# A faster direct sampling algorithm for equilateral closed polygons

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We present a faster direct sampling algorithm for random equilateral closed polygons in three-dimensional space. This method improves on the moment polytope sampling algorithm of Cantarella, Duplantier, Shonkwiler, and Uehara [4] and has (expected) time per sample quadratic in the number of edges in the polygon.

Equilateral polygons in $\mathbb{R}^3$—that is, polygonal walks in 3-space forming closed loops and consisting of unit-length steps—provide a standard, if highly simplified, model of ring polymers under "$\theta$-conditions" (see, e.g., the survey [22], which gives a number of applications of these models in physics and biology). The closure condition imposes subtle global correlations between edge directions, which means it is not obvious how to generate random equilateral polygons. Indeed, algorithms have been proposed for at least 4 decades [1, 5, 7–9, 13, 18–20, 25, 26], though most are numerically unstable or have not been proved to sample from the correct probability distribution.

In previous work [4], we introduced the *action-angle method*, which is a numerically stable and provably correct algorithm for generating random equilateral $n$-gons in $\mathbb{R}^3$ based on rejection sampling the hypercube. The action-angle method is the fastest extant method: it produces samples in expected time $\Theta(n^{5/2})$.

The purpose of this paper is to give a $\sqrt{n}$ speedup for the action-angle method, yielding an algorithm which produces random equilateral $n$-gons in expected time $\Theta(n^2)$. It is based on rejection sampling the same subset of the hypercube as in the action-angle method; the speedup comes from progressively checking the defining inequalities as we generate coordinates rather than checking all the inequalities in a batch. Hence, we call this algorithm the *progressive action-angle method*. The main challenge is to prove that the progressive action-angle method really gives a $\sqrt{n}$ speedup over the action-angle method, which we do in Proposition 4, Proposition 5, and Proposition 6 by reducing to the computation of the volume of a certain convex polytope.

We begin by establishing notation. For an $n$-gon in $\mathbb{R}^3$, let $v_1, \ldots, v_n \in \mathbb{R}^3$ be the coordinates of its vertices, and let $e_1, \ldots, e_n$ be the edge vectors, meaning that $e_i = v_{i+1} - v_i$ for $i = 1, \ldots, n-1$ and $e_n = v_1 - v_n$. We will assume throughout that our polygons are equilateral, so that $|e_i| = 1$ for all $i$; equivalently, $e_1, \ldots, e_n \in S^2$, the unit sphere in $\mathbb{R}^3$. The space $\operatorname{Pol}(n)$ consists of sets of edge vectors in $(S^2)^n$ which obey the closure condition $\sum_{i=1}^n e_i = 0$. One can show that the set

$$\operatorname{Pol}(n)^\times := \{\vec{e} \in (S^2)^n : \textstyle\sum_{i=1}^n e_i = 0 \text{ and for all } i \neq j\text{: } e_i \neq e_j\}$$

is a $(2n-3)$-dimensional submanifold of $(S^2)^n$ and that the $(2n-3)$-dimensional Hausdorff measure

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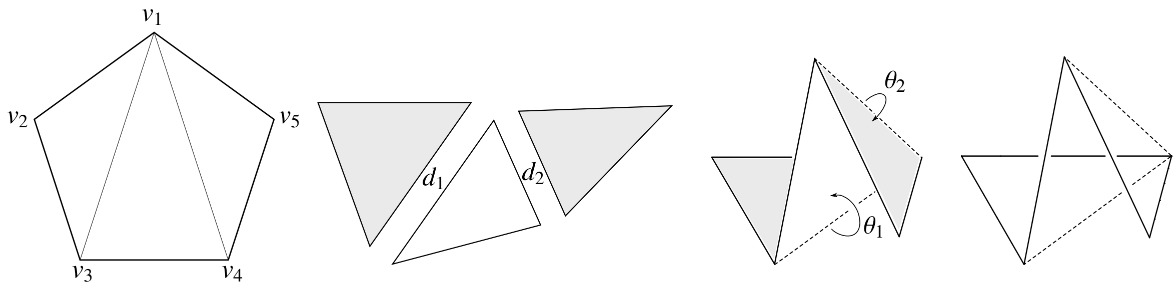


FIG. 1: Constructing an equilateral pentagon from diagonals and dihedrals. The far left shows the fan triangulation of an abstract pentagon. Given diagonal lengths $d_1$ and $d_2$ of the pentagon which obey the triangle inequalities, build the three triangles in the triangulation from their side lengths (middle left). Given dihedral angles $\theta_1$ and $\theta_2$, embed these triangles as a piecewise-linear surface in space (middle right). The far right shows the final space polygon, which is the (solid) boundary of this triangulated surface.

of $\mathrm{Pol}(n) \setminus \mathrm{Pol}(n)^\times$ vanishes. In this sense $\mathrm{Pol}(n)$ is almost everywhere a submanifold of $(S^2)^n$. We may give it the submanifold metric and corresponding volume; it is equivalent to take the $(2n-3)$-dimensional Hausdorff measure on $\mathrm{Pol}(n)$ with respect to the metric on $(S^2)^n$.

