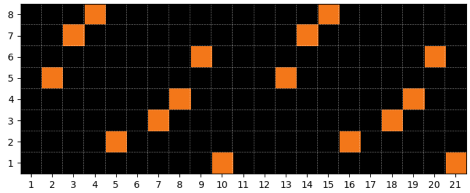

FIGURE 2.1. Plot of $\mathbb{P}'$ for $m = 8, n = 2\lceil 8 \rceil_p - 1 = 21$. Note how the maximum possible of 16 points placed is achieved.[1]

[1] Note that the x and y axes have been swapped in the figure to save space.

A corollary of this construction is as follows:

Theorem 2.1.4. Given $m < n < 2\lceil m \rceil_p - 1$, f_{mn} is at least equal to

$$2m - (2\lceil m \rceil_p - 1 - n) \approx n - O\left(m^{\theta}\right), \text{ where } \theta < 1$$

.

Proof. Our construction method places at most 1 point on each row as proved in 2.1.4. We also know that $2m$ points can be placed if $n = 2\lceil m \rceil_p - 1$, so the maximum number of points that are removed by truncating the construction at some $n < 2\lceil m \rceil_p - 1$ is equal to $2\lceil m \rceil_p - 1 - n$, therefore obtaining a minimum of $2m - (2\lceil m \rceil_p - 1 - n) = n - O(m^{\theta})$ points, where we invoked the order of magnitude of prime gaps in the last step again. ■

2.2. Preliminaries for counting collinear triples.

The main goal of this section will be to find a counting function $S(p, q)$ that counts the total number of collinear triples with slope equal to $\frac{q}{p}$. We will use the properties derived in subsection 2.2.1 to count the number of unique lines that pass through a certain number of points on the grid, and from there derive an expression for $S(p, q)$.

2.2.1. *Properties of lines in the rectangular grid.*

Definition 2.2.1. Define $l_{(a,b)}$ as a line that passes through (a, b) with slope $\frac{q}{p}$, where $(a, b) \in \mathbb{L}_{mn}$ and p and q are coprime integers.

We shall assume p and q to be constants throughout this section, and the word "line" will denote lines of slope $\frac{q}{p}$ unless otherwise specified.

Proposition 2.2.1. There exists an integer k such that $(x, y) = (a + kp, b + kq)$ if and only if $l_{(a,b)}$ passes through $(x, y) \in \mathbb{L}_{mn}$.

Proof. If $l_{(a,b)}$ passes through (x, y) ,

$$\frac{y-b}{x-a} = \frac{q}{p} \tag{2.4}$$

where $x-a$ and $y-b$ are both integers. Since p and q are coprime, it suffices that $x-a = kp$ and $y-b = kq$ where k is an integer. Rearranging gives $x = a+kp$ and $y = b + kq$.

The converse also holds, which we can see by substituting $x = a+kp$ and $y = b+kq$ into Equation 2.4.

With this in mind, we will impose the limits $1 \leqslant p \leqslant m-1$ and $1 \leqslant q \leqslant n-1$ in what follows, since these are the only lines with positive slope which pass through more than one point in $\mathbb{L}_{mn}$ and are thus the only lines which are meaningful to consider. All the proofs for lines of negative slope are analogous and can be obtained simply by reflecting the board with respect to either the x or y axis. We shall consider vertical and horizontal lines separately from other lines in Section 2.3. ■

Definition 2.2.2. Define the variable r

$$r \stackrel{\text{def}}{=} \min\left(\left\lfloor \frac{m-1}{p} \right\rfloor, \left\lfloor \frac{n-1}{q} \right\rfloor\right) \tag{2.5}$$

Hence, $r \leqslant \dfrac{m-1}{p}$ and $r \leqslant \dfrac{n-1}{q}$. Besides, in what follows, we assume $\dfrac{m-1}{p} \leqslant \dfrac{n-1}{q}$ and hence $r+1 = \left\lfloor \dfrac{m-1}{p} \right\rfloor + 1 > \dfrac{m-1}{p}$. The proofs when $\left\lfloor \dfrac{m-1}{p} \right\rfloor \geqslant \left\lfloor \dfrac{n-1}{q} \right\rfloor$ are analogous.

The geometric meaning of r is as follows:

Proposition 2.2.2. There exists no line $l_{(a,b)}$ that passes through more than $r+1$ lattice points in $\mathbb{L}_{mn}$.

Proof. Assume there exists a line that passes through at least $r+2$ lattice points. Then there exists a point $(a, b) \in \mathbb{L}_{mn}$ such that $(a + kp, b + kq) \in \mathbb{L}_{mn}$, where $k = 0, 1, 2, \cdots, r+1$. However,

$$m < (r+1)p + 1 \leqslant (r+1)p + a$$

Therefore, $(a + (r+1)p, b + (r+1)q)$ cannot lie in $\mathbb{L}_{mn}$. A contradiction arises. ■

Definition 2.2.3. Define the set $\mathbb{G}_i$, where $1 \leqslant i \leqslant r-1$, to be the union of two $p \times q$ rectangular sets of lattice points

$$\mathbb{G}_{i,1} = \left\{ (x, y) \in \mathbb{Z}^2 : \begin{array}{c} 1 \leqslant x \leqslant p \\ n - iq + 1 \leqslant y \leqslant n - (i-1)q \end{array} \right\} \tag{2.6}$$

$$\mathbb{G}_{i,2} = \left\{ (x, y) \in \mathbb{Z}^2 : \begin{array}{c} m - ip + 1 \leqslant x \leqslant m - (i-1)p \\ 1 \leqslant y \leqslant q \end{array} \right\} \tag{2.7}$$

We shall establish that a line of slope $\dfrac{q}{p}$ passes through i points in $\mathbb{L}_{mn}$ if and only if it passes through a point in $\mathbb{G}_i$.

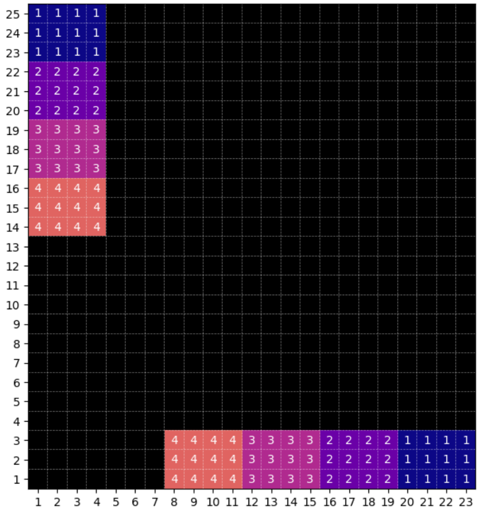

FIGURE 2.2. Visualisation of $\mathbb{G}_{1,2,3,4}$ for $m = 23, n = 25, p = 4, q = 3$. Points in $\mathbb{G}_i$ are labelled with the corresponding i.

Proposition 2.2.3. $\mathbb{G}_i \subset \mathbb{L}_{mn}$, i.e. the defined set lies entirely within the rectangular lattice.

Proof. In $\mathbb{G}_{i,1}$, $1 \leqslant x \leqslant p < m$. Meanwhile, the bounds imposed in $\mathbb{L}_{mn}$ are $1 \leqslant x \leqslant m$, so the bounds on x are satisfied.
For y, we have:

$$1 \leqslant i < r \leqslant \frac{n-1}{q} \implies iq < n-1 \implies n - iq > 1$$
$$n-(i-1)q \leqslant n-(1-1)q = n$$

Therefore, for all values of i, we have $1 < y \leqslant n$. Meanwhile, the bounds imposed in $\mathbb{L}_{mn}$ are $1 \leqslant y \leqslant n$, so the bounds on y are satisfied. We conclude that all points in the first set must be in $\mathbb{L}_{mn}$. The proof for $\mathbb{G}_{i,2}$ is analogous. ■

Proposition 2.2.4. $\mathbb{G}_{i,1} \cap \mathbb{G}_{i,2} = \emptyset$, i.e. there is no overlap between the two rectangular sets of lattice points constituting $\mathbb{G}_i$.

Proof. It is known that $pr \leqslant m-1$. Hence, $(i+1)p \leqslant pr \leqslant m-1 < m+1$.

$$ip + p < m + 1$$
$$p < m - ip + 1$$

For all points in $\mathbb{G}_{i,1}$, $x \leqslant p$, but for all points in $\mathbb{G}_{i,2}$, $x \geqslant m - ip + 1$. This is true regardless of the value of i. No x can satisfy both inequalities, so $\mathbb{G}_{i,1}$ and $\mathbb{G}_{i,2}$ are non-intersecting.

■

Proposition 2.2.5. If $(a, b) \in \mathbb{G}_i$, $l_{(a,b)}$ passes through i lattice points in $\mathbb{L}_{mn}$.

Proof. Define $P_k \overset{\text{def}}{=} (a + kp, b + kq)$. We only consider the set $\mathbb{G}_{i,1}$; For $\mathbb{G}_{i,2}$, the proof is analogous.
Note that $a \leqslant p$ in $\mathbb{G}_{i,1}$. When $k < 0$, we have $a + kp \leqslant a - p \leqslant 0$, which implies that P_k does not lie in $\mathbb{L}_{mn}$ if $k < 0$ as its x-coordinate is out of range. Additionally, since $\mathbb{G}_i \subset \mathbb{L}_{mn}$, $P_0 = (a, b)$ must lie in $\mathbb{L}_{mn}$. If $l_{(a,b)}$ passes through i lattice points, it then follows that $P_1, P_2, P_3, \cdots, P_{i-1} \in \mathbb{L}_{mn}$, but $P_i, P_{i+1}, \cdots \notin \mathbb{L}_{mn}$.

$$\begin{cases} 1 \leqslant a \leqslant p \\ n - iq + 1 \leqslant b \leqslant n - (i-1)q \end{cases} \implies \begin{cases} (i-1)p + 1 \leqslant a + (i-1)p \leqslant ip \\ n - q + 1 \leqslant b + (i-1)q \leqslant n \end{cases}$$

$$r \leqslant \left\lfloor \frac{n-1}{q} \right\rfloor \leqslant \left\lfloor \frac{m-1}{p} \right\rfloor \implies rp \leqslant m - 1$$
$$ip \leqslant (r-1)p \leqslant m - p < m$$

Hence, $1 \leqslant b + (i-1)q \leqslant n$ and $1 \leqslant a + (i-1)p < m$. Therefore, $P_{i-1} = (a+(i-1)p, b+(i-1)q) \in \mathbb{L}_{mn}$. The same argument is analogous for all $k \in [0, i-1]$. Then, we consider when $k = i$.

$$\begin{cases} 1 \leqslant a \leqslant p \\ n - iq + 1 \leqslant b \leqslant n - (i-1)q \end{cases} \implies \begin{cases} ip + 1 \leqslant a + ip \leqslant (i+1)p \\ n + 1 \leqslant b + iq \leqslant n + q \end{cases}$$

It is obvious that the y-coordinate of $(a+ip, b+iq)$ will be out of range. Therefore, $P_i \notin \mathbb{L}_{mn}$. The same argument holds for all $k \in [i, \infty)$.

■

Proposition 2.2.6. If a line $l_{(x,y)}$ passes through i lattice points on $\mathbb{L}_{mn}$, where $1 \leqslant i \leqslant r - 1$, it must pass through a lattice point $(a, b) \in \mathbb{G}_i$. (Converse of Proposition 2.2.5)

Proof. If a line $l_{(x,y)}$ passes through i lattice points on $\mathbb{L}_{mn}$, there exists a point $(a, b) \in \mathbb{L}_{mn}$ such that $(a + kp, b + kq) \in \mathbb{L}_{mn}$ only when $k \in [0, i-1]$, i.e. the following conditions are satisfied:
(1) $(a + (i-1)p, b + (i-1)q) \in \mathbb{L}_{mn}$ but $(a + ip, b + iq) \notin \mathbb{L}_{mn}$
(2) $(a - p, b - q) \notin \mathbb{L}_{mn}$
It then suffices to prove that $(a, b) \in \mathbb{G}_i$ if these conditions are satisfied.
Case I:$(a + ip, b + iq) \notin \mathbb{L}_{mn}$ because its x-coordinate exceeds the bound. This implies

$$a + (i-1)p \leqslant m < a + ip \implies m - ip + 1 \leqslant a \leqslant m - (i-1)p$$

Condition (2) implies that

$$1 \leqslant a \leqslant p \text{ or } 1 \leqslant b \leqslant q$$

Since $ip \leqslant m - p$, or equivalently $p < m - ip + 1$, $1 \leqslant a \leqslant p$ is never satisfied due to the constraint $m - ip \leqslant a$. Therefore, we conclude $1 \leqslant b \leqslant q$. The inequalities are reduced to those defining Equation 2.7.

$$\begin{cases} m - ip + 1 \leqslant a \leqslant m - (i-1)p \\ 1 \leqslant b \leqslant q \end{cases}$$

Therefore, $(a, b) \in \mathbb{G}_{i,2}$.
CASE II:Analogously, which exists when $(a + ip, b + iq) \notin \mathbb{L}_{mn}$ because its y-coordinate exceeds the bound, gives another possible set

$$\begin{cases} 1 \leqslant a \leqslant p \\ n - iq + 1 \leqslant b \leqslant n - (i-1)q \end{cases}$$

Therefore, $(a, b) \in \mathbb{G}_{i,1}$. The line must pass through a point $(a, b) \in \mathbb{G}_i$. ■

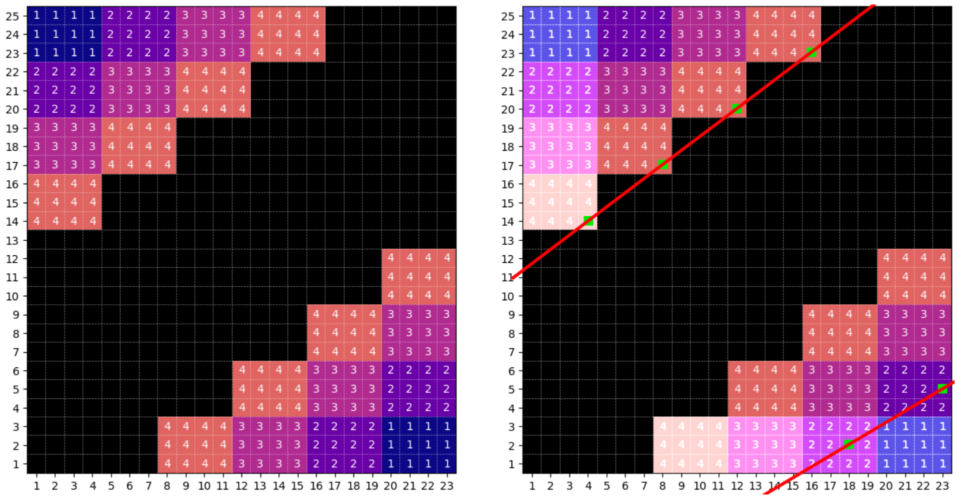

FIGURE 2.3. Each point (a, b) is labelled with a number showing how many lattice points $l_{(a,b)}$ passes through. Lines through the black points do not pass through any points in any $\mathbb{G}_i$. The original sets $\mathbb{G}_i$ are highlighted. It is obvious that a line passes through i points if and only if it passes through $\mathbb{G}_i$. $(m = 23, n = 25, p = 4, q = 3)$

Proposition 2.2.7. For two points A and $B \in \mathbb{G}_i$, the slope of AB is never equal to $\dfrac{q}{p}$ for any $1 \leqslant i \leqslant r - 1$.

Proof. $\mathbb{G}_i$ is a union of two subsets, each of which is a $p \times q$ rectangular lattice. We define two points $A(x_a, y_a)$ and $B(x_b, y_b)$ both in $\mathbb{G}_i$. When A and B belong to the same subset, $|x_a - x_b| \leqslant p - 1$ and $|y_a - y_b| \leqslant q - 1$. Since p and q are coprime, $\dfrac{q}{p}$ is irreducible, hence the numerator must be equal to or larger than q for the slope to equal $\dfrac{q}{p}$. However, since $|y_a - y_b| \leqslant q - 1$, the maximum value of the numerator of the slope cannot be larger than $q - 1$, and hence the slope can never be $\dfrac{q}{p}$.

When A and B belong to different subsets, we assume $A \in \mathbb{G}_{i,1}$ and $B \in \mathbb{G}_{i,2}$ without loss of generality. Since it is proved in Proposition 2.2.4 that $x_a < x_b$ and (analogously to the first proof) $y_a > y_b$,

$$\frac{y_a - y_b}{x_a - x_b} < 0 < \frac{q}{p}$$

Hence, the slope of AB is not equal to $\frac{q}{p}$. This implies that each line of slope $\frac{q}{p}$ passes through a point in $\mathbb{G}_i$ at most once.

■

Definition 2.2.4. Define the set $\mathbb{O} \subset \mathbb{L}_{mn}$ to be a rectangular set of lattice points satisfying

$$\{(x, y) \in \mathbb{L}_{mn} : 1 \leqslant x \leqslant m - rp, 1 \leqslant y \leqslant n - rq\} \tag{2.8}$$

We shall show below that a line of slope $\frac{q}{p}$ passes through $r + 1$ points in $\mathbb{L}_{mn}$ if and only if it passes through a point in $\mathbb{O}$.

Proposition 2.2.8. If $(a, b) \in \mathbb{O}$, $l_{(a,b)}$ passes through $r + 1$ lattice points in $\mathbb{L}_{mn}$.

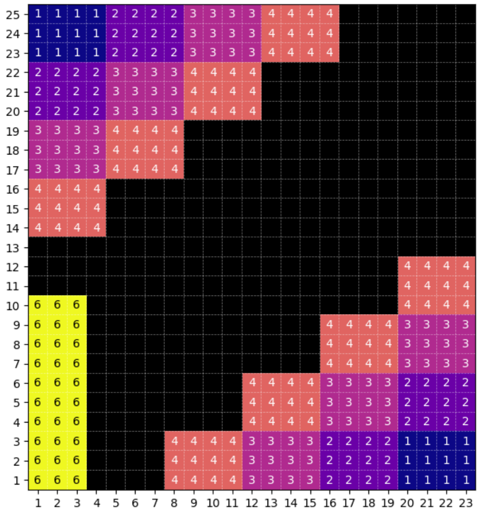

FIGURE 2.4. We add on the set $\mathbb{O}$ to Figure 2.3. Points in $\mathbb{O}$ are marked with a "6", since lines through $\mathbb{O}$ must pass through $r + 1 = \left\lfloor \frac{m-1}{p} \right\rfloor + 1 = 6$ points as proved later.

Proof. Define $P_k \stackrel{\text{def}}{=} (a + kp, b + kq)$. Since $r + 1 > \frac{m-1}{p}$, we have $rp > m - 1 - p$, giving $a < p$. For $k < 0$, the y-coordinate of P_k must be out of range, since

$P_{k,y} = a - kp \leqslant p - kp \leqslant 0 < 1$. Therefore, $P_k \in \mathbb{L}_{mn}$ only if $k \geqslant 0$. Analogously to Proposition 2.2.5, it suffices to prove that $P_r \in \mathbb{L}_{mn}$, but $P_{r+1} \notin \mathbb{L}_{mn}$.
If we add rp and rq respectively to the first and second inequalities in Equation 2.8, we obtain

$$\begin{cases} rp + 1 \leqslant a + rp \leqslant m \\ rq + 1 \leqslant b + rq \leqslant n \end{cases}$$

Therefore, $P_r = (a + rp, b + rq) \in \mathbb{L}_{mn}$.
When $k = r + 1$,

$$\begin{cases} (r+1)p + 1 \leqslant a + (r+1)p \leqslant m + p \\ (r+1)q + 1 \leqslant b + (r+1)q \leqslant n + q \end{cases}$$

Since $a + (r+1)p > \dfrac{m-1}{p}p + a \geqslant m$, the x-coordinate of P_{r+1} is out of range and we conclude that $P_{r+1} \notin \mathbb{L}_{mn}$. Therefore, $l_{(a,b)}$ passes through $r + 1$ lattice points $P_{0,1,\cdots,r}$.

