Probabilistic estimates of the diameters of the Rubik's Cube groups

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I. OBJECTIVE

The diameter of the Cayley graph of the Rubik's Cube^{1–4} group (hereafter the diameter) is the fewest number of turns to solve the Cube from any initial configuration. This number is also colloquially referred to as God's number. Here, a configuration denotes a unique arrangement of sticker colors of the Cube reachable by a series of turns from the solved configuration, while holding the orientation of the whole Cube fixed.

After decades of research by the community of mathematicians and computer scientists, $^{5-8}$ culminating in a Herculean computational effort by Rokicki *et al.*, $^{9-11}$ the diameter of the $3\times3\times3$ Cube was determined to be 20 in the half-turn metric or 26 in the quarter-turn metric. $^{9-11}$ The corresponding number for the $2\times2\times2$ Cube is 11 in the half-turn metric and 14 in the quarter-turn metric. 4 See below for the definitions of different metrics and other technical details.

The objective of this study is to examine to what extent a simple probabilistic argument can predict the diameters for different Rubik's Cube groups in various metrics, and to offer our best probabilistic estimates of the diameters for the $4\times4\times4$ and $5\times5\times5$ Cubes, whose brute-force determination is presently unthinkable.

II. BACKGROUND

Rubik's Cube¹⁻⁴ has long been a popular testbed for computer science research since the pioneering study by Korf, ^{12,13} especially in the areas of artificial intelligence and optimization theory. It has also fascinated mathematicians working on group theory. ^{3,14-19} Furthermore, its similarities with problems appearing in quantum mechanics, ²⁰ statistical mechanics, ²¹⁻²³ high-energy physics, ²⁴ and cryptography ^{25,26} have been noted.

The research on Rubik's Cube may be largely divided into three groups by their distinct objectives. The first group aims at determining the diameters described above as a mathematical question. The present study belongs to this group.

The second group's objective is to discover or develop an optimization method that is powerful enough to solve the Cube in any configurations efficiently. The method may also be general enough to do so without any domain knowledge, so that it can be applied to other puzzles. Machine Learning algorithms tend to fail^{27–29} because a required fitness function is hard to identify or define. Successful strategies first discover a good fitness function computationally³⁰ and/or to rely on large pattern databases,^{31–34} both of which are not meant to help a human player. So far the most effective method—the reinforcement learning algorithm recently developed by Agostinelli *et al.*³⁵—can solve the 3×3×3 Cube 100% of cases; with 60% of cases it discovers the most efficient solutions, underscoring its potential utility in determining the diameters of higher-order Cubes.

The third group computationally searches for the so-called "macros" or a series of turns that a human player can potentially master in a stepwise solution of the Cube. Such a solution is neither expected nor required to be efficient, but it may possibly contain some general principles or strategies for solutions, which may be applied to higher-order Cubes or other related puzzles. These studies, therefore, belong to the developments of expert systems³⁶ or discovery systems. These studies are discovery systems. Such as groundbreaking computational study 2,13 on Rubik's Cubes falls into this category, which exhaustively and systematically lists macros for both 2×2×2 and 3×3×3 Cubes. As a by-product, they also set the (albeit conservative) upper bounds for the diameters, spurring many subsequent studies.

III. PROBABILISTIC ESTIMATE

Let N be the total number of configurations. Consider a brute-force enumeration of configurations by performing all possible turns at each step, starting from the initial, solved configuration. Generated configurations are recorded in a non-duplicate list, and after a certain number of steps, all N configurations have been generated and no new configuration

can be added to the list. This number is equal to the diameter. This brute-force algorithm is as faultless as it is intractable for all but the $2\times2\times2$ Cube.

We shall instead estimate this number by simulating the above brute-force algorithm under the assumption that all generated configurations are random and independent of the previous "seed" configurations (this non-Markovian assumption is clearly not obeyed in reality and is a major approximation). We can then view this problem as a modified version of the coupon collector's problem^{39–42} in probabilistic theory (see Appendix A).

The coupon collector's problem asks the following question: Let T_N be the number of uniformly random integers in the range of 1 through N that need to be generated until every integer 1 through N is realized at least once. What is the expectation value of T_N ? The answer is

$$E[T_N] = N \ln N + \gamma N, \tag{1}$$

where $\gamma = 0.5772$ is the Euler–Mascheroni constant. The standard deviation of T_N is

$$\sigma[T_N] = 1.28 N. \tag{2}$$

See Appendix A for derivations.

The central limit theorem does not apply to T_N , whose distribution is said to be the Siobhan distribution, ⁴⁰ which is related to the Gumbel distributions. ³⁹ As per Dawkins, ⁴⁰ the probability of all integers occurring by the time T random integers have been generated is given asymptotically as

$$\Pr(T_N \le T) \approx e^{-Ne^{-T/N}}.$$
 (3)

The difference between the coupon collector's problem and the probabilistic estimation of the diameters is that in the latter the random configurations are generated in batches or stepwise. We therefore propose modifying the original problem as follows:

Let C(t) be the number of configurations generated in the tth step by performing all possible k turns to each of non-redundant "seed" configurations in the previous step t-1. Let the number of these seed configurations be S(t-1). Here, "non-redundant" means that no two configurations in the set are the same (lest the configurations generated from them are highly redundant and less uniformly random).

In the *t*th step, from each of the S(t-1) non-redundant seed configurations, r new configurations are generated by performing all k turns, but excluding some combinations of turns ("spurious turns"; see the following sections for examples) that predictably and immediately give rise to duplicate configurations:

$$C(t) = rS(t-1). (4)$$

Here, r (the branching ratio) is a real positive number that is less than k, and this condition r < k effectively excludes the spurious turns. The value of r is determined from the average growth ratio of the number of configurations generated in the first few steps (see the following sections). The purpose of this exclusion is not to eliminate any duplicate entries

in the set of C(t) newly generated configurations (the set is supposed to be redundant and increaingly more so as its size approaches or exceeds N); rather, it is to minimize the hysteresis in the generation and to make the generated configurations more uniformly random.

Collecting only the non-redundant configurations among the C(t) generated ones, we obtain a new set of seed configurations used in the next step. The size S(t) of this non-redundant set is related to the size C(t) of the original set by

$$S(t) = N(1 - e^{-C(t)/N}),$$
 (5)

whose derivation is given in Appendix B. The seed configurations should be non-redundant in that no two configurations in it are the same, ensuring more uniform randomness of the generated configurations, but some of them are certainly repeated from the seed sets of previous steps.

Because the seed set is non-redundant, its size S(t) cannot exceed N. This is ensured by Eq. (5). Furthermore, in earlier steps, $C(t) \ll N$ and because the use of r effectively eliminates spurious turns, there is a vanishing probability that two generated configurations are the same, implying $S(t) \approx C(t)$. This is also consistent with the first-order Taylor-series approximation of the exponential in Eq. (5).

The total number of redundantly generated configurations,

$$T(t) = C(0) + \dots + C(t), \tag{6}$$

will be compared with $E[T_N]$. When T(t) exceeds $E[T_N]$ for the first time, t is the probabilistic best estimate of the diameter. Nowhere in this estimation do actual configurations need to be generated; nor is a random number needed. The whole analysis proceeds by computing only the estimated sizes of various sets of configurations.