Since we are interested in shapes of polygons, we focus on the quotient space $\widehat{\mathrm{Pol}}(n) = \mathrm{Pol}(n)/\,\mathrm{SO}(3)$. This space has a Riemannian metric—defined by the condition that the quotient map $\mathrm{Pol}(n) \to \widehat{\mathrm{Pol}}(n)$ is a Riemannian submersion—and hence a natural probability measure after normalizing the Riemannian volume form.

Now we introduce some new coordinates on this space. Connecting the vertices $v_3, \ldots, v_{n-1}$ to $v_1$, as in Figure 1 (far left), produces a collection of $n-3$ triangles. The shape of the triangulated surface determined by these triangles (and hence also its boundary, which is the $n$-gon) is completely determined by the lengths $d_i$ of the diagonals joining $v_1$ and $v_{i+2}$ and the dihedral angles between triangles meeting at each diagonal. Hence, we can reconstruct the surface (and hence the polygon) up to orientation from the data $d_1, \ldots, d_{n-3}, \theta_1, \ldots, \theta_{n-3}$, and so these give a system of coordinates for $\widehat{\mathrm{Pol}}(n)$.

Indeed, as we have shown [5], these coordinates are natural from the symplectic geometry point of view: in that context, they are called *action-angle coordinates*. Note that, while the dihedral angles can be chosen completely independently, the diagonal lengths cannot: they must obey the system of triangle inequalities

$$0 \leq d_1 \leq 2 \qquad \begin{array}{c} 1 \leq d_i + d_{i+1} \\ -1 \leq d_{i+1} - d_i \leq 1 \end{array} \qquad 0 \leq d_{n-3} \leq 2. \tag{1}$$

Let $\mathcal{P}_n \subset [-1,1]^{n-3}$ be the polytope defined by the inequalities (1). If $T^{n-3} = (S^1)^{n-3}$ is the $(n-3)$-dimensional torus realized as the product of unit circles, then the action-angle coordinates are defined on $\mathcal{P}_{n-3} \times T^{n-3}$, and we have previously shown that the standard probability measure on this space—that is, the one coming from the product of Lebesgue measure on $\mathcal{P}_n$ and the standard product measure on $T^{n-3}$—is measure-theoretically equivalent to $\widehat{\mathrm{Pol}}(n)$:

**Theorem 1** (Cantarella–Shonkwiler [5])**.** *The reconstruction map $\alpha : \mathcal{P}_n \times T^{n-3} \to \widehat{\mathrm{Pol}}(n)$ defining action-angle coordinates (i.e., the procedure illustrated in Figure 1) is measure-preserving.*

Therefore, to sample points in $\widehat{\mathrm{Pol}}(n)$ (that is, equilateral $n$-gons), it suffices to sample $\vec{d}$ from Lebesgue measure on $\mathcal{P}_n$ and $\vec{\theta}$ uniformly from $T^{n-3}$. Of course, the only challenge is to produce the sample $\vec{d} \in \mathcal{P}_n$.

In [4], we showed how to do this efficiently. The key observation is that the consecutive differences $s_i := d_{i+1} - d_i$ lie in the hypercube $[-1, 1]^{n-3}$. Therefore, we can generate points in $\mathcal{P}_n$ by rejection sampling: generate proposed differences $(s_0, \ldots, s_{n-4})$ uniformly from $[-1, 1]^{n-3}$, and simply check whether the proposed diagonal lengths $(d_1, \ldots, d_{n-3})$ given by $d_{i+1} = d_i + s_i$ with $d_0 = |v_2 - v_1| = 1$ satisfy (1). This is surprisingly efficient:

**Theorem 2** (Cantarella–Duplantier–Shonkwiler–Uehara [4])**.** *The probability that a random point $(s_0, \ldots, s_{n-4}) \in [-1, 1]^{n-3}$ produces a valid collection of diagonal lengths $(d_1, \ldots, d_{n-3}) \in \mathcal{P}_n$ is asymptotically equivalent to $\frac{6\sqrt{6}}{\sqrt{\pi}} \frac{1}{n^{3/2}}$ as $n \to \infty$.*

In the above and throughought the rest of the paper, we say that $g(n)$ and $h(n)$ are *asymptotically equivalent*, denoted $g(n) \sim h(n)$, if $\lim_{n\to\infty} \frac{g(n)}{h(n)} = 1$.