■

Proposition 2.2.9. If a line passes through $r + 1$ lattice points on $\mathbb{L}_{mn}$, it must pass through a lattice point $(a, b) \in \mathbb{O}$. (Converse of Proposition 2.2.8)

Proof. Similar to Proposition 2.2.6, there exists a point $(a, b) \in \mathbb{L}_{mn}$ such that $(a + rp, b + rq) \in \mathbb{L}_{mn}$ but $(a + (r+1)p, b + (r+1)q) \notin \mathbb{L}_{mn}$.
This condition implies that the line passes through at least $r+1$ points; and due to Proposition 2.2.2, the line must pass through exactly $r+1$ points. It again suffices to prove that $(a, b) \in \mathbb{O}$ if the condition is met.
Case I: $(a + (r+1)p, b + (r+1)q) \notin \mathbb{L}_{mn}$ because its x-coordinate exceeds the bound.

$$\begin{cases} a + rp \leqslant m < a + (r+1)p \\ b + rq \leqslant n \\ a \geqslant 1 \text{ and } b \geqslant 1 \end{cases}$$

Rearranging gives

$$\begin{cases} \max(m - (r+1)p + 1, 1) \leqslant a \leqslant m - rp \\ 1 \leqslant b \leqslant n - rq \end{cases}$$

Case II: $(x + (r+1)p, y + (r+1)q) \notin \mathbb{L}_{mn}$ because its y-coordinate exceeds the bound. We obtain the equations

$$\begin{cases} 1 \leqslant a \leqslant m - rp \\ \max(n - (r+1)q + 1, 1) \leqslant b \leqslant n - rq \end{cases}$$

A line passes through $r + 1$ points only if it satisfies either Case I or Case II. Combining the two inequalities:

$$\begin{cases} 1 \leqslant a \leqslant m - rp \\ 1 \leqslant b \leqslant n - rq \end{cases}$$

These are identical to the inequalities defining $\mathbb{O}$; Therefore, the line must pass through a point $(a, b) \in \mathbb{O}$.

■

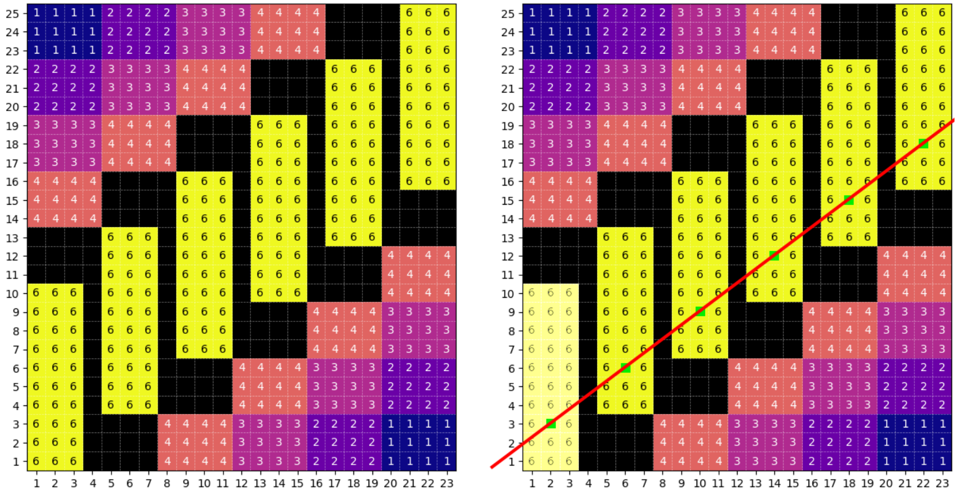

FIGURE 2.5. Similar to Figure 2.3, but including lines passing through $\mathbb{O}$. The original set $\mathbb{O}$ is highlighted. One sees immediately that lines pass through $r+1$ points if and only if they pass through $\mathbb{O}$. Lines through the remaining unlabelled points pass through 5 lattice points.

2.2.2. *Defining the counting function.*

Definition 2.2.5. Define $N_{(p,q)}(i)$ as the number of distinct lines with slope $\frac{q}{p}$ that pass through i lattice points lying on $\mathbb{L}_{mn}$.

Proposition 2.2.10. $N_{(p,q)}(i) = 2pq$ for $i \in [1, r-1]$

Proof. Proposition 2.2.7 shows that there is an injection from points in $\mathbb{G}_i$ to lines passing through i points, for the same line cannot pass through more than one point in the same $\mathbb{G}_i$.
In Proposition 2.2.6, it was proved that if a line passes through i lattice points lying on $\mathbb{L}_{mn}$, it must pass through at least one point $(a, b) \in \mathbb{G}_i$, i.e. there is a surjection from points in $\mathbb{G}_i$ to lines passing through i points. If both an injection and surjection exist from one set to another, there must be a bijection between them; We conclude that $N_{(p,q)}(i) = |\mathbb{G}_i|$. As visualised in Figure 2.2, each of $\mathbb{G}_{i,1}$ and $\mathbb{G}_{i,2}$ is a $p \times q$ rectangle of lattice points and hence $|\mathbb{G}_{i,1}| = |\mathbb{G}_{i,2}| = pq$; From Proposition 2.2.4, we have $|\mathbb{G}_i| = |\mathbb{G}_{i,1}| + |\mathbb{G}_{i,2}| - |\mathbb{G}_{i,1} \cap \mathbb{G}_{i,2}| = pq + pq - 0 = 2pq$. The bijection between then is intuitively $(a, b) \in \mathbb{G}_i \to l_{(a,b)}$.

∎

Proposition 2.2.11. $N_{(p,q)}(r+1) = (m - rp)(n - rq)$

Proof. $\mathbb{O}$ is a $(m - rp) \times (n - rq)$ rectangular lattice, so the maximum difference in y-coordinate between any two points is $n - rq - 1$. We note that

$n - rq - 1 < n - 1 - \left(\frac{n-1}{q} - 1\right)q = q$, so the slope of the line passing through any two points in $\mathbb{O}$ cannot equal $\frac{q}{p}$.

From Propositions 2.2.8 and 2.2.9, we then conclude that $N_{(p,q)}(r+1) = |\mathbb{O}| = (m - rp)(n - rq)$. The proof is analogous to that in Proposition 2.2.10. ∎

Proposition 2.2.12. $N_{(p,q)}(r) = pq - mn + mqr + mq - 2pqr + npr + np - pqr^2$

Proof. For every lattice point (a, b), there is one and only one unique line $l_{(a,b)}$ that passes through it. Therefore, the total number of lattice points should equal the sum of the number of points each unique line passes through.

$$\sum_{i=1}^{r-1} iN_{(p,q)}(i) + rN_{(p,q)}(r) + (r+1)N_{(p,q)}(r+1) = mn$$

Where we can be sure that $N_{(p,q)}(i) = 0$ for $i > r+1$ due to Proposition 2.2.2. After simplification,

$$N_{(p,q)}(r) = pq - mn + mqr + mq - 2pqr + nqr + np - pqr^2$$

∎

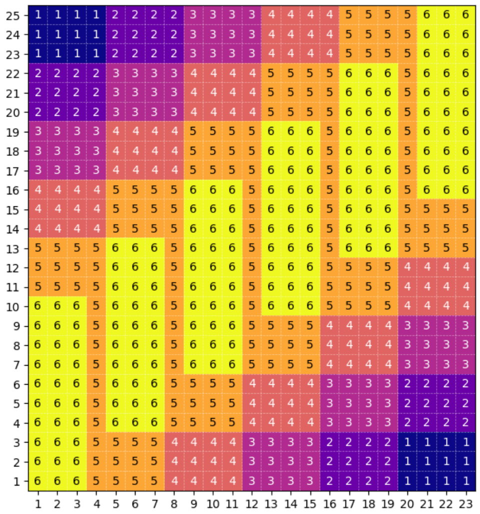

FIGURE 2.6. Figure 2.5 with the rest of the lattice points labelled.

Definition 2.2.6. Define $S(p, q)$ as the total number of collinear triples in $\mathbb{L}_{mn}$ such that the slope of line joining them is $\frac{q}{p}$. p and q are assumed to be positive coprime integers.

Theorem 2.2.1.

$$S(p,q) = \frac{r(r-1)}{12}[6mn - 4(qm+pn)(r+1) + pq(r+1)(3r+2)]$$

Proof. If a line passes through i points, collinear triples can be formed by choosing 3 points out of the i points arbitrarily. Therefore the total number of collinear triples is

$$S(p,q) = \sum_{i=3}^{r+1} \binom{i}{3} N_{(p,q)}(i)$$

After simplification,

$$S(p,q) = \frac{r(r-1)}{12}[6mn - 4(qm+pn)(r+1) + pq(r+1)(3r+2)] \tag{2.9}$$

■

2.3. Evaluating the probability of collinearity.

Definition 2.3.1. Define N_{col} to be the number of collinear triples in $\mathbb{L}_{mn}$ that do not lie on a vertical or horizontal line.

$$N_{\text{col}} \stackrel{\text{def}}{=} \sum_{\substack{p\in[1,\lfloor\frac{m-1}{2}\rfloor] \\ q\in[1,\lfloor\frac{n-1}{2}\rfloor] \\ gcd(p,q)=1}} 2S(p,q) \tag{2.10}$$

The upper bounds on p and q are defined as such, since if p and q are any larger, the line will not pass through more than 2 points and hence no collinear triples are possible. The factor of 2 is to count the negative slopes as well (for each line with positive slope, there is exactly one corresponding line with negative slope).

$S(p,q)$ is piecewise, as $r = \min\left(\left\lfloor\frac{m-1}{p}\right\rfloor, \left\lfloor\frac{n-1}{q}\right\rfloor\right)$ shows different behaviour in two regions of p,q-space where $\frac{m-1}{p} \leqslant \frac{n-1}{q}$ and where $\frac{m-1}{p} \geqslant \frac{n-1}{q}$ respectively. We shall define the crossover point q_{max} as the maximum q for which the first inequality holds:

$$q_{max} = \left\lfloor \frac{n-1}{m-1} p \right\rfloor \tag{2.11}$$

Therefore, we split the summation into two regions, then subtract double counted parts where $\frac{m-1}{p} = \frac{n-1}{q}$ *exactly*. There is only one double-counted coordinate, which is at $p' = \frac{m-1}{\gcd(m-1,n-1)}$ and $q' = \frac{n-1}{\gcd(m-1,n-1)}$.

$$\left(\sum_{p=1}^{\lfloor\frac{m-1}{2}\rfloor} \sum_{\substack{q=1 \\ gcd(p,q)=1}}^{\lfloor\frac{n-1}{m-1}p\rfloor} S(p,q)\right) + \left(\sum_{q=1}^{\lfloor\frac{n-1}{2}\rfloor} \sum_{\substack{p=1 \\ gcd(p,q)=1}}^{\lfloor\frac{m-1}{n-1}q\rfloor} S(p,q)\right) - S(p',q') \tag{2.12}$$

We will consider only the first term of the summation. The derivation for the second term is similar. We shall prove the last term is negligible (as well as justify other approximations we make) in Appendix A.
We are evaluating the sum in the asymptotic limit where m and n are very large; Therefore, we assume $m-1 \approx m$, $n-1 \approx n$, and $r = \left\lfloor \frac{m-1}{p} \right\rfloor \approx \frac{m}{p}$. This leaves us with

$$\begin{aligned}
&\sum_{p=1}^{\left\lfloor \frac{m-1}{2} \right\rfloor} \sum_{\substack{q=1 \\ gcd(p,q)=1}}^{\left\lfloor \frac{n-1}{m-1} p \right\rfloor} S(p,q) \\
\approx &\sum_{p=1}^{\left\lfloor \frac{m-1}{2} \right\rfloor} \sum_{\substack{q=1 \\ gcd(p,q)=1}}^{\left\lfloor \frac{n}{m} p \right\rfloor} \frac{r(r-1)}{12}(6mn - (4(qm+pn) + pq(3r+2))(r+1)) \\
\approx &\sum_{p=1}^{\left\lfloor \frac{m-1}{2} \right\rfloor} \sum_{\substack{q=1 \\ gcd(p,q)=1}}^{\left\lfloor \frac{n}{m} p \right\rfloor} \frac{m^2}{12p^2}\left(6mn - \frac{4(qm+pn)m}{p} + \frac{3m^2q}{p}\right) \\
= &\sum_{p=\left\lceil \frac{m}{n} \right\rceil}^{\left\lfloor \frac{m-1}{2} \right\rfloor} \sum_{\substack{q=1 \\ gcd(p,q)=1}}^{\left\lfloor \frac{n}{m} p \right\rfloor} \left(\frac{m^3n}{6p} - \frac{m^4q}{12p^2}\right)
\end{aligned}$$

We have replaced the lower bound in the summation of p because $\left\lfloor \frac{n}{m} p \right\rfloor = 0$ if $p < \left\lceil \frac{m}{n} \right\rceil$.
This sum is intractable without approximations. We shall employ the following theorem:

Theorem 2.3.1. We can make the approximation that

$$\sum_{\substack{q=1 \\ gcd(p,q)=1}}^{q_{max}} \left(\frac{m^3n}{6p} - \frac{m^4q}{12p^2}\right) \approx \frac{\varphi(p)}{p} \sum_{q=1}^{q_{max}} \left(\frac{m^3n}{6p} - \frac{m^4q}{12p^2}\right) \tag{2.13}$$

Where $\varphi(p)$, Euler's totient function, counts the number of integers less than p which are coprime to it. It can be defined by a product over the prime numbers

$$\varphi(n) = n \prod_{p|n} \left(1 - \frac{1}{p}\right) \tag{2.14}$$

This approximation basically assumes that the distribution of integers coprime to p is uniform. A full proof of this theorem is given in Appendix A.3, as it is quite lengthy.

The sum now becomes

$$\sum_{p=\lceil \frac{m}{n} \rceil}^{\lfloor \frac{m-1}{2} \rfloor} \sum_{\substack{q=1 \\ \gcd(p,q)=1}}^{\lfloor \frac{n}{m}p \rfloor} \left(\frac{m^3 n}{6p} - \frac{m^4 q}{12p^2} \right) \approx \sum_{p=\lceil \frac{m}{n} \rceil}^{\lfloor \frac{m-1}{2} \rfloor} \frac{m^3 \varphi(p)}{6p^2} \sum_{q=1}^{\lfloor \frac{n}{m}p \rfloor} \left(n - \frac{mq}{2p} \right)$$

$$\approx \sum_{p=\lceil \frac{m}{n} \rceil}^{\lfloor \frac{m-1}{2} \rfloor} \frac{m^3 \varphi(p)}{6p^2} \left(n \left\lfloor \frac{n}{m} p \right\rfloor - \frac{m \left\lfloor \frac{n}{m} p \right\rfloor^2}{4p} \right)$$

$$\approx \sum_{p=\lceil \frac{m}{n} \rceil}^{\lfloor \frac{m-1}{2} \rfloor} \frac{m^2 n^2 \varphi(p)}{8p^2}$$

Theorem 2.3.2. (Proved in [5])

$$\sum_{m=1}^{n} \frac{\varphi(m)}{m^2} = \frac{6}{\pi^2} \ln n + O(1)$$

Therefore, the final sum works out to be

$$\sum_{p=\lceil \frac{m}{n} \rceil}^{\lfloor \frac{m-1}{2} \rfloor} \frac{m^2 n^2 \varphi(p)}{8p^2} = \frac{m^2 n^2}{8} \left(\sum_{p=1}^{\lfloor \frac{m-1}{2} \rfloor} \frac{\varphi(p)}{p^2} - \sum_{p=1}^{\lceil \frac{m}{n} \rceil - 1} \frac{\varphi(p)}{p^2} \right)$$

$$\approx \frac{3m^2 n^2}{4\pi^2} \left(\ln \left\lfloor \frac{m-1}{2} \right\rfloor - \ln \left\lceil \frac{m}{n} \right\rceil + O(1) \right)$$

$$\approx \frac{3m^2 n^2}{4\pi^2} \left(\ln \frac{m}{\lceil \frac{m}{n} \rceil} + O(1) \right)$$

$$\approx \frac{3m^2 n^2}{4\pi^2} \ln(\min(m,n)) + O(m^2 n^2)$$

A full analysis of all errors introduced in the approximations is given in Appendix A, where we prove that the total order of errors is still $O(m^2 n^2)$.

Now, consider the second double-summation term in Equation 2.12. The derivation is completely the same and we arrive at

$$\sum_{q=1}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{\substack{p=1 \\ gcd(p,q)=1}}^{\lfloor \frac{m-1}{n-1} q \rfloor} S(p,q) = \frac{3m^2 n^2}{4\pi^2} \ln(\min(m,n))$$

$$N_{\text{col}} = 2 \left(\sum_{p=1}^{\lfloor \frac{m-1}{2} \rfloor} \sum_{\substack{q=1 \\ gcd(p,q)=1}}^{\lfloor \frac{n-1}{m-1} p \rfloor} S(p,q) + \sum_{q=1}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{\substack{p=1 \\ gcd(p,q)=1}}^{\lfloor \frac{m-1}{n-1} q \rfloor} S(p,q) \right)$$

$$= 2 \left(\frac{3m^2 n^2}{4\pi^2} \ln(\min(m,n)) + \frac{3m^2 n^2}{4\pi^2} \ln(\min(m,n)) \right) + O(m^2 n^2)$$

$$= \frac{3m^2 n^2}{\pi^2} \ln(\min(m,n)) + O(m^2 n^2)$$

Without loss of generality, we assume $m < n$ to reduce the equation to

$$N_{\text{col}} = \frac{3}{\pi^2} m^2 n^2 \ln m + O(m^2 n^2) \tag{2.15}$$

Definition 2.3.2. Define P_{col} to be the probability that three randomly chosen points from $\mathbb{L}_{mn}$ is a collinear triple which is not horizontal or vertical.

Substituting our result for N_{col}, we get

$$P_{\text{col}} = \frac{N_{\text{col}}}{\binom{mn}{3}} = \frac{18}{\pi^2} \frac{\ln m}{mn} + O\left(\frac{1}{mn}\right) \tag{2.16}$$

2.3.1. *Probabilistic lower bound on n for maximal solutions to exist.*

Definition 2.3.3. Define Ω be the number of ways to place 2 points on each column such that no rows have more than 2 points on them.