IV. THE 2×2×2 CUBE

One of the eight corner cubies (say, the front-top-left one) of the $2\times2\times2$ Cube is held fixed as the orientation anchor of the whole Cube (here, a "cubie" stands for a $1\times1\times1$ constituent cube). The remaining seven cubies' positions can be permuted in 7! ways and their orientations can take 3^7 ways, except the last (seventh) cubie's orientation is fixed by the first six (it is said¹ that the "sanity" of the seven cubies is maintained by only one of three orbits). Therefore, the total number of configurations N is

$$N = \frac{7! \cdot 3^7}{3} = 3.67 \times 10^6. \tag{7}$$

According to Eqs. (1) and (2), the expected number of random configurations $E[T_N]$ that need to be generated before each of N configurations occurs at least once (and its standard deviation $\sigma[T_N]$) is

$$E[T_N] \pm \sigma[T_N] = (15.7 \pm 1.3)N.$$
 (8)

It thus suggests that before the most stubborn one of all 3.67 million configurations is finally realized, an average configuration has to recur as many as 16 times on average.

TABLE I: The probabilistic estimates of the numbers of non-redundant seed configurations S(t), redundant configurations C(t), and cumulative redundant configurations T(t) as a function of step (t) in the half-turn metric of the $2\times2\times2$ Cube. N=3674160, $E[T_N]=15.7$ N, and therefore the predicted diameter is 12 for $T(12) > E[T_N] > T(11)$, while the correct diameter is 11.

t	S(t)	C(t)	T(t)
0	1	1	1
1	9	9	10
2	54	54	64
3	321	321	385
4	0.001N	0.001 N	0.001 N
5	0.003 N	0.003 N	0.004 N
6	0.018 N	0.018 N	0.022 N
7	0.102 N	0.108 N	0.130 N
8	0.454 N	0.606 N	0.735 N
9	0.933 N	2.699 N	3.435 N
10	0.996 N	5.540 N	8.975 N
11	0.997 N	5.917 N	14.892 N
12	0.997 N	5.924 N	20.816 N

A. Half-turn metric

With the front-top-left cubie held fixed, only the right (R), downward (D) and back (B) layers can be rotated. In the half-turn metric, the Cube can undergo one of the three (3) clockwise 90° turns (R, D, B), three (3) counterclockwise 90° turns (R^{-1}, D^{-1}, B^{-1}) , and three (3) 180° turns (R^2, D^2, B^2) in the Singmaster notation.²

In the first step, all nine (9) turns lead to distinct configurations. In the second and subsequent steps, X, X^{-1} , and X^2 immediately following the same (where X = R, D, or B) only produce the configurations that have already occurred. Therefore, $r \le 6$. An explicit enumeration indicates

$$S(0) = C(0) = 1, (9)$$

$$S(1) = C(1) = 9, (10)$$

$$S(2) = C(2) = 54,$$
 (11)

$$S(3) = C(3) = 321.$$
 (12)

The precise evaluation of S(t) at arbitrary value of t is still feasible for the $2\times2\times2$ Cube, and it is tantamount to determining the diameter by a brute-force enumeration.

Instead, starting with t = 4, we approximate the number of redundant random configurations C(t) in the tth step generated by performing all possible turns to the S(t-1) non-redundant seed configurations in the previous step, excluding the turns that predictably and immediately lead to the already realized configurations. Adopting the branching ratio of r = 321/54 = 5.94 to effectuate this exclusion, we use Eq. (4) to determine C(t) from S(t-1). The seed configurations of the subsequent (tth) step are then obtained by deleting all duplicate entries in the C(t) set. The size of this set S(t) is estimated by Eq. (5). The total number of redundantly generated configurations T(t) is then given by Eq. (6) and will be compared with $E[T_N]$.

Table I lists S(t), C(t), and T(t) thus computed as a function of t up to t = 12, where the cumulative number of configurations T(12) = 20.8 N exceeds $E[T_N] = 15.7 N$ for the first time. Therefore, the predicted diameter of the $2 \times 2 \times 2$ Cube in the half-turn metric is 12, which overshoots the correct diameter of 11.4

According to the Siobhan distribution [Eq. (3)], the probabilities that all configurations have been realized at t = 11 and 12 are

$$Pr(T_N \le T(11)) = 0.286,$$
 (13)

$$Pr(T_N \le T(12)) = 0.997, \tag{14}$$

respectively. Hence, the present probabilistic argument predicts that there is a fair (28.6%) chance that the diameter is correctly 11, which is consistent with the fact that T(11) is within one standard deviation $\sigma[T_N]$ from $E[T_N]$; the predicted diameter's overestimation is not severe. Correspondingly, according to Appendix B, the expected numbers of configurations that have *not* been realized after t = 11 and 12 are

$$Ne^{-T(11)/N} = 1.2,$$
 (15)

$$Ne^{-T(12)/N} = 0.0034,$$
 (16)

respectively.

B. Quarter-turn metric

In this metric, there are only six (6) valid 90° turns: R, D, B and their inverses R^{-1} , D^{-1} , B^{-1} . An explicit evaluation gives

$$S(0) = C(0) = 1, (17)$$

$$S(1) = C(1) = 6, (18)$$

$$S(2) = C(2) = 27,$$
 (19)

$$S(3) = C(3) = 120,$$
 (20)

suggesting r = 120/27 = 4.44. Using this r in conjunction with Eqs. (4)–(6), we obtain Table II. T(t) exceeds $E[T_N] = 15.7 N$ for the first time at t = 14, and therefore the predicted diameter of the $2\times2\times2$ Cube in the quarter-turn metric is 14, which agrees with the correct diameter of 14.4

As per Eq. (3), the probabilities that all configurations have been generated by t = 13, 14, and 15 are, respectively,

$$Pr(T_N \le T(13)) = 5 \times 10^{-6},$$
 (21)

$$Pr(T_N \le T(14)) = 0.859,$$
 (22)

$$Pr(T_N \le T(15)) = 0.998.$$
 (23)

Correspondingly, the estimated numbers of the unrealized configurations at t = 13, 14, and 15 are

$$Ne^{-T(13)/N} = 12,$$
 (24)

$$Ne^{-T(14)/N} = 0.15,$$
 (25)

$$Ne^{-T(15)/N} = 0.002.$$
 (26)

Hence, there is a negligible chance that the predicted diameter is actually 13 (not 14), but a small (14%) probability that

TABLE II: Same as Table I but in the quarter-turn metric. The predicted diameter is 14 for $T(14) > E[T_N] > T(13)$, while the correct diameter is also 14.

t	S(t)	C(t)	T(t)
0	1	1	1
1	6	6	7
2	27	27	34
3	120	120	154
4	533	533	687
5	0.001 N	0.001 N	0.001 N
6	0.003 N	0.003 N	0.004 N
7	0.013 N	0.013 N	0.016 N
8	0.055 N	0.056 N	0.073 N
9	0.221 N	0.250 N	0.323 N
10	0.626 N	0.983 N	1.306 N
11	0.938 N	2.778 N	4.084 N
12	0.984 N	4.164 N	8.248 N
13	0.987 N	4.371 N	12.619 N
14	0.988 N	4.384 N	17.003 N
15	0.988 N	4.385 N	21.388 N

it is 15. In this case, the predicted most likely (86%) value of the diameter (14) proves to be exact. See Sec. VIII C for our analysis of the metric-dependence of the accuracy of the probabilistic estimation.

