HÁSKÓLINN Í REYKJAVÍK
REYKJAVIK UNIVERSITY

ICE-TCS
Icelandic Centre of Excellence
in Theoretical Computer Science

Combinatorial Structures for CSP

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Outline

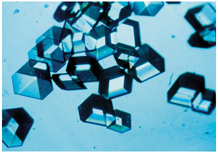
This Talk is split into three sections:

1. Background on both the chemical motivation behind this talk, and 1D necklaces.
2. An introduction to **multidimensional necklaces** as a combinatorial object.
3. A set of results on several fundamental problems associated with 1D necklace objects when generalised to the multidimensional setting.

Why Crystals?

- New materials are needed to deal with the challenges of the 21st century, from strong materials for manufacturing to better conductors for electrical systems.
- Crystals are a fundamental, and very common form of matter.
- Importantly, Crystals are **periodic** - meaning that a lot of the properties of a crystaline material can be determined from a relatively small amount of information.

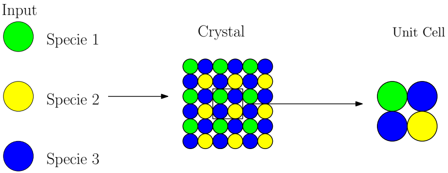
Crystals are everywhere

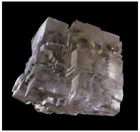


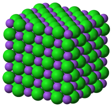
Crystals

Definition (Crystals)

A **Crystal** is a material composed of an (infinitely) repeating **Unit Cell**.



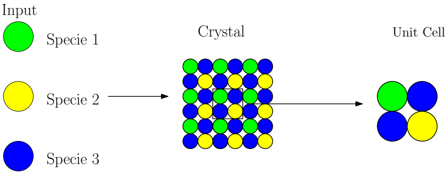


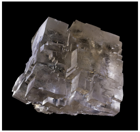


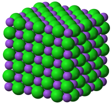
Crystals

Definition (Unit Cells)

A **Unit Cell** is a contiguous region of space containing some set of **Ions**.

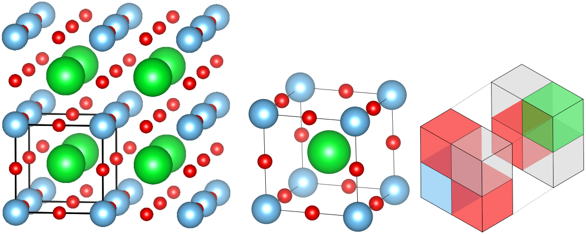






Discrete Crystals

- In this talk we are interested in **Discrete Crystals**, i.e. crystals where every ion is placed on a grid.
- In this model, every cell is either empty, or wholly occupied by an ion.
- For simplicity we assume that each cell can contain only 1 ion, and that each ion can fit into a single cell.



Goals

We want to:

- **Count** the number of potential (discrete) crystal structures from some set of ions and given size.
- **Generate** the complete set of (discrete) crystal structures from some set of ions and given size.
- **Sample** crystals from the space of potential structures with uniform probability.

Discrete Crystals as Multidimensional Words

- Multidimensional words are a natural object for representing discrete crystals.
- Here the alphabet Σ represents the set of ions plus some symbol for empty space.
- The size of the word is the dimensions of the unit cell.

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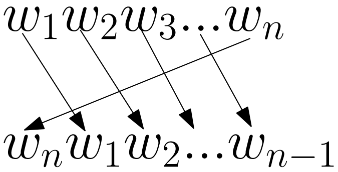
- The size of the word is the dimensions of the unit cell.
- **Advantages**: Multidimensional words are well studied objects, with results on counting, generating, and sampling.
- **Problem**: Crystals have **translational symmetry**.