Theorem 2.3.3. $\ln \Omega = 2m \ln n + O(m)$

Proof. There are $\binom{n}{2}$ ways to choose 2 points on each column. Neglecting the requirement on rows, the upper bound on $\ln \Omega$ is

$$\ln \Omega = \ln \binom{n}{2}^m \approx 2m \ln n - m \ln 2 = 2m \ln n + O(m) \tag{2.17}$$

Now, suppose that we place $2m$ points, 2 on each column, sequentially from the top to the bottom. We call a row "occupied" if it already has 2 points placed on it. The maximum number of occupied rows when placing points on the k-th column (starting from column 0) is k, so the lower bound for $\ln \Omega$ is

$$\begin{aligned}
\ln \Omega = \ln \prod_{k=0}^{m} \binom{n-k}{2} &\approx \sum_{k=0}^{m} (2 \ln(n-k) - \ln 2) \\
&\approx -m \ln 2 + 2 \int_{n-m}^{n} \ln(u) du \\
&= 2(n \ln n - (n-m) \ln(n-m)) - (2 + \ln 2)m \\
&= 2\left(m \ln n - (n-m) \ln\left(1 - \frac{m}{n}\right)\right) + O(m)
\end{aligned}$$

Note that the upper bound established in Theorem 2.1.3 implies that m and n differ by at most a factor of around 2, so $(n-m) \ln \left(1 - \frac{m}{n}\right)$ is at most an $O(m)$ term (save for a singularity that only occurs if $m = n$). Both methods therefore yield, without conflict,

$$\ln \Omega \approx 2m \ln n + O(m) \tag{2.18}$$

■

Theorem 2.3.4. We follow Guy and Kelly's argument in [4] that the expected number of ways to place $2m$ points on an $m \times n$ grid such that no three points are collinear is estimated by

$$\omega = \Omega(1 - P_{\text{col}})^{\binom{2m}{3}}$$

where the second term is the probability that all placed points are not collinear, assuming that the probability that any 3 chosen points are not collinear is independent.

While the assumption of independence is obviously incorrect, it would be unfeasible to do the calculations taking into account the correlation; Further analysis conducted in [5] suggests that approximating the events as independent provides a good upper bound.

We extend the result of [5], simulating the placement of n points in an $n \times n$ grid and calculating the empirical probability P_{actual} that no collinear triples exist in the set of points. Noting that only $\ln \omega$ will be considered below, we find the relative error between $\ln P_{predicted} \overset{\text{def}}{=} \binom{n}{3} \ln(1 - P_{\text{col}})$ and $\ln P_{actual}$. The code for this is given in Appendix C.1.

n	$-\ln P_{predicted}$	$-\ln P_{actual}$	Relative Error
8	1.03	2.15	-52.0%
10	1.71	3.37	-49.2%
12	2.49	4.65	-46.4%
14	3.42	6.07	-43.7%
16	4.42	7.48	-41.0%
18	5.50	9.02	-39.0%
20	6.63	10.50	-36.9%
22	7.88	12.18	-35.3%
24	9.12	13.78	-33.8%
26	10.49	15.62	-32.9%

The relative error can be seen to decrease as n becomes larger, and possibly approaching 0 asymptotically as $n \to \infty$; Testing for $n > 26$ or Points Placed $> n$ is unfortunately unfeasible due to hardware limitations.

Here, we can begin our argument in favour of Conjecture 1.

Note that, if a solution to the problem is to be expected, we have $\omega \approx 1$, i.e. $\ln \omega = 0$. We may use this fact to solve for the critical value of n. First, suppose $n = \beta m$ for some $\beta > 1$. It is known from the prerequisites section that $\beta < 2 + o(1)$ as m, n become very large.

$$\begin{aligned}
2m \ln \beta m + O(m) + \binom{2m}{3} \ln(1 - P_{\text{col}}) &= 0 \\
12m \ln m + 12m \ln \beta + O(m) - (8m^3)(P_{\text{col}} + O(P_{\text{col}}^2)) &= 0 \\
3 \ln m + O(1) - 2m^2 \left(\frac{18}{\pi^2} \frac{\ln m}{\beta m^2} \right) &= 0
\end{aligned}$$

$$1-\frac{12}{\pi^2\beta}+O\left(\frac{1}{\ln m}\right)=0$$

$$\beta=\frac{12}{\pi^2}+O\left(\frac{1}{\ln m}\right)\approx 1.2159 \tag{2.19}$$

Thus, maximal solutions should be expected to exist only for $n>\frac{12}{\pi^2}m$ as m becomes very large.

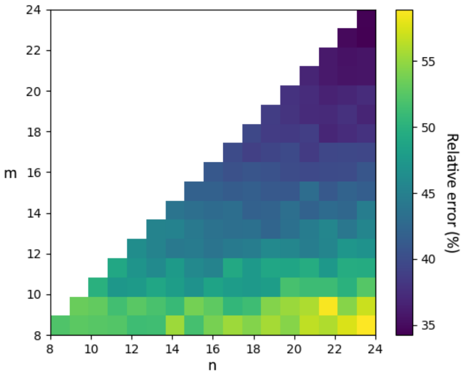

FIGURE 2.7. Plot of the relative error between $\ln P_{predicted}$ and $\ln P_{actual}$ for $n\in[8,24]$ and $m\in[8,n]$. It can be seen that the relative error increases as the ratio $\frac{n}{m}$ increases, i.e. we overestimate the expected number of solutions by a wider margin, and the real number of solutions expected should be even lower than our estimate. This suggests that $\frac{12}{\pi^2}m$ is a valid lower bound, although again empirical testing for large m,n is not possible due to hardware limitation. Code for the testing is given in Appendix C.1.

2.3.2. *Probabilistic bound on the number of points that can be placed on any rectangular board.*

If $n>\frac{12}{\pi^2}m$, the expected number of points is simply the trivial bound $f_{mn}=2m$, so we look only at $m\leqslant n\leqslant\frac{12}{\pi^2}m$.

Definition 2.3.4. Define Ω' to be the number of ways to place f_{mn} points on the grid such that no three points lie on the same row or column.

As established in Equation 2.18, the order of $\ln\Omega$ does not change significantly if we count contributions from the rows or columns. Therefore, we can approximate $\ln\Omega'\approx\ln\binom{mn}{f_{mn}}$. Using Stirling's approximation:

$$
\begin{aligned}
&\ln \Omega' \\
&= mn\ln(mn) - f_{mn}\ln f_{mn} - (mn - f_{mn})\ln(mn - f_{mn}) + O(\ln(mn)) \\
&= mn\ln(mn) - f_{mn}\ln f_{mn} - (mn - f_{mn})\left(\ln(mn) + O\left(\frac{f_{mn}}{mn}\right)\right) + O(\ln(mn)) \\
&= f_{mn}\ln(mn) - f_{mn}\ln f_{mn} + O(f_{mn})
\end{aligned}
$$

We begin our argument in favour of Conjecture 2.

Proof. We repeat a similar derivation to the argument in favour of the first part of the conjecture:

$$
\begin{aligned}
f_{mn}\ln(mn) - f_{mn}\ln f_{mn} + O(f_{mn}) + \binom{f_{mn}}{3}\ln(1 - P_{\text{col}}) = 0 \\
6(\ln(mn) - \ln f_{mn}) + O(1) - f_{mn}^2\left(\frac{18}{\pi^2}\frac{\ln m}{mn} + O\left(\frac{1}{mn}\right)\right) = 0
\end{aligned}
$$

Note that m and n differ by at most a constant factor of $\frac{12}{\pi^2}$, so we can suppose $2\ln m = \ln mn + O(1)$, which does not change the order of the error. Let $f_{mn} = \sqrt{\gamma mn}$. Then the expression simplifies to

$$
g(\gamma) \overset{\text{def}}{=} 1 - \frac{\ln\gamma}{\ln(mn)} - \frac{3}{\pi^2}\gamma + \frac{C_1 + C_2\gamma}{\ln(mn)} = 0
$$

Where C_1 and C_2 are bounds for the error terms. We can solve the above equation for γ using Newton's method. We define $\frac{1}{\eta} \overset{\text{def}}{=} \ln(mn)$ and make an initial guess $\gamma_0 = \frac{\pi^2}{3}$.

$$
\begin{aligned}
g'(\gamma) &= -\frac{\eta}{\gamma} - \frac{3}{\pi^2} + \eta C_2 \\
\gamma_1 &= \gamma_0 + \eta\frac{C_1 + C_2\gamma_0 - \ln\gamma_0}{\frac{3}{\pi^2} + \eta(\frac{1}{\gamma_0} - C_2)} \\
&= \gamma_0 + O\left(\frac{1}{\ln(mn)}\right)
\end{aligned}
$$

Therefore, we conclude that $\gamma = \gamma_0 + O\left(\frac{1}{\ln(mn)}\right)$. Thus, we have $f_{mn} = \frac{\pi}{\sqrt{3}}\sqrt{mn} + O\left(\frac{\sqrt{mn}}{\ln mn}\right)$. If we solve $\frac{\pi}{\sqrt{3}}\sqrt{mn} = 2m$ for n, we obtain $n = \frac{12}{\pi^2}m$, which agrees with Conjecture 1. If we substitute $n = m$, we return Guy and Kelly's result in [4] that the expected value of f_{nn} is $\frac{\pi}{\sqrt{3}}n$ for large n. (An arithmetic error was made by Guy and Kelly, so the result written in [4] is not $\frac{\pi}{\sqrt{3}}n$; A corrected version is mentioned in [5].)

■

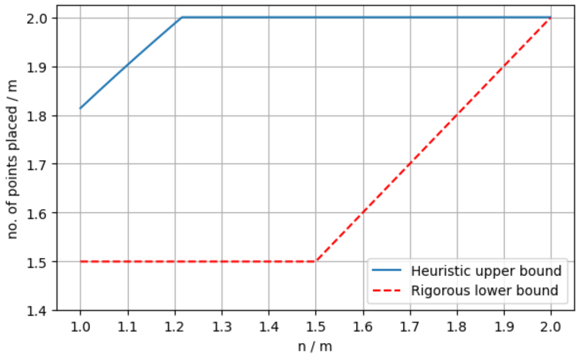

FIGURE 2.8. The solid line shows a plot of the expected upper bound on the number of points that can be placed based on Conjecture 2, while the dashed line shows the highest known lower bound based on Theorems 2.1.2 and 2.1.3

3. No-Three-in-Line problem in 3D

3.1. Preliminaries for counting collinear triples in 3D.

In the investigation of collinear triples for 2D rectangular lattice in Section 2.2, we focused only on the behaviour of lines with a specific slope. Analogously, we only focus on lines with a specific direction vector in this section.

Definition 3.1.1. We define $l_{(a,b,c)}$ as a line that passes through $(a, b, c) \in \mathbb{T}_n$ with direction vector $\vec{s} = (s_1, s_2, s_3)$, where $s_1, s_2, s_3 \in \mathbb{Z}^+$ and $\gcd(s_1, s_2, s_3) = 1$.

Similar to Section 2.2, we only consider lines with $1 \leqslant s_1, s_2, s_3 \leqslant n - 1$.

Proposition 3.1.1. $l_{(a,b,c)}$ passes through another $(x, y, z) \in \mathbb{T}_n$ if and only if there exists a integer k such that $(x, y, z) = (a, b, c) + \vec{s}k$.

Proof. If $l_{(a,b,c)}$ passes through (x, y, z), there exists a *real number* k such that

$$\frac{x-a}{s_1} = \frac{y-b}{s_2} = \frac{z-c}{s_3} = k$$

Suppose k is not an integer. Since $a, b, c, x, y, z, s_1, s_2, s_3 \in \mathbb{Z}$, k must at least be rational and may be expressed as an irreducible fraction $\frac{q}{p}$. This implies that $p|s_1$, $p|s_2$ and $p|s_3$, violating the definition that s_1, s_2, s_3 must be coprime unless $p = 1$, i.e. $k \in \mathbb{Z}$. The converse can be proved trivially, by substituting $(a + ks_1, b + ks_2, c + ks_3)$ into the equation of $l_{(a,b,c)}$. ∎

Definition 3.1.2. We define, analogously to Definition 2.2.2,

$$r = \min\left(\left\lfloor \frac{n-1}{s_1} \right\rfloor, \left\lfloor \frac{n-1}{s_2} \right\rfloor, \left\lfloor \frac{n-1}{s_3} \right\rfloor\right) \tag{3.1}$$

Without loss of generality, we may assume $s_1 \leqslant s_2 \leqslant s_3$. Hence, $r = \lfloor \frac{n-1}{s_3} \rfloor$. It follows that

$$s_3(r+1) > n-1 \tag{3.2}$$

Proposition 3.1.2. There exists no $l_{(a,b,c)}$ that passes through more than $r+1$ points in $\mathbb{T}_n$.

Proof. The proof is analogous to Proposition 2.2.2. Assume there exists a line that passes through at least $r+2$ lattice points. Then there exists a point $(a,b,c) \in \mathbb{T}_n$ such that $(a+ks_1, b+ks_2, c+ks_3) \in \mathbb{T}_n$, where $k = 0,1,2,\cdots,r+1$. However,

$$n < (r+1)s_3 + 1 \leqslant c + (r+1)s_3$$

Therefore, $(a+(r+1)s_1, b+(r+1)s_2, c+(r+1)s_3) \notin \mathbb{T}_n$. A contradiction arises. ■

Definition 3.1.3. Define the set $\mathbb{G}_i$ $(1 \leqslant i \leqslant r-1)$ to be the union of 6 cuboid sets of lattice points, one for each permutation π of $1,2,3$. This is analogous to Definition 2.2.3 for the 2D case.

$$\mathbb{G}_{i,\pi} = \left\{ (x_1,x_2,x_3) \in \mathbb{T}_n : \begin{array}{r} 1 \leqslant x_{\pi(1)} \leqslant n-(i-1)s_{\pi(1)} \\ 1 \leqslant x_{\pi(2)} \leqslant s_{\pi(2)} \\ n-is_{\pi(3)}+1 \leqslant x_{\pi(3)} \leqslant n-(i-1)s_{\pi(3)} \end{array} \right\} \tag{3.3}$$

Proposition 3.1.3. $\mathbb{G}_i \subset \mathbb{T}_n$. The proof follows analogously from Proposition 2.2.3.

Proposition 3.1.4. Consider two different permutations π_1 and π_2; $\mathbb{G}_{i,\pi_1}$ and $\mathbb{G}_{i,\pi_2}$ are non-intersecting if $\pi_1(3) = \pi_2(2)$ or $\pi_1(2) = \pi_2(3)$.

Proof. We consider only $\pi_1 = (1,2,3)$; The proof is analogous for other choices of π_1.
For any point in $\mathbb{G}_{i,\pi_1}$, we have $x_2 \leqslant s_2$. This rules out possible intersections with the the sets where $\pi_2(3) = 2$, since $n - is_2 + 1 \geqslant n - (r-1)s_2 + 1 \geqslant n + 1 - (n-1) + s_2 = s_2 + 2$, i.e. $x_2 \geqslant s_2 + 2$ for any point in $\mathbb{G}_{i,\pi_2}$ regardless of i. Obviously, this contradicts $x_2 \leqslant s_2$. Similarly, $x_3 \geqslant s_3 + 2$ for any point in $\mathbb{G}_{i,\pi_1}$ regardless of i. This rules out intersections with any sets where $\pi_2(2) = 3$, since in that case $x_3 \leqslant s_3$ for any i. ■

Proposition 3.1.5. $|\mathbb{G}_i| = 2n(s_1s_2 + s_1s_3 + s_2s_3) - 6is_1s_2s_3$

Proof. Again, we consider only $\pi_1 = (1,2,3)$; The proof is analogous for other choices of π_1. As established in Proposition 3.1.4, there are only two sets whose intersection we need to consider: The permutations $(3,2,1)$ and $(2,1,3)$.
For the permutation $(2,1,3)$, we take the intersection of two sets of inequalities:

$$\mathbb{G}_{i,\pi_1} \cap \mathbb{G}_{i,\pi_2} = \left\{ \begin{array}{c} 1 \leqslant x_1 \leqslant n-(i-1)s_1 \\ 1 \leqslant x_2 \leqslant s_2 \\ n-is_3+1 \leqslant x_3 \leqslant n-(i-1)s_3 \end{array} \right\}$$

$$\cap \left\{ \begin{array}{c} 1 \leqslant x_1 \leqslant s_1 \\ 1 \leqslant x_2 \leqslant n-(i-1)s_2 \\ n-is_3+1 \leqslant x_3 \leqslant n-(i-1)s_3 \end{array} \right\}$$

Noticing again that $s_k < n-(i-1)s_k$, this is reduced to

$$\begin{array}{c} 1 \leqslant x_1 \leqslant s_1 \\ 1 \leqslant x_2 \leqslant s_2 \\ n-is_3+1 \leqslant x_3 \leqslant n-(i-1)s_3 \end{array}$$

Repeating the same procedure for permutation $(3,2,1)$, we have:

$$\begin{array}{c} n-is_1+1 \leqslant x_1 \leqslant n-(i-1)s_1 \\ 1 \leqslant x_2 \leqslant s_2 \\ n-is_3+1 \leqslant x_3 \leqslant n-(i-1)s_3 \end{array}$$

Repeating this for all permutations π_1, we get 6 such sets of $s_1 \times s_2 \times s_3$ overlapping lattice points.

■

We shall make the following definition to facilitate the proof of the proposition:

Definition 3.1.4. Define the set $\mathbb{G}_\cap(a_1,a_2,a_3)$, where $a_1,a_2,a_3 \in \{0,1\}$ as follows:

$$\left\{ (x_1,x_2,x_3) \in \mathbb{T}_n : \begin{array}{cc} 1 \leqslant x_k \leqslant s_k & \text{if } a_k = 0 \\ n-is_k+1 \leqslant x_k \leqslant n-(i-1)s_k & \text{if } a_k = 1 \end{array} \ \forall\, k \in \{1,2,3\} \right\}$$

Each $\mathbb{G}_\cap(\{0,1\}^3)$ corresponds to one set of overlapping lattice points, except for $\mathbb{G}_\cap(0,0,0)$ and $\mathbb{G}_\cap(1,1,1)$ which do not correspond to any.
Note that two of the sets are different if at least one of a_1,a_2,a_3 are different between them. Suppose we have $a_u = 0$ in the first and $a_u = 1$ in the second, with $u \in \{1,2,3\}$. For all points in the first set, we have $x_u \leqslant s_u$, and for all points in the second set, we have $x_u \geqslant n - is_u + 1$; As established, $s_u < n - is_u + 1$ in all cases, so a point cannot be in both sets simultaneously. More generally,

$$(a_1,a_2,a_3) \neq (b_1,b_2,b_3) \implies \mathbb{G}_\cap(a_1,a_2,a_3) \cap \mathbb{G}_\cap(b_1,b_2,b_3) = \emptyset$$

i.e. No point in $\mathbb{T}_n$ can be in more than two $\mathbb{G}_{i,\pi}$. Therefore, invoking the inclusion-exclusion principle: $|\mathbb{G}_i|$

$$= 2((n-(i-1))s_1)s_2s_3 + (n-(i-1))s_2)s_1s_3 + (n-(i-1))s_3)s_1s_2) - 6s_1s_2s_3$$
$$= 2n(s_1s_2 + s_1s_3 + s_2s_3) - 6is_1s_2s_3$$

Proposition 3.1.6. A line of direction vector $\vec{s}$ passes through i points in $\mathbb{T}_n$, where $1 \leqslant i \leqslant r-1$, if and only if it passes through a point in $\mathbb{G}_i$.

The proof follows analogously from Propositions 2.2.5 and 2.2.6.

Proposition 3.1.7. A line with direction vector $\vec{s}$ only passes through at most 1 point in $\mathbb{G}_i$.

