# THE GEOMETRY OF CONSTRAINED RANDOM WALKS AND AN APPLICATION TO FRAME THEORY

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## ABSTRACT

Random walks in $\mathbb{R}^3$ are classical objects in geometric probability which have, over the last 70 years, been rather successfully used as models of polymers in solution. Modifying the theory to apply to topologically nontrivial polymers, such as ring polymers, has proven challenging, but several recent breakthroughs have been made by thinking of random walks as points in some nice conformation space and then exploiting the geometry of the space. Using tools from symplectic geometry, this approach yields a fast algorithm for sampling loop random walks. Such walks can be lifted via the Hopf map to finite unit norm tight frames (FUNTFs) in $\mathbb{C}^2$, producing an algorithm for randomly sampling FUNTFs in $\mathbb{C}^2$ as well as a mechanism for searching for FUNTFs with nice properties. In general, symplectic geometry seems like a promising tool for understanding the space of FUNTFs in $\mathbb{C}^d$ for any $d$.

***Index Terms—*** Random polygons, finite frames, polymers, Hopf map

## 1. INTRODUCTION

A polymer – like a protein or strand of DNA – is a long chain formed from (near-)identical pieces, called monomers, and so a plausible model of an ideal polymer is a chain of rigid rods connected by universal joints. This model dates back to the 1930s [1, 2], and has provided the mathematical framework for the study of polymers since the pioneering work of Flory [3, 4]; as Grosberg et al. say [5], "Modern polymer physics is based on the analogy between a polymer chain and a random walk." In mathematical terms, an ideal chain is a random walk in $\mathbb{R}^3$.

However, classical random walk models are only directly applicable to so-called linear polymers which form open chains: they cannot incorporate topological constraints as in ring polymers which form closed loops. As such, there is an extensive literature on closed random walks, or *random polygons*, and their applications to modeling ring polymers [6, 7].

Nonetheless, progress in this area has been frustratingly slow, especially in terms of developing provably correct sampling and numerical integration algorithms. However, in work with various coauthors over the last few years, we have transformed this field by thinking about the *moduli space* of possible polygon conformations and exploiting the geometry of this space to develop sampling algorithms and numerical integration methods as well as to prove theorems.

Much of our work in this area has been inspired by developments in the realm of symplectic and algebraic geometry, especially work of Kapovich–Millson [8] and Hausmann–Knutson [9]. In short, polygon spaces can be interpreted as highly-symmetric symplectic manifolds and projective varieties, their natural probability measure is unique with respect to this extra structure, and it can be accessed using symplectic and algebraic techniques. Sections 2 and 3 survey some recent results in this area.

The theory of polygons relates, somewhat surprisingly, to *frame theory*, which might rather glibly be described as the study of redundant bases which are useful for reconstructing noisy or lossy signals. Frames have a long history in the signal processing literature, dating back to Duffin–Schaefer [10], and have come into vogue in recent years for their applications to, e.g., wireless communications [11].

By way of the construction given in Section 2, which depends fundamentally on the Hopf map, polygons in $\mathbb{R}^3$ can be lifted to so-called *tight frames* in $\mathbb{C}^2$. This lifting is described in Section 4 and applied to highly symmetric polygons to produce frames of low coherence. The main result of that section and of this paper is Theorem 4, which gives an algorithm for generating random *finite unit norm tight frames* (FUNTFs) in $\mathbb{C}^2$. This seems to be the first algorithm for sampling FUNTFs in any Hilbert space.

Finally, this paper concludes with some speculation about how to generalize these results to frames in $\mathbb{C}^d$ for $d > 2$.

## 2. STIEFEL MANIFOLDS AND SPACE POLYGONS

An $n$-gon in $\mathbb{R}^3$ is a piecewise-linear closed curve of $n$ steps in $\mathbb{R}^3$. While it is traditional to represent an $n$-gon by a list of vertices $v_1, \ldots, v_n$, we can get a translation-invariant representation by instead considering the edge vectors $e_i = v_{i+1} - v_i$, where the subscripts are taken modulo $n$. In this representation, the closure condition is equivalent to the vector equation $e_1 + \ldots + e_n = 0$.

While this is a concise description, it does not readily lend

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itself to sampling or numerical integration, but, following Hausmann–Knutson [9] and Howard–Manon–Millson [12], in [13] we described a way to lift $n$-gons in $\mathbb{R}^3$ to points on the Stiefel manifold $\mathrm{St}_2(\mathbb{C}^n)$ of orthonormal pairs of vectors in $\mathbb{C}^n$. The construction is based on the simple observation that applying the Hopf map to a vector $\vec{w} \in \mathbb{C}^2$ produces a vector $\vec{x} \in \mathbb{R}^3$.