C. Semi-quarter-turn metric

In this newly introduced metric, only three (3) clockwise 90° turns (R, D, and B) are allowed in each step. With an explicit enumeration, we find

$$S(0) = C(0) = 1, (27)$$

$$S(1) = C(1) = 3,$$
 (28)

$$S(2) = C(2) = 9, (29)$$

$$S(3) = C(3) = 27, (30)$$

$$S(4) = C(4) = 78,$$
 (31)

$$S(5) = C(5) = 216,$$
 (32)

suggesting r = 216/78 = 2.77. Using Eqs. (4)–(6) with this r for $t \ge 6$, we obtain Table III. T(21) exceeds $E[T_N]$ for the first time and therefore the predicted diameter is 21, which is too large as compared with the correct diameter of 19.

The probabilities that all configurations have been generated by t = 20, 21, and 22 are, respectively,

$$Pr(T_N \le T(20)) = 0.0097, \tag{33}$$

$$Pr(T_N \le T(21)) = 0.697, \tag{34}$$

$$Pr(T_N \le T(22)) = 0.972,$$
 (35)

with the estimated numbers of the non-generated configurations being

$$Ne^{-T(20)/N} = 4.6,$$
 (36)

$$Ne^{-T(21)/N} = 0.36,$$
 (37)

$$Ne^{-T(22)/N} = 0.03. (38)$$

TABLE III: Same as Table I but in the semi-quarter-turn metric. The predicted diameter is 21 for $T(21) > E[T_N] > T(20)$, while the correct diameter is 19.

t	S(t)	C(t)	T(t)
0	1	1	1
1	3	3	4
2	9	9	13
3	27	27	40
4	78	78	118
5	216	216	334
6	583	583	917
7	1546	1546	2463
8	0.001 N	0.001 N	0.002 N
9	0.003 N	0.003 N	0.005 N
10	0.010 N	0.010 N	0.015 N
11	0.026 N	0.026 N	0.041 N
12	0.070 N	0.072 N	0.113 N
13	0.175 N	0.193 N	0.306 N
14	0.384 N	0.485 N	0.791 N
15	0.655 N	1.065 N	1.856 N
16	0.837 N	1.815 N	3.671 N
17	0.902 N	2.319 N	5.990 N
18	0.918 N	2.498 N	8.488 N
19	0.921 N	2.542 N	11.030 N
20	0.922 N	2.552 N	13.582 N
21	0.922 N	2.554 N	16.136 N
22	0.922 N	2.555 N	18.691 N

In this case, the probabilistic estimate misses the mark completely, predicting that there is zero probability that the diameter is correctly 19.

D. Bi-quarter-turn metric

In this another new metric, all nine (9) turns in the half-turn metric plus six (6) additional bi-quarter turns (RD, $R^{-1}D^{-1}$, DB, $D^{-1}B^{-1}$, BR, $B^{-1}R^{-1}$) are elementary operations. This metric is intentionally highly redundant.

In the first few steps, the numbers of configurations are

$$S(0) = C(0) = 1, (39)$$

$$S(1) = C(1) = 15.$$
 (40)

$$S(2) = C(2) = 144,$$
 (41)

$$S(3) = C(3) = 1324.$$
 (42)

Using r = 1324/144 = 9.19, we can generate the numbers of configurations compiled in Table IV. The first time T(t) exceeds $E[T_N]$ is t = 9, predicting the diameter of 9, which is too small as compared with the correct diameter of 10.

As per Eq. (3),

$$Pr(T_N \le T(9)) = 0.9916, \tag{43}$$

$$Pr(T_N \le T(10)) = 0.9999,$$
 (44)

implying that there is slightly less than 1% chance that the diameter is 10. No configuration has been unrealized by t = 9

TABLE IV: Same as Table I but in the bi-quarter-turn metric. The predicted diameter is 9 for $T(9) > E[T_N] > T(8)$, while the correct diameter is 10.

t	S(t)	C(t)	T(t)
0	1	1	1
1	15	15	16
2	144	144	160
3	1324	1324	1484
4	0.003 N	0.003 N	0.004 N
5	0.030 N	0.030 N	0.034 N
6	0.240 N	0.275 N	0.309 N
7	0.890 N	2.210 N	2.519 N
8	1.000 N	8.182 N	10.700 N
9	1.000 N	9.187 N	19.888 N
10	1.000 N	9.189 N	29.077 N
11	1.000 N	9.189 N	38.266 N

since

$$Ne^{-T(9)/N} = 0.008,$$
 (45)

which is also inferred from the fact that T(9) exceeds $E[T_N]$ by $3\sigma[T_N]$.

V. THE 3×3×3 CUBE

The central cubie on each of the six faces of the $3\times3\times3$ Cube is held fixed as the orientation anchor. The number of configurations is¹

$$N = \frac{8! \cdot 3^8}{3} \frac{12! \cdot 2^{12}}{4} = 4.33 \times 10^{19}.$$
 (46)

The first fraction denotes the number of ways in which the eight corner cubies can be positioned (8!) and oriented (3^8) divided by the three orbits, only one of which maintains the sanity. The second fraction is the number of ways in which the twelve edge cubies can be placed (12!) and oriented (2^{12}) divided by the four orbits, only one of which has the sanity. The expected number of random configurations to generate all N configurations is therefore

$$E[T_N] \pm \sigma[T_N] = (45.8 + 1.3)N,$$
 (47)

as per Eqs. (1) and (2).

A. Half-turn metric

TABLE V: The probabilistic estimates of the numbers of non-redundant seed configurations S(t), redundant configurations C(t), and cumulative redundant configurations T(t) as a function of step (t) in the half-turn metric of the $3\times3\times3$ Cube. $N=4.33\times10^{19}$, $E[T_N]=45.8$ N, and the predicted diameter is 22 for $T(22) > E[T_N] > T(21)$, while the correct diameter is 20.

t	S(t)	C(t)	T(t)
0	1	1	1
1	18	18	19
2	243	243	262
3	3240	3240	3502
4	43217	43189	46691
5	576232	576088	622780
6	7683099	7681178	8303957
7	102415704	102415704	110719662
8	1365200187	1365201339	1475921001
9	1.820×10^{10}	1.820×10^{10}	1.967×10^{10}
10	2.426×10^{11}	2.426×10^{11}	2.623×10^{11}
11	3.234×10^{12}	3.234×10^{12}	3.496×10^{12}
12	4.310×10^{13}	4.310×10^{13}	4.660×10^{13}
13	5.746×10^{14}	5.746×10^{14}	6.212×10^{14}
14	0.0002 N	0.0002 N	0.0002 N
15	0.0024 N	0.0024 N	0.0026 N
16	0.0309 N	0.0314 N	0.0340 N
17	0.3379 N	0.4124 N	0.4464 N
18	0.9889 N	4.5046 N	4.9510 N
19	1.0000N	13.1826 N	18.1336 N
20	1.0000N	13.3300 N	31.4635 N
21	1.0000 N	13.3300 N	44.7935 N
22	1.0000 N	13.3300 N	58.1235 N

only produce the configurations that are already visited. Furthermore, repeated commutative turns such as RL and LR lead to the same configurations, together indicating r < 15.