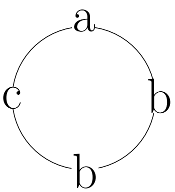
Translational Symmetry

$$\begin{bmatrix} a & a & a \\ a & b & b \\ c & c & b \end{bmatrix}, \quad \begin{bmatrix} a & a & a \\ b & b & a \\ c & b & c \end{bmatrix}, \quad \begin{bmatrix} a & a & a \\ b & a & b \\ b & c & c \end{bmatrix},$$
$$\begin{bmatrix} a & b & b \\ c & c & b \\ a & a & a \end{bmatrix}, \quad \begin{bmatrix} b & b & a \\ c & b & c \\ a & a & a \end{bmatrix}, \quad \begin{bmatrix} b & a & b \\ b & c & c \\ a & a & a \end{bmatrix},$$
$$\begin{bmatrix} c & c & b \\ a & a & a \\ a & b & b \end{bmatrix}, \quad \begin{bmatrix} c & b & c \\ a & a & a \\ b & b & a \end{bmatrix}, \quad \begin{bmatrix} b & c & c \\ a & a & a \\ b & a & b \end{bmatrix}$$

Necklaces

- In 1D the problem of translational symmetry is solved using **Necklaces**.
- Informally a necklace is a set of words that can be reached from each other by some **translation**.
- The **translation** (or cyclic shift) of a word w by some integer i returns the word w' where $w'_j = w_{j-i \bmod n}$.





abbc
bbca
bcab
cabb

Periodicity

- A necklace of length n containing the word w is **periodic** if there is a subword of w that can be repeated to make w.
- A necklace is **aperiodic** if it is not periodic.
- An aperiodic necklace is called a **Lyndon word**.

abab	**aaab**
baba	aaba
abab	abaa
baba	baaa

Some Notation for 1D Necklaces

For the remainder of this talk we use the following assumptions:

- Σ to denotes an alphabet, which we assume has size q.
- The **Canonical form** of a necklace ω (denoted $\langle\omega\rangle$) is the **Lexicographically smallest** word $w \in \omega$.
- $\mathcal{N}_q^n$ denotes the set of necklaces of length n over an alphabet of size q.
- $\mathcal{L}_q^n$ denotes the set of Lyndon words (aperiodic necklaces) in $\mathcal{N}_q^n$.

Results for Necklaces

Necklaces are a well studied object, of note to us are the results on:

- **Counting** the sizes of $\mathcal{N}_q^n$ and $\mathcal{L}_q^n$.
- **Generating** the sets $\mathcal{N}_q^n$ and $\mathcal{L}_q^n$ in order.
- **Ranking** a necklace within the sets $\mathcal{N}_q^n$ and $\mathcal{L}_q^n$.
- **Unranking** a necklace from the sets $\mathcal{N}_q^n$ and $\mathcal{L}_q^n$.

Counting Necklaces and Lyndon words

- The most fundamental result for both necklaces and Lyndon words are the closed from formulas for counting.
- These results follow from the Pólya enumeration and the Möbius inversion formula respectively.

$$\begin{aligned}
|\mathcal{N}_q^n| &= \sum_{d|n} |\mathcal{L}_q^d| &&= \frac{1}{n} \sum_{d|n} \phi\left(\frac{n}{d}\right) q^d \\
|\mathcal{L}_q^n| &= \sum_{d|n} \mu\left(\frac{n}{d}\right) |\mathcal{N}_q^d| &&= \frac{1}{n} \sum_{d|n} \mu\left(\frac{n}{d}\right) q^d
\end{aligned}$$

Where:

- $\phi(x)$ is Euler's totient function.
- $\mu(x)$ is the Möbius function.

Generating Necklaces and Lyndon words

- There have been several algorithms for generating both the sets of necklaces and Lyndon words.
- Fredricksen and Kessler[1] provided an algorithm to generate $\mathcal{N}_q^n$ in $O(n)$ time (proven by Ruskey et al.[2]).
- Catel et. al.[3] provided an $O(n)$ time algorithm to generate only $\mathcal{L}_q^n$.

[1] Harold Fredricksen and Irving J Kessler. "An algorithm for generating necklaces of beads in two colors". In: *Discrete mathematics* 61.2-3 (1986), pp. 181–188.

