Enumeration of the Building Game

Daniel Johnson & Govind Menon
Division of Applied Mathematics
Brown University

June 23, 2014

Abstract

The Building Game is a sequential coloring process on polyhedra. We enumerate the Building Game state space for all polyhedra in the Platonic, Archimedean, and Catalan solids classes of up to 30 faces. By putting a probability distribution on each step of the Building Game process, a distribution is induced on the entire state space. With the help of a finite group theoretic identity, we find the explicit form of these distributions. Finally, we examine the properties of the resulting distributions.

1 Introduction

The Building Game (BG) was first considered by Zlotnick [9] as a model for the assembly of polyhedral viral capsids. We formalize the idea as a sequential coloring process that progresses from a polyhedron $\mathscr{P}$ with each face colored white, through a number of intermediate states each having a mix of white and black faces, and ending with all of the faces colored black.

Definition 1. *A Building Game* ***intermediate*** *x is a function from the faces of $\mathscr{P}$, $F(\mathscr{P})$, to a color in $\{white, black\}$ such that the set $\{f_m \in F(\mathscr{P}) : x(f_m) = black\}$ is edge connected along with the equivalence relation $x \sim x'$ if there is an element g of $\mathscr{P}$'s rotation group G that satisfies $x(f_m) = x'(g.f_m)$ for every $f_m \in F(\mathscr{P})$.*

For ease of exposition, we use the notational shorthand $(x)_m$ for $x(f_m)$ and $x = g.x'$ when $x(f_m) = x'(g.f_m)$ for every $f_m \in F(\mathscr{P})$. Additionally, we denote the intermediate satisfying $(x)_m = \mathit{white}$ for all $f_m \in F(\mathscr{P})$ as x^w and similarly x^b is the intermediate with $(x)_m = \mathit{black}$ for all $f_m \in F(\mathscr{P})$. The function counting the number of black faces an intermediate has is denoted $h(x) \doteq |\{f_m \in F(\mathscr{P}) : (x)_m = \mathit{black}\}|$.

Definition 2. *Two intermediates x^j and x^k are **connected** ($x^j \leftrightarrow x^k$) if $(x^j)_m = (x^k)_m$ for all $f_m \in F(\mathscr{P})$ except for exactly one face f_n that has $(x^j)_n \neq (x^k)_n$.*

Definition 3. *A Building Game **pathway** is a sequence of intermediates $x^{p_0}, x^{p_1}, x^{p_2}, \ldots, x^{p_N}$ such that $x^{p_0} = x^w$, $x^{p_N} = x^b$, x^{p_i} is connected to $x^{p_{i+1}}$ and $h(x^{p_i}) = i$.*

In this way it is useful to think of intermediates as connected if it is possible to color one face of the first intermediate to get the second and a pathway as a sequence of these connections between x^w and x^b. Figure 1 shows a Building Game pathway for the dodecahedron using Schlegel diagrams. The pathways has 13 intermediates since there must be exactly one intermediate x^{p_i} satisfying $h(x^{p_i}) = i$ for each $i = 0, 1, 2, \ldots, 12$.

Figure 1: One Building Game pathway on the dodecahedron.

With many pairs of connected intermediates, we organize these relations in a graph.

Definition 4. *The Building Game **state space** for a polyhedron $\mathscr{P}$ is a graph in which the nodes are $\mathscr{P}$'s intermediates and a graph edge exists between two intermediates if and only if they are connected.*

When the intermediates are partitioned by their value of h, it is natural to arrange the state space as a tiered graph according to this partition. Figure 2 shows the Building Game state space for the cube. As seen, each tier has intermediates with the same number of blackfaces and connections thus exist with intermediates that are either in the tier directly above or below them. We can also see that there are three distinct pathways contained in the state space.

Interestingly, it is not the case that the recoloring of each face of x^j results in a distinct intermediate.

Figure 2: The Building Game state space of the cube.

Definition 5. *The number of different faces* $\left|\left\{f_m \in F\left(\mathscr{P}\right) : x^j + e^m \in \left[x^k\right]\right\}\right|$ *of* x^j *that can be colored to form* x^k *is called the* ***degeneracy number*** S_{jk}.

It is important to note that in general the degeneracy number is not symmetric, i.e. $S_{jk} \neq S_{kj}$ for some connections $x^j \leftrightarrow x^k$ in the state space. Both figures 1 and 1 show the forward and backward degeneracy numbers for each connection.