With explicit evaluation, we find

$$S(0) = C(0) = 1, (48)$$

$$S(1) = C(1) = 18,$$
 (49)

$$S(2) = C(2) = 243,$$
 (50)

$$S(3) = C(3) = 3240,$$
 (51)

suggesting r = 3240/243 = 13.33. Table V lists S(t), C(t), and T(t) as a function of t. For small t, S(t) and C(t) coincide with the "positions" listed in Table 5.1 of Ref. 9, but they are distinct quantities and deviate from each other as t increases. At t = 22, T(t) exceeds $E[T_N]$ for the first time and by a wide margin and, therefore, 22 is the predicted value of the diameter, which overestimates the correct value of 20 (Ref. 9) by two.

Since T(21) = 44.8 N is within $\sigma[T_N]$ of $E[T_N] = 45.8 N$, Eq. (3) places about a 22% chance that the diameter is actually 21, still overestimating the correct diameter by one.

$$Pr(T_N \le T(21)) = 0.218,$$
 (52)

$$Pr(T_N \le T(22)) = 0.9999998.$$
 (53)

The chance that the predicted diameter agrees with the correct value of 20 is zero, which underscores the limitation of

TABLE VI: Same as Table V but in the quarter-turn metric. The predicted diameter is 26 for $T(26) > E[T_N] > T(25)$, while the correct diameter is also 26.

			= (1)
t	S(t)	C(t)	T(t)
0	1	1	1
1	12	12	13
2	114	114	127
3	1068	1068	1195
4	9604	10007	11202
5	91237	89988	101190
6	854745	854889	956079
7	8009630	8008958	8965037
8	75049468	75050236	84015273
9	703214807	703213511	787228784
10	6589121400	6589122744	7376351528
11	6.174×10^{10}	6.174×10^{10}	6.912×10^{10}
12	5.785×10^{11}	5.785×10^{11}	6.476×10^{11}
13	5.421×10^{12}	5.421×10^{12}	6.068×10^{12}
14	5.079×10^{13}	5.079×10^{13}	5.686×10^{13}
15	4.759×10^{14}	4.759×10^{14}	5.328×10^{14}
16	0.0001N	0.0001N	0.0001N
17	0.0010 N	0.0010 N	0.0011 N
18	0.0090 N	0.0090 N	0.0101 N
19	0.0809 N	0.0844 N	0.0945 N
20	0.5315 N	0.7583 N	0.8528 N
21	0.9931 N	4.9804 N	5.8332 N
22	0.9999 N	9.3056 N	15.1388 N
23	0.9999 N	9.3691 N	24.5079 N
24	0.9999 N	9.3692 N	33.8771 N
25	0.9999 N	9.3692 N	43.2463 N
26	0.9999 N	9.3692 N	52.6155 N

the present probabilistic estimation. The expected numbers of remaining unrealized configurations are

$$Ne^{-T(21)/N} = 1.5,$$
 (54)

$$Ne^{-T(22)/N} = 2 \times 10^{-6}.$$
 (55)

B. Quarter-turn metric

In this metric, twelve (12) 90° turns R, D, B, L, U, F, R^{-1} , D^{-1} , B^{-1} , L^{-1} , U^{-1} , and F^{-1} are valid. With an explicit evaluation, we find

$$S(0) = C(0) = 1, (56)$$

$$S(1) = C(1) = 12, (57)$$

$$S(2) = C(2) = 114,$$
 (58)

$$S(3) = C(3) = 1068,$$
 (59)

suggesting r = 1068/114 = 9.37. Table VI predicts how these numbers grow in subsequent steps. It indicates that at t = 26, T(t) is expected to exceed $E[T_N]$ for the first time and hence the predicted diameter is 26, which agrees with the correct diameter determined by Rokicki *et al.*⁹

The probability that the diameter is actually 25 is less than 0.1%; there is a 99.9% probability that the diameter is cor-

rectly 26 according to Eq. (3).

$$Pr(T_N \le T(25)) = 8 \times 10^{-4},$$
 (60)

$$Pr(T_N \le T(26)) = 0.9994.$$
 (61)

The estimated numbers of configurations that have not been realized after t = 25 and 26 are, respectively,

$$Ne^{-T(25)/N} = 7.2,$$
 (62)

$$Ne^{-T(26)/N} = 6 \times 10^{-4}.$$
 (63)

Therefore, for the quarter-turn metric, just as in the case of the $2\times2\times2$ Cube, the probabilistic estimate proves to be exact (see more on this in Sec. VIII A).

VI. THE 4×4×4 CUBE

The number of configurations of the $4\times4\times4$ Cube is 43

$$N = \frac{7! \cdot 3^7}{3} 24! \frac{24!}{(4!)^6} = 7.40 \times 10^{45}.$$
 (64)

The first fraction is the number of ways in which seven of the eight corner cubies can be placed and oriented, while the last (eighth) one is held fixed as the orientation anchor. This fraction is therefore equal to the number of configurations of the $2\times2\times2$ Cube [Eq. (7)]. The second factor (24!) is the number of ways in which twenty-four edge cubies can be permuted, which are distinguishable and cannot be freely oriented. The last fraction is the number of ways in which six quadruplicate center cubies can be positioned, whose orientations cannot be freely changed.

The number of random configurations that needs to be generated before all *N* configurations occur is

$$E[T_N] \pm \sigma[T_N] = (106.2 \pm 1.3)N.$$
 (65)

according to Eqs. (1) and (2).

A. Half-turn metric

There are twenty-seven (27) turns, which are clockwise 90° turns R_1 , D_1 , B_1 , R_2 , D_2 , B_2 , R_3 , D_3 , B_3 and their inverses R_1^{-1} , D_1^{-1} , B_1^{-1} , etc. as well as the corresponding 180° turns R_1^2 , D_1^2 , B_1^2 , etc., where the subscript i in X_i refers to the ith layer rotated with i = 1 being the face (exterior) layer (and hence R_3 is alternatively denoted by L_2^{-1}).

For the first few steps, we can explicitly compute

$$S(0) = C(0) = 1, (66)$$

$$S(1) = C(1) = 27,$$
 (67)

$$S(2) = C(2) = 567,$$
 (68)

$$S(3) = C(3) = 11721,$$
 (69)

and, therefore, we adopt r = 11721/567 = 20.67. Table VII estimates S(t), C(t), and T(t) for $t \ge 4$ using Eqs. (4)–(6). At

TABLE VII: The probabilistic estimates of the non-redundant seed configurations S(t), redundant configurations C(t), and cumulative redundant configurations T(t) as a function of step (t) in the half-turn metric of the $4\times4\times4$ Cube. $N=7.40\times10^{45}$, $E[T_N]=106.2$ N, and the predicted diameter is 41 since $T(41)>E[T_N]>T(40)$. The correct diameter is unknown.

t	S(t)	C(t)	T(t)
0	1	1	1
1	27	27	28
2	567	567	595
3	11721	11721	12316
4	242273	242273	254589
5	5007784	5007784	5262373
6	103510903	103510903	108773276
7	2139570358	2139570358	2248343634
8	44224919298	44224919298	46473262932
32	0.0002 N	0.0002 N	0.0002 N
33	0.0046 N	0.0046 N	0.0048 N
34	0.0899 N	0.0942 N	0.0990 N
35	0.8442 N	1.8590 N	1.9581 N
36	1.0000 N	17.4491 <i>N</i>	19.4072 N
37	1.0000 N	20.6700 N	40.0772 N
38	1.0000 N	20.6700 N	60.7472 N
39	1.0000 N	20.6700 N	81.4172 N
40	1.0000 N	20.6700 N	102.0872 N
41	1.0000 N	20.6700 N	122.7572 N

 $t=41,\,T(t)$ becomes greater than $E[T_N]$ for the first time, predicting the diameter of 41 for the 4×4×4 Cube in the half-turn metric. The correct diameter is unknown and its brute-force computational determination seems out of the question in the foreseeable future.