[2] F. Ruskey, C. Savage, and T. Min Yih Wang. "Generating necklaces". In: *Journal of Algorithms* 13.3 (1992), pp. 414–430. ISSN: 01966774.

[3] K. Cattell et al. "Fast Algorithms to Generate Necklaces, Unlabeled Necklaces, and Irreducible Polynomials over GF(2)". In: *Journal of Algorithms* 37.2 (2000), pp. 267–282.

Ranking necklaces

Definition (Rank)

The **Rank** of a necklace ω in the set $\mathcal{N}_q^n$ is the number of necklaces with a canonical form that is less than or equal to the canonical form of ω.

1.	aaaaaa	2.	aaaaab	3.	aaaabb	4.	aaabab
5.	aaabbb	6.	aabaab	7.	aababb	**8.**	**aabbab**
9.	aabbbb	10.	ababab	11.	ababbb	12.	abbabb
13.	abbbbb	14.	bbbbbb				

Example of the set $\mathcal{N}_2^6$. In bold, the necklace represented by the word aabbab with a rank of 8.

Ranking Necklaces

- The problem of ranking necklaces originates from the problem of ranking de Bruijn Sequences[4].
- The first class of necklaces to be ranked was Lyndon words.
- This was generalised to ranking general necklaces[5],[6] in $O(n^2)$ time.

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[4] T. Kociumaka, J. Radoszewski, and W. Rytter. "Computing k-th Lyndon word and decoding lexicographically minimal de Bruijn sequence". In: *Symposium on Combinatorial Pattern Matching*. Springer International Publishing, 2014, pp. 202–211.

[5] S. Kopparty, M. Kumar, and M. Saks. "Efficient indexing of necklaces and irreducible polynomials over finite fields". In: *Theory of Computing* 12.1 (2016), pp. 1–27.

[6] J. Sawada and A. Williams. "Practical algorithms to rank necklaces, Lyndon words, and de Bruijn sequences". In: *Journal of Discrete Algorithms* 43 (2017), pp. 95–110. ISSN: 15708667.

Unranking Necklaces

Definition (Uranking Problem)

Given a set of necklaces $\mathcal{N}_q^n$ and an integer i, the unranking problem asks for the necklace with a rank of i.

1.	aaaaaa	2.	aaaaab	3.	aaaabb	4.	aaabab
5.	aaabbb	6.	aabaab	7.	aababb	**8.**	**aabbab**
9.	aabbbb	10.	ababab	11.	ababbb	12.	abbabb
13.	abbbbb	14.	bbbbbb				

Why do we care about ranks?

- Going back to our goal of sampling, note that while randomly sampling words may lead to some necklaces (Lyndon words in particular) being over represented, choosing a rank at random and unranking the corresponding necklaces allows for a uniform distribution.

aaaa	**aaab**	**aabb**	**ab**ab	**abbb**	**b**bbb
-	aaba	abba	baba	bbba	-
-	abaa	bbaa	-	bbab	-
-	baaa	baab	-	babb	-

Example of the set of words of length 4 over the alphabet $\Sigma = \{a, b\}$ *split into the 6 necklaces in* $\mathcal{N}_2^4$. *Highlighted are the periods of the words, corresponding to the number of words in the corresponding necklace.*

Multidimensional Necklaces (almost)

- To define multidimensional necklaces we need three more things:
  1. Notation for multidimensional words.
  2. A formal definition of translational equivalence.
  3. Some notion over ordering over the set of multidimensional words.

Notation for multidimensional words

- We treat d dimensional words as d-dimensional arrays of symbols over some alphabet Σ.
- Given a word w, the notation $w[x_1, x_2, \ldots, x_d]$ is used to denote the symbol at position $x_1, x_2, \ldots, x_d$ in w.
- Given a word w of size $n_1 \times n_2 \times \ldots \times n_d$, the notation w_i is used denote the word v of size $n_1 \times n_2 \times \ldots \times n_{d-1}$ where $v[x_1, x_2, \ldots, x_{d-1}] = w[x_1, x_2, \ldots, x_{d-1}, i]$. We call w_i the i^{th} slice of w.