1.1 Related Work

–Like polyominos on polyhedra

1.2 Applications

–Viral capsid assembly
–Self-assembly of molecular cages
–Self assembly for manufacturing purposes

1.3 Paper Overview

– Summary of subsequent sections

2 Enumerative Results

As we consider polyhedra with more and more faces, there is a combinatorial explosion in the number intermediates in state space. While the 6-faced cube state space has only 8 nodes and 9 nodes, the 20-faced icosahedron state space has 2,649 nodes and 17,241 nodes and the 26-faced truncated cuboctahedron state space has 1,525,605 nodes and 17,672,377. Figure 3 details state space sizes of all polyhedra in the Platonic, Archimedean, and Catalan solid classes of up to 26 faces.

Also something about pathway statistics.

Polyhedra Name	Class	F($\mathscr{P}$)	E($\mathscr{P}$)	V($\mathscr{P}$)	Intermediates	Connections	Pathways
Tetrahedron	P	4	6	4	5	4	1
Cube	P	6	12	8	9	10	3
Octahedron	P	8	12	6	15	22	14
Dodecahedron	P	12	30	20	74	264	17,696
Icosahedron	P	20	30	12	2,650	17,242	57,396,146,640
Truncated Tetrahedron	A	8	18	12	29	65	402
Cuboctahedron	A	14	24	12	341	1,636	10,170,968
Truncated Cube	A	14	36	24	500	2,731	101,443,338
Truncated Octahedron	A	14	36	24	556	3,071	68,106,377
Rhombicuboctahedron	A	26	48	24	638,851	6,459,804	16,494,392,631,838,879,380
Truncated Cuboctahedron	A	26	72	48	1,525,605	17,672,377	?
Icosidodecahedron	A	32	60	30	?	?	?
Truncated Dodecahedron	A	32	90	60	?	?	?
Truncated Icosahedron	A	32	90	60	?	?	?
Triakis Tetrahedron	C	12	18	8	99	319	38,938
Rhombic Dodecahedron	C	12	24	14	128	494	76,936
Triakis Octahedron	C	24	36	14	12,749	81,297	169,402,670,046,670
Tetrakis Hexahedron	C	24	36	14	50,768	394,278	4,253,948,297,210,346
Deltoidal Icositetrahedron	C	24	48	26	209,676	1,989,549	?
Pentagonal Icositetrahedron	C	24	60	38	345,939	3,544,988	2,828,128,000,716,774,492
Rhombic Triacontahedron	C	30	60	32	?	?	5,266,831,101,345,821,968

Figure 3: Table of polyhedra in the Platonic (P), Archimedean (A), and Catalan (C) solid classes of up to 32 faces and their Building Game state space statistics.

2.1 Bounds and Asymptotics

Have upper, but what about lower?

2.2 Methods

3 The Building Game as a Stochastic Process

Since the Building Game is a sequential process with several choices at each step, it is natural to consider it as a stochastic process. By putting a distribution on all possible faces that can be colored black at each step of the Building game, a distribution on the space of pathways is implicitly defined. Thus, for a choice of this transition rule, we can ask questions about the likelihood of the different pathways.

–Math and graphical results about putting a distribution on pathways

3.1 Forward and Backward Transitions

If we allow faces be changed both from white to black and from black to white, the process consists of transitions from intermediate to intermediate along

Polyhedra Name	Class	F($\mathscr{P}$)	E($\mathscr{P}$)	V($\mathscr{P}$)	Intermediates	Connections	Pathways
Tetrahedron	P	4	6	4	5	4	1
Cube	P	6	12	8	8	8	2
Octahedron	P	8	12	6	12	12	14
Dodecahedron	P	12	30	20	53	156	2166
Icosahedron	P	20	30	12	468	1984	105999738
Truncated Tetrahedron	A	8	18	12	22	42	174
Cuboctahedron	A	14	24	12	137	470	477776
Truncated Cube	A	14	36	24	248	1002	5232294
Truncated Octahedron	A	14	36	24	343	1466	5704138
Rhombicuboctahedron	A	26	48	24	70836	462149	48399693494788840
Truncated Cuboctahedron	A	26	72	48	?	?	?
Icosidodecahedron	A	32	60	30	?	?	?
Truncated Dodecahedron	A	32	90	60	?	?	?
Truncated Icosahedron	A	32	90	60	?	?	?
Triakis Tetrahedron	C	12	18	8	49	116	5012
Rhombic Dodecahedron	C	12	24	14	68	196	6258
Triakis Octahedron	C	24	36	14	667	2383	15255459
Tetrakis Hexahedron	C	24	36	14	4220	21079	5854799360107
Deltoidal Icositetrahedron	C	24	48	26	?	?	?
Pentagonal Icositetrahedron	C	24	60	38	95127	654537	5607231936129109
Rhombic Triacontahedron	C	30	60	32	97368	697623	6889989896241902854