T(41) exceeds $E[T_N]$ by a wide margin and hence the probability that the diameter is actually 40 is zero.

$$Pr(T_N \le T(40)) = 1 \times 10^{-15}, \tag{70}$$

$$Pr(T_N \le T(41)) = 1.$$
 (71)

However, these probabilities are predicated on the validity of the assumptions underlying our probabilistic predictions, which may well overestimate the diameters judging from the results for the $2\times2\times2$ and $3\times3\times3$ Cubes in the half-turn metric. The estimated numbers of unrealized configurations after t=40 and 41 are

$$Ne^{-T(40)/N} = 34,$$
 (72)

$$Ne^{-T(41)/N} = 4 \times 10^{-8},$$
 (73)

reiterating the fact that the present probabilistic estimate of 41 is rather definitive because the stepwise growth of T(t) for large t is 20.7 N, which is an order of magnitude greater than $\sigma[T_N] = 1.3 N$.

TABLE VIII: Same as Table VII but in the quarter-turn metric. The predicted diameter is 48 since $T(48) > E[T_N] > T(47)$. The correct diameter is unknown.

t	S(t)	C(t)	T(t)
0	1	1	1
1	18	18	19
2	261	261	280
3	3732	3732	4012
4	53368	53368	57380
5	763157	763157	820536
6	10913141	10913141	11733677
7	156057909	156057909	167791586
8	2231628106	2231628106	2399419692
9	31912281912	31912281912	34311701604
36	0.0001 N	0.0001 N	0.0001N
37	0.0010 N	0.0010 N	0.0010 N
38	0.0137 N	0.0138 N	0.0148 N
39	0.1777 N	0.1957 N	0.2105 N
40	0.9213 N	2.5417 N	2.7522 N
41	1.0000 N	13.1741 N	15.9264 N
42	1.0000 N	14.3000 N	30.2264 N
43	1.0000 N	14.3000 N	44.5263 N
44	1.0000 N	14.3000 N	58.8263 N
45	1.0000 N	14.3000 N	73.1263 N
46	1.0000 N	14.3000 N	87.4263 N
47	1.0000 N	14.3000 N	101.7263 N
48	1.0000 N	14.3000 N	116.0263 N

B. Quarter-turn metric

There are eighteen (18) turns in this metric, which are clockwise 90° turns R_1 , D_1 , B_1 , R_2 , D_2 , B_2 , and R_3 , D_3 , B_3 as well as their inverses.

An explicit enumeration shows

$$S(0) = C(0) = 1, (74)$$

$$S(1) = C(1) = 18,$$
 (75)

$$S(2) = C(2) = 261,$$
 (76)

$$S(3) = C(3) = 3732.$$
 (77)

We adopt r = 3732/261 = 14.30. Using the identical probabilistic logic in the foregoing sections, we obtain Table VIII. At t = 48, T(t) exceeds $E[T_N]$ for the first time, and therefore the predicted diameter is 48, whereas the correct value is unknown.

The probabilities that the diameter is 47 or 48 are, respectively,

$$Pr(T_N \le T(47)) = 5 \times 10^{-22},$$
 (78)

$$Pr(T_N \le T(48)) = 0.99997. \tag{79}$$

The estimated numbers of unrealized configurations are

$$Ne^{-T(47)/N} = 49,$$
 (80)

$$Ne^{-T(48)/N} = 3 \times 10^{-5},$$
 (81)

meaning that the predicted diameter of 48 is definitive, which however does not imply the accuracy of the prediction.

VII. THE 5×5×5 CUBE

The number of configurations of the $5\times5\times5$ Cube is ⁴³

$$N = \frac{8! \cdot 3^8}{3} \frac{12! \cdot 2^{12}}{4} 24! \frac{24!}{(4!)^6} \frac{24!}{(4!)^6} = 2.83 \times 10^{74}.$$
 (82)

The center cubie of each face is held fixed as the orientation anchor. The first two fractions are, respectively, the number of ways in which the eight corner cubies are placed and oriented and the number of ways in which the twelve center-edge cubies are positioned and oriented. They are the same as the corresponding factors for the 3×3×3 Cube [Eq. (46)]. The third factor (24!) is the number of ways in which twenty-four non-central-edge cubies are permuted, which are distinguishable and cannot be freely oriented. The last two fractions are, respectively, the number of ways in which six quadruplicate diagonal center cubies are positioned and the number of ways in which six quadruplicate remaining cubies are placed.

Therefore, the expected number of configurations that need to be generated before every configuration is realized is

$$E[T_N] \pm \sigma[T_N] = (172.0 \pm 1.3)N.$$
 (83)

A. Half-turn metric

The thirty-six (36) turns in this metric are face (exterior) layer clockwise 90° turns R_1 , D_1 , B_1 , L_1 , U_1 , F_1 , interior layer clockwise 90° turns R_2 , D_2 , B_2 , L_2 , U_2 , F_2 , and their inverses as well as the corresponding 180° turns.

In the first few steps, the numbers of configurations can be determined exactly as

$$S(0) = C(0) = 1, (84)$$

$$S(1) = C(1) = 36,$$
 (85)

$$S(2) = C(2) = 1026,$$
 (86)

$$S(3) = C(3) = 28812,$$
 (87)

suggesting r = 28812/1026 = 28.08. In the subsequent steps, they are estimated probabilistically, and the result is given in Table IX. It shows that T(58) is greater than $E[T_N]$ for the first time and hence the predicted diameter is 58. The correct value of the diameter is unknown.

Owing to the large number of configurations (28.1 N) generated in each of the later steps as compared with the fixed standard deviation of $\sigma[T_N] = 1.3 N$, the probability that the predicted diameter is shifted by one is essentially zero.

$$Pr(T_N \le T(57)) = 0,$$
 (88)

$$Pr(T_N \le T(58)) = 0.996.$$
 (89)

Correspondingly, many configurations are expected to remain unrealized after t = 57, all of which are however recuperated in the next step.

$$Ne^{-T(57)/N} = 7 \times 10^9,$$
 (90)
 $Ne^{-T(58)/N} = 4 \times 10^{-3}.$ (91)

$$Ne^{-T(58)/N} = 4 \times 10^{-3}$$
. (91)

Therefore, the present probabilistic estimate is definitive, saying nothing about its accuracy.