$$w = \begin{bmatrix} a & a & b \\ a & a & c \\ a & b & c \end{bmatrix}$$

$$w_1 = \begin{bmatrix} a & a & b \end{bmatrix}$$
$$w_2 = \begin{bmatrix} a & a & c \end{bmatrix}$$
$$w_3 = \begin{bmatrix} a & b & c \end{bmatrix}$$

Translational Equivalence

- Let w be a 2D word of size $n_1 \times n_2$ and let (i, j) be a pair of integers such that $0 \leq i \leq n_1 - 1$ and $0 \leq j \leq n_2 - 1$.
- The *translation* of w by (i, j) returns the word v where $w[x, y] = v[x + i \bmod n_1, y + j \bmod n_2]$.
- More generally, given a d-dimensional word w of size $n_1 \times n_2 \times \dots n_d$, the translation by $(t_1, t_2, \dots, t_d)$ returns the word v such that $w[x_1, x_2, \dots, x_d] = v[x_1 + t_1 \bmod n_1, x_2 + t_2 \bmod n_2, \dots, x_d + t_d \bmod n_d]$.
- The notation $w \circ (t_1, t_2, \dots, t_d)$ is used to denote the shift of w by $(t_1, t_2, \dots, t_d)$.

$$\begin{bmatrix} a & a & b \\ a & a & b \\ a & b & c \end{bmatrix} \circ (1, 1) = \begin{bmatrix} a & b & a \\ b & c & a \\ a & b & a \end{bmatrix}$$

Translational Equivalence

- We define the set of translations for words of size $\vec{n} = (n_1, n_2, \ldots, n_d)$, $Z_{\vec{n}}$ by the direct product of the cyclic groups $Z_{n_1} \times Z_{n_2} \times \ldots \times Z_{n_d}$.
- We order the set of translations $Z_{\vec{n}}$ such that $(i, j) < (x, y)$ if and only if $i < x$ or $i = x$ and $j < y$.

$$\begin{bmatrix} (0,0) & (0,1) & (0,2) & (0,3) \\ (1,0) & (1,1) & (1,2) & (1,3) \\ (2,0) & (2,1) & (2,2) & (2,3) \\ (3,0) & (3,1) & (3,2) & (3,3) \end{bmatrix} = \begin{bmatrix} 0\cdot 4+0 & 0\cdot 4+1 & 0\cdot 4+2 & 0\cdot 4+3 \\ 1\cdot 4+0 & 1\cdot 4+1 & 1\cdot 4+2 & 1\cdot 4+3 \\ 2\cdot 4+0 & 2\cdot 4+1 & 2\cdot 4+2 & 2\cdot 4+3 \\ 3\cdot 4+0 & 3\cdot 4+1 & 3\cdot 4+2 & 3\cdot 4+3 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 & 2 & 3 \\ 4 & 5 & 6 & 7 \\ 8 & 9 & 10 & 11 \\ 12 & 13 & 14 & 15 \end{bmatrix}$$

Ordering Multidimensional Words

- We order multidimensional words using **Necklace recursive order**.
- This order works by comparing each slice in order.
- Let $\langle w \rangle$ denote the canonical representation of the necklace containing the word w, and let $T(w)$ denote the translation $t \in Z_{\vec{n}}$ such that $\langle w \rangle \circ t = w$.

Definition (Necklace Recursive Order)

Given two words w, v of size $n_1 \times n_2 \times \ldots \times n_d$ over the alphabet Σ, $w \leq v$ if and only if for the smallest i such that $w_i \neq v_i$, either $\langle w_i \rangle < \langle v_i \rangle$ or $\langle w_i \rangle = \langle v_i \rangle$ and $T(w_i) < T(v_i)$.