Proof. Suppose a point $\vec{r} = (x_1, x_2, x_3) \in \mathbb{G}_{i,\pi}$ for some π. We know that other points on the line $l_{\vec{r}}$ are of the form $\vec{P}_k \overset{\text{def}}{=} \vec{r}+\vec{s}k$ for some integer k. Note that points with $k < 0$ are not in $\mathbb{G}_i$, since then $x_{\pi(2)} - ks_{\pi(2)} \leqslant x_{\pi(2)} - s_{\pi(2)} \leqslant s_{\pi(2)} - s_{\pi(2)} = 0$, which implies that $\vec{P}_k$ must lie outside $\mathbb{T}_n$ and hence outside $\mathbb{G}_i$ as well. Also, note that we have the condition

$$\max_{(x_1,x_2,x_3)\in\mathbb{G}_i} x_{\pi(3)} \leqslant n - (i-1)s_{\pi(3)}$$

regardless of what π is. This also implies that $\vec{P}_k$ does not lie in $\mathbb{G}_i$ for $k > 0$, since then $x_{\pi(3)} + ks_{\pi(3)} \geqslant x_{\pi(3)} + s_{\pi(3)} \geqslant n - (i-1)s_{\pi(3)} + 1 > n - (i-1)s_{\pi(3)}$. It then follows that $\vec{P}_0$ is the only point in the family of points $\vec{P}$ which is in $\mathbb{G}_i$, thus proving the proposition. ∎

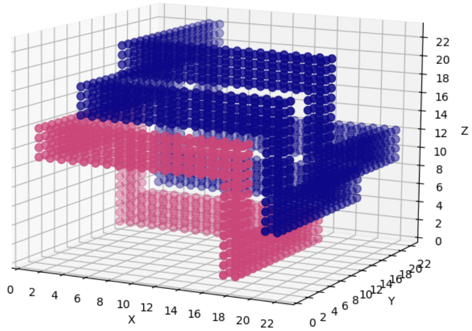

FIGURE 3.1. For each point (a, b, c) on the graph, $l_{(a,b,c)}$ passes through 3 points in $\mathbb{T}_n$. $\mathbb{G}_3$ is highlighted with a light shade of pink. Note the staircase-like structure of the points. ($n = 22$, $\vec{s} = (2, 3, 4)$)

Definition 3.1.5. Define the set $\mathbb{O} \subset \mathbb{T}_n$ to be a cuboid set of lattice points satisfying

$$\{(x_1, x_2, x_3) \in \mathbb{T}_n : 1 \leqslant x_k \leqslant n - rs_k \ \forall\ k \in \{1, 2, 3\}\} \tag{3.4}$$

Proposition 3.1.8. A line of direction vector $\vec{s}$ passes through $r+1$ points in $\mathbb{T}_n$, if and only if it passes through a point in $\mathbb{O}$.

The proof is analogous to Propositions 2.2.8 and 2.2.9.

Definition 3.1.6. Define $N_{(s_1,s_2,s_3)}(i)$ to be the number of unique lines passing through i points in $\mathbb{T}_n$.

We will derive formulae for $N_{(s_1,s_2,s_3)}(i)$ below.

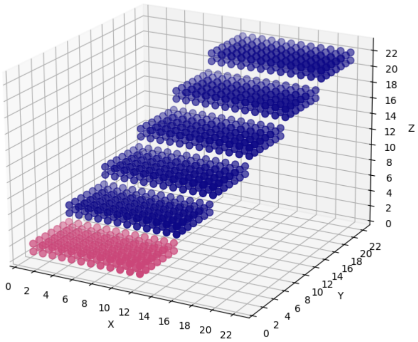

FIGURE 3.2. For each point (a, b, c) on the graph, $l_{(a,b,c)}$ passes through $r+1 = 6$ points in $\mathbb{T}_n$. $\mathbb{O}$ is highlighted with a light shade of pink. $(n = 22,\ \vec{s} = (2, 3, 4))$

Proposition 3.1.9. $N_{(s_1,s_2,s_3)}(i) = 2n(s_1s_2 + s_1s_3 + s_2s_3) - 6is_1s_2s_3$ for $i \in [1, r-1]$.

Proof. Propositions 3.1.6 and 3.1.7 imply a bijection between points in $\mathbb{G}_i$ and line passing through i points, the proof being completely analogous to Proposition 2.2.10. Thus, $N_{(s_1,s_2,s_3)}(i) = |\mathbb{G}_i| = 2n(s_1s_2 + s_1s_3 + s_2s_3) - 6is_1s_2s_3$. ∎

Proposition 3.1.10. $N_{(s_1,s_2,s_3)}(r+1) = (n - rs_1)(n - rs_2)(n - rs_3)$

Proof. Note that we have, from 3.2, $s_3(r+1) > n-1 \implies n - rs_3 \leqslant s_3$. Therefore, it is obvious that any line of direction vector $\vec{s}$ only passes through at most one point in $\mathbb{O}$. Along with Proposition 3.1.8, this implies that a bijection between points in $\mathbb{O}$ and lines passing through $r+1$ points in $\mathbb{T}_n$, analogous to Proposition 2.2.11. Therefore, we have $N_{(s_1,s_2,s_3)}(r+1) = |\mathbb{O}| = (n - rs_1)(n - rs_2)(n - rs_3)$. ∎

Proposition 3.1.11. Define the function $\sigma(k)$ for $k \in \{1, 2, 3\}$ to be the coefficient of the n^{3-k} term in $(n + s_1)(n + s_2)(n + s_3)$, i.e.

$$(n + s_1)(n + s_2)(n + s_3) \equiv n^3 + \sigma(1)n^2 + \sigma(2)n + \sigma(3)$$

Then we have

$$N_{(s_1,s_2,s_3)}(r) = ((r+1)^3 - 6r)\sigma(3) - ((r+1)^2 - 2)\sigma(2)n + (r+1)\sigma(1)n^2 - n^3$$

Proof. The derivation is similar to 2.2.12. We set up the equation

$$\sum_{i=1}^{r-1} iN_{(s_1,s_1,s_3)}(i) + rN_{(s_1,s_1,s_3)}(r) + (r+1)N_{(s_1,s_1,s_3)}(r+1) = n^3$$

From which we obtain the equation above after solving. ∎

Definition 3.1.7. Define $S(s_1, s_2, s_3)$ to be the total number of collinear triples of direction vector $\vec{s}$.

Theorem 3.1.1. $S(s_1, s_2, s_3)$

$$= \frac{r(r-1)}{60}\left(30n^3 - (r+1)[20\sigma(1)n^2 - 5(3r+2)\sigma(2)n + (12r^2+15r+2)\sigma(3)]\right)$$

Proof. Similar to the 2D case,

$$S(s_1, s_2, s_3) = \sum_{i=3}^{r+1} \binom{i}{3} N_{(s_1,s_2,s_3)}(i)$$

from which the above equation is obtained after working through the algebra. ■

3.2. **Counting collinear triples in 3D.**

We now evaluate the total number of collinear triples in an $n \times n \times n$ lattice. Analogous to the double summation in the 2D case, we have

$$N_{\mathrm{col},\,3D} = \sum_{\substack{s_1,s_2,s_3 \in [1, \lfloor \frac{n-1}{2} \rfloor] \\ \gcd(s_1,s_2,s_3)=1}} 4\,S(s_1, s_2, s_3). \tag{3.5}$$

Extracting the constant from Equation 3.5 , the summation can be reorganized as

$$\begin{aligned}\sum_{\substack{s_1,s_2,s_3 \in [1, \lfloor \frac{n-1}{2} \rfloor] \\ \gcd(s_1,s_2,s_3)=1}} S(s_1, s_2, s_3) = 6 &\sum_{\substack{1 \leqslant s_1 < s_2 < s_3 \leqslant \lfloor \frac{n-1}{2} \rfloor \\ \gcd(s_1,s_2,s_3)=1}} S(s_1, s_2, s_3) \\ &+ 3 \sum_{\substack{1 \leqslant s_1 < s_2 \leqslant \lfloor \frac{n-1}{2} \rfloor \\ \gcd(s_1,s_2)=1}} \Big(S(s_1, s_2, s_2) + S(s_1, s_1, s_2)\Big) \\ &+ S(1,1,1).\end{aligned} \tag{3.6}$$

Cases where one of s_1, s_2, or s_3 equals zero reduce to the two-dimensional situation and will be treated separately.

Consider the first summation term. Since s_3 is the largest among (s_1, s_2, s_3), set

$$r = \left\lfloor \frac{n-1}{s_3} \right\rfloor, \qquad \delta \overset{\text{def}}{=} \left\lfloor \frac{n-1}{s_3} \right\rfloor - \frac{n}{s_3}.$$

Expanding $S(s_1, s_2, s_3)$, we have

$$\begin{aligned} &S(s_1, s_2, s_3) \\ &= n^5 \left(\frac{1}{6s_3^2} - \frac{s_1+s_2}{12s_3^3} + \frac{s_1 s_2}{20 s_3^4}\right) \\ &\quad + n^4 \left(-\frac{1}{2s_3} + \frac{s_1+s_2}{6s_3^2} - \frac{s_1 s_2}{12 s_3^3}\right) \\ &\quad + n^3 \left[\frac{s_1 s_2}{s_3^2}\left(-\frac{\delta^2}{2} - \frac{\delta}{2} - \frac{1}{12}\right) + \frac{s_1+s_2}{s_3}\left(\frac{\delta^2}{2} + \frac{\delta}{2} + \frac{1}{12}\right) - \frac{\delta^2}{2} - \frac{\delta}{2} + \frac{1}{3}\right] \end{aligned}$$

$$
\begin{aligned}
&+ n^2 \Bigg[\frac{s_1 s_2}{s_3} \left(-\delta^3 - \delta^2 + \frac{1}{12} \right) + (s_1 + s_2) \left(\frac{2}{3}\delta^3 + \frac{1}{2}\delta^2 - \frac{1}{6}\delta - \frac{1}{6} \right) \\
&+ s_3 \left(-\frac{1}{3}\delta^3 + \frac{1}{3}\delta \right) \Bigg] \\
&+ n \Bigg[s_1 s_2 \left(-\frac{3}{4}\delta^4 - \frac{5}{6}\delta^3 + \frac{1}{4}\delta^2 + \frac{1}{3}\delta + \frac{1}{30} \right) \\
&+ s_3(s_1 + s_2) \left(\frac{1}{4}\delta^4 + \frac{1}{6}\delta^3 - \frac{1}{4}\delta^2 - \frac{1}{6}\delta \right) \Bigg] \\
&+ s_1 s_2 s_3 \left(-\frac{1}{5}\delta^5 - \frac{1}{4}\delta^4 + \frac{1}{6}\delta^3 + \frac{1}{4}\delta^2 + \frac{\delta}{30} \right)
\end{aligned}
$$

Unlike the 2D case, all terms must be taken into account when computing the final sum. We will apply the following theorems, where the proof is given in Appendix B.1. Note that $\mu(d)$ denotes the Möbius function, which is defined as:

$$
\mu(n) = \begin{cases} 1 & \text{if } n = 1, \\ 0 & \text{if } n \text{ is divisible by a square } (p^2 \mid n \text{ for some prime } p), \\ (-1)^k & \text{if } n \text{ is the product of } k \text{ distinct primes.} \end{cases}
$$

Definition 3.2.1. Define the indicator function

$$
\mathbf{1}_{\text{condition}} = \begin{cases} 1 & \text{if the condition is true} \\ 0 & \text{otherwise} \end{cases}
$$

Definition 3.2.2. Define the set

$$
\mathbb{A} = \{(s_1, s_2, s_3) \in \mathbb{Z}^3 : 1 \leqslant s_1 < s_2 < s_3 \leqslant \left\lfloor \frac{n-1}{2} \right\rfloor \text{ and } \gcd(s_1, s_2, s_3) = 1\}
$$

Theorem 3.2.1.

$$
\sum_{s_2=2}^{s_3-1} \sum_{s_1=1}^{s_2-1} \mathbf{1}_{\gcd(s_1,s_2,s_3)=1} = \sum_{d \mid s_3} \mu(d) \left(\frac{s_3^2}{2d^2} + O\left(\frac{s_3}{d} \right) \right)
$$

Theorem 3.2.2.

$$
\sum_{s_2=2}^{s_3-1} \sum_{s_1=1}^{s_2-1} (s_1 + s_2)\, \mathbf{1}_{\gcd(s_1,s_2,s_3)=1} = \sum_{d \mid s_3} \mu(d) \left(\frac{s_3^3}{2d^2} + O\left(\frac{s_3^2}{d} \right) \right)
$$

Theorem 3.2.3.

$$
\sum_{s_2=2}^{s_3-1} \sum_{s_1=1}^{s_2-1} s_1 s_2\, \mathbf{1}_{\gcd(s_1,s_2)=1} = \sum_{d \mid s_3} \mu(d) \left(\frac{s_3^4}{8d^2} + O\left(\frac{s_3^3}{d} \right) \right)
$$

Consider the terms with coefficient n^5 in $S(s_1, s_2, s_3)$. We have

$$\begin{aligned}
&\sum_{\vec{s}\in\mathbb{A}} n^5 \left(\frac{1}{6s_3^2} - \frac{s_1+s_2}{12s_3^3} + \frac{s_1s_2}{20s_3^4}\right)\\
&= n^5 \sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor} \sum_{d|s_3} \mu(d)\left(\frac{23}{480d^2} + O\!\left(\frac{1}{s_3 d}\right)\right)
\end{aligned}$$

We invoke the following theorems to extract the leading term and the error term:

Theorem 3.2.4. For any non-negative integer k,

$$\sum_{s_3=3}^{m} \sum_{d|s_3} \frac{s_3^k\,\mu(d)}{d^2} = \frac{m^{k+1}}{(k+1)\zeta(3)} + O(m^k)$$

Substituting $m = \left\lfloor \dfrac{n-1}{2} \right\rfloor$, we obtain

$$\sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor} \sum_{d|s_3} \frac{s_3^k\,\mu(d)}{d^2} = \frac{n^{k+1}}{2^k(k+1)\zeta(3)} + O(n^k).$$

Theorem 3.2.5.

$$\sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor} \sum_{d|s_3} \frac{s_3^k\,\mu(d)}{d} = \begin{cases} O(n^{k+1}), & k \geq 0,\\ O(\log n), & k=-1.\end{cases}$$

Hence, the sum of n^5 terms becomes

$$n^5 \sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor} \sum_{d|s_3} \mu(d)\left(\frac{23}{480d^2} + O\!\left(\frac{1}{s_3 d}\right)\right) = \frac{23}{960\,\zeta(3)} n^6 + O\big(n^5 \ln n\big)\,.$$

Similarly, the sum of n^4 terms is

$$\begin{aligned}
&\sum_{\vec{s}\in\mathbb{A}} n^4 \left(-\frac{1}{2s_3} + \frac{s_1+s_2}{6s_3^2} - \frac{s_1s_2}{12s_3^3}\right)\\
&= n^4 \sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor} \sum_{d|s_3} \mu(d)\left(-\frac{17s_3}{96d^2} + O\!\left(\frac{1}{d}\right)\right)\\
&= -\frac{17}{768\,\zeta(3)} n^6 + O(n^5).
\end{aligned}$$

Contrary to the 2D case, when computing the sum of terms below order n^4, we cannot directly apply Theorem 3.2.4 and Theorem 3.2.5. This is because these sums involve δ, which depends on both n and s_3.

To handle δ, we substitute

$$\delta = -\frac{1}{s_3} - \left\{\frac{n-1}{s_3}\right\},$$

where $\{x\}$ denotes the fractional part of x. Since $\left\{\dfrac{n-1}{s_3}\right\} = O(1)$ dominates $O\left(\dfrac{1}{s_3}\right)$, we can approximate

$$\delta \approx -\left\{\frac{n-1}{s_3}\right\}.$$

Applying Theorem 3.2.4 with s_3^k replaced by s_3^{k-1}, the resulting error term of the approximation is one polynomial order lower than the leading term of the sum. Moreover, we shall apply the following theorem to handle δ:

Theorem 3.2.6. Let $f(t)$ be a polynomial of degree T, i.e., $f(t) = \sum_{i=0}^{T} a_i t^i$. If $k - T \geqslant 0$, then

$$\sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{s_3^k \mu(d)}{d^2} f\left(\left\{\frac{n-1}{s_3}\right\}\right) = \frac{n^{k+1}}{\zeta(3)} \int_0^1 f(t)\, \zeta_H(k+2, t+2)\, dt + O(n^k \ln n),$$

where $\zeta_H(s,a)$ denotes the Hurwitz zeta function

$$\zeta_H(s,a) = \sum_{m=0}^{\infty} \frac{1}{(m+a)^s}, \qquad \operatorname{Re}(s) > 1,\ a > 0.$$

Now we proceed to handle terms below n^4. For the summation of n^3 terms, by applying Theorem 3.2.2 and Theorem 3.2.3, we have

$$\sum_{\vec{s} \in \mathbb{A}} n^3 \left[\frac{s_1 s_2}{s_3^2}\left(-\frac{\delta^2}{2} - \frac{\delta}{2} - \frac{1}{12}\right) + \frac{s_1 + s_2}{s_3}\left(\frac{\delta^2}{2} + \frac{\delta}{2} + \frac{1}{12}\right) - \frac{\delta^2}{2} - \frac{\delta}{2} + \frac{1}{3}\right]$$
$$= n^3 \sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \mu(d) \left(\frac{s_3^2}{d^2} + O\left(\frac{s_3}{d^2}\right)\right)\left(-\frac{\delta^2}{16} - \frac{\delta}{16} + \frac{19}{96}\right).$$

By Theorem 3.2.6, the main term reduces to

$$\frac{n^6}{\zeta(3)} \int_0^1 f(t)\, \zeta_H(4, t+2)\, dt + O(n^5 \ln n), \quad \text{where } f(t) = -\frac{1}{16}t^2 + \frac{1}{16}t + \frac{19}{96}.$$

Evaluating the integral gives

$$\frac{8\pi^2 - 59}{2304\zeta(3)} n^6 + O(n^5 \ln n).$$

Similarly, for the n^2 term:

$$\begin{aligned}
&\sum_{\vec{s}\in\mathbb{A}} n^2\left[\frac{s_1s_2}{s_3}\left(-\delta^3-\delta^2+\frac{1}{12}\right)+(s_1+s_2)\left(\frac{2}{3}\delta^3+\frac{1}{2}\delta^2-\frac{1}{6}\delta-\frac{1}{6}\right)\right.\\
&\left.+s_3\left(-\frac{1}{3}\delta^3+\frac{1}{3}\delta\right)\right]\\
&=n^2\sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor}\sum_{d|s_3}\mu(d)\left(\frac{s_3^3}{d^2}+O\left(\frac{s_3^2}{d}\right)\right)\left(\frac{1}{24}\delta^3+\frac{1}{8}\delta^2+\frac{1}{12}\delta-\frac{7}{96}\right)\\
&=\frac{n^6}{\zeta(3)}\int_0^1\left(-\frac{1}{24}t^3+\frac{1}{8}t^2-\frac{1}{12}t-\frac{7}{96}\right)\zeta_H(5,t+2)\,dt+O(n^5\ln n)\\
&=\frac{32\pi^2-109-192\zeta(3)}{18432\,\zeta(3)}n^6+O(n^5\ln n).
\end{aligned}$$