Figure 4: Table of polyhedra in the Platonic (P), Archimedean (A), and Catalan (C) solid classes of up to 32 faces and their Building Game state space shellability statistics.

state space connections. By specifying a distribution on these transitions, it will induce a stationary measure on the state space.

We define the Markov process X_t by the transition rate matrix Q, with the heuristic that the rate of transition to an intermediate $x^k$from an intermediate x^kshould be proportional to the number of faces of x^jthat can be colored to reach the intermediate x^k. For this reason, we include the degeneracy number S_{jk} as a factor in the transition rate matrix. Furthermore, we model the process after and energetic model in which each intermediate has an energy and to transtion between intermediates, an energy barrier $E_{jk} = E_{kj}$ must be overcome.

$$Q_{jk} = S_{jk} e^{-\beta\left(E_{jk}-E_j\right)} \tag{1}$$

$$Q_{jj} = -z_j \tag{2}$$

$$\tag{3}$$

Here, $z_j \doteq \sum_{\ell:\ell\neq j} S_{j\ell} e^{-\beta\left(E_{j\ell}-E_j\right)}$ is the rate at which the process leaves x^j.

Theorem 1. *If the transition rate matrix Q can be decomposed as $Q = DC$ where D is diagonal with each entry of the diagonal positive and C is a non-negative symmetric matrix with $C_{jk} > 0$ if and only if x^j and x^k are connected, then X_t has the unique stationary distribution $\pi = \operatorname{diag}\left(D^{-1}\right)$.*

Proof. First, we show Q and π satisfy detailed balance.

$$\pi_j Q_{jk} = \left(\frac{1}{D_{jj}}\right)(D_{jj} C_{jk}) \tag{4}$$
$$= C_{jk} \tag{5}$$
$$= C_{kj} \tag{6}$$
$$= \left(\frac{1}{D_{kk}}\right)(D_{kk} C_{kj}) \tag{7}$$
$$= \pi_k Q_{kj} \tag{8}$$

– Prove aperiodicity – Prove positive reccurence

□

In order to use theorem 1 to find the stationary distribution for the transition rule **??**, we must be able to decompose the degeneracy number S_{jk} to fit the template of **C** and **D**. In the following section we derive group theoretic identities to show that this is possible.

3.2 Hitting Times

$$\tau_j^A \doteq \inf\left\{t \geq 0 : X_t \in A, X_0 = x^j\right\} \tag{9}$$

$$\nu_j^A \doteq \inf\left\{n \geq 0 : Y_n \in A, Y_0 = x^j\right\} \tag{10}$$

For $j \notin A$.

$$\begin{aligned}
E\left[\tau_j^A\right] &= E\left[E\left[\tau_j^A | Y_1\right]\right] && (11)\\
&= E\left[Exp\left(z_j\right) + \tau_{Y_1}^A\right] && (12)\\
&= \frac{1}{z_j} + E\left[\sum_k \tau_{Y_1}^A \mathbb{1}_{Y_1=k}\right] && (13)\\
&= \frac{1}{z_j} + \sum_{k:k\neq j} E\left[\tau_k^A\right] P\left(Y_1 = k\right) && (14)\\
&= \frac{1}{z_j}\left(1 + \sum_{k:k\neq j} q_{jk} E\left[\tau_k^A\right]\right) && (15)\\
\sum_k q_{jk} E\left[\tau_k^A\right] &= 1 && (16)\\
& && (17)
\end{aligned}$$

For $j \in A$.