We can define the Hopf map as follows: identify $\mathbb{C}^2$ with the skew-field $\mathbb{H}$ of quaternions via $(u, v) \leftrightarrow u + v\mathbf{j}$. Then the Hopf map $\mathbb{H} \to \mathbb{R}^3$ is given by $q \mapsto \bar{q}\mathbf{i}q$. Applying this map column-wise to a $2 \times n$ matrix defines a map $\mathbb{C}^{2\times n} \to (\mathbb{R}^3)^n$, and a straightforward calculation shows:

**Theorem 1 ([9, 12, 13])** *The inverse image of the closed polygons is the collection of* $2 \times n$ *matrices with orthogonal rows of the same norm, which is a cone over the Stiefel manifold* $\mathrm{St}_2(\mathbb{C}^n)$.

In many cases we are only interested in polygons up to similarity, so it is convenient to fix a scale. At the level of $2 \times n$ matrices with orthogonal rows of the same norm, we can fix the scale by choosing the rows to have common norm $r > 0$; after applying the map, this produces polygons of length $2r^2$. Choosing $r = 1$ is natural, producing a copy of the Stiefel manifold $\mathrm{St}_2(\mathbb{C}^n)$ sitting over polygons of length 2 in $\mathbb{R}^3$.

The Stiefel manifold is extremely well-studied (see, for example, [14]) and very easy to sample: choosing a pair independent standard Gaussian vectors and applying Gram–Schmidt gives a linear-time algorithm for sampling directly from the Haar measure [15]. Moreover, passing to the Grassmannian $\mathrm{Gr}_2(\mathbb{C}^n) = \mathrm{St}_2(\mathbb{C}^n)/U(2)$ has the effect of taking the quotient of $n$-gon space by the rotation group $SO(3)$ and hence gives an *orientation-independent* representation of polygons. This is quite useful in a polymer modeling context since polymers in solution appear in random orientations yet nonetheless need to be compared. In this way, the theory gives a *shape theory* of curves in $\mathbb{R}^3$. See [13, 16, 17] for various applications to random polygons, and [18] for an extension to continuous curves.

## 3. EQUILATERAL POLYGONS

In polymer physics models it is traditional to fix not only the total length of an $n$-gon in $\mathbb{R}^3$, but to make all individual edges the same (typically unit) length. In other words, each edge vector in such an equilateral polygon has norm 1. Up in the land of $2 \times n$ matrices, this corresponds to elements of the scaled Stiefel manifold $\sqrt{n/2}\,\mathrm{St}_2(\mathbb{C}^n)$ with unit columns. In other words, lifts of equilateral polygons in $\mathbb{R}^3$ are matrices $A$ such that

$$AA^* = \begin{bmatrix} n/2 & 0 \\ 0 & n/2 \end{bmatrix} \quad \text{and} \quad (A^*A)_{ii} = 1 \text{ for all } i. \qquad (1)$$

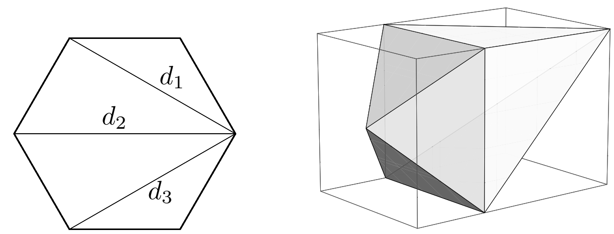


**Fig. 1**. The three diagonals of a triangulation of a 6-gon and the corresponding convex polytope.

As will be described in more detail in Section 4, this space has recently come to prominence as the space of *finite unit norm tight frames* of length $n$ in $\mathbb{C}^2$.

For polymers, as described above, we can mod out by rotations by passing to the quotient of the $U(2)$ action on this subset of the Stiefel manifold. The quotient is the inverse image of the moment map of a Hamiltonian $(n-1)$-torus action on the Grassmannian $\mathrm{Gr}_2(\mathbb{C}^n)$, which is a Kähler manifold. Taking the quotient by the torus action is equivalent to taking the Kähler reduction of the Grassmannian and produces exactly the space of shapes of equilateral $n$-gons in $\mathbb{R}^3$ [9, 12].