Ordering Examples

$$w = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} a & a & a & b \\ a & a & b & a \\ a & a & a & b \\ b & a & a & a \end{bmatrix}, u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} a & a & a & b \\ a & a & b & a \\ b & a & a & a \\ b & a & a & a \end{bmatrix},$$

$$v = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} a & a & a & b \\ a & a & b & a \\ a & a & b & b \\ b & a & a & a \end{bmatrix}$$

Figure 1: An example of three words, w, u, and v, ordered as follows $w < u < v$. Note that $w_1 : w_2 = v_1 : v_2 = u_1 : u_2$. However, $\langle w_3 \rangle = \langle u_3 \rangle = aaab$, which is smaller than $\langle v_3 \rangle = aabb$. Further, $w_3 < u_3$ as $G(w_3, \langle w_3 \rangle) = 2$ and $G(u_3, \langle u_3 \rangle) = 3$, which is larger than 2.

Multidimensional Necklace

Definition (Multidimensional Necklace)

A **Multidimensional Necklace** ω of size $n_1 \times n_2 \times \ldots \times n_d$ over an alphabet Σ is a set of d-dimensional words of size $n_1 \times n_2 \times \ldots \times n_d$ over an alphabet Σ that are equal under the set of translations $Z_{(n_1, n_2, \ldots, n_d)}$. The set of all such necklaces is denoted $\mathcal{N}_q^{(n_1, n_2, \ldots, n_d)}$.

Definition (Canonical Form)

The **Canonical Form** of a necklace ω, denoted $\langle \omega \rangle$, is the smallest word $w \in \omega$ under the **necklace recursive order**.

Definition (Comparing Necklaces)

Let ω, υ be a pair of necklaces of size $n_1, n_2, \ldots, n_d$ over the alphabet Σ. $\omega < \upsilon$ if and only if $\langle \omega \rangle < \langle \upsilon \rangle$.

Examples of Multidimensional Necklaces

$\begin{bmatrix} a & a \\ a & a \end{bmatrix}$	$\begin{bmatrix} a & a \\ a & b \end{bmatrix}$	$\begin{bmatrix} a & a \\ b & b \end{bmatrix}$	$\begin{bmatrix} a & b \\ a & b \end{bmatrix}$	$\begin{bmatrix} a & b \\ b & a \end{bmatrix}$	$\begin{bmatrix} a & b \\ b & b \end{bmatrix}$	$\begin{bmatrix} b & b \\ b & b \end{bmatrix}$
-	$\begin{bmatrix} a & a \\ b & a \end{bmatrix}$	-	$\begin{bmatrix} b & a \\ b & a \end{bmatrix}$	$\begin{bmatrix} b & a \\ a & b \end{bmatrix}$	$\begin{bmatrix} b & a \\ b & b \end{bmatrix}$	-
-	$\begin{bmatrix} a & b \\ a & a \end{bmatrix}$	$\begin{bmatrix} b & b \\ a & a \end{bmatrix}$	-	-	$\begin{bmatrix} b & b \\ a & b \end{bmatrix}$	-
-	$\begin{bmatrix} b & a \\ a & a \end{bmatrix}$	-	-	-	$\begin{bmatrix} b & b \\ b & a \end{bmatrix}$	-

Aperiodicity in Multidimensional Necklaces

- As in the 1D case, multidimensional necklaces (and words) can be **Aperiodic**.
- A multidimensional necklace ω is **Periodic** if there exists some subword of ω that can be used to tile the space equivalently to ω.
- A multidimensional necklace ω is **Aperiodic** if there exists no such subword.
- An aperiodic multidimensional necklace is called a multidimensional **Lyndon Word**. The set of Lyndon Words of size $n_1 \times n_2 \times \ldots \times n_d$ over an alphabet of size q is denoted $\mathcal{L}_q^{(n_1,n_2,\ldots,n_d)}$.

Aperiodicity in Multidimensional Necklaces

$$\langle \omega \rangle = \begin{bmatrix} \color{blue}{a} & \color{blue}{b} & a & b \\ \color{blue}{b} & \color{blue}{a} & b & a \\ a & b & a & b \\ b & a & b & a \end{bmatrix}, \langle \upsilon \rangle = \begin{bmatrix} a & a & a & b \\ a & a & a & b \\ a & a & a & b \\ a & a & b & a \end{bmatrix}$$

- As in 1D, the number of words in a necklace is bounded from above by the size of the period.