$$\begin{aligned}
E\left[\tau_j^A\right] = 0 && (18)\\
&& (19)
\end{aligned}$$

As a linear system:

$$\begin{aligned}
\left(\mathrm{diag}\left(\mathbb{1}_A\right) - \mathrm{diag}\left(\mathbb{1}_{A^c}\right) Q\right) E\left[\tau^A\right] = \mathbb{1}_{A^c} && (20)\\
&& (21)
\end{aligned}$$

$$\begin{aligned}
\psi_j^A\left(t\right) &\doteq P\left(\tau_j^A \leq t\right) && (22)\\
\psi_j^A\left(0\right) &= \mathbb{1}_{j\in A} && (23)\\
\psi_j^A\left(t\right) &= 0 \forall j \in A && (24)\\
& && (25)
\end{aligned}$$

For $j \notin A$.

$$
\begin{aligned}
\psi_j^A(t) &\doteq P\left(\tau_j^A \le t\right) && (26)\\
&= \sum_k P\left(\tau_j^A \le t | Y_1 = x^k\right) P\left(Y_1 = x^k\right) && (27)\\
&= \frac{1}{z_j} \sum_{k:k\neq j} q_{jk} P\left(Exp\left(z_j\right) \tau_j^A \le t\right) && (28)\\
&= \frac{1}{z_j} \sum_{k:k\neq j} q_{jk} \int_0^t P\left(\tau_j^A \le t - s\right) z_j e^{-z_j s} ds && (29)\\
&= \sum_{k:k\neq j} q_{jk} \int_0^t \psi_k^A\left(t-s\right) e^{-z_j s} ds && (30)\\
&= \sum_{k:k\neq j} q_{jk} \int_0^t \psi_k^A\left(r\right) e^{-z_j (t-r)} dr && (31)\\
e^{z_j t}\psi_j^A(t) &= \sum_{k:k\neq j} q_{jk} \int_0^t e^{z_j r}\psi_k^A\left(r\right) dr && (32)\\
e^{z_j t}\frac{d\psi_j^A}{dt} + z_j e^{z_j t}\psi_j^A(t) &= \sum_{k:k\neq j} q_{jk} e^{z_j t}\psi_k^A(t) && (33)\\
\frac{d\psi_j^A}{dt} &= \sum_k q_{jk}\psi_k^A(t) && (34)
\end{aligned}
$$

Combining both cases, we get the linear system and solution.

$$
\begin{aligned}
\frac{d\psi^A}{dt} &= \operatorname{diag}\left(\mathbb{1}_{A^c}\right) Q\psi^A && (35)\\
\psi^A(0) &= \mathbb{1}_A && (36)\\
\psi^A(t) &= e^{\operatorname{diag}\left(\mathbb{1}_{A^c}\right)Qt}\mathbb{1}_A && (37)\\
& && (38)
\end{aligned}
$$

This is the solution for the CDF of the stopping time τ^A, but we can also compute the PDF explicitly for $t > 0$.

$$
\begin{aligned}
p\left(\tau^{A}=t\right) &= \frac{d\psi^{A}}{dt} && (39)\\
&= \operatorname{diag}\left(\mathbb{1}_{A^{c}}\right) Q\psi^{A} && (40)
\end{aligned}
$$

4 A Finite Geometric Result

Since we define Building Game intermediates as rotationally unique from each other, it is useful to think about the problem in the context of $\mathscr{P}$'s rotational symmetry group $G \doteq G(\mathscr{P})$ and group actions. For an intermediate x^{j}, the number of symmetries r_j is the order of the stabilizer subgroup $G_{x^j} \doteq \{g \in G : g.x^{j} = x^{j}\}$ of G that fixes x^{j}. Suppose x^{j} and x^{k} are connected in the state space and φ is one of the S_{jk} faces that, when added to x^{j}, forms x^{k}. We say $x^{j}+\varphi = x^{k}$. The degeneracy number S_{jk} can then be expressed as the order of the orbit $(G_{x^j}).\varphi$ of φ with respect to x^{j}'s stabilizer subgroup. Analogously, we define the reverse degeneracy number as $S_{kj} \doteq |(G_{x^k}).\varphi|$

Lemma 1. *For Building Game intermediates x^{j} and x^{k} connected in the state space and a face $f_m \in F(\mathscr{P})$ satisfying $x^{j}+e^{m} = x^{k}$, the stabilizer subgroup G_{x^j,e^m} that fixes both x^{j} and e^{m} is the same stabilizer subgroup G_{x^k,e^m} that fixes x^{k} and e^{m}.*