Since the time it takes to generate points in $[-1, 1]^{n-3}$ is linear in $n$, rejection sampling the hypercube yields a valid point in $\mathcal{P}_n$ in expected time $\Theta(n^{5/2})$. The steps of generating dihedral angles and assembling the $n$-gon from $(d_1, \ldots, d_{n-3})$ and $(\theta_1, \ldots, \theta_{n-3})$ do not affect the time bound since they are both linear in $n$. Therefore, this gives a numerically stable algorithm for generating random equilateral $n$-gons in expected time $\Theta(n^{5/2})$ which we called the *action-angle method*.

Recently, one of us (Schumacher) created a new implementation of the action-angle sampler which, in practice, seemed to scale quadratically in $n$ rather than as $n^{5/2}$. While we were initially worried that there was a mistake in our analysis of the action-angle method, it turns out that some clever programming led to a $\sqrt{n}$ speedup: our goal now is to explain and justify this.

By fixing $d_0 = 1$ and generating proposed consecutive differences $s_i$ uniformly from $[-1, 1]^{n-3}$, the inequalities $0 \leq d_1 \leq 2$ and $-1 \leq d_{i+1} - d_i \leq 1$ for $i = 1, \ldots, n-4$ are automatically satisfied. Of course, the final inequality $0 \leq d_{n-3} \leq 2$ can only be checked at the very end, but the inequalities $1 \leq d_i + d_{i+1}$ can be checked one at a time as each $s_i$ is generated, and we can abort and start over as soon as one of these inequalities fails. Naively, one might expect to have to check, on average, some constant fraction of the inequalities. This would speed up the algorithm by a constant factor, but not change the complexity bound. However, as we will show below, the expected number of coordinates that get generated before failure is actually $\Theta(\sqrt{n})$, yielding an overall time bound of $\Theta(n^2)$. Algorithm 1 summarizes our algorithm, which we call the *progressive action-angle method*. A reference C implementation of this algorithm is included in `plCurve` [2], where it is now the default algorithm for producing random equilateral polygons in $\mathbb{R}^3$.

**Algorithm 1** Progressive action-angle method

```
procedure ProgressiveActionAngleMethod(n)          ▷ Generate closed equilateral n-gon
    d_0 ← 1
    i ← 0
    repeat
        repeat
            s_i ← UniformRandom([−1, 1])
            d_{i+1} ← d_i + s_i
            if d_i + d_{i+1} < 1 then
                i ← 0
            else
                i ← i + 1
            end if
        until i = n − 3
    until 0 ≤ d_{n−3} ≤ 2
    Sample n − 3 i.i.d. dihedral angles θ_i uniformly from [0, 2π).
    Reconstruct P from diagonals d_1, ..., d_{n−3} and dihedrals θ_1, ..., θ_{n−3}.
end procedure
```

Let $\mathcal{I}(n)$ be the expected number of iterations in the inner loop of the progressive action-angle method: that is, $\mathcal{I}(n)$ is the number of coordinates $s_i$ that we expect to generate before failing one of the $d_i+d_{i+1} \geq 1$ inequalities. Since we know from Theorem 2 that the overall acceptance probability is $\sim \frac{6\sqrt{6}}{\sqrt{\pi}} \frac{1}{n^{3/2}}$, the expected number of iterations of the outermost loop is $\Theta(n^{3/2})$. Multiplying the time per iteration by the number of iterations yields $\Theta(n^{3/2}\mathcal{I}(n))$ for the expected time to produce a valid list of diagonals. The postprocessing steps of generating dihedral angles and assembling the polygon are both linear in $n$, so do not affect the overall time bound. Hence, our goal is to understand how $\mathcal{I}(n)$ scales.

**Definition 3.** Let $p(k)$ be the probability that the proposed diagonal lengths generated by a random point in $\vec{s} \in [-1, 1]^{n-3}$ satisfy each of the first $k$ inequalities $d_0 + d_1 \geq 1, \ldots, d_{k-1} + d_k \geq 1$. In other words, $p(k)$ (thought of as a function of $k$) is the survival function for the distribution of the index of the first inequality which fails. For ease of notation, we also declare $p(0) := 1$.