Aperiodicity in Multidimensional Necklaces

$$\langle \omega \rangle = \begin{bmatrix} a & b & a & b \\ b & a & b & a \\ a & b & a & b \\ b & a & b & a \end{bmatrix}, \langle \upsilon \rangle = \begin{bmatrix} a & a & a & b \\ a & a & a & b \\ a & a & a & b \\ a & a & b & a \end{bmatrix}$$

- As in 1D, the number of words in a necklace is bounded from above by the size of the period.
- Unlike in 1D, the number of words may be less than the size of the period.

Atranslational Multidimensional Necklaces

- A necklace of size $n_1 \times n_2 \times \ldots \times n_d$ is **atranslational** if it contains $n_1 \cdot n_2 \cdot \ldots \cdot n_d$ words.
- A word w is atranslational if $w \circ t \neq w \circ r$ for every pair of translations $t, r \in Z_{\vec{n}}$ where $t \neq r$.
- Every atranslational word is aperiodic, however not every aperiodic word is atranslational.
- The set of atranslational necklaces of size $n_1 \times n_2 \times \ldots \times n_d$ over an alphabet of size q is denoted $\mathcal{A}_q^{(n_1, n_2, \ldots, n_d)}$.

Atranslational Multidimensional Necklaces

$$\langle \omega \rangle = \begin{bmatrix} a & a & a & b \\ a & a & b & a \\ a & b & a & a \\ b & a & a & a \end{bmatrix}, \langle \upsilon \rangle = \begin{bmatrix} a & a & a & b \\ a & a & a & b \\ a & a & a & b \\ a & a & b & a \end{bmatrix}$$

- ω is aperiodic, but not atranslational as it only contains 4 words, υ is both aperiodic and atranslational.

Atranslational Multidimensional Necklaces

$\begin{bmatrix} a & a \\ a & b \end{bmatrix}$	$\begin{bmatrix} a & b \\ b & a \end{bmatrix}$	$\begin{bmatrix} a & b \\ b & b \end{bmatrix}$
$\begin{bmatrix} a & a \\ b & a \end{bmatrix}$	$\begin{bmatrix} b & a \\ a & b \end{bmatrix}$	$\begin{bmatrix} b & a \\ b & b \end{bmatrix}$
$\begin{bmatrix} a & b \\ a & a \end{bmatrix}$	$\begin{bmatrix} b & a \\ a & b \end{bmatrix}$	$\begin{bmatrix} b & b \\ a & b \end{bmatrix}$
$\begin{bmatrix} b & a \\ a & a \end{bmatrix}$	$\begin{bmatrix} a & b \\ b & a \end{bmatrix}$	$\begin{bmatrix} b & b \\ b & a \end{bmatrix}$

- Example of the set of aperiodic 2×2 words over a binary alphabet sorted into necklace classes.
- Note that $\begin{bmatrix} a & b \\ b & a \end{bmatrix}$ is aperiodic, as it can be represented using any subword (without applying some translation), but it is not atranslational, as there are only two unique translations.

Results Overview

Let $\vec{n} = (n_1, n_2, \ldots, n_d)$, $N = \prod_{i=1}^{d} n_i$ and q be the size of the alphabet Σ. We obtain the following results for multidimensional necklaces, Lyndon words, and atranslational necklaces of size $n_1 \times n_2 \times \ldots \times n_d$ over Σ:

- Closed from formulae for counting the sizes of $\mathcal{N}_q^{\vec{n}}, \mathcal{L}_q^{\vec{n}}$, and $\mathcal{A}_q^{\vec{n}}$.
- An $O(N)$ amortised time algorithm for generating the set $\mathcal{N}_q^{\vec{n}}$ in Necklace recursive order.
- An $O(N^5)$ time algorithm for ranking necklaces within the sets $\mathcal{N}_q^{\vec{n}}, \mathcal{L}_q^{\vec{n}}$, and $\mathcal{A}_q^{\vec{n}}$.
- An $O(N^{6(d+1)} \cdot \log^d(q))$ time unranking algorithm for the sets $\mathcal{N}_q^{\vec{n}}, \mathcal{L}_q^{\vec{n}}$, and $\mathcal{A}_q^{\vec{n}}$.

