SFWRENG 6O03 Final Report: Combinatorial optimization formulations with applications to theoretical physics

William Luders
001403581

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1 Introduction

Consider the following combinatorial structure: for a given integer d, let R_d be the set of all non-zero $\{0,1\}^d$ vectors. By excluding the $\{0\}^d$ vector we get $|R_d| = 2^d - 1$ such vectors. Let S_d be the set of possible $\{0,1\}$ vector sub-sums of R_d. There are $|S_d| = 2^{|R_d|} = 2^{2^d-1}$ such sub-sums. We will study the convex hull of S_d, specifically considering the number of vertices of the convex hull. Let H_d represent the subset of S_d whose members are vertices of the convex hull of S_d. Let $a(d) = |H_d|$ represent the number of vertices of the described d-dimensional hull.

The sequence $a(d)$ is described in the OEIS with its relevance to quantum field theory [1].

1.1 Example

For $d = 2$, we have $|R_2| = 2^2-1 = 3$. These vectors are: $R_2 = \{\{0,1\},\{1,0\},\{1,1\}\}$. We have $|S_2| = 2^3 = 8$. These points are:

$$0 \times \{0,1\} + 0 \times \{1,0\} + 0 \times \{1,1\} = \{0,0\}$$

$$0 \times \{0,1\} + 0 \times \{1,0\} + 1 \times \{1,1\} = \{1,1\}$$

$$0 \times \{0,1\} + 1 \times \{1,0\} + 0 \times \{1,1\} = \{1,0\}$$

$$0 \times \{0,1\} + 1 \times \{1,0\} + 1 \times \{1,1\} = \{2,1\}$$
$$1 \times \{0,1\} + 0 \times \{1,0\} + 0 \times \{1,1\} = \{0,1\}$$
$$1 \times \{0,1\} + 0 \times \{1,0\} + 1 \times \{1,1\} = \{1,2\}$$
$$1 \times \{0,1\} + 1 \times \{1,0\} + 0 \times \{1,1\} = \{1,1\}$$
$$1 \times \{0,1\} + 1 \times \{1,0\} + 1 \times \{1,1\} = \{2,2\}$$

$\{1,1\}$ occurs twice in S_2. By plotting the convex hull of S_2 in figure 1, we can see that $\{1,1\}$ is not a member of H_d, but all other points are. Therefore $a(2) = |H_2| = |S_2| - 2 = 6$, and we can equivalently visually verify there are 6 vertices of S_2.