TABLE IX: The probabilistic estimates of the non-redundant seed configurations S(t), redundant configurations C(t), and cumulative redundant configurations T(t) as a function of step (t) in the quarter-turn metric of the $5 \times 5 \times 5$ Cube. $N = 2.83 \times 10^{74}$, $E[T_N] = 172.0 N$, and the predicted diameter is 58 since $T(58) > E[T_N] > T(57)$. The correct diameter is unknown.

t	S(t)	C(t)	T(t)
0	1	1	1
1	36	36	37
2	1026	1026	1063
3	28812	28812	29875
4	809041	809041	838916
5	22717870	22717870	23556786
6	637917794	637917794	661474580
7	17912731656	17912731656	18574206236
49	0.0004 N	0.0004 N	0.0004 N
50	0.0120 N	0.0121 N	0.0125 N
51	0.2864 N	0.3374 N	0.3499 N
52	0.9997 N	8.0413 N	8.3912 N
53	1.0000 N	28.0710 N	36.4621 N
54	1.0000 N	28.0800 N	64.5421 N
55	1.0000 N	28.0800 N	92.6221 N
56	1.0000 N	28.0800 N	120.7021 N
57	1.0000 N	28.0800 N	148.7821 N
58	1.0000 N	28.0800 N	176.8621 <i>N</i>

Quarter-turn metric

The twenty-four (24) turns in this metric are exterior-layer clockwise 90° turns, interior-layer clockwise 90° turns, and their inverses. An explicit enumeration gives

$$S(0) = C(0) = 1, (92)$$

$$S(1) = C(1) = 24,$$
 (93)

$$S(2) = C(2) = 468,$$
 (94)

$$S(3) = C(3) = 9000,$$
 (95)

suggesting r = 9000/468 = 19.23. Table X indicates that the predicted diameter is 68 because $T(68) > E[T_N] > T(67)$.

In this case also, the probability that the diameter is 67 instead of 68 is virtually zero.

$$Pr(T_N \le T(67)) = 2 \times 10^{-5}, \tag{96}$$

$$Pr(T_N \le T(68)) = 1.$$
 (97)

There expected to be an appreciable number of configurations that have not been realized after t = 67, but none at t = 68.

$$Ne^{-T(67)/N} = 11,$$
 (98)

$$Ne^{-T(68)/N} = 5 \times 10^{-8}. (99)$$

VIII. DISCUSSION

Table XI summarizes the size and metric dependence of the actual (if available) and predicted diameters of the $n \times n \times n$

TABLE X: Same as Table IX but in the quarter-turn metric. The predicted diameter is 68 since $T(68) > E[T_N] > T(67)$. The correct diameter is unknown.

t	S(t)	C(t)	T(t)
0	1	1	1
1	24	24	25
2	468	468	493
3	9000	9000	9493
4	173070	173070	182563
5	3328136	3328136	3510699
6	64000057	64000057	67510756
7	1230721100	1230721100	1298231856
8	23666766753	23666766753	24964998610
9	455111924665	455111924665	480076923275
55	0.0002 N	0.0002 N	0.0002 N
56	0.0036 N	0.0036 N	0.0038 N
57	0.0663 N	0.0686 N	0.0724 N
58	0.7207 N	1.2755 N	1.3479 N
59	1.0000 N	13.8593 N	15.2072 N
60	1.0000 N	19.2300 N	34.4371 N
61	1.0000 N	19.2300 N	53.6671 N
62	1.0000 N	19.2300 N	72.8971 N
63	1.0000 N	19.2300 N	92.1271 N
64	1.0000 N	19.2300 N	111.3571 N
65	1.0000 N	19.2300 N	130.5871 N
66	1.0000 N	19.2300 N	149.8171 N
67	1.0000 N	19.2300 N	169.0471 N
68	1.0000 N	19.2300 N	188.2771 <i>N</i>

TABLE XI: Actual and predicted diameters of the $n \times n \times n$ Rubik's Cube group $(2 \le n \le 5)$ in various metrics.

			Diameter		
Cube	Metric	r^{a}	Actual	Predicted ^b	Predicted ^c
$2\times2\times2$	Half	5.94	11 ^d	12	11
$2\times2\times2$	Quarter	4.44	14 ^d	14	14
$2\times2\times2$	Semi-quarter	2.77	19 ^e	21	20
$2\times2\times2$	Bi-quarter	9.19	10 ^e	9	9
$3\times3\times3$	Half	13.33	$20^{\rm f}$	22	21
$3\times3\times3$	Quarter	9.37	$26^{\rm f}$	26	25
$4\times4\times4$	Half	20.67		41	40
$4\times4\times4$	Quarter	14.30		48	47
$5 \times 5 \times 5$	Half	28.08		58	58
5×5×5	Quarter	19.23		68	67

^a Branching ratio. See Eq. (4).

Rubik's Cube groups $(2 \le n \le 5)$. This table's predictions can be easily extended to greater n, different metrics, or other types of Cubes with essentially little additional computational cost, but determining actual values will be formidable.

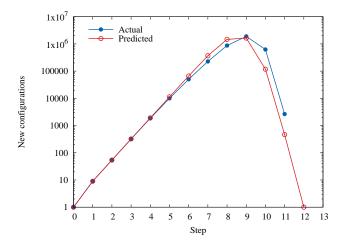


FIG. 1: The number of new (non-redundant) configurations of the 2×2×2 Cube generated in each step in the half-turn metric. A terminal plot (step 11 for the actual) corresponds to the diameter.

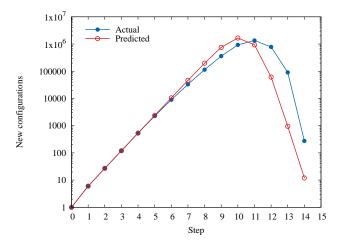


FIG. 2: Same as Fig. 1 for the quarter-turn metric.

A. Comparison between predicted and actual results

For the $2\times2\times2$ Cube, one can easily perform the brute-force enumeration of configurations as a function of the number of turns applied to the solved configuration, in nearly but not exactly the same way the probabilistic estimation's hypothetical algorithm generates configurations.

In Figs. 1–4 are plotted the number of new, non-redundant configurations generated ("Actual") in each step for the half-turn, quarter-turn, semi-quarter-turn, and bi-quarter-turn metrics, respectively, which are compared with the probabilistic estimates ("Predicted"). The "Actual" numbers were determined by a computer program.⁴⁴ The "Predicted" numbers were obtained as

$$N\left(e^{-T(t-1)/N} - e^{-T(t)/N}\right),$$
 (100)

which is consistent with Appendix B. A terminal point corresponds to the diameter at which all configurations have been

b Probabilistic estimate based on a modified version of the coupon collector's problem (this work).

^c Equation (101) (this work).

d Reference 4.

^e This work.

f Rokicki et al. 9-11

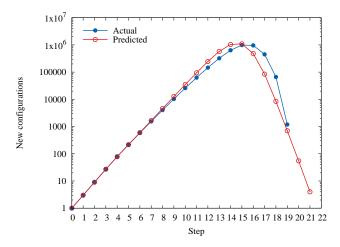


FIG. 3: Same as Fig. 1 for the semi-quarter-turn metric.

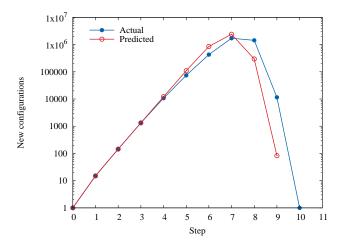


FIG. 4: Same as Fig. 1 for the bi-quarter-turn metric.

generated and no new ones can be added in the subsequent steps.