This space of equilateral polygons inherits an almost toric structure from the Gel'fand-Tsetlin system on the Grassmannian equivalent to Kapovich and Millson's [8] bending flows. More precisely, the space of equilateral $n$-gon shapes is $(2n-6)$-dimensional and there is an $(n-3)$-dimensional torus action defined almost everywhere by bending the polygon around the $n-3$ diagonals of any triangulation; see Fig. 1.

These $n-3$ symmetries of the space have $n-3$ associated conserved quantities (or *momenta*), namely the lengths $d_1, \ldots, d_{n-3}$ of the diagonals. In turn, each $d_i$ is involved in two triangles in the triangulation, and thus must satisfy various triangle inequalities, and so the vector $(d_1, \ldots, d_{n-3})$ lies in some convex polytope in $\mathbb{R}^{n-3}$. In this way, sampling equilateral $n$-gons reduces to the problem of sampling a convex polytope. In [19] we describe a Markov chain sampler for equilateral polygons based on the hit-and-run algorithm [20, 21].

Even better, for the triangulation with all diagonals emanating from a single vertex, as shown in Fig. 1, we can define $d_0 = 1 = d_{n-2}$ and make the linear change of variables $s_i = d_i - d_{i-1}$. Then the triangle inequalities reduce to

$$-1 \leq s_i \leq 1 \quad \text{and} \quad \sum_{j=1}^{i} s_j + \sum_{j=1}^{i+1} s_j \geq -1 \text{ for all } i,$$

so rejection sampling the unit hypercube $[-1, 1]^{n-3}$ yields:

**Theorem 2 ([22])** *The space of equilateral* $n$*-gons in* $\mathbb{R}^3$ *can be directly sampled in expected* $\Theta(n^{5/2})$ *time.*

See [22] for an explicit description of this algorithm and [23] for an implementation.

## 4. UNIT NORM TIGHT FRAMES

As alluded to in the previous section, the lift of equilateral polygons in $\mathbb{R}^3$ to $2 \times n$ complex matrices is equivalent to the space of finite unit norm tight frames in $\mathbb{C}^2$.

**Definition 3** *A* frame *in a Hilbert space $\mathcal{H}$ is a collection $\{\varphi_i\}_{i\in\mathcal{I}}$ of vectors in $\mathcal{H}$ with $A, B > 0$ so that*

$$A\|x\|^2 \leq \sum_{i\in\mathcal{I}} |\langle x, \varphi_i\rangle|^2 \leq B\|x\|^2$$

*for all $x \in \mathcal{H}$. The frame is* finite *if $\mathcal{I}$ is finite (which implies $\mathcal{H}$ is finite-dimensional),* tight *if we can take $A = B$, and* unit norm *if $\|\varphi_i\| = 1$ for all $i \in \mathcal{I}$. We abbreviate a* finite unit norm tight frame *as FUNTF.*

Interpreting the vectors $\varphi_i$ of a finite frame in $\mathbb{C}^d$ as the columns of a $d \times n$ matrix $\Phi$, the frame is tight if and only if $\Phi\Phi^* = \lambda I_d$ for some constant $\lambda$, and the frame is unit norm if and only if the diagonal entries of $\Phi^*\Phi$ are all 1.

Notice that, with $d = 2$ and $\lambda = n/2$, these two conditions together are exactly the equations (1) defining the preimage of the equilateral $n$-gons in $\mathbb{R}^3$ under the column-wise Hopf map. This is the complex version of Goyal, Kovačević, and Kelner's [24] observation that tight frames in $\mathbb{R}^2$ are square roots of planar polygons, and it can also be seen from the perspective of Copenhaver et al.'s [25] diagram vectors.

This means we can translate fairly freely between equilateral polygons and FUNTFs in $\mathbb{C}^2$, which is promising since the space of FUNTFs is of considerable interest, but not particularly well-understood. For example, almost the simplest possible question one could ask about the space of FUNTFs is the so-called *frame homotopy problem* [26], which asks whether the space of FUNTFs is connected; this problem was only very recently answered in the affirmative [27].

(Incidentally, the frame homotopy problem becomes straightforward from the symplectic geometry perspective: the Hamiltonian torus action on the Grassmannian mentioned in Section 3 generalizes to arbitrary $d$ and a theorem of Atiyah [28] guarantees connectedness of the level sets of moment maps of Hamiltonian torus actions. This implies connectdness of the space of FUNTFs in $\mathbb{C}^d$ for any $d$ [29].)