For the n term:

$$\begin{aligned}
&\sum_{\vec{s}\in\mathbb{A}} n\left[s_1s_2\left(-\frac{3}{4}\delta^4-\frac{5}{6}\delta^3+\frac{1}{4}\delta^2+\frac{1}{3}\delta+\frac{1}{30}\right)\right.\\
&\left.+s_3(s_1+s_2)\left(\frac{1}{4}\delta^4+\frac{1}{6}\delta^3-\frac{1}{4}\delta^2-\frac{1}{6}\delta\right)\right]\\
&=n\sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor}\sum_{d|s_3}\mu(d)\left(\frac{s_3^4}{d^2}+O\left(\frac{s_3^3}{d}\right)\right)\left(\frac{1}{32}\delta^4-\frac{1}{48}\delta^3-\frac{3}{32}\delta^2-\frac{1}{24}\delta+\frac{1}{240}\right)\\
&=\frac{n^6}{\zeta(3)}\int_0^1\left(\frac{1}{32}t^4+\frac{1}{48}t^3-\frac{3}{32}t^2+\frac{1}{24}t+\frac{1}{240}\right)\zeta_H(6,t+2)\,dt+O(n^5\ln n)\\
&=\frac{781-40\pi^2-320\zeta(3)}{38400\zeta(3)}n^6+O(n^5\ln n)
\end{aligned}$$

For the constant term:

$$\begin{aligned}
&\sum_{\vec{s}\in\mathbb{A}} s_1s_2s_3\left(-\frac{1}{5}\delta^5-\frac{1}{4}\delta^4+\frac{1}{6}\delta^3+\frac{1}{4}\delta^2+\frac{\delta}{30}\right)\\
&=n\sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor}\sum_{d|s_3}\mu(d)\left(\frac{s_3^5}{d^2}+O\left(\frac{s_3^4}{d}\right)\right)\left(-\frac{1}{5}\delta^5-\frac{1}{4}\delta^4+\frac{1}{6}\delta^3+\frac{1}{4}\delta^2+\frac{1}{30}\delta\right)\\
&=\frac{n^6}{\zeta(3)}\int_0^1\left(\frac{1}{5}t^5-\frac{1}{4}t^4-\frac{1}{6}t^3+\frac{1}{4}t^2-\frac{1}{30}t\right)\zeta_H(7,t+2)\,dt+O(n^5\ln n)\\
&=\frac{-960\zeta(3)+4313-320\pi^2}{57600\,\zeta(3)}n^6+O(n^5\ln n).
\end{aligned}$$

All integration steps are included in Appendix B.2

Combining all the contributions of summation of n^0 to n^6 terms, we can calculate the first term of Equation 3.6

$$
\begin{aligned}
&6\sum_{\vec{s}\in\mathbb{A}} S(s_1,s_2,s_3)\\
&= n^6\left(\frac{23}{160\zeta(3)} - \frac{17}{128\zeta(3)} + \frac{8\pi^2-59}{384\zeta(3)} + \frac{32\pi^2-109-192\zeta(3)}{3072\zeta(3)}\right.\\
&\quad\left. + \frac{781-40\pi^2-320\zeta(3)}{6400\zeta(3)} + \frac{-960\zeta(3)+4313-320\pi^2}{9600\zeta(3)}\right) + O(n^5\ln n)\\
&= \frac{30191-16320\zeta(3)-640\pi^2}{76800\,\zeta(3)} n^6 + O(n^5\ln n)\\
&\approx 0.046111\, n^6 + O(n^5\ln n).
\end{aligned}
$$

The second term of Equation 3.6 has smaller order:

$$
\begin{aligned}
3\sum_{\substack{1\leqslant s_1<s_2\leqslant\lfloor\frac{n-1}{2}\rfloor\\ \gcd(s_1,s_2)=1}} S(s_1,s_2,s_2) &= \sum_{\substack{1\leqslant s_1<s_2\leqslant\lfloor\frac{n-1}{2}\rfloor\\ \gcd(s_1,s_2)=1}} n^5\left(\frac{s_1^2}{20s_2^4} - \frac{s_1}{s_2^3} - \frac{1}{4s_2^2}\right)\\
&= O(n^5\ln n).
\end{aligned}
$$

The third term, $S(1,1,1)$, is $O(n^5)$, which is smaller than $O(n^5\ln n)$ and thus does not change the total order of error.

When one of s_1, s_2 or s_3 is equal to zero, it reduces to the 2D square grid case. Using Equation 2.15 and taking $m = n$, the number of collinear triples in each layer is $O(n^4\ln n)$. Since there are n such layers in 3D, their contribution is $n\times O(n^4\ln n) = O(n^5\ln n)$, which does not affect the main term.

Finally, multiplying by the factor 4 from Equation 3.5 gives

$$
\begin{aligned}
N_{col,3D} &= \frac{30191-16320\zeta(3)-640\pi^2}{19200\,\zeta(3)} n^6 + O(n^5\ln n)\\
&\approx 0.18444\, n^6 + O(n^5\ln n)\\
&\stackrel{\text{def}}{=} \alpha n^6 + O(n^5\ln n)
\end{aligned}
$$

3.3. **Limitations of probabilistic heuristics in 3D.**

An unexpected feature of the 3D case is that Guy and Kelly's heuristic in [4] does not produce the correct result. We repeat the procedure in Section 2.3 to find the expected number of solutions using the same heuristic, applying Stirling's approximation. For brevity, define $f_n \stackrel{\text{def}}{=} f(\mathbb{T}_n)$

$$
\begin{aligned}
\binom{n^3}{f_n}\left(1-\frac{N_{col,3D}}{\binom{n^3}{3}}\right)^{\binom{f_n}{3}} &\approx 1 \\
\ln\binom{n^3}{f_n}+\binom{f_n}{3}\ln\left(1-\frac{N_{col,3D}}{\binom{n^3}{3}}\right) &= 0 \\
f_n(\ln n^3-\ln f_n)+O(f_n)+f_n^3\left(\frac{\alpha}{n^3}+O\left(\frac{\ln n}{n^4}\right)\right) &= 0 \\
f_n &= \sqrt{\frac{n^3\,O(\ln n)}{\alpha+O\left(\dfrac{\ln n}{n}\right)}} \\
f_n &= O\left(n^{1.5}(\ln n)^{0.5}\right)
\end{aligned}
$$

However, [8] provides a construction that guarantees $(1-o(1))n^2$ points can be placed; In particular, they proved that exactly n^2 points can be placed if n is a prime with $n \equiv 3 \pmod 4$, by placing points on the coordinates $(x, y, (x^2+y^2)) \pmod n$

As our analysis yields only $f_n = O\left(n^{1.5}(\ln n)^{0.5}\right)$ using Guy and Kelly's probabilistic heuristic method, it follows that this approach significantly underestimates the true rate of growth of f_n. It is possible that, because the structure of the distribution of collinear triples in $\mathbb{T}_n$ is much more complicated than in the 2D case, the heuristic underestimates the actual number of solutions as it is unable to take into account possible constructions which deterministically lead to solutions to the No-Three-in-Line problem. By contrast, in the 2D case, the paper [5] as well as some of our results in section 2.3 suggest that the heuristic tends to overestimate the number of solutions.

It is worth noting that while the probability of three points being collinear is correctly given by $\frac{N_{col,3D}}{\binom{n^3}{3}}$, the subsequent heuristic step where we assume independence of events is where the method fails. To illustrate the point, we implemented a Python simulation that randomly selects three points in a $n\times n\times n$ grid and checks the probability that they are collinear. We then compare this with the asymptotic estimate

$$\frac{N_{col,3D}}{\binom{n^3}{3}} \approx \frac{1.10664}{n^3}$$

In fact, from empirical testing, if $g(n)$ is of order $O(n)$, we conjecture that the probability that $g(n)$ points randomly placed on the grid contain no collinear triples can be well-approximated by the formula

$$\left(1-\frac{N_{col,3D}}{\binom{n^3}{3}}\right)^{\binom{g(n)}{3}}$$

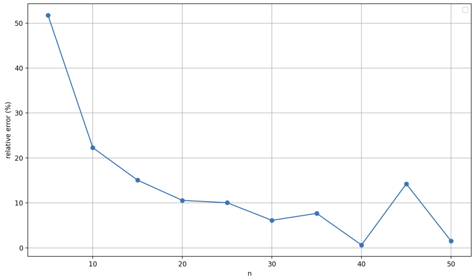

FIGURE 3.3. Relative error of our asymptotic estimate that 3 points are collinear against the empirical probability; It can be seen that the relative error decreases are n increases, until the probability becomes low enough at around $n = 40$ that random fluctuations occur in the empirical results. All the code of the simulation is given in Appendix C.2.

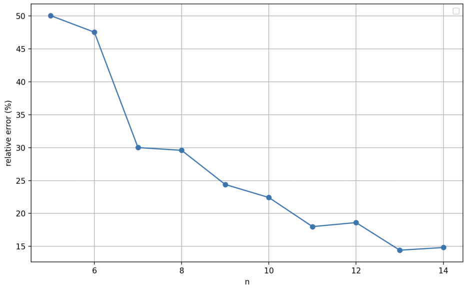

FIGURE 3.4. Relative error of our asymptotic estimate that n points are collinear against the empirical probability; Note that the number of iterations have been reduced to 10^6 and n has been limited to $n < 15$ due to hardware limitations. It can be seen that the relative error decreases as n increases, which is an argument in favour of Conjecture 3.

However, if $g(n) = O(n^2)$, our heuristics produce obviously incorrect results, showing that solutions will not exist for n^2 points for large n which contradicts constructions which have been shown to reach this bound.

Therefore, we have come to the conclusion that a completely probabilistic heuristic approach like Guy and Kelly's [4] **would not** yield a correct bound for the maximum number of points that can be placed in an $n \times n \times n$ grid without forming any collinear triples. Unfortunately, experimental testing of probabilities in 3D is not feasible as in the 2D case; Due to combinatorial explosion, simulating the placement of n^2 points on an $n \times n \times n$ grid and calculating the empirical probability that no collinear triples exist is not computationally feasible, taking a long time

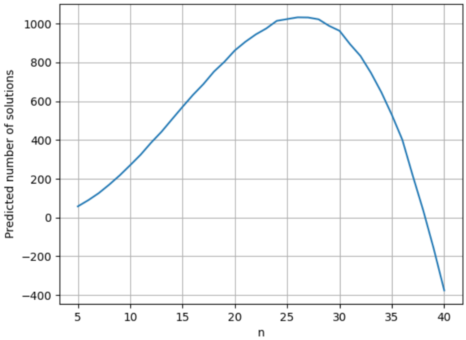

FIGURE 3.5. Logarithm of the predicted number of solutions for n^2 points to the 3D No-Three-in-Line problem as estimated by our heuristic. Note the (Incorrect) crossover point at $n > 38$ where it predicts no solutions will exist.

even for a very small n such as $n = 3$. Thus, developing a reliable heuristic bound for f_n in 3D remains an open question and will require further research.

Appendix A. Error analysis of $\sum S(p,q)$

Let $r = \left\lfloor \dfrac{m-1}{p} \right\rfloor = \dfrac{m}{p} + a$, where $a \in (-(1+\frac{1}{p}), 0)$.
Note that since $p \geqslant 1$, $a \in (-2, 0)$ regardless of the value of p. Therefore, it is an $O(1)$ term.
We first expand $S(p,q)$ using this new definition of r. In what follows, we only consider the region where $r = \left\lfloor \dfrac{m-1}{p} \right\rfloor$; The error terms corresponding to the other region can be derived via reflectional symmetry of m and n.

$$\begin{aligned}
S(p,q) &= \frac{mnr(r-1)}{2} - \frac{r(mq+pn)(r-1)(r+1)}{3} + \frac{pq(r+1)(3r+2)r(r-1)}{12} \\
&= \frac{1}{4}a^4pq + \frac{2}{3}a^3mq - \frac{1}{3}a^3np + \frac{1}{6}a^3pq + \frac{1}{2}\frac{a^2m^2}{pq} - \frac{1}{2}a^2mn + \frac{1}{2}a^2mq \\
&\quad - \frac{1}{4}a^2pq + \frac{1}{2}\frac{am^2q}{p} - \frac{1}{2}amn - \frac{1}{6}amq + \frac{1}{3}anp - \frac{1}{6}apq - \frac{1}{12}\frac{m^4q}{p^3} \\
&\quad + \frac{1}{6}\frac{m^3n}{p^2} + \frac{1}{6}\frac{m^3q}{p^2} - \frac{1}{2}\frac{m^2n}{p} + \frac{1}{12}\frac{m^2q}{p} + \frac{1}{3}mn - \frac{1}{6}mq
\end{aligned}$$

We can group the equation into different terms. Two of these terms, $\dfrac{1}{6}\dfrac{m^3n}{p^2}$ and $-\dfrac{1}{12}\dfrac{m^4q}{p^2}$, are main order terms that contribute to the final sum. We shall look at the other terms first.

A.1. **Error analysis of non-main-order terms.**

1.

$$mn\left(-\frac{a^2}{2} - \frac{a}{2} + \frac{1}{3}\right), pq\left(\frac{1}{4}a^4 + \frac{1}{6}a^3 - \frac{1}{4}a^2 - \frac{1}{6}a\right)$$
$$np\left(-\frac{1}{3}a^3 + \frac{1}{3}a\right), mq\left(\frac{2}{3}a^3 + \frac{1}{2}a^2 - \frac{1}{6}a - \frac{1}{6}\right)$$

These terms are all of the order $O(mn)$; Since $p < \dfrac{m}{2}$ and $q < \dfrac{n}{2}$, p and q are of order $O(m)$ and $O(n)$ respectively. Any multiplicative factors involving a are $O(1)$ terms. The summation area is $O(mn)$, so these terms all sum to $O(m^2n^2)$.

2. $-\dfrac{1}{2}\dfrac{m^2n}{p}$

$$\begin{aligned}
\sum_{p=\lceil \frac{m}{n} \rceil}^{\lfloor \frac{m-1}{2} \rfloor} \sum_{\substack{q=1 \\ gcd(p,q)=1}}^{\lfloor \frac{n}{m}p \rfloor} \frac{m^2n}{p} &< \sum_{p=1}^{\lfloor \frac{m-1}{2} \rfloor} \frac{m^2n}{p}\left\lfloor \frac{n-1}{m-1}p \right\rfloor \\
&< \sum_{p=1}^{\lfloor \frac{m-1}{2} \rfloor} \frac{m^2n^2}{m-1}
\end{aligned}$$

Therefore, the order is $O(m^2n^2)$.

3. $\dfrac{m^2q}{p}\left(\dfrac{a^2}{2}+\dfrac{1}{2}a+\dfrac{1}{12}\right)$
We note that $q<n$, so this term is at most of the same order as the previous term, so the order is also $O(m^2n^2)$.

4. $\dfrac{1}{6}\dfrac{m^3q}{p^2}$

$$\begin{aligned}\sum_{p=\lceil\frac{m}{n}\rceil}^{\lfloor\frac{m-1}{2}\rfloor}\sum_{\substack{q=1\\ gcd(p,q)=1}}^{\lfloor\frac{n}{m}p\rfloor}\frac{m^3q}{p^2} &< \sum_{p=\lceil\frac{m}{n}\rceil}^{\lfloor\frac{m-1}{2}\rfloor}\frac{m^3}{2p^2}\left(\left\lfloor\frac{n-1}{m-1}p\right\rfloor\right)\left(\left\lfloor\frac{n-1}{m-1}p\right\rfloor+1\right)\\ &< \sum_{p=\lceil\frac{m}{n}\rceil}^{\lfloor\frac{m-1}{2}\rfloor}\frac{m^3}{2p^2}\left(\frac{pn}{m-1}\right)\left(\frac{pn}{m-1}+1\right)\\ &= O(m^2n^2)+\sum_{p=\lceil\frac{m}{n}\rceil}^{\lfloor\frac{m-1}{2}\rfloor}\frac{m^3n}{2p(m-1)}\\ &= O(m^2n^2)+O(m^2n\ln\min(m,n))\\ &\sim O(m^2n^2)\end{aligned}$$

A.2. **Error in changing summation bounds.**
Justifying the approximation of $q_{max}=\left\lfloor\dfrac{n-1}{m-1}p\right\rfloor\approx\dfrac{np}{m}$,

$$\begin{aligned}\Delta &= \left\lfloor\frac{n-1}{m-1}p\right\rfloor-\frac{np}{m}\\ &= \frac{n-1}{m-1}p-\frac{np}{m}+O(1)\\ &= \frac{n-m}{m^2-m}p+O(1)\end{aligned}$$

The order of the total error is as follows:

$$\begin{aligned}&\sum_{p=\lceil\frac{m-1}{n-1}\rceil}^{\lfloor\frac{m-1}{2}\rfloor}\frac{m^3n}{6p^3}\left(\frac{n-m}{m^2-m}p+O(1)\right)\varphi(p)\\ &\approx \frac{m^3n\ O(1)}{6}\sum_{p=\lceil\frac{m-1}{n-1}\rceil}^{m}\frac{\varphi(p)}{p^3}+\sum_{p=\lceil\frac{m-1}{n-1}\rceil}^{m}\frac{m^2n(n-m)}{6(m-1)p^2}\varphi(p)\\ &< \frac{O(m^3n)}{6}\sum_{p=\lceil\frac{m-1}{n-1}\rceil}^{m}\frac{1}{p^2}+\sum_{p=\lceil\frac{m-1}{n-1}\rceil}^{m}\frac{m^2n(n-m)}{6(m-1)p}\\ &= O(m^2n^2)+O(mn\max(m,n)\ln\min(m,n))\\ &\sim O(m^2n^2)\end{aligned}$$

Therefore, the error in the approximation of q_{max} is $O(m^2n^2)$.