Counting Multidimensional Necklaces

- Our counting results are obtained using the Pólya enumeration and the Möbius inversion formulae for necklaces and Lyndon words respectively.

$$|\mathcal{N}_q^{\vec{n}}| = \frac{1}{N} \sum_{f_1 | n_1} \phi(f_1) \sum_{f_2 | n_2} \phi(f_2) \dots \sum_{f_d | n_d} \phi(f_d)\, q^{(N/lcm(f_1, f_2, \dots, f_d))}$$

$$|\mathcal{L}_q^{\vec{n}}| = \sum_{f_1 | n_1} \mu\left(\frac{n_1}{f_1}\right) \sum_{f_2 | n_2} \mu\left(\frac{n_2}{f_2}\right) \dots \sum_{f_d | n_d} \mu\left(\frac{n_d}{f_d}\right) |\mathcal{N}_q^{f_1, f_2 \dots f_d}|$$

Counting Multidimensional Necklaces

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$$|\mathcal{N}_q^{\vec{n}}| = \frac{1}{N} \sum_{f_1 | n_1} \phi(f_1) \sum_{f_2 | n_2} \phi(f_2) \dots \sum_{f_d | n_d} \phi(f_d)\, q^{(N/lcm(f_1, f_2, \dots, f_d))}$$

$$|\mathcal{L}_q^{\vec{n}}| = \sum_{f_1 | n_1} \mu\left(\frac{n_1}{f_1}\right) \sum_{f_2 | n_2} \mu\left(\frac{n_2}{f_2}\right) \dots \sum_{f_d | n_d} \mu\left(\frac{n_d}{f_d}\right) |\mathcal{N}_q^{f_1, f_2 \dots f_d}|$$

- Counting atranslational words is more complicated.

Intuition behind counting Atranslational Necklaces

- At a (very) high level, the idea behind counting atranslational necklaces is to determine the number of **translational, aperiodic necklaces**.
- This is done in a recursive manner, noting that every translational, aperiodic necklace is composed of some subword that has been repeated under a translation.
- By counting the number of such words, we are able to determine the number of aperiodic necklaces.

$$w = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} a & a & a & b \\ a & a & b & a \\ a & b & a & a \\ b & a & a & a \end{bmatrix} = \begin{bmatrix} w_1 \circ (0) \\ w_1 \circ (1) \\ w_1 \circ (2) \\ w_1 \circ (3) \end{bmatrix}$$

Counting Atranslational Necklaces

$$|L_q^{\vec{n}}| - \sum_{i \in [d]} \sum_{l | n_i} \begin{cases} 0 & l = n_i \\ \left(\prod_{t=i+1}^{d-1} -\mu(n_t) \right) \left(-\mu\left(\frac{n_i}{l}\right)\right) |\mathcal{A}_q^{n_1, n_2, \ldots, n_{d-1}, l}| \cdot H(i, l, \vec{n}, d) & 1 < l < n_d \end{cases}$$

Where:

- $H(i, l, \vec{n}, d) = \prod_{j=i}^{d} \begin{cases} 1 & i = d \\ (|\mathbf{G}(1, \vec{n})| - (I(i, l, \vec{n}))) \cdot (H(i, l, (n_1, n_2, \ldots, n_{d-1}), d-1)) & i < d \end{cases}$
- $I(i, l, (n_1, n_2, \ldots, n_d)) = \begin{cases} 0 & i = d \text{ or } l > 1 \\ 1 + I(i, l, (n_1, n_2, \ldots, n_{d-1})) & n_i = n_d \\ I(i, l, (n_1, n_2, \ldots, n_{d-1})) & n_i \neq n_d \end{cases}$

Generating Multidimensional Necklaces

- At a high level our algorithm works by generating the set of **Prenecklaces** (prefixes of necklaces) in order.
- Our generation algorithm relies on the Necklace Recursive Ordering as a means to do so.
- We show a worked example of how to generate the necklace in $\mathcal{N}_2^{(4,4)}$ following $\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ b & b & b & b \end{bmatrix}$.