By a standard integration by parts argument (see, for example, [11, Exercise 1.7.2]), the expected value of a non-negative random variate is the integral of the survival function, so we see that

$$\mathcal{I}(n) = \sum_{k=0}^{n-3} p(k). \tag{2}$$

Since our goal is to understand the asymptotics of $\mathcal{I}(n)$, we will proceed in the following steps:

- Find an exact expression for $p(k)$ (Proposition 4).
- Find an asymptotic approximation for $p(k)$ (Proposition 5).
- Plug this into (2) to get the desired asymptotic expression for $\mathcal{I}(n)$ (Proposition 6).

This will give us the desired complexity bound $\Theta(n^{3/2}\mathcal{I}(n))$ for the progressive action-angle method (Theorem 7).

**Proposition 4.** *For any nonnegative integer k,*

$$p(k) = \frac{2}{\pi}\int_0^\infty \operatorname{sinc}^{k+1}(t)\,\mathrm{d}t.$$

*Proof.* For each $k$, let $\mathcal{S}_k \subset [-1,1]^k$ be the subset of points $\vec{s}$ satisfying the in the definition of $p(k)$. As a simple calculation confirms, the affine transformation from $\vec{s}$ to $\vec{d}$ given by $d_i = 1 + \sum_{j=0}^{i-1} s_j$ is volume-preserving. Let $Q_k$ be the image of $\mathcal{S}_k$ under this map; i.e., $Q_k$ is the polytope of $(d_1,\ldots,d_k)$ satisfying the inequalities $d_0 + d_1 \geq 1, \ldots, d_{k-1} + d_k \geq 1$ (again, recall that $d_0 = 1$, which implies in particular that all the $d_i$ are nonnegative). Since $p(k) = \frac{\operatorname{Vol}(\mathcal{S}_k)}{\operatorname{Vol}([-1,1]^k)} = \frac{\operatorname{Vol}(\mathcal{S}_k)}{2^k}$, to prove the proposition it suffices to prove that

$$\operatorname{Vol}(Q_k) = 2^k\frac{2}{\pi}\int_0^\infty \operatorname{sinc}^{k+1}(t)\,\mathrm{d}t.$$

Notice that the defining inequalities for $Q_k$ are precisely the inequalities (1) *except* the last inequality $0 \leq d_k \leq 2$. This suggests that these inequalities may just be the diagonal lengths of an equilateral polygonal path in $\mathbb{R}^3$ which is not required to close up.

More precisely, let

$$\widehat{\operatorname{APol}}(k) := \left\{(e_1,\ldots,e_{k+1}) \in (S^2)^{k+1} : z_1 + \cdots + z_{k+1} = 0\right\}/\operatorname{SO}(2),$$

where $e_i = (x_i, y_i, z_i)$, so that the defining condition says that the path starts and ends in the $x$-$y$-plane, and SO(2) acts by simultaneously rotating all edges around the $z$-axis; this is the diagonal subgroup of the $T^{k+1} = \operatorname{SO}(2)^{k+1}$ action on $(S^2)^{k+1}$ which rotates edges around the $z$-axis. $\widehat{\operatorname{APol}}(k)$ is the space of *abelian polygons* introduced by Hausmann and Knutson [12], and we will see that it admits two different effective, Hamiltonian $T^k$ actions, as shown in Figure 2.

The first is the residual $T^{k+1}/\operatorname{SO}(2) \simeq T^k$ action above. The moment map for this action simply records the $z$-coordinates of the edges; since the defining equation $z_1 + \cdots + z_{k+1} = 0$ implies that $z_{k+1}$ is determined by the remaining $z_i$'s, the last coordinate can be dropped and we can think of the moment map as recording the vector $(z_1,\ldots,z_k)$. Let $\mathcal{H}_k$ be the image of this map; that is, the moment polytope for this torus action. Of course, $-1 \leq z_i \leq 1$ for all $i$, and, since $-1 \leq z_{k+1} \leq 1$, we see that the defining inequalities of $\mathcal{H}_k$ are

$$-1 \leq z_i \leq 1 \text{ for all } i = 1,\ldots,k \quad \text{and} \quad -1 \leq z_1 + \cdots + z_k \leq 1.$$