In each of the metrics, the actual curve in earlier steps displays a geometrical growth r^t with the step count t and is accurately reproduced by the probabilistically predicted curve. The peaks of the curves tend to occur one step too early in the predicted curves. The subsequent rapid falloffs of the actual curves seem super-exponential with their slopes in the logarithm scale becoming more negative for higher step counts. It may be imagined that in the final few steps of the diameter, the remaining unrealized configurations will be more efficiently exhausted than a random generation can. However, the predicted curves, owing to the non-Markovian assumption of the probabilistic estimation, will display an exponential and thus slower decay of the form e^{-rt} , where r is the branching ratio, taking more steps than reality to exhaust the remaining unrealized configurations.

In the half-turn and quarter-turn metrics, therefore, there seems to be a systematic cancellation of errors between the peak positions (occurring one step too early in the predicted curves) and the rate of decay (which is faster in the actual

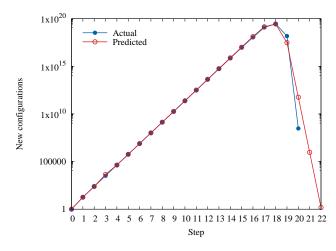


FIG. 5: The number of new (non-redundant) configurations of the 3×3×3 Cube generated in each step in the half-turn metric. The actual values (those in the last five steps were approximate) were taken from Table 5.1 of Rokicki *et al.*⁹

curves), although the predicted diameter in the half-turn metric is still overestimated by one. In the semi-quarter-turn metric, since r is small, there is a longer decay phase, causing the slow decay of the predicted curve to overshoot the diameter by as much as two, despite its peak position occurring one step too early. In the bi-quarter-turn metric, in contrast, r is large, which minimizes the error of the predicted decay rate, and underestimates the diameter by one.

Implicit in our probabilistic estimation logic is the assumption that the details of each metric are unimportant and all of its characteristics can be encapsulated into the branching ratio r, which is invariant of the step count. From Figs. 1–4, this assumption seems valid for the growth phase, but is no longer so in the decay phase. The fact that these curves show a super-exponential decay suggests that the effective value of r increases near the diameter and may even exceed the number of turns. In fact, the actual and predicted curves in Fig. 3 behave like $e^{-4.0t}$ and $e^{-2.6t}$ (where t is the number of steps) at the diameter, respectively, and the factor of 4.0 in the former exceeds r=2.77 or even the number of turns, which is three. There seems room for improvement in the probabilistic estimates in the peak position and decay rate of these curves.

For the $3\times3\times3$ Cube, Rokicki *et al.*⁹ gave the actual and estimated numbers ("positions") of new configurations generated at each step. They are compared with our predicted values in Fig. 5. In this case, the rising part and the peak of the actual curve is accurately reproduced by the prediction, but the falling part decays too slow in the latter, overestimating the diameter by two, although the Rokicki *et al.*'s values in the last five steps are approximate. The actual curve has a rapid falloff of $e^{-22.3t}$, although it likely decreases faster than exponentially. On the other hand, the predicted curve decays exponentially as $e^{-13.3t}$ corresponding to r=13.33. It again suggests that our probabilistic logic tends to underestimate the accerelated rate of exhausting remaining unrealized configurations in the final few steps. However, the exact agreement

of the predicted and actual diameters in the quarter-turn metric may contradict this view, given the smaller value of r = 9.37 and even slower decay of the predicted curve in this metric.

In the $4\times4\times4$ and $5\times5\times5$ Cubes, whose branching ratio r is small relative to the huge $E[T_N]$, there expected to be long decay phases, potentially causing noticeable overestimation of the diameters.

B. Size dependence

Demaine *et al.* ¹⁶ argued that the diameter is asymptotically proportional to $n^2/\log n$, where n denotes the Cube size. Under the assumption of the exact proportionality in the quarter-turn metric, their formula predicts the diameters of the 4×4×4 and 5×5×5 Cubes in the same metric to be 43 and 62, respectively, which are much smaller than our estimates (48 and 68).

Our probabilistic estimation suggests that a more meaningful closed-form expression may be a function of the number of configurations N (rather than of the Cube size n) and also of the metric. This is because there are complicated n dependencies (possibly including even-odd alternation) of N and also because it is N that dictates the complexity of the puzzle and thus the diameters more directly than n. Furthermore, as discussed below, the diameters may also depend on the metric in a nontrivial manner since some turns seem more useful than others.

With the branching ratio r and the number of configurations N, both of which can be relatively easily determined as has been done in the foregoing sections, the probabilistic estimate of the diameter (which must be distinguished from the correct diameter) is approximated by

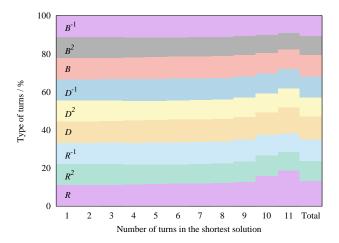
$$\frac{\ln N}{\ln r} + \frac{\ln N}{r}.\tag{101}$$

The first term counts the number of steps required for S(t) to increase geometrically and reach N, while the second term is the number of additional steps needed for T(t) to increase linearly and exceed $E[T_N] \approx N \ln N$, in both cases approximately. This formula gives the predicted value of the diameter within one from either the correct or probabilistically predicted value for any given Cube size n and metric.

C. Metric dependence

$$\frac{11}{9} \times 6 + \frac{11}{9} \times 3 \times 2 = 14.7,$$
 (102)

where the second term doubles the number of turns for each of the three X^2 compound turns. It slightly overestimates the



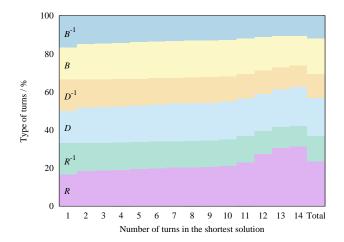


FIG. 7: Same as Fig. 6 for the quarter-turn metric.

correct diameter of 14. The diameter (19) in the semi-quarterturn metric is predicted as

$$\frac{11}{9} \times 3 + \frac{11}{9} \times 3 \times 2 + \frac{11}{9} \times 3 \times 3 = 22.0,$$
 (103)

which is too large by three. The diameter (26) of the $3\times3\times3$ Cube in the quarter-turn metric is obtainable from the same (20) in the half-turn metric as

$$\frac{20}{18} \times 12 + \frac{20}{18} \times 6 \times 2 = 26.7,\tag{104}$$

which is again overestimated slightly. These overestimations suggest that X^2 (180°) turns are less used especially near the diameter.

This is borne out in Fig. 6, where the numbers of types of turns in the half-turn metric used in the shortest solutions are

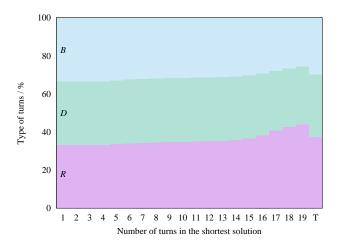


FIG. 8: Same as Fig. 6 for the semi-quarter-turn metric. "T" stands for "Total."