A.3. **Error in assuming uniform density of coprime integers.**
Let $p_1, p_2, p_3, ..., p_{\omega(u)}$ be the unique prime factors of u, $\omega(u)$ being the prime omega function. Let us denote the number of integers coprime to u up to some number v as $\varphi'_u(v)$. A number is *not* coprime to u if it is divisible by any of its prime factors; By the inclusion-exclusion principle, we arrive at the following expression for $\varphi'_u(v)$:
(A.1)

$$\begin{aligned}\varphi'_u(v) &= \sum_{i=1,\gcd(i,u)=1}^{u} 1 \\ &= v - \sum_{i=1}^{\omega(u)} \left\lfloor \frac{v}{p_i} \right\rfloor + \sum_{i=1}^{\omega(u)} \sum_{j=i+1}^{\omega(u)} \left\lfloor \frac{v}{p_i p_j} \right\rfloor - ... + (-1)^{\omega(u)} \left\lfloor \frac{v}{p_1 p_2 ... p_n} \right\rfloor \\ \text{e.g. } \varphi'_{84}(v) &= v - \left\lfloor \frac{v}{2} \right\rfloor - \left\lfloor \frac{v}{3} \right\rfloor - \left\lfloor \frac{v}{7} \right\rfloor + \left\lfloor \frac{v}{2\cdot 3} \right\rfloor + \left\lfloor \frac{v}{2\cdot 7} \right\rfloor + \left\lfloor \frac{v}{3\cdot 7} \right\rfloor - \left\lfloor \frac{v}{2\cdot 3\cdot 7} \right\rfloor\end{aligned}$$

Now, we approximate this sum by not flooring any of the terms. We arrive at part of Theorem 2.3.1:

$$\begin{aligned}\varphi'_u(v) &\approx v - \sum_{i=1}^{\omega(u)} \frac{v}{p_i} + \sum_{i=1}^{\omega(u)} \sum_{j=i+1}^{\omega(u)} \frac{v}{p_i p_j} - ... + (-1)^{\omega(u)} \frac{v}{p_1 p_2 ... p_n} \\ &= v \left(1 - \sum_{i=1}^{\omega(u)} \frac{1}{p_i} + \sum_{i=1}^{\omega(u)} \sum_{j=i+1}^{\omega(u)} \frac{1}{p_i p_j} - ... + (-1)^{\omega(u)} \frac{1}{p_1 p_2 ... p_n} \right) \\ &= v \left(\frac{\varphi(u)}{u} \right)\end{aligned}$$

Note that this result only applies to the first term of Theorem 2.3.1, where the summand is independent of the summation variable q. In the second term, the summand is linear in the summation variable q. Therefore, we shall consider the following sum:

$$\sum_{i=1,\gcd(i,u)=1}^{v} i \tag{A.2}$$

We observe that

$$\begin{aligned}\gcd(i,u) = 1 &\implies \varphi'_u(i) = \varphi'_u(i-1) + 1, \\ \gcd(i,u) \neq 1 &\implies \varphi'_u(i) = \varphi'_u(i-1)\end{aligned}$$

Therefore, the sum can be rewritten as follows:

$$\begin{aligned}\sum_{i=1,\gcd(i,u)=1}^{v} i &= \sum_{i=1}^{v} i(\varphi'_u(i) - \varphi'_u(i-1)) \\ &\approx \sum_{i=1}^{v} i(i-(i-1)) \frac{\varphi(u)}{u}\end{aligned}$$

$$= \frac{\varphi(u)}{u}\sum_{i=1}^{v} i$$

which applies to the second term of Theorem 2.3.1.
Now, we prove that the error terms are negligible compared to the main term.

Theorem A.3.1. Define $\delta \overset{\text{def}}{=} v\dfrac{\varphi(u)}{u} - \varphi'_u(v)$. We assert that

$$\delta \leqslant \min(v, 2^{\omega(u)}) \tag{A.3}$$

Proof: Since $x - \lfloor x \rfloor < 1$, making the approximation $\lfloor x \rfloor \approx x$ in any term of Equation A.1 introduces an error of at most 1. There are $2^{\omega(u)}$ terms in the summation, so the error must be smaller than $2^{\omega(u)}$. Also, we note that $\varphi'_u(v)$ is a counting function which counts the number of things from 1 to v which satisfy a certain condition. Therefore, $0 \leqslant \varphi'_u(v) \leqslant v$. We also note that $0 \leqslant v\dfrac{\varphi(u)}{u} \leqslant v$. This gives an upper bound on the error of v. Combining both results, we thus prove the theorem.
This result can be extended to the sum in Equation A.2. We rewrite the sum in the following way:

$$\begin{aligned}
\sum_{\gcd(i,u)=1, i=1}^{v} i &= \sum_{i=1}^{v} i(\varphi'_u(i) - \varphi'_u(i-1)) \\
&= \sum_{i=1}^{v} i\varphi'_u(i) - \sum_{i=0}^{v-1}(i+1)\varphi'_u(i) \\
&= v\varphi'_u(v) - \sum_{i=0}^{v-1}\varphi'_u(i)
\end{aligned}$$

The upper bound on the error in our approximation is

$$\begin{aligned}
& v\min(v, 2^{\omega(u)}) + \sum_{i=0}^{v-1}\min(i, 2^{\omega(u)}) \\
< {}& v\min(v, 2^{\omega(u)}) + \sum_{i=0}^{v-1}\min(v, 2^{\omega(u)}) \\
= {}& \min(v^2, v\,2^{\omega(u)})
\end{aligned}$$

Theorem A.3.1 implies that the error in our approximation of $\varphi'_u(v)$ is at most on the order of $O\left(\min\left(v, 2^{\omega(u)}\right)\right)$. However, this is useless without an estimate of the order of $2^{\omega(u)}$ as $u \to \infty$ which does not make explicit reference to the factorisation of u.

Theorem A.3.2. $2^{\omega(u)} < \sqrt{8u}$

The n-th prime number is strictly larger than $2n - 2$ for all n. Therefore, for all positive u, $u > 2^{\omega(u)-1}(\omega(u)-1)! \geqslant 2^{2\omega(u)-3}$ where the last inequality is a property of the factorial. Solving the inequality, we get $2^{\omega(u)} < \sqrt{8u}$, i.e. $2^{\omega(u)} \sim O(\sqrt{u})$

If a stricter upper bound on the error is needed, we shall invoke the following theorem:

Theorem A.3.3. (Theorem 8.30 of [7]) For every $\varepsilon > 0$, there is an $n_0(\varepsilon)$ such that if $n > n_0(\varepsilon)$ then $\omega(n) < \dfrac{(1+\varepsilon)(\ln n)}{\ln\ln n}$. This is best possible in the sense that there exist infinitely many n such that $\omega(n) > \dfrac{(1-\varepsilon)(\ln n)}{\ln\ln n}$.

From the upper bound given by the theorem we see that

$$2^{\omega(u)} < u^{\frac{(1+\varepsilon)\ln 2}{\ln\ln u}}$$

Therefore, the order of $2^{\omega(q)}$ is at most $O\left(u^{\frac{(1+\varepsilon)\ln 2}{\ln\ln u}}\right)$ for some finite number ε, which can be chosen so that $n_0(\varepsilon) < u$ for all values of u we are concerned with. Consider the original term, given in Theorem 2.3.1, whose error we were considering:

$$\sum_{p=\lceil \frac{m}{n} \rceil}^{\frac{m}{2}} \sum_{\substack{q=1 \\ gcd(p,q)=1}}^{\lfloor \frac{n}{m}p \rfloor} \frac{m^3 n}{6p^2} - \frac{m^4 q}{12p^3}$$

$$\text{Order of error in first term} = \sum_{p=\lceil \frac{m}{n} \rceil}^{\frac{m}{2}} \frac{m^3 n}{p^2} O\left(\min\left(2^{\omega(p)}, \frac{n}{m}p\right)\right)$$

$$\text{Order of error in second term} = \sum_{p=\lceil \frac{m}{n} \rceil}^{\frac{m}{2}} \frac{m^4}{p^3} O\left(\min\left(\frac{n}{m}p\, 2^{\omega(p)}, \left(\frac{n}{m}p\right)^2\right)\right)$$

Their orders are obviously the same and equal to

$$\sum_{p=\lceil \frac{m}{n} \rceil}^{\frac{m}{2}} O\left(\min\left(\frac{m^3 n\, 2^{\omega(p)}}{p^2}, \frac{m^2 n^2}{p}\right)\right)$$

We shall analyse the errors introduced due to our approximation in the cases below.
Case I: $m < n$
Theorem A.3.2 shall suffice. The error is on the order of

$$\begin{aligned}\sum_{p=\lceil \frac{m}{n} \rceil}^{\frac{m}{2}} O\left(\frac{m^3 n\sqrt{p}}{p^2}\right) &= m^3 n \sum_{p=1}^{\frac{m}{2}} O\left(p^{-\frac{3}{2}}\right) \\ &= m^3 n\; O(1^{-\frac{1}{2}}) \\ &= O(m^3 n)\end{aligned}$$

Case II: $\frac{m}{n} < A$, e.g. $A = 100$

The A is somewhat arbitrary; The purpose is purely to avoid possible singularities in Case III. We shall invoke Theorem A.3.2 as before. The error is on the order of

$$
\begin{aligned}
&O\left(\sum_{p=\lceil \frac{m}{n} \rceil}^{\frac{m}{2}} \min\left(\frac{m^3 n\sqrt{8p}}{p^2}, \frac{m^2n^2}{p}\right)\right)\\
&= O\left(\sum_{p=\lceil \frac{m}{n} \rceil}^{\frac{8m^2}{n^2}} \frac{m^2n^2}{p} + \sum_{p=\frac{8m^2}{n^2}}^{\frac{m}{2}} \frac{m^3 n\sqrt{8p}}{p^2}\right)\\
&= O\left(m^2n^2 \ln\frac{8m}{n} + m^3 n\left(\frac{m^2}{n^2}\right)^{-\frac{1}{2}}\right)\\
&= O\left(m^2n^2\ln\frac{m}{n} + m^2n^2\right) \sim O(m^2n^2)
\end{aligned}
$$

Case III: $\frac{m}{n} \geqslant A$

This case does not need to be considered in our current context, where $\frac{m}{n} < 2 + o(1)$; Nonetheless, a derivation of the error may be interesting for posterity. Using Theorem A.3.3, we have an error on the order of

$$
O\left(\sum_{p=\lceil \frac{m}{n} \rceil}^{\frac{m}{2}} \min\left(\frac{m^3 n p^{\frac{(1+\varepsilon)\ln 2}{\ln\ln p}}}{p^2}, \frac{m^2n^2}{p}\right)\right)
$$

We must first obtain an estimate of the crossover point. This occurs when

$$
\begin{aligned}
mp^{\frac{(1+\varepsilon)\ln 2}{\ln\ln p}} &= np\\
(\ln\ln p)\left(\ln\frac{n}{m}\right) + (\ln\ln p - (1+\varepsilon)\ln 2)(\ln p) &= 0
\end{aligned}
\tag{A.4}
$$

This equation cannot be solved with elementary methods, but a good estimate is available using Newton's method. We define $x \stackrel{\text{def}}{=} \ln p$ and $x_0 \stackrel{\text{def}}{=} \ln\frac{m}{n}$, and find the root of the function

$$
\begin{aligned}
f(x) &= -x_0 \ln x + x(\ln x - (1+\varepsilon)\ln 2)\\
f'(x) &= -\frac{x_0}{x} + \ln x - (1+\varepsilon)\ln 2 + 1
\end{aligned}
$$

In the subsequent derivation, we shall assume A is sufficiently large so that the inequalities $\ln x_0 - (1+\varepsilon)\ln 2 > 1$ and $\frac{\max(1, (1+\varepsilon)\ln 2))}{\ln x_0 - (1+\varepsilon)\ln 2} < 1$ are true. It is guaranteed that such an A exists; We can always choose a finite ε such that $n_0(\varepsilon) < A < \left\lceil \frac{m}{n} \right\rceil <$ any value of p we sum over. Then, we can simply solve these two inequalities for A.

For cleanliness of notation, we define $z \stackrel{\text{def}}{=} (1+\varepsilon)\ln 2$.

$$\begin{aligned}
x_1 &= x_0 - \frac{-x_0 \ln x_0 + x_0(\ln x_0 - z)}{-\frac{x_0}{x_0} + \ln x_0 - z + 1} \\
&= x_0 \left(1 + \frac{z}{\ln x_0 - z}\right) \\
\ln x_1 &= \ln x_0 + \frac{z}{\ln x_0 - z} + O\left(\left(\frac{z}{\ln x_0 - z}\right)^2\right) \\
x_2 &= x_1 - \frac{-x_0 \ln x_1 + (\ln x_1 - z)x_1}{-\frac{x_0}{x_1} + (\ln x_1 - z) + 1} \\
&= x_1 - x_0 \frac{-\ln x_1 + (\ln x_1 - z)\left(1 + \frac{z}{\ln x_0 - z}\right)}{-\frac{\ln x_0 - z}{\ln x_0} + \left(\ln x_0 + \frac{z}{\ln x_0 - z} + O\left(\left(\frac{z}{\ln x_0 - z}\right)^2\right) - z\right) + 1} \\
&= x_1 - z x_0 \frac{\left(\ln x_0 + \frac{z}{\ln x_0 - z} + O\left(\left(\frac{z}{\ln x_0 - z}\right)^2\right)\right) \frac{1}{\ln x_0 - z} - 1 - \frac{z}{\ln x_0 - z}}{\ln x_0 - z + O\left(\frac{z}{\ln x_0 - z}\right)} \\
&= x_1 - z x_0 \frac{\frac{z}{(\ln x_0 - z)^2} + O\left(\frac{z^2}{(\ln x_0 - z)^3}\right)}{\ln x_0 - z + O\left(\frac{z}{\ln x_0 - z}\right)} \\
&= x_0 \left(1 + \frac{z}{\ln x_0 - z} + O\left(\frac{z^2}{(\ln x_0 - z)^3}\right)\right)
\end{aligned}$$

We split the summation into two parts:

One part where $\min\left(\frac{m^3 np^{\frac{(1+\varepsilon)\ln 2}{\ln \ln p}}}{p^2}, \frac{m^2 n^2}{p}\right)$ equals the first term, and another part where it equals the second term, separated by the crossover point which we solved for. We shall first evaluate the summation assuming that the crossover point is not greater than m.

The first part of the summation equals roughly

$$\begin{aligned}
& O\left(\sum_{p=\lceil \frac{m}{n} \rceil}^{e^{x_2}} \frac{m^2 n^2}{p}\right) \\
&= O\left(m^2 n^2 \left(x_2 - \ln \frac{m}{n}\right)\right) \\
&= O\left(m^2 n^2 \ln \frac{m}{n} \left(\frac{(1+\varepsilon)\ln 2}{\ln \ln \frac{m}{n} - (1+\varepsilon)\ln 2} + O\left(\frac{((1+\varepsilon)\ln 2)^2}{\left(\ln \ln \frac{m}{n} - (1+\varepsilon)\ln 2\right)^3}\right)\right)\right) \\
&= O\left(m^2 n^2 \frac{\ln \frac{m}{n}}{\ln \ln \frac{m}{n}}\right)
\end{aligned}$$

An approximate solution to the transcendental equation in A.4 will not suffice for an accurate treatment of the second part. We must define the crossover point as $x_{cross} \stackrel{\text{def}}{=} kx_0$ for some k exactly. Substituting into A.4, we obtain

$$(\ln kx_0 - (1+\varepsilon)\ln 2)k = \ln kx_0$$
$$\frac{(1+\varepsilon)\ln 2}{\ln kx_0} = 1 - \frac{1}{k}$$

The second part of the summation can be evaluated as follows:

$$\begin{aligned}\sum_{p=(\frac{m}{n})^k}^{m} \frac{m^3 np^{\frac{(1+\varepsilon)\ln 2}{\ln\ln p}}}{p^2} &< \sum_{p=(\frac{m}{n})^k}^{\infty} \frac{m^3 np^{\frac{(1+\varepsilon)\ln 2}{\ln kx_0}}}{p^2} \\ &= \sum_{p=(\frac{m}{n})^k}^{\infty} \frac{m^3 np^{1-\frac{1}{k}}}{p^2} \\ &= O\left(m^3 n \left(\left(\frac{m}{n}\right)^k\right)^{(-1-\frac{1}{k}+1)}\right) \\ &= O(m^2n^2)\end{aligned}$$

Which is eclipsed by the order of the first part of the summation, so the total order of error is $O\left(m^2n^2\frac{\ln\frac{m}{n}}{\ln\ln\frac{m}{n}}\right)$. The order of error in this case is still less than the order of magnitude of the main term $O(m^2n^2\ln n)$.

In the event that the crossover point is greater than m, we obtain an error order of

$$O\left(\sum_{p=\lceil\frac{m}{n}\rceil}^{m} \frac{m^2n^2}{p}\right) = O(m^2n^2\ln n)$$

In which case it is possible that the approximation will fail to hold. (It should be noted that we have only arrived at an upper bound for the error; Since $\omega(u)$ is of order $\ln\ln u$ on average instead of the worst case $\dfrac{\ln u}{\ln\ln u}$ as stated in Theorem A.3.3, it is quite possible that the bound can be tightened further.) For the crossover point to be greater than m, we have $(1+\dfrac{z}{\ln\ln\frac{m}{n} - z})\ln\dfrac{m}{n} \approx \ln m$.

Suppose $m = n^{(\alpha+1)}$. We solve for α using an iterative method:

$$\left(1+\frac{z}{\ln\alpha + \ln\ln n - z}\right)\alpha\ln n = (\alpha+1)\ln n$$
$$\frac{z}{\ln\alpha+\ln\ln n - z} = \frac{1}{\alpha}$$
$$\alpha = \frac{1}{z}(\ln\alpha + \ln\ln n - z)$$

With an initial guess $\alpha_0 = \dfrac{1}{z}\ln\ln n - 1$, we obtain $\alpha \approx \dfrac{1}{z}(\ln\ln n + O(\ln\ln\ln n))$.

Note that $n^{\frac{1}{z}(\ln\ln n + O(\ln\ln\ln n))}$ grows faster than any polynomial function of n; This implies that the approximation is justified, i.e. the error is always smaller than the main term, as long as $m(n)$ is bounded by a polynomial function of n as $n \to \infty$.

A.4. **Error in neglecting the double count.**
As mentioned in Section 2.3, there is one double count term equal to $S(p', q')$, with $p' = \dfrac{m-1}{\gcd(m-1, n-1)}$ and $q' = \dfrac{n-1}{\gcd(m-1, n-1)}$. For ease of computation, we define $u = \gcd(m-1, n-1) \sim O(\min(m, n))$.

$$\begin{aligned} S(p', q') &= u(u-1)\left[\frac{mn}{2} - \left(\frac{(n-1)m + (m-1)n}{3u}\right.\right. \\ &\qquad \left.\left. + \frac{(m-1)(n-1)}{12u^2}(3u+2)\right)(u+1)\right] \\ &= O(mnu^2) \end{aligned}$$

This is eclipsed by other $O(m^2n^2)$ terms, so it is negligible.

A.5. **Summary.**
In our current context, where m and n differ by at most a factor of $2+o(1)$, the order of error in all error terms considered in this section is at most $O(m^2n^2)$, which is of an order less than the main order term of $\sum S(p, q)$ which is $O(m^2n^2 \ln\min(m, n))$. Therefore, the approximations we made were justified.