Prenecklaces

Definition (Prefix)

A word w of size $n_1 \times n_2 \times \ldots \times n_d$ is a **prefix** of the word v of size $n_1 \times n_2 \times \ldots \times n_{d-1} \times m$ if $m \geq n_d$ and $w_i = v_i$ for every $i \in 1, 2, \ldots, n_d$.

Definition (Prenecklaces)

A word w of size $n_1 \times n_2 \times \ldots \times n_d$ is a **prenecklace** if there exists a word v of size $n_1 \times n_2 \times \ldots \times n_{d-1} \times m$ such that $v = \langle v \rangle$ and w is a prefix of v.

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ b & b & b & b \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & a \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & b \end{bmatrix}$$

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ \mathbf{b} & \mathbf{b} & \mathbf{b} & \mathbf{b} \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & a \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & b \end{bmatrix}$$

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ \mathbf{b} & \mathbf{b} & \mathbf{b} & \mathbf{b} \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & a \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & b \end{bmatrix}$$

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ b & b & b & b \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & a \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & b \end{bmatrix}$$

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ b & b & b & b \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & a \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & b \end{bmatrix}$$

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ b & b & b & b \end{bmatrix} \rightarrow \begin{bmatrix} \mathbf{a} & \mathbf{a} & \mathbf{a} & \mathbf{a} \\ a & a & a & b \\ b & a & a & a \\ \mathbf{a} & \mathbf{a} & \mathbf{a} & \mathbf{a} \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & b \end{bmatrix}$$

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ b & b & b & b \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & a \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & b \end{bmatrix}$$

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ b & b & b & b \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ \mathbf{a} & \mathbf{a} & \mathbf{a} & \mathbf{a} \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ \mathbf{a} & \mathbf{a} & \mathbf{a} & \mathbf{b} \end{bmatrix}$$

Necklace Generation Example

$$\begin{bmatrix} a & a & a & a \\ a & a & a & b \\ a & b & a & a \\ b & b & b & b \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & a \end{bmatrix} \rightarrow \begin{bmatrix} a & a & a & a \\ a & a & a & b \\ b & a & a & a \\ a & a & a & b \end{bmatrix}$$

Ranking

- Let ω be the necklace we are ranking and $\mathcal{N}_q^{\vec{n}}$ be the set we are ranking ω in.
- The high level idea behind our ranking algorithm is to compute the number of words belonging to a necklace class that is smaller than $\langle \omega \rangle$.
- This is transformed first into the number of Atranslational necklaces smaller than ω, then into the number of Lyndon words smaller than ω.
- Our recursive ordering allows this process to be handled recursively.

Unranking

- Let i be the rank of the necklace in $\mathcal{N}_q^{\vec{n}}$ and let $\omega, \upsilon \in \mathcal{N}_q^{\vec{n}}$ be a pair of necklaces such that:
  - $\omega \leq \upsilon$.
  - w is the longest prefix that is shared by both $\langle \omega \rangle$ and $\langle \upsilon \rangle$.
  - ω is the smallest necklace such that w is a prefix of $\langle \omega \rangle$.
  - υ is the largest necklace such that w is a prefix of $\langle \upsilon \rangle$.
- Then the number of necklaces sharing w as a prefix is given by $Rank(\upsilon) - Rank(\omega)$ and further the necklace with a rank of i has w as a prefix if and only if $Rank(\omega) \leq i \leq Rank(\upsilon)$.
- This can be used with a binary search to determine the i^{th} necklace by determining the prefix iteratively.

Open Problems

- Can de Bruijn Tori be found efficiently?
- Can multidimensional necklaces be ranked in $O(N^2)$.
- Can our results be extended to other notions of symmetry?