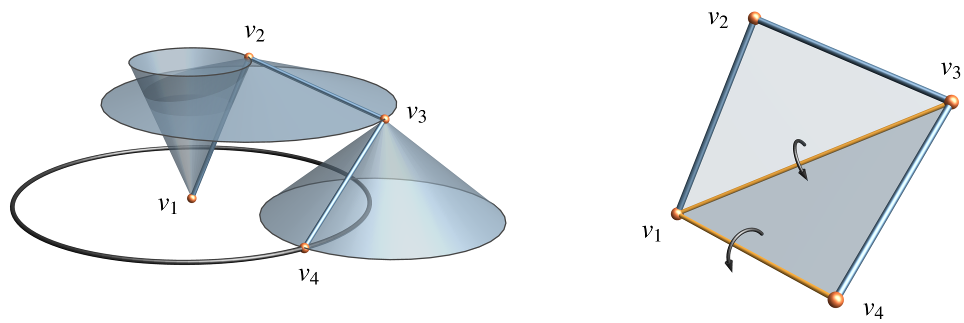


FIG. 2: Here we see both torus actions on the space $\widehat{\mathrm{APol}}(2)$. On the left, we may rotate each of the three edges (independently) around the $z$-axis, sweeping out three cones. Then we identify configurations which are the same under the diagonal circle action rotating the entire configuration around the $z$-axis (indicated by the dark circle in the $xy$-plane). On the right, we may rotate the first two edges around the diagonal joining vertices $v_1$ and $v_3$ or rotate the entire polygon around the diagonal joining $v_1$ and $v_4$. In each case, this is a Hamiltonian 2-torus action on $\widehat{\mathrm{APol}}(2)$.

In other words, $\mathcal{H}_k$ is the central slab of the hypercube $[-1, 1]^k$ of points whose coordinates sum to between $-1$ and 1. This is a well-studied polytope, and its volume has been known at least since Pólya [23] to be

$$\mathrm{Vol}(\mathcal{H}_k) = 2^k \frac{2}{\pi} \int_0^\infty \mathrm{sinc}^{k+1}(t)\,\mathrm{d}t,$$

where $\mathrm{sinc}(t) = \frac{\sin(t)}{t}$ for $t \neq 0$ and $\mathrm{sinc}(0) = 1$ is the sinc function (see also Borwein, Borwein, and Mares [3] for generalizations of the above formula).

On the other hand, we get a $T^k$ action on $\widehat{\mathrm{APol}}(k)$ which is analogous to the bending flows on $\widehat{\mathrm{Pol}}(n)$ described above and in more detail in [5]. Specifically, the $i$-th SO(2) factor acts by rotating the first $i+1$ edges of the polygonal arm around the $i$-th diagonal, which is the axis through $v_1$ and $v_{i+1}$. Just as in the case of $\widehat{\mathrm{Pol}}(n)$, the moment map records the lengths $d_1, \ldots, d_k$ of the diagonals, and the image of the moment map is precisely $Q_k$.

But now we've realized $\widehat{\mathrm{APol}}(k)$ as a toric symplectic manifold in 2 ways, with moment polytopes $\mathcal{H}_k$ and $Q_k$. Since the Duistermaat–Heckman theorem [10] implies that the volume of $\widehat{\mathrm{APol}}(k)$ must be the product of the volume $(2\pi)^k$ of the torus $T^k$ and the volume of either of its moment polytopes, it follows that

$$\mathrm{Vol}(Q_k) = \mathrm{Vol}(\mathcal{H}_k) = 2^k \frac{2}{\pi} \int_0^\infty \mathrm{sinc}^{k+1}(t)\,\mathrm{d}t,$$

as desired. □

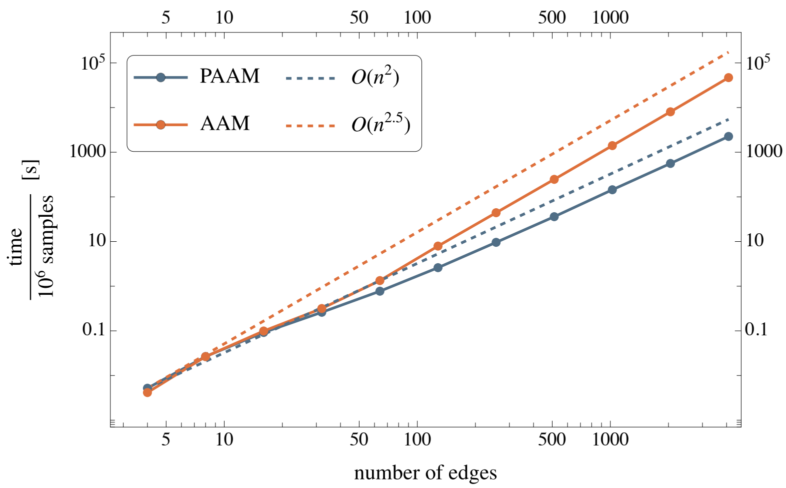


FIG. 3: This plot compares average time per sample for random equilateral $n$-gons with $n = 2^2, 2^3, \ldots, 2^{12}$ using the action-angle method (AAM) and the progressive action-angle method (PAAM). The time needed to generate samples scales as predicted by Theorem 2 and Theorem 7.