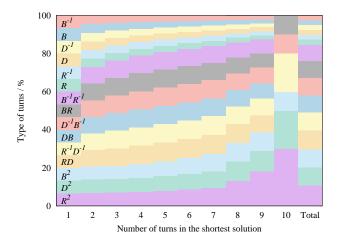


FIG. 9: Same as Fig. 6 for the bi-quarter-turn metric.

shown as histograms. While the contributions of nine turns are comparable with one another in all the solutions (in the rightmost column "Total"), the contribution of X^2 is less than those of X and X^{-1} in the last few steps of the diameter. In particular, the contribution of R becomes progressively more important near the diameter. This is primarily because R happens to be the first turn applied in our computer program, and other subsequent turns have greater probabilities of generating redundant configurations as the remaining unrealized configurations become fewer.

One might expect that the more uneven the contributions of different types of turns are, the less accurate our probabilistic estimates of the diameters become, since the latter are oblivious of the different types of turns. This expectation is not necessarily supported by our data in Figs. 6–9. The most erroneous prediction for the 2×2×2 Cube is in the semi-quarter-turn metric, but this metric has one of the most uniform usage of its three turns (Fig. 8). In contrast, Fig. 9 shows that the bi-quarter-turn metric is superfluous with the 90° turns less and less used near the diameter. However, the error in the

predicted diameter is less than that in the semi-quarter-turn metric. The most accurate prediction is for the quarter-turn metric, but the use of different turns seems no more uniform (Fig. 7) than in the other metrics. It may be concluded that the present probabilistic estimation is largely insensitive to the metrics.

ACKNOWLEDGMENTS

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Appendix A: Coupon collector's problem³⁹⁻⁴²

Suppose that m (out of total N) non-redundant configurations have been generated so far. How many (t_m) random configurations need to be generated before one more non-redundant configuration is added? Let $E[t_m]$ be the expectation value of this number. The probability that the first randomly generated configuration is non-redundant is

$$p_m = \frac{N - m}{N}. (A1)$$

The probability that the *k*th randomly generated configuration is non-redundant for the first time is

$$(1-p_m)^{k-1}p_m. (A2)$$

Writing $q_m = 1 - p_m$, the expected value $E[t_m]$ is then an infinite sum,

$$E[t_m] = 1 \cdot p_m + 2 \cdot q_m p_m + 3 \cdot q_m^2 p_m + \dots$$

$$= p_m \frac{d}{dq_m} \left(q_m + q_m^2 + q_m^3 + \dots \right)$$

$$= p_m \frac{d}{dq_m} \frac{q_m}{1 - q_m}$$

$$= p_m \frac{1}{(1 - q_m)^2} = \frac{1}{p_m}, \tag{A3}$$

where we used $\lim_{k\to\infty} q_m^k = 0$. Variance $V[t_m]$ is also evaluated similarly as

$$V[t_{m}] = (E[t_{m}^{2}]) - (E[t_{m}])^{2}$$

$$= (1^{2} \cdot p_{m} + 2^{2} \cdot q_{m}p_{m} + 3^{2} \cdot q_{m}^{2}p_{m} + \dots) - \frac{1}{p_{m}^{2}}$$

$$= p_{m} \frac{d}{dq_{m}} (q_{m} + 2q_{m}^{2} + 3q_{m}^{3} + \dots) - \frac{1}{p_{m}^{2}}$$

$$= p_{m} \frac{d}{dq_{m}} q_{m} \frac{d}{dq_{m}} (q_{m} + q_{m}^{2} + q_{m}^{3} + \dots) - \frac{1}{p_{m}^{2}}$$

$$= p_{m} \frac{d}{dq_{m}} q_{m} \frac{d}{dq_{m}} \frac{q_{m}}{1 - q_{m}} - \frac{1}{p_{m}^{2}}$$

$$= p_{m} \frac{d}{dq_{m}} \frac{q_{m}}{(1 - q_{m})^{2}} - \frac{1}{p_{m}^{2}}$$

$$= \frac{1}{p_{m}^{2}} - \frac{1}{p_{m}}.$$
(A4)

Let $E[T_N]$ be the expected number of random configurations that need to be generated so that every one of N configurations occurs at least once. It should be the sum of $E[t_m]$ over $0 \le m \le N - 1$.

$$E[T_N] = E[t_0] + E[t_1] + E[t_2] + \dots + E[t_{N-1}]$$

$$= \frac{N}{N} + \frac{N}{N-1} + \frac{N}{N-2} + \dots + \frac{N}{1}$$

$$= N\left(\frac{1}{1} + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{N}\right)$$

$$= N \ln N + \gamma N, \tag{A5}$$

where γ is the Euler–Mascheroni constant. The corresponding variance $V[T_N]$ is

$$V[T_N] \equiv V[t_0] + V[t_1] + V[t_2] + \dots + V[t_{N-1}]$$

$$= \frac{N^2}{N^2} + \frac{N^2}{(N-1)^2} + \frac{N^2}{(N-2)^2} + \dots + \frac{N^2}{1^2} - E[T_N]$$

$$= N^2 \left(\frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \dots + \frac{1}{N^2}\right) - E[T_N]$$

$$\approx \frac{\pi^2 N^2}{6} - N \ln N - \gamma N, \tag{A6}$$

where we used

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}.$$
 (A7)

For large N, the standard deviation $\sigma[T_N]$ is

$$\sigma[T_N] = \sqrt{V[T_N]} \approx 1.28 \, N.$$
 (A8)

Appendix B: Derivation of Eq. (5)

What is the expected number $E[N_T]$ of non-redundant configurations among T randomly generated configurations, when the total number of possible configurations is N? Let p_t be the probability that the tth randomly generated configuration is distinct from all previously generated configurations. Furthermore, let N_t be the number of non-redundant configurations after t random configurations are generated. We have

$$p_{t+1} = \frac{N - N_t}{N},\tag{B1}$$

which can be rearranged to

$$N_t = N(1 - p_{t+1}). (B2)$$

On the other hand,

$$N_t = p_t (N_{t-1} + 1) + (1 - p_t) N_{t-1} = N_{t-1} + p_t.$$
 (B3)

Substituting Eq. (B2) into Eq. (B3), we obtain

$$p_{t+1} = \left(1 - \frac{1}{N}\right) p_t = \left(1 - \frac{1}{N}\right)^t,$$
 (B4)

where we used $p_1 = 1$ and $N_0 = 0$. Therefore, after T random configurations are generated, the expected number of only the non-redundant configurations among all the generated configurations is

$$E[N_T] = N(1 - p_{T+1})$$

$$= N\left\{1 - \left(1 - \frac{1}{N}\right)^T\right\}$$

$$\approx N\left(1 - e^{-T/N}\right), \tag{B5}$$

in the large *N* limit.

For $T \ll N$, approximating the exponential by its first-order Taylor expansion, we have

$$E[N_T] = N(1 - e^{-T/N}) \approx N\{1 - (1 - \frac{T}{N})\} = T,$$
 (B6)

indicating that most of all T generated configurations are non-redundant.

The expected number of configurations that are not realized even once is

$$N - E[N_T] = N - N(1 - e^{-T/N}) = Ne^{-T/N}.$$
 (B7)

which is consistent with the Siobhan distribution [Eq. (3)]. When this number is smaller than one, it is expected that all of the N configurations have been realized (the coupon collector's problem).

$$Ne^{-T/N} < 1, (B8)$$

which implies

$$N \ln N < T. \tag{B9}$$

This is consistent with (if not identical to) the solution of the coupon collector's problem given in Appendix A.

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