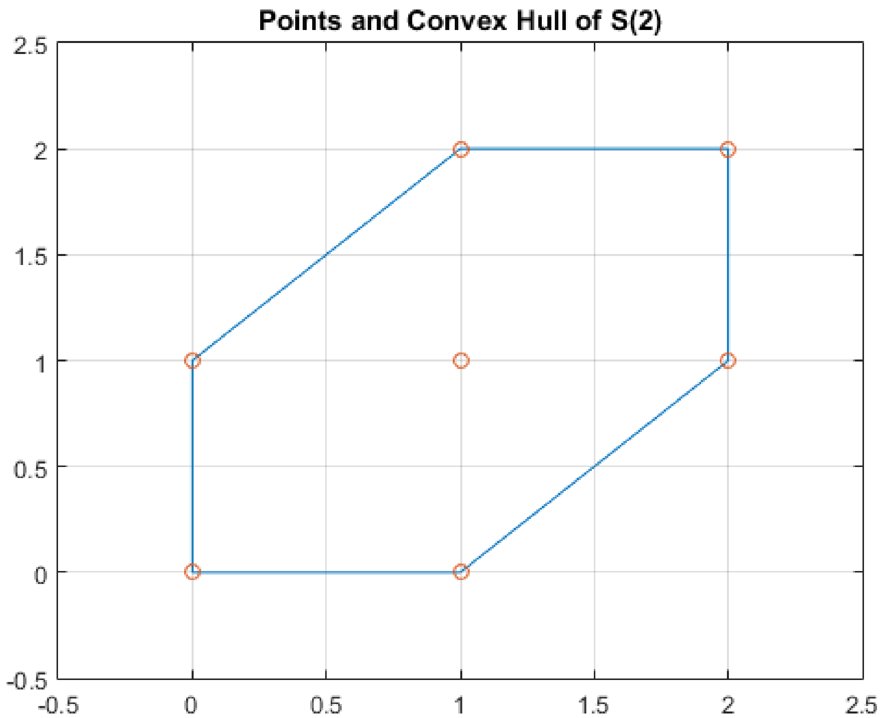


Figure 1: Cartesian Representation of S_2

Any member of S that can be generated uniquely in the fashion described above is a vertex. The converse is also true. We can use these facts to determine vertices of S by generating S and finding its members that occur only once.

The vertices for $d = 2$ are $\{0,0\}$, $\{0,1\}$, $\{1,0\}$, $\{1,2\}$, $\{2,1\}$ and $\{2,2\}$. There are only 2 vertices we care about: $\{0,0\}$ and $\{0,1\}$. All others can be deduced from permutation and symmetry arguments. $\{1,0\}$ is a permutation of $\{0,1\}$. Symmetrical vertices (the latter three) are obtained by subtracting known vertices from $\{2,2\}$. In any d, symmetrical vertices are obtained by subtracting known vertices from $\{2^{d-1}\}^d$. Considering only the number of vertices whose coordinates average to 2^{d-2} or less, and multiplying by 2 accounts for all symmetric vertices.

2 Calculation

Let $\boldsymbol{R}$ be the a $d \times (2^d - 1)$ matrix in which each row contains a unique non-zero $\{0,1\}^d$ vector. Let $\boldsymbol{W}$ be a $(2^{2^d-1}) \times (2^d - 1)$ 'weight' matrix in which each row contains a unique $\{0,1\}^{2^d-1}$. Let $\boldsymbol{S} = \boldsymbol{W}\boldsymbol{R}$. Each row of $\boldsymbol{S}$ will contain a member of S_d. Unique rows are vertices of the convex hull of S_d.

This method is prohibitive for $d > 4$ due to memory constraints. Smarter methods can be used; since $\boldsymbol{R}$ and $\boldsymbol{W}$ contain only 0 and 1, once can perform bitwise operations on bit arrays or integers and iterate through them rather than storing them as a matrix. Since $\boldsymbol{S}$ will contain duplicates, it would be a better use of memory to store members of S in a dictionary, with the key being the member and its value being the count.

Calculation of vertices for $d = 3$ and $d = 4$ were done with the above primary described method with a Matlab program. Figures 1 and 2 were generated with Matlab also.

3 Permutation and Symmetry

Representing H_3 in Cartesian space further displays the arguments of permutation and symmetry (See figure 2).

It is noted that all 6 vertices from $d = 2$ exist as vertices with a prepended 0 for $d = 3$, such as $\{0,1,2\}$ and $\{0,2,2\}$. Their permutations (e.g. $\{2,0,1\}$) and symmetries (e.g. $\{4,4,4\} - \{0,1,2\} = \{4,3,2\}$) are also vertices. Thus $\{0,1,2\}$ has 6 permutations and contributes a total of 12 vertices to a(d) by symmetry. However, one new vertex exists: $\{1,1,3\}$. Identification of these vertices becomes particularly challenging as d grows.