Appendix B. Calculations involved in 3D No-Three-in-Line

B.1. **Proof of Theorems 3.2.1 to 3.2.6.**
We shall use the indicator function as defined in 3.2.1.
1. Proof of Theorem 3.2.1
Using the following property of the Möbius function (Theorem 4.7 of [7]),

$$\sum_{d|n} \mu(d) = \begin{cases} 1 & \text{if } n = 1 \\ 0 & \text{if } n > 1 \end{cases}$$

we can rewrite the indicator function with the Möbius function

$$\begin{aligned}\sum_{s_2=2}^{s_3-1} \sum_{s_1=1}^{s_2-1} \mathbf{1}_{\gcd(s_1,s_2,s_3)=1} &= \sum_{s_2=2}^{s_3-1} \sum_{s_1=1}^{s_2-1} \sum_{d|\gcd(s_1,s_2,s_3)} \mu(d) \\ &= \sum_{s_2=2}^{s_3-1} \sum_{s_1=1}^{s_2-1} \sum_{d|s_3} \mu(d)(\mathbf{1}_{d|s_1})(\mathbf{1}_{d|s_2}) \\ &= \sum_{d|s_3} \left(\mu(d) \sum_{s_2=2}^{s_3-1} \left(\mathbf{1}_{d|s_2} \sum_{s_1=1}^{s_2-1} \mathbf{1}_{d|s_1} \right) \right)\end{aligned}$$

Note that $\sum_{s_1=1}^{s_2-1} \mathbf{1}_{d|s_1}$ is equivalent to counting how many integers from 1 to $s_2 - 1$ are divisible by d. Hence, it is equal to $\lfloor \frac{s_2-1}{d} \rfloor$.
Therefore, the expression becomes

$$\sum_{d|s_3} \left(\mu(d) \sum_{s_2=2}^{s_3-1} \mathbf{1}_{d|s_2} \left\lfloor \tfrac{s_2-1}{d} \right\rfloor \right).$$

Since $\lfloor \frac{s_2-1}{d} \rfloor = \frac{s_2}{d} + O(1)$, we can rewrite this as

$$\sum_{d|s_3} \left(\mu(d) \sum_{s_2=2}^{s_3-1} \mathbf{1}_{d|s_2} \left(\tfrac{s_2}{d} + O(1) \right) \right).$$

By a similar reasoning, $\sum_{s_2=2}^{s_3-1} s_2 \cdot \mathbf{1}_{d|s_2}$ sums up the integers s_2 from 2 to $s_3 - 1$ that are divisible by d. Applying the formula for the summation of natural numbers and factorising, we get $\sum_{s_2=2}^{s_3-1} s_2 \cdot \mathbf{1}_{d|s_2} = \frac{1}{2} d \left(\left\lfloor \frac{s_3-1}{d} \right\rfloor - \left\lfloor \frac{1}{d} \right\rfloor \right) \left(\left\lfloor \frac{s_3-1}{d} \right\rfloor + \left\lfloor \frac{1}{d} \right\rfloor + 1 \right)$.
Hence,

$$\sum_{d|s_3}\mu(d)\sum_{s_2=2}^{s_3-1}\mathbf{1}_{d|s_2}\Big(\tfrac{s_2}{d}+O(1)\Big)=\sum_{d|s_3}\mu(d)\Bigg[\frac{d\left(\lfloor\frac{s_3-1}{d}\rfloor-\lfloor\frac{1}{d}\rfloor\right)\left(\lfloor\frac{s_3-1}{d}\rfloor+\lfloor\frac{1}{d}\rfloor+1\right)}{2} + O\left(\frac{s_3}{d}\right)\Bigg]$$

$$=\sum_{d|s_3}\mu(d)\left(\frac{s_3^2}{2d^2}+O\Big(\frac{s_3}{d}\Big)\right)$$

2. Proof of Theorem 3.2.2

The outline of the proof is similar to that of Theorem 3.2.1.

$$\sum_{s_2=2}^{s_3-1}\sum_{s_1=1}^{s_2-1}(s_1+s_2)\mathbf{1}_{\gcd(s_1,s_2,s_3)=1}$$

$$=\sum_{s_2=2}^{s_3-1}\sum_{s_1=1}^{s_2-1}\sum_{d|\gcd(s_1,s_2,s_3)}(s_1+s_2)\mu(d)$$

$$=\sum_{s_2=2}^{s_3-1}\sum_{s_1=1}^{s_2-1}\sum_{d|s_3}(s_1+s_2)\mu(d)(\mathbf{1}_{d|s_1})(\mathbf{1}_{d|s_2})$$

$$=\sum_{d|s_3}\mu(d)\left(\sum_{s_2=2}^{s_3-1}\left(\mathbf{1}_{d|s_2}\sum_{s_1=1}^{s_2-1}s_1\,\mathbf{1}_{d|s_1}\right)+\sum_{s_2=2}^{s_3-1}\left(s_2\,\mathbf{1}_{d|s_2}\sum_{s_1=1}^{s_2-1}\mathbf{1}_{d|s_1}\right)\right)$$

$$=\sum_{d|s_3}\mu(d)\left(\sum_{s_2=2}^{s_3-1}\mathbf{1}_{d|s_2}\left(\frac{3s_2^2}{2d}+O(s_2)\right)\right)$$

Analogous to the proof of Theorem 3.2.1, we have the equality

$$\sum_{s_2=2}^{s_3-1}s_2^2\,\mathbf{1}_{d|s_2}=\frac{d^2}{6}\Bigg[\left\lfloor\frac{s_3-1}{d}\right\rfloor\left(\left\lfloor\frac{s_3-1}{d}\right\rfloor+1\right)\left(2\left\lfloor\frac{s_3-1}{d}\right\rfloor+1\right) - \left\lfloor\frac{1}{d}\right\rfloor\left(\left\lfloor\frac{1}{d}\right\rfloor+1\right)\left(2\left\lfloor\frac{1}{d}\right\rfloor+1\right)\Bigg]$$

Obtaining the final expression

$$\sum_{s_2=2}^{s_3-1}\sum_{s_1=1}^{s_2-1}(s_1+s_2)\mathbf{1}_{\gcd(s_1,s_2,s_3)=1}=\sum_{d|s_3}\mu(d)\left(\frac{s_3^3}{2d^2}+O\Big(\frac{s_3^2}{d}\Big)\right)$$

3. Proof of Theorem 3.2.3

$$\sum_{s_2=2}^{s_3-1}\sum_{s_1=1}^{s_2-1}s_1s_2\,\mathbf{1}_{\gcd(s_1,s_2,s_3)=1}=\sum_{s_2=2}^{s_3-1}\sum_{s_1=1}^{s_2-1}\sum_{d|\gcd(s_1,s_2,s_3)}s_1s_2\mu(d)$$

$$=\sum_{d|s_3}\mu(d)\left(\sum_{s_2=2}^{s_3-1}s_2\,\mathbf{1}_{d|s_2}\left(\sum_{s_1=1}^{s_2-1}s_1\,\mathbf{1}_{d|s_1}\right)\right)$$

$$= \sum_{d|s_3} \mu(d) \left(\sum_{s_2=2}^{s_3-1} \mathbf{1}_{d|s_2} \left(\frac{s_2^3}{2d} + O\left(s_2^2\right) \right) \right)$$

Using the fact that

$$\sum_{s_2=2}^{s_3-1} s_2^3 \, \mathbf{1}_{d|s_2} = d^3 \left[\left(\frac{\lfloor \frac{s_3-1}{d} \rfloor \left(\lfloor \frac{s_3-1}{d} \rfloor + 1 \right)}{2} \right)^2 - \left(\frac{\lfloor \frac{1}{d} \rfloor \left(\lfloor \frac{1}{d} \rfloor + 1 \right)}{2} \right)^2 \right]$$

We get the final expression

$$\sum_{d|s_3} \mu(d) \left(\frac{s_3^4}{8d^2} + O\left(\frac{s_3^3}{d} \right) \right)$$

4. Proof of Theorem 3.2.4

Let $s_3 = dq$ for some integer q. The equation simplifies to

$$\sum_{s_3=3}^{m} \sum_{d|s_3} \frac{s_3^k \mu(d)}{d^2} = \sum_{d=1}^{m} \left(\frac{\mu(d)}{d^2} \sum_{q=\lceil \frac{3}{d} \rceil}^{\lfloor \frac{m}{d} \rfloor} (dq)^k \right)$$

$$= \sum_{d=1}^{m} \mu(d) d^{k-2} \left(\sum_{q=1}^{\lfloor \frac{m}{d} \rfloor} q^k - \sum_{q=1}^{\lceil \frac{3}{d} \rceil - 1} q^k \right)$$

$$= \sum_{d=1}^{m} \mu(d) d^{k-2} \left(\frac{\lfloor \frac{m}{d} \rfloor^{k+1}}{k+1} + O\left(\frac{m^k}{d^k} \right) \right) \tag{B.1}$$

$$= \sum_{d=1}^{m} \left(\frac{m^{k+1} \mu(d)}{(k+1) d^3} + \mu(d) O\left(\frac{m^k}{d^2} \right) \right)$$

We invoke Theorem 8.15 of [7], which says that, for every $s > 1$,

$$\sum_{d=1}^{\infty} \frac{\mu(d)}{d^s} = \frac{1}{\zeta(s)}$$

Hence,

$$\sum_{d=1}^{m} \frac{\mu(d)}{d^s} = \frac{1}{\zeta(s)} + \sum_{d=m+1}^{\infty} \frac{\mu(d)}{d^2}$$

Note that

$$\left| \sum_{d=m+1}^{\infty} \frac{\mu(d)}{d^s} \right| \leqslant \sum_{d=m+1}^{\infty} \frac{1}{d^s} \leqslant \int_m^{\infty} \frac{1}{x^s} dx = O(m^{1-s})$$

Therefore, the original expression simplifies to

$$\frac{m^{k+1}}{(k+1)\zeta(3)} + O(m^k)$$

For improved accuracy, which will be only be used in the proof of Theorem 3.2.6, one can see that the constant multiplicative factor of the $O(\frac{m^k}{d^k})$ term at Equation B.1 is equal to $\frac{1}{2}$. Hence, the multiplicative constant of the $O(m^k)$ error term is $\frac{1}{2\zeta(2)} = \frac{3}{\pi^2}$.

5. Proof of Theorem 3.2.5

Firstly, consider the case when $k \geqslant 0$. The proof is very similar to that of Theorem 3.2.4. By letting $s_3 = dq$, we get

$$\sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{s_3^k \mu(d)}{d} \approx \sum_{d=1}^{\lfloor \frac{n-1}{2} \rfloor} \frac{n^{k+1}\mu(d)}{2^{k+1}(k+1)d^2}$$
$$= O(n^{k+1})$$

Special care must be taken for the case $k = -1$, using the harmonic series:

$$\sum_{q=1}^{q'} \frac{1}{q} = O(\ln q')$$

Therefore, we arrive at the following result:

$$\sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{\mu(d)}{s_3 d} \approx \sum_{d=1}^{\lfloor \frac{n-1}{2} \rfloor} \frac{\mu(d)}{d^2} \ln(n)$$
$$= O(\ln n)$$

6. Proof of Theorem 3.2.6

We will first prove the following proposition

Proposition B.1.1. Let i be a non-negative integer and $k - i \geqslant 0$, then

$$\sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{s_3^k \mu(d)}{d^2} \left\{\frac{n-1}{s_3}\right\}^i = \frac{(n-1)^{k+1}}{\zeta(3)} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \int_0^1 t^i (r+t)^{-(k+2)} dt + O(n^k \ln n)$$

Proof: Recall that $r = \left\lfloor \frac{n-1}{s_3} \right\rfloor$. Note that

$$\left\{\frac{n-1}{s_3}\right\} = \frac{n-1}{s_3} - \left\lfloor \frac{n-1}{s_3} \right\rfloor = \frac{1}{s_3}(n-1-s_3 r)$$

The original expression is thus equal to

$$\sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{s_3^{k-i}\mu(d)}{d^2} (n-1-s_3 r)^i$$

Applying the Binomial Theorem, we can further expand $(n-1-s_3r)^i$

$$\sum_{s_3=3}^{\lfloor\frac{n-1}{2}\rfloor}\sum_{d|s_3}\frac{s_3^{k-i}\mu(d)}{d^2}\sum_{h=0}^{i}\binom{i}{h}(n-1)^{i-h}(-r)^h s_3^h$$

Note that r is constant for all s_3 in $\left\lfloor\frac{n-1}{r+1}\right\rfloor < s_3 \leqslant \left\lfloor\frac{n-1}{r}\right\rfloor$. Therefore, we can rewrite the outer summation by r instead of s_3. The upper bound of the summation is given by the maximum value of r, which is $\left\lfloor\frac{n-1}{3}\right\rfloor$, as the minimum value of s_3 is 3. Similarly, the lower bound of the summation is 2.

$$\sum_{r=2}^{\lfloor\frac{n-1}{3}\rfloor}\sum_{s_3=\lfloor\frac{n-1}{r+1}\rfloor+1}^{\lfloor\frac{n-1}{r}\rfloor}\sum_{d|s_3}\frac{s_3^{k-i}\mu(d)}{d^2}\sum_{h=0}^{i}\binom{i}{h}(n-1)^{i-h}(-r)^h s_3^h$$

Swapping the order of summation, we get

$$\begin{aligned}
&\sum_{r=2}^{\lfloor\frac{n-1}{3}\rfloor}\sum_{h=0}^{i}\binom{i}{h}(n-1)^{i-h}(-r)^h\sum_{s_3=\lfloor\frac{n-1}{r+1}\rfloor+1}^{\lfloor\frac{n-1}{r}\rfloor}\sum_{d|s_3}\frac{s_3^{k-i+h}\mu(d)}{d^2}\\
&=\sum_{r=2}^{\lfloor\frac{n-1}{3}\rfloor}\sum_{h=0}^{i}\binom{i}{h}(n-1)^{i-h}(-r)^h\left(\sum_{s_3=1}^{\lfloor\frac{n-1}{r}\rfloor}\sum_{d|s_3}\frac{s_3^{k-i+h}\mu(d)}{d^2}\right.\\
&\qquad\left.-\sum_{s_3=1}^{\lfloor\frac{n-1}{r+1}\rfloor}\sum_{d|s_3}\frac{s_3^{k-i+h}\mu(d)}{d^2}\right)
\end{aligned}$$

We can apply Theorem 3.2.4 to handle the inner summation terms, since $k-i+h\geqslant 0$. We will separately handle the main term and error term in 3.2.4. For the main term,

$$\begin{aligned}
&\sum_{r=2}^{\lfloor\frac{n-1}{3}\rfloor}\sum_{h=0}^{i}\binom{i}{h}(n-1)^{i-h}(-r)^h\frac{(n-1)^{k-i+h+1}}{(k-i+h+1)\zeta(3)}\left(\frac{1}{r^{k-i+h+1}}-\frac{1}{(r+1)^{k-i+h+1}}\right)\\
&=\sum_{r=2}^{\lfloor\frac{n-1}{3}\rfloor}\sum_{h=0}^{i}\binom{i}{h}(n-1)^{i-h}(-r)^h\frac{(n-1)^{k-i+h+1}}{\zeta(3)}\int_0^1\frac{dt}{(r+t)^{k-i+h+2}}\\
&=\frac{(n-1)^{k+1}}{\zeta(3)}\sum_{r=2}^{\lfloor\frac{n-1}{3}\rfloor}\sum_{h=0}^{i}\binom{i}{h}(-r)^h\int_0^1\frac{dt}{(r+t)^{k-i+h+2}}\\
&=\frac{(n-1)^{k+1}}{\zeta(3)}\sum_{r=2}^{\lfloor\frac{n-1}{3}\rfloor}\int_0^1\frac{1}{(r+t)^{k-i+2}}\left(\sum_{h=0}^{i}\binom{i}{h}\left(\frac{-r}{r+t}\right)^h\right)dt
\end{aligned}$$

$$= \frac{(n-1)^{k+1}}{\zeta(3)} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \int_0^1 \frac{1}{(r+t)^{k-i+2}} \left(1 + \frac{-r}{r+t}\right)^i dt$$

$$= \frac{(n-1)^{k+1}}{\zeta(3)} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \int_0^1 t^i (r+t)^{-(k+2)} dt$$

For the error term,

$$\sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \sum_{h=0}^{i} \binom{i}{h} (n-1)^{i-h} (-r)^h \left(\frac{3}{\pi^2}\right) \left(\frac{n^{k-i+h}}{r^{k-i+h}} - \frac{n^{k-i+h}}{(r+1)^{k-i+h}}\right)$$

$$= \frac{3}{\pi^2} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \sum_{h=0}^{i} \binom{i}{h} \frac{n^k((r+1)^{k-i} - r^{k-i})}{r^{k-i}(r+1)^{k-i}}$$

$$\leqslant \frac{3}{\pi^2} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \sum_{h=0}^{i} \binom{i}{h} \frac{n^k r^{k-i-1}}{r^{k-i}(r+1)^{k-i}}$$

$$= \frac{3(2^i)}{\pi^2} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \frac{n^k}{r(r+1)^{k-i}}$$

$$\leqslant \frac{3(2^i)}{\pi^2} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \frac{n^k}{r}$$

$$= O(n^k \ln n)$$

Thus proving the proposition.

We shall apply the proposition in the proof of Theorem 3.2.6,

$$\sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{s_3^k \mu(d)}{d^2} f\left(\left\{\frac{n-1}{s_3}\right\}\right)$$

$$= \sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{s_3^k \mu(d)}{d^2} \sum_{i=0}^{T} a_i \left\{\frac{n-1}{s_3}\right\}^i$$

$$= \sum_{i=0}^{T} a_i \sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{s_3^k \mu(d)}{d^2} \left\{\frac{n-1}{s_3}\right\}^i$$

$$= \sum_{i=0}^{T} a_i \frac{(n-1)^{k+1}}{\zeta(3)} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \int_0^1 t^i (r+t)^{-(k+2)} dt + O(n^k \ln n)$$

$$= \frac{(n-1)^{k+1}}{\zeta(3)} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \int_0^1 \sum_{i=0}^{T} a_i t^i (r+t)^{-(k+2)} dt + O(n^k \ln n)$$

$$= \frac{(n-1)^{k+1}}{\zeta(3)} \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} \int_0^1 f(t)(r+t)^{-(k+2)} dt + O(n^k \ln n)$$

$$= \frac{(n-1)^{k+1}}{\zeta(3)} \int_0^1 f(t) \sum_{r=2}^{\lfloor \frac{n-1}{3} \rfloor} (r+t)^{-(k+2)} dt + O(n^k \ln n)$$

We approximate the innermost summation as $\zeta_H(k+2, t+2)$. The error in this approximation is given by

$$\begin{aligned}(n-1)^{k+1} \sum_{r=\lfloor \frac{n-1}{3} \rfloor + 1}^{\infty} (r+t)^{-(k+2)} &\approx (n-1)^{k+1} \int_{\frac{n}{3}}^{\infty} (r+t)^{-(k+2)} dr \\ &= \frac{3^{k+1}(n-1)^{k+1}}{(k+1)(3t+n)^{k+1}} \\ &= O(1)\end{aligned}$$

which can be neglected in the limit $n \to \infty$, as it is of a lesser order than the other error term $O(n^k \ln n)$. Therefore, the approximation is justified, and the theorem holds true, i.e.

$$\sum_{s_3=3}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{d|s_3} \frac{s_3^k \mu(d)}{d^2} f\left(\left\{\frac{n-1}{s_3}\right\}\right) = \frac{n^{k+1}}{\zeta(3)} \int_0^1 f(t)\, \zeta_H(k+2, t+2)\, dt + O(n^k \ln n),$$

B.2. **Evaluating integrals.**

For the integrals in Theorem 3.2.6 the detailed steps are as follows :

Integral 1.

$$\frac{n^6}{\zeta(3)} \int_0^1 \left(-\frac{1}{16}t^2 + \frac{1}{16}t + \frac{19}{96}\right) \zeta_H(4, t+2)\, dt$$

Consider:

$$\begin{aligned}&\int_0^1 \left(-\frac{1}{16}t^2 + \frac{1}{16}t + \frac{19}{96}\right) \zeta_H(4, t+2)\, dt \\ &= \int_0^1 \left(-\frac{1}{16}t^2 + \frac{1}{16}t + \frac{19}{96}\right) \sum_{k=0}^{\infty} \frac{1}{(k+t+2)^4} dt \\ &= \frac{1}{96} \sum_{k=0}^{\infty} \int_0^1 \frac{-6t^2 + 6t + 19}{(k+t+2)^4} dt\end{aligned}$$