Proof.

$$
\begin{aligned}
G_{x^j,e^m} &\doteq \left\{g \in G | g.x^{j} = x^{j}, g.e^{m} = e^{m}\right\} && (41)\\
&= \left\{g \in G | g.\left(x^{k}-e^{m}\right) = x^{k}-e^{m}, g.e^{m} = e^{m}\right\} && (42)\\
&= \left\{g \in G | g.x^{k} = x^{k}, g.e^{m} = e^{m}\right\} && (43)\\
&\doteq G_{x^k,e^m} && (44)
\end{aligned}
$$

□

Theorem 2. *For two Building Game intermediates x^{j} and x^{k} are connected in the BG state space, $r_k S_{jk} = r_j S_{kj}$.*

Proof. Let e^{m} be a face such that $x^{k} = x^{j}+e^{m}$. Then, by the orbit-stabilizer theorem, Lagrange's Theorem and lemma 1 we have the following [7].

$$
\begin{aligned}
\frac{r_j}{S_{jk}} &\doteq \frac{|G_{x^j}|}{|(G_{x^j}).e^m|} && (45)\\
&= [G_{x^j} : (G_{x^j}).e^m] && (46)\\
&= \left|G_{x^j,e^m}\right| && (47)\\
&= \left|G_{x^k,e^m}\right| && (48)\\
&= [G_{x^k} : (G_{x^k}).e^m] && (49)\\
&= \frac{|G_{x^k}|}{|(G_{x^k}).e^m|} && (50)\\
&\doteq \frac{r_k}{S_{kj}} && (51)
\end{aligned}
$$

The result $r_k S_{jk} = r_j S_{kj}$ follows. □

5 Stationarity

Theorem 3. *The Markov process X_t defined by the transition rate matrix Q in equation 1 admits the unique stationary distribution $\frac{1}{zr_j}e^{-\beta E_j}$ where $z \doteq \sum_\ell \frac{1}{r_\ell}e^{-\beta E_\ell}$ is the partition function.*

Proof. We take $C_{jk} \doteq \frac{S_{jk}}{zr_j}e^{-\beta E_{jk}}$ and notice that it is symmetric by theorem 2. With $D_{jj} \doteq zr_j e^{\beta E_j}$ we have our partition.

$$
\begin{aligned}
Q_{jk} &= S_{jk}e^{-\beta\left(E_{jk}-E_j\right)} && (52)\\
&= \left(zr_j e^{\beta E_j}\right)\left(\frac{S_{jk}}{zr_j}e^{-\beta E_{jk}}\right) && (53)\\
&= D_{jj}C_{jk} && (54)
\end{aligned}
$$

Thus, by theorem 1, $\pi_j = \frac{1}{D_{jj}} = \frac{1}{zr_j}e^{-\beta E_j}$. □

6 Discussion

6.1 Nonenumerative Approaches

Acknowledgments

Supported by NSF grants DMS 07-48482 and EFRI 10-22638

7 Potential Citations (temp)

[1] [6] [2] [8] [4] [3] [5]

References

[1] H Coxeter. *Regular Polytopes*. Dover Publications, Inc., New York, NY, 1973.

[2] P Cromwell. *Polyhedra*. Cambridge University Press, Cambridge, UK, 1997.

[3] M Eden. A two-dimensional growth process. pages 223–239.

[4] B Gidas. *Topics in contemporary probability and its application*, chapter Metropolis-type Monte Carlo simulation algorithms and simulated annealing. CDC Press, Boca Raton, FL, 1995.

[5] N Grayson. *Models of molecular self-assembly for RNA viruses and synthetic DNA cages*. PhD thesis, University of York, 2012.

[6] B Grunbaum. *Convex Polytopes*. Springer-Verlag New York, Inc., New York, NY, 2003.

[7] J Rotman. *An Introduction to the Theory of Groups*. Springer-Verlag, New York, NY, fourth edition, 1995.

[8] G Ziegler. *Lectures on Polytopes*. Springer-Verlag, New York, NY, 1995.

[9] A Zlotnick. An equilibrium model of the self assembly of polyhedral protein complexes. *Journal of Molecular Biology*, 241:59–67, 1994.