Permutations and symmetry provide an easy way to calculate $a(d)$. Provided

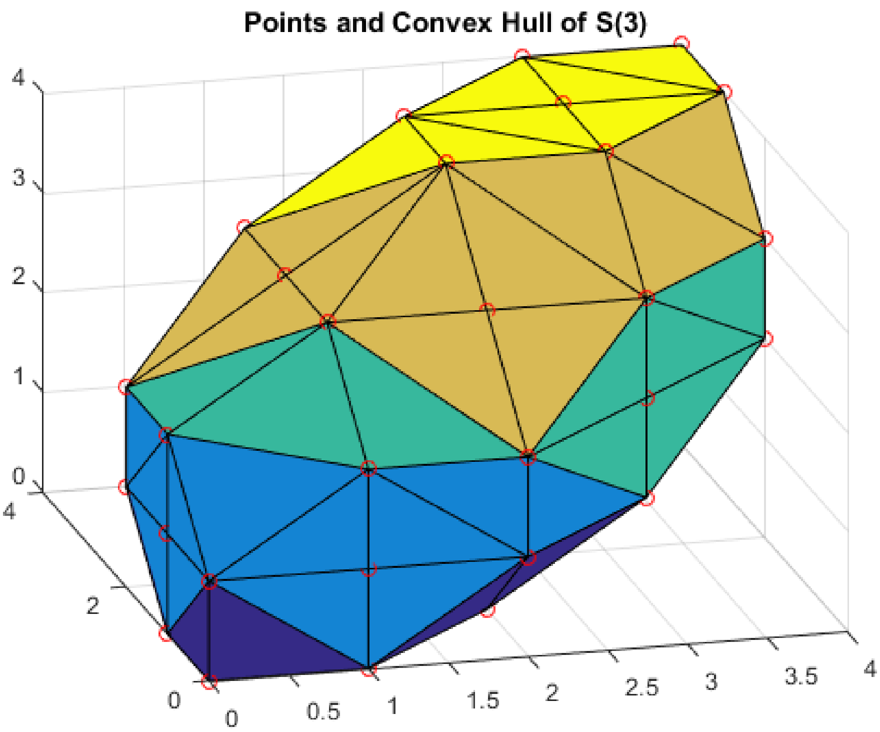


Figure 2: Cartesian Representation of S_3

a comprehensive list of unpermuted vertices, a(3) can be calculated as seen in Table 1.

Unpermuted Vertex	Total Vertices
$\{0, 0, 0\}$	2
$\{0, 0, 1\}$	6
$\{0, 1, 2\}$	12
$\{0, 2, 2\}$	6
$\{1, 1, 3\}$	6
Sum:	32

Table 1: Count of vertices of H_3 by permutation and symmetry

4 Representation for arbitrary d

Visualising H_d is obviously prohibitive for $d > 3$. However, any vertex v of H_d can be represented compactly in the form of a hypergraph. The nodes of the hypergraph represent the coordinates of v, and the set of hyperedges represents the members of set R_d that were used in the sub-sum that created v. For any member of $R_d = \{r_1, .., r_d\}$, the hyperedge touches the coordinates $\{v_1, .., v_d\}$ where $r_i = 1$. The number of hyperedges touching a given node is that node's coordinate value. For example, in $d = 3$, the vertex $\{1, 1, 3\}$ is uniquely composed of $\{0, 0, 1\} + \{0, 1, 1\} + \{1, 0, 1\}$ and its hypergraph appears in figure 3.

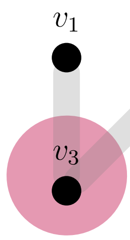


Figure 3: Hypergraph representation of $\{1, 1, 3\}$ vertex

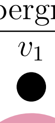
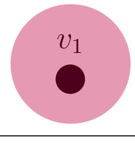
5 Hypergraph Representation of $H(d)$, $d \leq 4$