Let $u = k+t+2 \Rightarrow du = dt$. Then we continue the integration:

$$\begin{aligned}&\frac{1}{96} \sum_{k=0}^{\infty} \int_{k+2}^{k+3} \frac{-6(u-k-2)^2 + 6(u-k-2) + 19}{u^4} du \\ &= \frac{1}{96} \sum_{k=0}^{\infty} \int_{k+2}^{k+3} \left(-\frac{6}{u^2} + \frac{12k+30}{u^3} - \frac{6k^2+30k+17}{u^4}\right) du\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{96}\sum_{k=0}^{\infty}\left[\left(\frac{6}{k+3}-\frac{6k+15}{(k+3)^2}+\frac{6k^2+30k+17}{3(k+3)^3}\right)\right. \\
&\qquad\left.-\left(\frac{6}{k+2}-\frac{6k+15}{(k+2)^2}+\frac{6k^2+30k+17}{3(k+2)^3}\right)\right] \\
&= \frac{1}{96}\sum_{k=0}^{\infty}\left(\frac{2}{k+3}+\frac{1}{(k+3)^2}-\frac{19}{3(k+3)^3}\right. \\
&\qquad\left.-\frac{2}{k+2}+\frac{1}{(k+2)^2}+\frac{19}{3(k+2)^3}\right) \\
&= \frac{1}{96}\left(\frac{\pi^2}{3}-\frac{59}{24}\right)
\end{aligned}
$$

Therefore, we have

$$
\begin{aligned}
&\frac{n^6}{\zeta(3)}\int_0^1\left(-\frac{1}{16}t^2+\frac{1}{16}t+\frac{19}{96}\right)\zeta_H(4,t+2)\,dt+O(n^5\ln n) \\
&= \frac{8\pi^2-59}{2304\zeta(3)}n^6+O(n^5\ln n)
\end{aligned}
$$

Integral 2.

$$
\frac{n^6}{\zeta(3)}\int_0^1\left(-\frac{1}{24}t^3+\frac{1}{8}t^2-\frac{1}{12}t-\frac{7}{96}\right)\zeta_H(5,t+2)\,dt+O(n^5\ln n)
$$

Consider:

$$
\begin{aligned}
&\int_0^1\left(-\frac{1}{24}t^3+\frac{1}{8}t^2-\frac{1}{12}t-\frac{7}{96}\right)\zeta_H(5,t+2)\,dt \\
&= \int_0^1\left(-\frac{1}{24}t^3+\frac{1}{8}t^2-\frac{1}{12}t-\frac{7}{96}\right)\sum_{k=0}^{\infty}\frac{1}{(k+t+2)^5}\,dt \\
&= \frac{1}{96}\sum_{k=0}^{\infty}\int_0^1\frac{-4t^3+12t^2-8t-7}{(k+t+2)^5}\,dt
\end{aligned}
$$

Let $u=k+t+2 \Rightarrow du=dt$. Then we continue the integration:

$$
\begin{aligned}
&\frac{1}{96}\sum_{k=0}^{\infty}\int_{k+2}^{k+3}\frac{4\big((u-k-2)^3-3(u-k-2)^2+2u\big)-8k-9}{u^5}\,du \\
&= \frac{1}{96}\sum_{k=0}^{\infty}\int_{k+2}^{k+3}\left(\frac{4}{u^2}-\frac{12k+36}{u^3}+\frac{12k^2+72k+104}{u^4}\right. \\
&\qquad\left.-\frac{4k^3+36k^2+104k+89}{u^5}\right)du \\
&= \frac{1}{96}\sum_{k=0}^{\infty}\left[-\frac{4}{u}+\frac{6k+18}{u^2}-\frac{12k^2+72k+104}{3u^3}+\frac{4k^3+36k^2+104k+89}{4u^4}\right]_{k+2}^{k+3}
\end{aligned}
$$

$$= \frac{1}{96}\sum_{k=0}^{\infty}\Bigg(\Bigg(-\frac{4}{k+3}+\frac{6k+18}{(k+3)^2}-\frac{12k^2+72k+104}{3(k+3)^3}+\frac{4k^3+36k^2+104k+89}{4(k+3)^4}\Bigg)$$

$$-\Bigg(-\frac{4}{k+2}+\frac{6k+18}{(k+2)^2}-\frac{12k^2+72k+104}{3(k+2)^3}+\frac{4k^3+36k^2+104k+89}{4(k+2)^4}\Bigg)\Bigg)$$

$$= \frac{1}{96}\sum_{k=0}^{\infty}\Bigg(-\frac{1}{k+3}+\frac{1}{3(k+3)^3}-\frac{7}{4(k+3)^4}+\frac{1}{k+2}-\frac{1}{(k+2)^2}$$

$$+\frac{2}{3(k+2)^3}+\frac{7}{4(k+2)^4}\Bigg)$$

$$= \frac{32\pi^2-109-192\,\zeta(3)}{18432}$$

Therefore, we have

$$\frac{n^6}{\zeta(3)}\int_0^1\left(-\frac{1}{24}t^3+\frac{1}{8}t^2-\frac{1}{12}t-\frac{7}{96}\right)\zeta(5,t+2)\,dt+O(n^5\ln n)$$

$$= \frac{32\pi^2-109-192\,\zeta(3)}{18432\,\zeta(3)}\,n^6+O(n^5\ln n).$$

Integral 3.

$$\frac{n^6}{\zeta(3)}\int_0^1\left(\frac{1}{32}t^4+\frac{1}{48}t^3-\frac{3}{32}t^2+\frac{1}{24}t+\frac{1}{240}\right)\zeta_H(6,t+2)\,dt+O(n^5\ln n)$$

Consider:

$$\int_0^1\left(\frac{1}{32}t^4+\frac{1}{48}t^3-\frac{3}{32}t^2+\frac{1}{24}t+\frac{1}{240}\right)\zeta_H(6,t+2)\,dt$$

$$=\int_0^1\left(\frac{1}{32}t^4+\frac{1}{48}t^3-\frac{3}{32}t^2+\frac{1}{24}t+\frac{1}{240}\right)\sum_{k=0}^{\infty}\frac{1}{(k+t+2)^6}\,dt$$

$$=\frac{1}{480}\sum_{k=0}^{\infty}\int_0^1\frac{15t^4+10t^3-45t^2+20t+2}{(k+t+2)^6}\,dt$$

Let $u=k+t+2\Rightarrow du=dt$. Then we continue the integration:

$$\frac{1}{480}\sum_{k=0}^{\infty}\int_{k+2}^{k+3}\frac{1}{u^6}\Big[5\big(3(u-k-2)^4+2(u-k-2)^3$$

$$-9(u-k-2)^2+4u\big)-20k-38\Big]\,du$$

$$=\frac{1}{480}\sum_{k=0}^{\infty}\int_{k+2}^{k+3}\left(\frac{15}{u^2}-\frac{60k+110}{u^3}+\frac{90k^2+330k+255}{u^4}\right.$$

$$-\frac{60k^3+330k^2+510k+160}{u^5}$$

$$\left.+\frac{15k^4+110k^3+255k^2+160k-58}{u^6}\right)du$$

$$= \frac{1}{480}\sum_{k=0}^{\infty}\Bigg[-\frac{15}{u}+\frac{60k+110}{2u^2}-\frac{90k^2+330k+255}{3u^3} + \frac{60k^3+330k^2+510k+160}{4u^4} - \frac{15k^4+110k^3+255k^2+160k-58}{5u^5}\Bigg]_{k+2}^{k+3}$$

$$= \frac{1}{480}\sum_{k=0}^{\infty}\Bigg[-\frac{2}{5(k+3)^5}-\frac{1}{(k+3)^4}-\frac{5}{2(k+3)^3} - \frac{7}{2(k+3)^2}-\frac{3}{k+3} - \left(-\frac{2}{5(k+2)^5}-\frac{1}{(k+2)^4}+\frac{3}{2(k+2)^3} - \frac{1}{2(k+2)^2}-\frac{3}{k+2}\right)\Bigg]$$

$$= \frac{1}{480}\left(-4\zeta(3)-\frac{\pi^2}{2}+\frac{781}{80}\right)$$

Therefore, we have

$$\frac{n^6}{\zeta(3)}\int_0^1\left(\frac{1}{32}t^4+\frac{1}{48}t^3-\frac{3}{32}t^2+\frac{1}{24}t+\frac{1}{240}\right)\zeta_H(6,t+2)\,dt+O(n^5\ln n)$$
$$= \frac{781-40\pi^2-320\zeta(3)}{38400\zeta(3)}n^6+O(n^5\ln n)$$

Integral 4.

$$\frac{n^6}{\zeta(3)}\int_0^1\left(\frac{1}{5}t^5-\frac{1}{4}t^4-\frac{1}{6}t^3+\frac{1}{4}t^2-\frac{1}{30}t\right)\zeta_H(7,t+2)\,dt$$

Consider:

$$\int_0^1\left(\frac{1}{5}t^5-\frac{1}{4}t^4-\frac{1}{6}t^3+\frac{1}{4}t^2-\frac{1}{30}t\right)\zeta_H(7,t+2)\,dt$$
$$= \sum_{k=0}^{\infty}\int_0^1\frac{12t^5-15t^4-10t^3+15t^2-2t}{60(k+t+2)^7}\,dt$$

Let $u=k+t+2 \implies du=dt$. Then we continue the integration:

$$\frac{1}{60}\sum_{k=0}^{\infty}\int_{k+2}^{k+3}\frac{12t^5-15t^4-10t^3+15t^2-2t}{u^7}\,dt$$
$$= \frac{1}{60}\sum_{k=0}^{\infty}\int_{k+2}^{k+3}\Bigg(\frac{12}{u^2}-\frac{60k+135}{u^3}+\frac{120k^2+540k+590}{u^4} - \frac{120k^3+810k^2+1770k+1245}{u^5}+\frac{60k^4+540k^3+1770k^2+2490k+1258}{u^6}$$

$$- \frac{12k^5 + 135k^4 + 590k^3 + 1245k^2 + 1258k + 480}{u^7}\Bigg) \, dt$$

$$= \frac{1}{60} \sum_{k=0}^{\infty} \Bigg[- \frac{12}{u} + \frac{60k + 135}{2u^2} - \frac{120k^2 + 540k + 590}{3u^3}$$
$$+ \frac{120k^3 + 810k^2 + 1770k + 1245}{4u^4} - \frac{60k^4 + 540k^3 + 1770k^2 + 2490k + 1258}{5u^5}$$
$$+ \frac{12k^5 + 135k^4 + 590k^3 + 1245k^2 + 1258k + 480}{6u^6} \Bigg]_{k+2}^{k+3}$$

$$= \frac{1}{60} \sum_{k=0}^{\infty} \Bigg(- \frac{2}{k+3} - \frac{3}{2(k+3)^2} - \frac{5}{6(k+3)^3} - \frac{1}{4(k+3)^4} + \frac{1}{15(k+3)^5}$$
$$+ \frac{2}{k+2} - \frac{1}{2(k+2)^2} - \frac{1}{6(k+2)^3} + \frac{1}{4(k+2)^4} - \frac{1}{15(k+2)^5} \Bigg)$$

$$= \frac{1}{60} \left(\frac{4313}{960} - \frac{\pi^2}{3} - \zeta(3) \right)$$

$$= \frac{4313 - 320\pi^2 - 960\zeta(3)}{57600}$$

Therefore, we have

$$\frac{n^6}{\zeta(3)} \int_0^1 \left(\frac{1}{5}t^5 - \frac{1}{4}t^4 - \frac{1}{6}t^3 + \frac{1}{4}t^2 - \frac{1}{30}t \right) \zeta_H(7, t+2) \, dt + O(n^5 \ln n)$$
$$= \frac{-960\zeta(3) + 4313 - 320\pi^2}{57600\,\zeta(3)} n^6 + O(n^5 \ln n)$$

Appendix C. Code

C.1. Empirical testing of independence of probabilities. For the case $m = n$:

```
import random
import itertools

for n in range(8, 27):
  grid = [(x, y) for x in range(n) for y in range(n)]

  iters = 0
  collinearCount = 0
  while iters - collinearCount < 100:
    iters += 1
    coordinates = random.sample(grid, n)
    x = [0] * n
    y = [0] * n
    trivial = 0
    for (x1, y1) in coordinates:
      x[x1] += 1
      y[y1] += 1
      if x[x1] > 2 or y[y1] > 2:
        collinearCount += 1
        trivial = 1
        break
    if trivial:
      continue
    for (a, b, c) in itertools.combinations(coordinates, 3):
      if (a[0] * (b[1] - c[1]) + b[0] * (c[1] - a[1]) + c[0] * (a[1] -
     b[1]) == 0):
        collinearCount += 1
        break
  actual = 1 - collinearCount / iters
  print("---- n =", n, "----")
  print("chance =", actual)
```

```
from math import log, gcd

def nC3(n):
  return n * (n - 1) * (n - 2) / 6

chances = [[8, 0.11648223645893996],
       [10, 0.03441274648129666],
       [12, 0.009561234929103435],
       [14, 0.0023081201976674626],
       [16, 0.0005618324727932889],
       [18, 0.00012113136696745297],
       [20, 2.7662333638711623e-05],
       [22, 5.129161519512593e-06],
       [24, 1.0324466065414484e-06],
```

```
    [26, 1.6383958867383086e-07]
]

def S(n, p, q):
  r = min((n - 1) // p, (n - 1) // q)
  return r * (r - 1) / 12 * (6 * n * n + (r + 1) * (p * q * (3 * r +
    2) - 4 * n * (p + q)))

for (n, actual) in chances:
  n_collinear = 0
  for p in range(1, (n - 1) // 2 + 1):
    for q in range(1, (n - 1) // 2 + 1):
      if gcd(p, q) == 1:
        n_collinear += 2 * S(n, p, q)
  # Add rows and columns
  n_collinear += 2 * nC3(n)
  predicted = (1 - n_collinear / nC3(n * n)) ** nC3(n)
  print(n,
     "&",
     "{0:.2f}".format(log(1 / predicted)),
     "&",
     "{0:.2f}".format(log(1 / actual)),
     "&",
     "{0:.1f}\%".format((log(1 / predicted) - log(1 / actual)) / log(1
     / actual) * 100))
  print("\\\\")
  print("\hline")
```

For general m and n:

```
import random
import itertools

def nCr(n, r):
  a = 1
  for i in range(r):
    a *= (n - i)
    a //= (i + 1)
  return a

for n in range(8, 25):
  for m in range(8, n + 1):
    iters = 0
    collinearCount = 0
    base_rate = nCr(m * n, 3)
    while iters - collinearCount < 300:
      iters += 1
      # generate list of ways to choose 0-2 points on each column;
    index means # of columns with 2
      ways = []
      total_non_trivial_ways = 0
```

```
      for i in range(m // 2):
        # m - i columns to choose from
        column_choice = nCr(m, i)
        # choose which of those columns has 2 points
        column_choice_2 = nCr(m - i, i)
        ways.append(column_choice * column_choice_2)
        total_non_trivial_ways += column_choice * column_choice_2
      choice = random.randint(0, total_non_trivial_ways - 1)
      for i in range(len(ways)):
        choice -= ways[i]
        if choice < 1:
          choice = i
          break
      coordinates = []
      put_on_these_columns = random.sample(range(m), m - choice)
      for i in range(choice):
        y1, y2 = random.sample(range(n), 2)
        coordinates.append((put_on_these_columns[i], y1))
        coordinates.append((put_on_these_columns[i], y2))
      for i in range(choice):
        y1, y2 = random.sample(range(n), 2)
        coordinates.append((put_on_these_columns[i], y1))
        coordinates.append((put_on_these_columns[i], y2))
      for (a, b, c) in itertools.combinations(coordinates, 3):
        if (a[0] * (b[1] - c[1]) + b[0] * (c[1] - a[1]) + c[0] * (a[1]
     - b[1]) == 0):
          collinearCount += 1
          break
    actual = 1 - collinearCount / iters
    print("[{0}, {1}, {2}],".format(m, n, actual))
```

```
from math import log, gcd
import matplotlib.pyplot as plt
import numpy as np

def nC3(n):
  return n * (n - 1) * (n - 2) / 6

# Data generated from first file
chances = []

def S(m, n, p, q):
  r = min((m - 1) // p, (n - 1) // q)
  return r * (r - 1) / 12 * (6 * n * m + (r + 1) * (p * q * (3 * r +
    2) - 4 * (p * n + q * m)))

z = np.zeros((25 - 8, 25 - 8))
for (m, n, actual) in chances:
  n_collinear = 0
  for p in range(1, (m - 1) // 2 + 1):
```

```
    for q in range(1, (n - 1) // 2 + 1):
      if gcd(p, q) == 1:
        n_collinear += 2 * S(m, n, p, q)
  # Add rows and columns
  n_collinear += nC3(n) + nC3(m)
  predicted = (1 - n_collinear / nC3(n * m)) ** nC3(min(m,n))
  z[m - 8, n - 8] = -(log(1 / predicted) - log(1 / actual)) / log(1 /
    actual) * 100


im = plt.imshow(np.ma.masked_where(z == 0, z), extent=[8,24,8,24],
    origin="lower") # drawing the function
plt.colorbar(im)
plt.show()
```

```
import random

def are_collinear_3d(p1, p2, p3):
    ab = (p2[0]-p1[0], p2[1]-p1[1], p2[2]-p1[2])
    ac = (p3[0]-p1[0], p3[1]-p1[1], p3[2]-p1[2])

    cross = (
        ab[1]*ac[2] - ab[2]*ac[1],
        ab[2]*ac[0] - ab[0]*ac[2],
        ab[0]*ac[1] - ab[1]*ac[0]
    )

    return cross == (0, 0, 0)

def probabilistic_3d(max_n, points=10, iterations=10):
    ns = list(range((max_n // points), max_n + 1, max_n // points))
    for n in ns:
        collinear_count = 0
        coordinates = [(x, y, z) for x in range(n) for y in range(n)
    for z in range(n)]

        for _ in range(iterations):
            selected = random.sample(coordinates, 3)
            if are_collinear_3d(selected[0], selected[1], selected[2])
    :
                collinear_count = collinear_count + 1

        actual_value = collinear_count / iterations
        asymptotic_value = 1.10664 / (n ** 3) # ~ 0.18444n^6 / (n^3C3)

        error = (asymptotic_value - actual_value) / actual_value * 100
        print(f"relative error at n = {n}: {error}%")

max_n = 50
points = 10
```

```
probabilistic_3d(max_n=max_n, points=points, iterations=100000000)
```

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EDITOR'S COMMENTS

The classical No-Three-in-Line problem asks for the largest number of points on an $n \times n$ grid with no three in a line. This paper extends it in two directions: to rectangular $m \times n$ grids, and to the three-dimensional cubic grid. The team gives construction-based bounds for rectangles, probabilistic estimates in the style of Guy and Kelly, and an asymptotic count of collinear triples in 3D. Extending the collinear-triple heuristic to rectangles, and especially into three dimensions, is a worthwhile and non-obvious step, and the exact asymptotic $N_{\mathrm{col}}(\mathbb{T}_n) \approx 0.18444\, n^6$—with an explicit constant involving $\zeta(3)$ and π^2—is a concrete and pleasing result.

The 3D collinear-triple computation is the technical highlight, and the team conducted careful error analysis by covering the coprime-density assumptions, double-counting, and summation-bound errors in a substantial appendix. They are also admirably honest about explaining why the heuristic cannot simply be carried over into 3D, which shows good understanding of the method's limits. It is a strong paper in the interface of combinatorics and analysis.