We have the following estimate for $p(k)$, which goes back at least to Laplace [16, pp. 172–173] (see also [17]):

**Proposition 5.** $p(k) = \sqrt{\frac{6}{\pi k}} + O\left(\frac{1}{k^{3/2}}\right)$.

Now we can easily get the desired asymptotic expression for $\mathcal{I}(n)$:

**Proposition 6.** $\mathcal{I}(n) \sim \sqrt{\frac{24n}{\pi}}$.

*Proof.* By Proposition 5, $p(k) = \sqrt{\frac{6}{\pi k}} + O\left(\frac{1}{k^{3/2}}\right)$, so, from (2),

$$\mathcal{I}(n) = \sum_{k=0}^{n-3} p(k) = 1 + \sum_{k=1}^{n-3} \left[ \sqrt{\frac{6}{\pi k}} + O\left(\frac{1}{k^{3/2}}\right) \right] = 1 + \sum_{k=1}^{n-3} \sqrt{\frac{6}{\pi k}} + \sum_{k=1}^{n-3} O\left(\frac{1}{k^{3/2}}\right).$$

The first sum is asymptotic to $\sqrt{\frac{24n}{\pi}}$ by the integral test. The rest of this expression has order $O(1)$ since the second sum is a partial sum of a convergent series, and the result follows. $\square$

Therefore, $\Theta(n^{3/2}\mathcal{I}(n)) = \Theta(n^2)$ and we have proved a sharp complexity bound on the progressive action-angle method:

**Theorem 7.** *The progressive action-angle method generates uniform random samples of closed, equilateral $n$-gons in expected time $\Theta(n^2)$.*

This agrees with the behavior we see in practice; see Figure 3.

### Discussion

Since it requires listing $n$ edges (or vertices), the time needed to generate random equilateral $n$-gons must be at least linear in $n$. Theorem 7 shows that the optimal bound is no worse than quadratic in $n$. It would be interesting to see if even the quadratic bound can be improved.

In the proof of Proposition 4, we showed that $\mathrm{Vol}(Q_k) = \mathrm{Vol}(\mathcal{H}_k)$ by showing that $Q_k$ and $\mathcal{H}_k$ are moment polytopes for different toric structures on the manifold $\widehat{\mathrm{APol}}(k)$. In fact, some additional analysis indicates that if one could generate polygons in $\widehat{\mathrm{APol}}(n-3)$ directly, their diagonals would *automatically* obey $0 \leq d_1 \leq 2$, $1 \leq d_i + d_{i+1}$, and $-1 \leq d_{i+1} - d_i \leq 1$ for $i \in 1, \ldots, n-2$, but still have probability only $\sim \frac{6}{n}$ of satisfying the final inequality $0 \leq d_{n-3} \leq 2$ and lying in the moment polytope $\mathcal{P}_n$. This (hypothetical) algorithm would be faster by a constant factor, but still quadratic in $n$. This may indicate that a new idea is required, but it also seems plausible that the moment polytope $\mathcal{P}_n$ could be transformed more cleverly to occupy a larger fraction of an even smaller polytope.

We note that the equivalence $\mathrm{Vol}(Q_k) = \mathrm{Vol}(\mathcal{H}_k)$ seems potentially interesting as a statement in combinatorics. We could not find a more elementary proof, which leads us to ask: Are there other pairs of polytopes which can be identified as moment polytopes for the same toric symplectic manifold which are difficult to prove equivalent otherwise?

As in the case of the action-angle method [24], the progressive action-angle method can easily be modified to give an algorithm for sampling so-called *unit-norm tight frames* in $\mathbb{C}^2$. Unit-norm tight frames in $\mathbb{C}^d$ are of considerable interest for applications in signal processing, compressed sensing, and quantum information (see [6, 14, 15, 27] for introductions to this area). It would be very interesting to generalize the approach from this paper to the $d > 2$ setting.

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