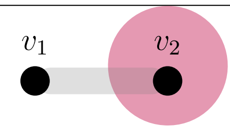
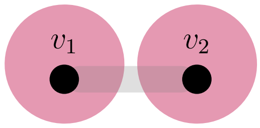
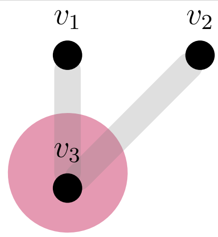
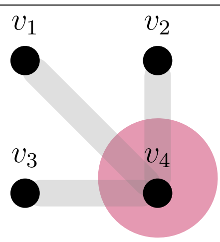
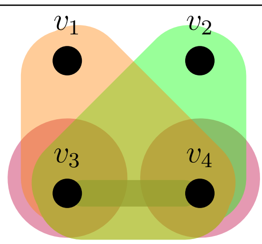
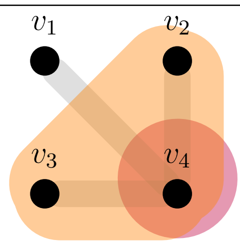
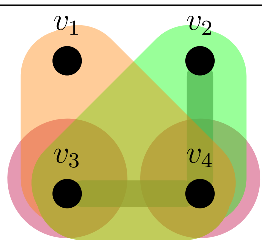
Table 2 shows the unpermuted vertices of S_d for $d \leq 4$, as well as the count of their permutations and symmetries. Table 3 shows the vertices of H_d in hypergraph form from $d = 1$ to $d = 4$. For $d = 3$ and $d = 4$, vertices that are obtained by adding a prepended 0 are ignored as the hypergraph has already been shown for lower d, but without the additional unused vertices. For example, $\{0, 0, 1\}$ has a similar hypergraph to $\{0, 1\}$ but has one extra node with no hyperedges attached to it. Equivalently, $\{4, 4, 4\}$ is a vertex by symmetry in $d = 3$, so in $d = 4$ we will not display $\{0, 4, 4, 4\}$. Vertices obtained by symmetry are not shown as their hyperedges are the complement of the hyperedges of the symmetric vertex. For example, the complement of the empty hypergraph for $\{0, 0, 0\}$ is a hypergraph with hyperedges corresponding to the power set of $\{1, 2, 3\}$: edges $\{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}$ and $\{1, 2, 3\}$

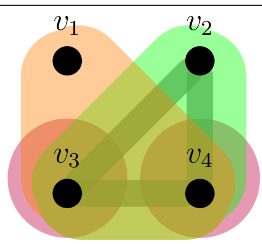
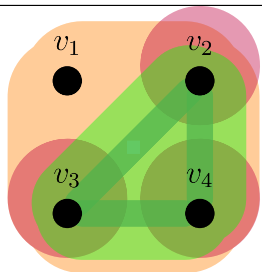
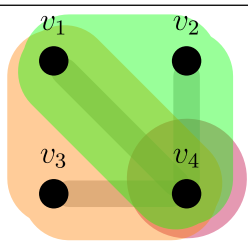
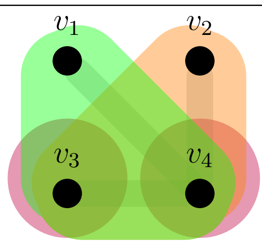
Table 2: Count of vertices of H_d by permutation and symmetry

Dimension	Unpermuted Vertex	Total Vertices	$a(d)$
1	$\{0\}$	2	=2
2	$\{0,0\}$	2	
	$\{0,1\}$	+4	=6
3	$\{0,0,0\}$	2	
	$\{0,0,1\}$	6	
	$\{0,1,2\}$	12	
	$\{0,2,2\}$	6	
	$\{1,1,3\}$	+6	=32
4	$\{0,0,0,0\}$	2	
	$\{0,0,0,1\}$	8	
	$\{0,0,1,2\}$	24	
	$\{0,0,2,2\}$	12	
	$\{0,1,1,3\}$	24	
	$\{0,1,3,3\}$	24	
	$\{0,2,2,4\}$	24	
	$\{0,2,3,4\}$	48	
	$\{0,3,4,4\}$	24	
	$\{0,4,4,4\}$	8	
	$\{1,1,1,4\}$	8	
	$\{1,1,4,4\}$	12	
	$\{1,2,2,5\}$	24	
	$\{1,2,4,5\}$	48	
	$\{1,3,5,5\}$	24	
	$\{1,5,5,5\}$	8	
	$\{2,2,3,6\}$	24	
	$\{2,2,4,6\}$	+24	=370

Table 3: Unpermuted vertices and hypergraphs of H_d.

Dimension	Vertex	Hypergraph
1	$\{0\}$	
	$\{1\}$	

2	$\{1,2\}$	
	$\{2,2\}$	
3	$\{1,1,3\}$	
4	$\{1,1,1,4\}$	
	$\{1,1,4,4\}$	
	$\{1,2,2,5\}$	
	$\{1,2,4,5\}$	

	$\{1,3,5,5\}$	
	$\{1,5,5,5\}$	
	$\{2,2,3,6\}$	
	$\{2,2,4,6\}$	

6 Bibliography

1 Tim S. Evans (2019), The On-Line Encyclopedia of Integer Sequences, http://oeis.org/A034997.