The natural measure on the space of FUNTFs in $\mathbb{C}^d$ is induced by the Riemannian metric inherited from the standard Riemannian metric on the (scaled) Stiefel manifold. When $d = 2$, building on the equilateral polygon sampler from Theorem 2 and using the fact that the Hopf preimage of each edge is a great circle on the 3-sphere $S^3 \subset \mathbb{R}^4$ which can be uniformly sampled, this yields:

**Theorem 4** *There exists an explicit algorithm for uniformly sampling the space of length-$n$ FUNTFs in $\mathbb{C}^2$ in expected $\Theta(n^{5/2})$ time.*

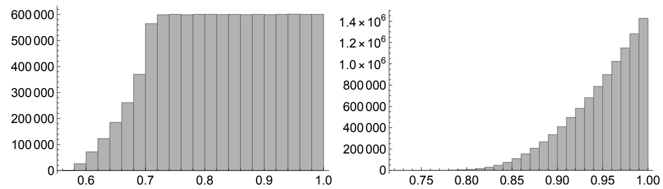


**Fig. 2**. Histogram of the coherences of 10,000,000 randomly sampled length-4 (left) and length-6 FUNTFs in $\mathbb{C}^2$.

With a uniform sampler in hand, it is interesting to explore some of the features of the spaces of FUNTFs in $\mathbb{C}^2$. For example, from a signal reconstruction perspective, there is particular interest in frames $\{\varphi_i\}_{i\in[n]}$ of low *coherence*, defined as

$$\mu(\{\varphi_i\}_{i\in[n]}) := \max_{i\neq j} |\langle \varphi_i, \varphi_j\rangle|.$$

Low-coherence frames can sometimes be found on an *ad hoc* basis using special configurations or symmetry, but in general are challenging to come up with, suggesting that they are rare. In support of this hypothesis, Fig. 2 shows a histogram of the coherences of 10,000,000 random length-6 FUNTFs in $\mathbb{C}^2$ sampled using the algorithm from Theorem 4. The smallest observed coherence in this sample was 0.7284, which is surprisingly close to the optimal coherence $\frac{1}{\sqrt{2}} \approx 0.7071$. However, only about 1 in 1000 samples had coherence less than 0.8, and in general similar experiments with varying $n$ suggest that FUNTFs in $\mathbb{C}^2$ with small coherence are exceedingly rare.

An interesting phenomenon occurs for $n = 4$: as the histogram in Fig. 2 shows, all coherences between $\frac{1}{\sqrt{2}}$ and 1 seem to be equally likely, with the density then rapidly dying off between $\mu = \frac{1}{\sqrt{2}}$ and the minimum achievable value of $\frac{1}{\sqrt{3}} \approx 0.5773$.

Given sufficient patience, the random sampler from Theorem 4 will eventually find a FUNTF of relatively small coherence, but it can be quicker to lift particularly symmetric equilateral polygons in $\mathbb{R}^3$. For example, interpreting the vertices of a Platonic solid as edge vectors produces an equilateral polygon in $\mathbb{R}^3$, and these lift to frames with low coherence. Indeed, the tetrahedron, octahedron, and icosahedron all lift to so-called *Grassmannian frames* which have the smallest possible coherence. In each case the resulting frame saturates the Toth bound [30, 31]

$$\mu \geq \frac{1}{2}\csc\left(\frac{n\pi}{6(n-2)}\right).$$

The vertices of the tetrahedron, octahedron, and icosahedron all solve the *Tammes problem*, which is to place $n$ points on the sphere $S^2$ which maximize the minimum distance between them. The fact that these polyhedra all lift to Grassmannian frames suggests that in general solutions of the

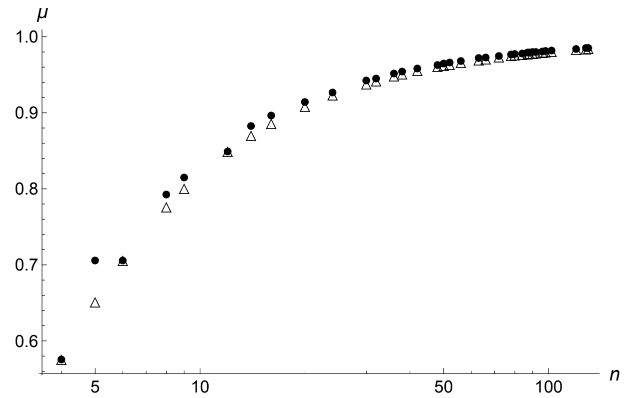


**Fig. 3**. Coherences of lifts of the Sloane sphere packings giving closed polygons (•) compared to the Toth bound (△).

Tammes problem may correspond to FUNTFs of low coherence in $\mathbb{C}^2$. In fact, the $n = 2$ and $n = 3$ solutions also lift to Grassmannian frames, namely the standard basis and the Mercedes–Benz frame, respectively.

For $4 \leq n \leq 130$, Neil Sloane has compiled a list of (proved for $n \leq 14$ and $n = 24$, otherwise putative) solutions to the Tammes problem on $S^2$ [32]. Not all of these solutions form the edges of a closed polygon, but those that do necesarily lift to FUNTFs, and their coherences compare quite favorably to the Toth bound, as seen in Fig. 3, supporting the idea that these FUNTFs may have optimal or at least nearly-optimal coherence. It is worth pointing out that the lift of the bipyramid, which is the $n = 5$ solution of the Tammes problem, saturates the orthoplex bound $\mu \geq \frac{1}{\sqrt{2}}$ and hence is also a Grassmannian frame; it agrees with Casazza and Haas's Example 4.2 from [31].

## 5. A LOOK AHEAD

The individual elements of a FUNTF in $\mathbb{C}^2$ are simply unit vectors in $\mathbb{C}^2$, or points on the unit sphere $S^3 \subset \mathbb{C}^2$. Applying the Hopf map produces points on $S^2 \subset \mathbb{R}^3$, and a minor algebraic miracle translates the tight frame condition upstairs into the closed polygon condition. This allows results on equilateral polygons in $\mathbb{R}^3$ to be ported to the world of FUNTFs in $\mathbb{C}^2$, which is the source of Theorem 4.

More generally, the elements of a FUNTF in $\mathbb{C}^d$ for $d \geq 2$ are points on the unit sphere $S^{2d-1} \subset \mathbb{C}^d$, and there is always a Hopf fibration $S^1 \hookrightarrow S^{2d-1} \to \mathbb{CP}^{d-1}$, so the frame vectors can be mapped to points in $\mathbb{CP}^{d-1}$. Of course, the identification $\mathbb{CP}^1 \simeq S^2$ is a one-shot deal: even $\mathbb{CP}^2$ is quite different from $S^4$ (for example, it has nontrivial 2-dimensional homology).

This begs the question of whether there is a corresponding generalization of the tight frame condition on collections of (unit) frame vectors in $\mathbb{C}^d$ to some natural geometric condition on collections of points in $\mathbb{CP}^{d-1}$. Adding points in $\mathbb{CP}^{d-1}$ (as in the closure condition on edge vectors in $\mathbb{CP}^1$) does not really make sense, but some further manipulations reveal that there is a natural generalization.

Given a unit vector $\varphi \in S^{2d-1} \subset \mathbb{C}^d$, the projection matrix $\varphi\varphi^*$ is a rank-one $d \times d$ Hermitian matrix. Since $\varphi\varphi^*$ is invariant under phase changes to $\varphi$, the space of such matrices can be identified with $\mathbb{CP}^{d-1}$, and the map $\varphi \mapsto \varphi\varphi^*$ is a version of the Hopf map. As in [31], it is convenient to make a slight adjustment and consider the map $H : \varphi \mapsto \varphi\varphi^* - \frac{1}{d} I_d$ to the traceless part, where $I_d$ is the $d \times d$ identity matrix. If $\{\varphi_i\}_{i \in [n]}$ is a FUNTF in $\mathbb{C}^d$, then the $H(\varphi_i)$ are rank-one, traceless, Hermitian matrices and satisfy the equation $H(\varphi_1) + \ldots + H(\varphi_n) = 0$: in other words, FUNTFs in $\mathbb{C}^d$ correspond to equilateral polygons in the space of traceless Hermitian matrices!

The space of such polygons, which is a direct generalization of the space of equilateral polygons in $\mathbb{R}^3$, is described by Flaschka and Millson [33], who show that it can be constructed as the symplectic reduction of the Grassmannian $G_d(\mathbb{C}^n)$ by the action of the torus of diagonal matrices in $U(n)$, just as in Section 3. In particular, it is almost toric and hence, as in Theorem 2, sampling it reduces to sampling a convex polytope, in this case determined by interlacing inequalities in the eigenvalues of the partial sums $\sum_{i=1}^{j} H(\varphi_i)$. Given an algorithm for sampling this polytope, then, it should be possible to prove analogs of Theorems 2 and 4, producing algorithms for sampling random complex FUNTFs in any dimension.

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